La Transformée de Legendre–Fenchel et la convexifiée d'une fonction : algorithmes rapides de calcul, analyse et régularité du second ordre

The Legendre–Fenchel Transform and the Convex Hull of a Function: Fast Computational Algorithms, Second-Order Smoothness and Analysis

Mots-Clés : Transformée de Legendre–Fenchel, enveloppe convexe, régularisée de Moreau–Yosida, analyse au second ordre, épi-dérivée, dérivée directionnelle seconde, fonction marginale, conjuguée, biconjuguée.

Keywords and phrases: Legendre–Fenchel Transform, Convex Hull, Moreau–Yosida Approximate, Second-Order Analysis, Epi-Derivative, Second-Order Directional Derivative, Marginal Function, Conjugate, Biconjugate, Convex Envelope.

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Introduction

La *transformée de Legendre–Fenchel* d'un fonction u :

$$u^*(s) = \sup_x [\langle s, x \rangle - u(x)] \tag{1}$$

est fondamentale en analyse convexe [17, 32]. Certains auteurs [26, 30] ont comparé son rôle à celui de la transformée de Fourier.

Considérant la diversité des domaines où elle apparaît, il nous semble primordial de **disposer d'algorithmes efficaces pour la calculer numériquement**. Nous nous sommes ainsi intéressés —dans la première partie de notre travail— à *la transformée de Legendre–Fenchel Discrète* :

$$u_X^*(s) = \max_{x \in X} [\langle s, x \rangle - u(x)], \tag{2}$$

où X est un ensemble fini de points de $\mathbb{R}^d$.

Nous montrons que lorsque u est semi-continue supérieurement, la transformée de Legendre–Fenchel discrète converge ponctuellement vers la transformée de Legendre–Fenchel. Cette convergence est d'autant plus rapide que u est régulière.

Après avoir établi la convergence, nous avons étudié deux algorithmes de calcul numérique de la transformée de Legendre–Fenchel discrète.

Le premier —*l'algorithme de transformation de Legendre rapide*, introduit par Brenier [4]— utilise la monotonie du sous-différentiel de l'analyse convexe pour accélérer autant les calculs que la transformée de Fourier rapide accélère les calculs de la transformation de Fourier.

Le second —*l'algorithme de transformation de Legendre en temps linéaire*— atteint une complexité linéaire quand l'ensemble X est ordonné, hypothèse toujours vérifiée dans le cadre de notre étude.

Le pré-traitement des données par des d'algorithmes classiques de géométrie combinatoire (« Beneath-Beyond [9, 29], Ultimate Planar Convex Hull Algorithm [23] ») permet d'obtenir une complexité *optimale* par rapport au nombre de points de X et au nombre de sommets de l'enveloppe convexe de X.

L'algorithme de transformation de Legendre rapide a été appliqué à la résolution d'équations d'Hamilton–Jacobi par Corrias [8] et à la résolution d'équations de Burger par Noullez et Vergassola [27]. Leurs résultats peuvent être obtenus plus rapidement avec notre algorithme de transformation de Legendre en temps linéaire.

Si on applique deux fois la transformée de Legendre–Fenchel à une fonction $E : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$, on obtient l'*enveloppe convexe semi-continue inférieure* de E [17, 32] qui est à la fois la plus grande fonction convexe semi-continue inférieure minorant E et l'enveloppe semi-continue inférieure de

$$\text{co}\, E(x) = \inf\{\sum_{i=1}^{p} \lambda_i E(x_i) \ : \ \sum_{i=1}^{p} \lambda_i x_i = x, \quad \lambda_i \geq 0 \quad \text{et} \ \sum_{i=1}^{p} \lambda_i = 1\}. \tag{3}$$

Son importance n'est plus a démontrer dans des domaines très divers, dont l'optimisation globale et la thermodynamique. La deuxième partie de notre travail est consacrée à **l'étude de la régularité au second ordre de l'enveloppe convexe semi-continue inférieure**.

L'enveloppe convexe d'une fonction très régulière (et 1-coercive) est continûment différentiable [2] mais presque jamais deux fois différentiable. Nous présentons diverses approches pour étudier sa régularité au second ordre.

Le cas unidimensionnel est entièrement traité en utilisant les dérivées secondes directionnelles. En dimension supérieure nous avons obtenu des résultats partiels en utilisant des techniques très variées :

– *Une généralisation du cas unidimensionnel* permet, pour certaines directions, de prouver l'existence et de calculer la dérivée seconde directionnelle.

– *L'étude des simplexes de phases* (les phases de x sont les points x_i pour lesquels l'infimum (3) est atteint) nous permet de généraliser certains résultats de Griewank et Rabier [14, 31] et de caractériser l'unicité du minimum (3).

- *La théorie des multifonctions* [1, 24] permet de clarifier la régularité de la multifonction qui à un point associe l'ensemble de ses phases. L'existence d'une sélection lipschitzienne donnerait des résultats sur la régularité au second ordre de $\bar{\text{co}}E$, mais nous construisons une fonction E pour laquelle cette multifonction n'admet pas de sélection continue. Nous montrons ainsi les limites de cette approche géométrique.

- Considérant l'enveloppe convexe comme une *fonction marginale* [6, 7, 13, 10, 11, 12, 15, 16, 18], nous appliquons des résultats sur le calcul des dérivées d'une fonction marginale et retrouvons ainsi certaines propriétés de régularité au premier ordre. Les récents travaux sur la régularité au second ordre d'une fonction marginale [5, 19, 20, 21, 22] —en particulier sur l'effet d'enveloppe— illustrent la difficulté de notre problème qui se décompose en deux fonctions marginales : l'une à données régulières sur un domaine non borné et l'autre à données non régulière sur un domaine borné.

Dans une troisième partie nous utilisons la transformée de Legendre–Fenchel pour étudier **la régularité au second ordre de la régularisée de Moreau–Yosida** :

$$F(x) = \min_{y \in \mathbb{R}^n} [f(y) + \frac{1}{2}\|x - y\|^2],$$

qui apparaît dans les algorithmes de minimisation de type méthodes de faisceaux.

En utilisant des techniques d'épi-différentiation seconde [33, 34, 35] nous retrouvons la caractérisation du Hessien [3]. De plus, nous obtenons une formule explicite du Hessien de F en fonction de l'épi-différentielle seconde de f. Ce travail a été réalisé à la suite de discussions avec C. Lemaréchal. Ces résultats ont été obtenus indépendamment par Poliquin et Rockafellar [28].

Remarques bibliographiques

La première partie de ce travail a fait l'objet de deux articles présentés aux journées MODE (Mathématiques de l'Optimisation de la DÉcision) en Novembre

1993 et en Mars 1996. Le premier —« a fast computational algorithm for the Legendre–Fenchel transform [25] »— est paru dans « Computational Optimization and Applications ». Le dernier chapitre a été présenté lors des journées MODE en Mars 1995 sous le titre « Formule explicite du Hessien de la régularisée de Moreau–Yosida d'une fonction convexe f en fonction de l'épi-différentielle seconde de f ». Tous ces manuscrits sont disponibles en tant que rapport de laboratoire. Ils peuvent être obtenus en écrivant au laboratoire ou directement par l'intermédiaire du réseau à :

– ftp ://ftp.cict.fr/pub/lao/LAO94-03a.ps.gz (version anglaise),

– ftp ://ftp.cict.fr/pub/lao/LAO94-03.ps.gz (version française),

– ftp ://ftp.cict.fr/pub/lao/LAO95-15.ps.gz,

– ftp ://ftp.cict.fr/pub/lao/LAO95-08.ps.gz.

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Chapter 1

Numerical computation of the Legendre–Fenchel transform

Introduction

What is the analog of the Fast Fourier transform (FFT) for the Legendre–Fenchel transform? Since both transforms have been known to share similar properties [13, 17], could one build an algorithm as fast as the FFT to compute the Legendre–Fenchel transform? Considering the fields of convex analysis and computational geometry, we clearly see the absence of such an algorithm.

The Legendre–Fenchel transform —also named conjugate or Legendre–Fenchel conjugate— is a well-known fundamental tool in convex analysis [7, 19]. It is defined by:

$$u^*(s) = \sup_x [\langle s, x\rangle - u(x)],$$

where u is a real-valued function, and $\langle ., .\rangle$ the standard scalar product on $\mathbb{R}^d$. In fact, applying twice the Legendre–Fenchel transform, we obtain the closed convex hull.

The convex hull problem —namely finding all vertices of the convex hull of a finite set of points— has been largely investigated in computational geometry [5, 16]. That geometric operation has an analytic counterpart: given a real-valued function u, compute its convex hull[1] $\operatorname{co} u$, *i.e.*, the largest convex function underestimating u. The convex hull —also named convex envelope— has also

[1]Alternatively, the convex hull may be defined geometrically by its epigraph: the epigraph of $\operatorname{co} u$ is the smallest convex set containing the epigraph of u, that is, $\operatorname{Epi} \operatorname{co} u = \operatorname{co} \operatorname{Epi} u$.

been much investigated in convex analysis [7, 19]. It has been used in numerous fields, especially in chemistry [8, 18].

Since the convex hull has a discrete counterpart —the convex hull problem— what is the discrete counterpart of the Legendre–Fenchel transform? Brenier [1] named it the *Discrete Legendre Transform* (DLT).

In section 1.1 we prove that the DLT converges towards the Legendre–Fenchel transform, and we overestimate the rate of convergence. We then present two algorithms to compute the DLT.

The *Fast Legendre Transform* (FLT) algorithm was introduced by Brenier [1] and studied by Corrias [3]. It shares the same basic idea and the complexity of the FFT. Noullez and Vergassola [14] proposed a similar algorithm not only taking into account worst-case time complexity but also space complexity (the amount of memory used when running the algorithm). We present our results on the DLT and on the FLT algorithm. They complete those of Corrias.

Even if the FLT algorithm is worst-case time optimal, we present a new faster algorithm that runs in linear time under rather general assumptions. Indeed, we noted that, as far as worst-case time complexity is involved, the DLT and the convex hull problems are equivalent. Since there are several linear-time convex hull algorithms [5, 16], we can assume our data is convex. Then we show that only linear time is needed to obtain the DLT. We name our two-step algorithm the Linear-time Legendre Transform (LLT) algorithm.

In section 1.2.2 we study the LLT algorithm. Complexity calculation and numerical tests clearly show that our two-step method —first computing the convex hull, next the DLT— is faster than applying the FLT algorithm. Interestingly we use convex hull computations to compute the Legendre–Fenchel transform, whereas one usually uses the Legendre–Fenchel transform to obtain the convex hull.

Section 1.3 ends this chapter with straightforward applications of the DLT in convex analysis.

In what follows, we introduce our notation. Since we deal with asymptotic analysis and mainly worst-case time complexity, we adopt the notational devices introduced in [11]. Throughout the paper, whenever we compute a lower bound, we use the d^{th}-order algebraic decision-tree computational model (see section 1.4 in [16] for justifications for choosing that model). Our notation is closed to that of [16].

We let $O(f(n))$ denote the set of all functions $g(n)$ such that there exist positive constants C and n_0 with $|g(n)| \leq Cf(n)$, for all $n \geq n_0$. It is used to describe upper bounds.

The set of all functions $g(n)$ such that there exist positive constants C and n_0 with $|g(n)| \geq Cf(n)$, for all $n \geq n_0$ is denoted by $\Omega(f(n))$. It is used to describe lower bounds.

To indicate functions of the same order as $f(n)$ (the concept needed to describe "optimal algorithms"), we define $\Theta(f(n))$: the set of all functions $g(n)$ such that there exist positive constants C_1, C_2 and n_0 with $C_1 f(n) \leq g(n) \leq C_2 f(n)$, for all $n \geq n_0$.

We do not address here the problem of space complexity. Instead, we concentrate on time complexity. To sum up our goal, "we are essentially interested in the general functional dependence of computation time upon problem size, that is, how fast the computation time grows with the problem size." In our setting, "optimal" means that the asymptotic worst-case time complexity is attained for some input data.

1.1 The Discrete Legendre Transform: theoretical study

We consider an extended real-valued function $u : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ finite on a non-empty subset of $\mathbb{R}$. We define its domain: $\mathrm{Dom}(u) = \{x \in \mathbb{R} \ : \ u(x) < +\infty\}$. We name the indicator function of $[a, b]$:

$$I_{[a,b]}(x) = \begin{cases} 0 & \text{if } x \in [a,b], \\ +\infty & \text{otherwise;} \end{cases},$$

and $u_{[a,b]} = u + I_{[a,b]}$. The function $u_{[a,b]}$ is equal to u on $[a, b]$ and to $+\infty$ outside of $[a, b]$.

The Legendre–Fenchel transform of $u_{[a,b]}$ is:

$$u^*_{[a,b]}(s) = \sup_{x\in[a,b]}[sx - u(x)] = (u + I_{[a,b]})^*(s);$$

the set of points —possibly empty— where the supremum is attained is:

$$H^*_{[a,b]}(s) = \operatorname*{Argmax}_{x\in[a,b]}[sx - u(x)] = \{x \in [a,b] \ : \ sx - u(x) = u^*_{[a,b]}(s)\}.$$

We approximate the interval $[a,b]$ with the finite set:
$X = \{x_i \ : \ a \leq x_1 < x_2 < \cdots < x_n \leq b\}$. We denote $|X|$ the number of elements in X (here, $|X| = n$). We define:

$$u^*_X(s) = (u + I_X)^*(s) = \max_{x\in X}[sx - u(x)],$$

and its associated set-valued function:

$$H^*_X(s) = \operatorname*{Argmax}_{x\in X}[sx - u(x)] = \{x \in X \ : \ sx - u(x) = u^*_X(s)\}.$$

We name h^*_X a function taking values in H^*_X (for all s, we have $h^*_X(s) \in H^*_X(s)$).

The idea is to approximate $[a,b]$ by a finite set X which satisfies $X \to [a,b]$ when $|X| \to +\infty$, that is, for any point y in $[a,b]$, $\inf_{x\in X}\|x - y\| \to 0$. Section 1.1.2 shows that u^*_X (resp. $u^*_{[-a,a]}$) converges when $|X| \to +\infty$ (resp. $a \to +\infty$) under a weak smoothness assumption on u.

1.1.1 Basic properties

We define the inverse mapping $(H^*_{[a,b]})^{-1}$ by $s \in (H^*_{[a,b]})^{-1} \Leftrightarrow x \in H^*_{[a,b]}(s)$.

The set-valued function $H^*_{[a,b]}$ (resp. $(H^*_{[a,b]})^{-1}$) is closely related to the subdifferential of $u^*_{[a,b]}$ (resp. $u_{[a,b]}$).

Proposition 1.1. *If u is lower semi-continuous (lsc), then the following holds at any x, s in $\mathbb{R}$:*

i). $\mathrm{Dom}(H^*_{[a,b]}) = \{s \in \mathbb{R} \ : \ H^*_{[a,b]}(s) \neq \emptyset\} = \mathbb{R}$,

ii). $(H^*_{[a,b]})^{-1}(x) = \partial u_{[a,b]}(x) \subset \partial u^{**}_{[a,b]}(x)$, *iii).* $H^*_{[a,b]}(s) \subset \partial u^*_{[a,b]}(s)$, *and*

iv). $\mathrm{co}\, H^*_{[a,b]}(s) = \partial u^*_{[a,b]}(s)$,

where $\partial u(x) = \{s \in \mathbb{R} \ : \ \forall y \in \mathbb{R}\ ,\ u(y) \geq u(x) + s(y-x)\}$ is the subdifferential of u in the sense of convex analysis.

Proof. i). First, since $u^*_{[a,b]}$ is clearly 1-coercive, we have $\mathrm{Dom}(u^*_{[a,b]}) = \mathbb{R}$ (see Corollary 13.3.1 in [19] or Proposition 1.3.8 of Chap. X in [7]). We then note that $u_{[a,b]}$ is lsc on the compact set $\mathrm{Dom}(u_{[a,b]}) = [a,b] \cap \mathrm{Dom}(u)$. Consequently, for all s in $\mathbb{R}$, the supremum in $u^*_{[a,b]}(s)$ is attained at some point x, that is, $H^*_{[a,b]}(s)$ is nowhere empty.

ii). First, we suppose $(H^*_{[a,b]})^{-1}(x)$ is empty: there is no s such that x belongs to $H^*_{[a,b]}(s)$, that is, for all s, $u^*_{[a,b]}(s) > sx - u_{[a,b]}(x)$. For $\epsilon > 0$ small enough, there is y in $\mathbb{R}$ such that:

$$sx - u_{[a,b]}(x) < u^*_{[a,b]}(s) - \epsilon \leq sy - u_{[a,b]}(y) \leq u^*_{[a,b]}(s),$$

that is to say, $u_{[a,b]}(y) < s(y-x) + u(x)$. In other words, $\partial u_{[a,b]}(x)$ is empty.

Now we assume there is s in $(H^*_{[a,b]})^{-1}(x)$. For all y, we have

$$sx - u_{[a,b]}(x) \geq sy -_{[a,b]} u(y).$$

Hence s belongs to $\partial u_{[a,b]}(x)$.

Similar arguments prove the reverse inclusion.

iii). For x in $H^*_{[a,b]}(s)$ and for all y in $\mathbb{R}$, we have

$$u^*_{[a,b]}(s) = sx - u_{[a,b]}(x) \geq sy - u_{[a,b]}(y).$$

Hence x is in $\partial u^*_{[a,b]}(s)$.

iv). From iii) and the convexity of $\partial u^*_{[a,b]}(s)$ we deduce $\mathrm{co}\, H^*_{[a,b]}(s) \subset \partial u^*_{[a,b]}(s)$. Now, let x belongs to $\partial u^*_{[a,b]}(s)$. To apply Proposition 1.5.4 of Chap. X in [7], we note that the function $u_{[a,b]}$ is proper, lsc, underestimated by an affine function and 1-coercive (its domain is bounded). It follows that there exist $x_1, x_2 \in \mathbb{R}$, and two nonnegative numbers $\alpha_1, \alpha_2 \in \mathbb{R}$ with $\alpha_1 + \alpha_2 = 1$ such that:

$$\begin{aligned} x &= \alpha_1 x_1 + \alpha_2 x_2, \\ u^{**}_{[a,b]}(x) &= \alpha_1 u_{[a,b]}(x_1) + \alpha_2 u_{[a,b]}(x_2), \\ s \in \partial u^{**}_{[a,b]}(x) &= \partial u_{[a,b]}(x_1) \cap \partial u_{[a,b]}(x_2), \\ \text{and } u_{[a,b]}(x_i) &= u^{**}_{[a,b]}(x_i), \text{ for } i = 1, 2. \end{aligned}$$

We deduce:

$$u^*_{[a,b]}(s) = sx_i - u^{**}_{[a,b]}(x_i) = sx_i - u_{[a,b]}(x_i).$$

Consequently x is a convex combination of points in $H^*_{[a,b]}(s)$. □

We end this subsection with several remarks.

Remark 1.1. Property ii) and iii) hold even if u is not lower semi-continuous.

Remark 1.2. Equality does not always hold in $H^*_{[a,b]}(s) \subset \partial u^*_{[a,b]}(s)$. Indeed, consider $u_{[-1,1]}(x) = (x^2 - 1)^2 + I_{[-1,1]}(x)$. Its Legendre–Fenchel transform is $u^*_{[-1,1]}(s) = |s|$. Although equality holds in the above inclusion for $s \neq 0$ ($H^*_{[-1,1]}(s) = \{s/|s|\} = \partial u^*_{[-1,1]}(s)$), for $s = 0$ we have:

$$H^*_{[-1,1]}(0) = \{-1, 1\} \subsetneq [-1, 1] = \partial u^*_{[-1,1]}(0).$$

Remark 1.3. Since the subdifferential is a monotone set-valued function [Proposition 6.1.1 of Chap. VI in [7]], and since we can write:

$$\begin{aligned} H^*_X(s) &= \operatorname*{Argmax}_{x \in \mathbb{R}} \left[sx - (u(x) + I_X)(x)\right] \subset \partial \left(u + I_X\right)^*(s), \\ H^*_{[a,b]}(s) &= \operatorname*{Argmax}_{x \in \mathbb{R}} \left[sx - \left(u(x) + I_{[a,b]}\right)(x)\right] \subset \partial \left(u + I_{[a,b]}\right)^*(s); \end{aligned}$$

both set-valued functions, H^*_X and $H^*_{[a,b]}$, are monotone. That is, for all x_1 in $H^*_X(s_1)$ and x_2 in $H^*_X(s_2)$, $\langle x_1 - x_2, s_1 - s_2 \rangle \geq 0$. This property will be the key idea of the FLT algorithm.

Remark 1.4. Since our algorithm computes *both* $u^*_X(s)$ and $H^*_X(s)$, we obtain as output data: $\operatorname{co} H^*_X(s) = \partial(u + I_X)^*(s) = \partial u^*_X(s)$. Corrias [3] proved that $\partial u^*_X(s)$ converges towards $\partial u^*_{[a,b]}(s)$ when $|X| \to +\infty$. Hence not only do we get an approximation of u^* but also of its subdifferential ∂u^*.

1.1.2 Convergence results

First, we prove the pointwise convergence of u_X^*, next the pointwise convergence of $u_{[-a,a]}^*$.

Convergence of u_X^* towards $u_{[a,b]}^*$

For the sake of simplicity we consider equidistant points:

$$X = \{a + i\frac{b-a}{n} \ : \ i = 1, 2, \ldots, n\}.$$

We will name $\varphi(x) = sx - u(x)$.

We first give minimal assumptions to ensure convergence:

Proposition 1.2. *If $u_{[a,b]}$ is upper semi-continuous on $[a,b]$ then u_X^* converges pointwisely to $u_{[a,b]}^*$ when $n = |X|$ goes to infinity.*

Proof. Let $\epsilon > 0$. There is $\bar{x}$ in $[a,b]$ such that $u_{[a,b]}^*(s) - \epsilon \leq \varphi(\bar{x}) \leq u_{[a,b]}^*(s)$. As φ is lower semi-continuous, for any $\epsilon' > 0$ there is $\eta > 0$ such that if $|x - \bar{x}| < \eta$, $\varphi(\bar{x}) - \varphi(x) \leq \epsilon'$.

For n large enough, there is x^n in X for which $|\bar{x} - x^n| \leq (b-a)/n < \eta$. Now using $\varphi(x^n) \leq u_X^*(s)$, we obtain:

$$u_{[a,b]}^*(s) - \epsilon - u_X^*(s) \leq \varphi(\bar{x}) - \varphi(x^n)) \leq \epsilon'.$$

Consequently, $0 \leq u_{[a,b]}^*(s) - u_X^*(s) \leq \epsilon + \epsilon'$, which proves the proposition. □

Example 1.1. If u is not upper semi-continuous, u_X^* does not always converge pointwisely to $u_{[a,b]}^*$. Consider $[a,b] = [0,1]$, and let

$$u(x) = \begin{cases} \frac{1}{2}x^2 & \text{if} & x \in (0,1], \\ -1 & \text{if} & x = 0, \\ +\infty & \text{otherwise.} & \end{cases}$$

For all s in $[0,1]$, $u_{[a,b]}^*(s) = 1$ but $u_X^*(s)$ converges towards $1/2s^2$. Indeed, u_X^* does not take into account the value of u at the origin.

Remark 1.5. We take s in $\mathbb{R}$. Since X is a finite set, there is $\bar{x}^n$ in X such that $u_X^*(s) = \varphi(\bar{x}^n)$. When u is lower semi-continuous, there is also $\bar{x}$ in $[a,b]$ s.t. $u_{[a,b]}^*(s) = \varphi(\bar{x})$. Although the sequence $(\bar{x}^n)_n$ does not always converge to $\bar{x}$, there is x^n in X for which x^n converges to $\bar{x}$ and $\varphi(x^n)$ converges to $\varphi(\bar{x})$.

Next we study the rate of convergence.

Proposition 1.3. *We take s in $\mathbb{R}$. If u is twice continuously differentiable on a neighborhood of $[a,b]$, then there is K in $\mathbb{R}$ such that*

$$0 \le u^*_{[a,b]}(s) - u^*_X(s) \le \frac{K}{n^2}.$$

Moreover, K depends only on a, b, and u.

Proof. We recall that $\varphi(x) = sx - u(x)$. We name $\bar{x}^n$ (resp. $\bar{x}$) such that the maximum in $u^*_X(s)$ (resp. $u^*_{[a,b]}(s)$) is attained at $\bar{x}^n$ (resp. $\bar{x}$). There is x^n in X which satisfies $|x^n - \bar{x}| \le (b-a)/n$. We have

$$0 \le u^*_{[a,b]}(s) - u^*_X(s) = \varphi(\bar{x}) - \varphi(\bar{x}^n) \le \varphi(\bar{x}) - \varphi(x^n).$$

We apply Taylor–Lagrange's Theorem to φ at $\bar{x}$: there is $\tilde{x}^n$ between x^n and $\bar{x}$ such that: $\varphi(x^n) - \varphi(\bar{x}) = (x^n - \bar{x})\varphi'(\bar{x}) + \frac{1}{2}(x^n - \bar{x})^2\varphi''(\tilde{x}^n)$. We note that $\varphi'(\bar{x}) = 0$ and $\varphi''(\tilde{x}^n) = -u''(\tilde{x}^n)$. Consequently

$$u^*_{[a,b]}(s) - u^*_X(s) \le \frac{u''(\tilde{x}^n)}{2}(\bar{x} - x^n)^2 \le \frac{1}{2}\left(\frac{b-a}{n}\right)^2 u''(\tilde{x}^n).$$

Since u'' is continuous on $[a,b]$, the proposition holds with

$$K = \frac{(b-a)^2}{2} \max_{x \in [a,b]} u''(x) \quad \square$$

Remark 1.6. Corrias [3] proved additional convergence results under intermediate smoothness assumptions. Eventually, the smoother u, the faster the convergence.

Convergence of $u^*_{[-a,a]}$ towards u^*

In order to simplify the presentation, we consider a symmetric interval $[-a,a]$. We do not require any assumption on u to obtain the convergence.

Proposition 1.4. $(u^* \square a|.|) = \left(u + I_{[-a,a]}\right)^* = u^*_{[-a,a]}$ *converges pointwisely to u^* when a goes to infinity.*

This result is a consequence of the following proposition:

Proposition 1.5. *Let $f : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ be a lower semi-continuous, real-valued function, underestimated by some affine function. Then, for all s, we have*

$$f \square a|.|(s) \xrightarrow[a \to +\infty]{} f(s).$$

Proof. We give here an elementary proof of a more general result proved in [6]. First, we define $\varphi(x) = f(x) + a|s - x|$ with s in the domain of f. There exist α, β in $\mathbb{R}$ such that for all x in $\mathbb{R}$, $f(x) \geq \alpha x + \beta$.

Next, Let $\epsilon > 0$. There is $\bar{x}_{a,\epsilon}$ such that:

$$\inf_x [f(x) + a|s - x|\,] \leq f(\bar{x}_{a,\epsilon}) + a|s - \bar{x}_{a,\epsilon}| \leq \inf_x [f(x) + a|s - x|\,] + \epsilon. \tag{1.1}$$

First step. Let us prove by contradiction that $\bar{x}_{a,\epsilon}$ converges towards s when a goes to infinity. We suppose that there exist $M > 0$ and a sequence $(a_k)_{k \in \mathbb{N}}$ going to infinity such that for all k: $|s - \bar{x}_k| \geq M > 0$, with $\bar{x}_k = \bar{x}_{a_k,\epsilon}$.

We obtain the following stream of inequalities:

$$\begin{aligned} \alpha \bar{x}_k + \beta + a_k M &\leq \alpha \bar{x}_k + \beta + a_k |s - \bar{x}_k| \\ &\leq f(\bar{x}_k) + a_k |s - \bar{x}_k| \\ &\leq \inf_x [f(x) + a_k |s - x|] + \epsilon \\ &\leq f(s) + \epsilon < \infty. \end{aligned}$$

The convergence of $a_k M$ to $+\infty$ implies that $\alpha \bar{x}_k$ converges to $-\infty$. Thus $|\bar{x}_k|$ converges to $+\infty$ when k goes to infinity. Now from

$$-|\alpha||\bar{x}_k| + a_k(|\bar{x}_k| - |s|) + \beta \leq \alpha \bar{x}_k + \beta + a_k |\bar{x}_k - s| \leq f(s) + \epsilon,$$

we deduce

$$\beta + |\bar{x}_k| \left(\frac{a_k}{2} - |\alpha| \right) + a_k \left(\frac{|\bar{x}_k|}{2} - |s| \right) \leq f(s) + \epsilon.$$

The left-hand side goes to infinity when k increases, whereas the right-hand side is always bounded. That contradiction proves that $\bar{x}_{a,\epsilon}$ converges to s.

Last step. First we take $\epsilon' > 0$. We use the lower semi-continuity of f at s and the convergence of $\bar{x}_{a,\epsilon}$ to s: for a large enough we have $|\bar{x}_{a,\epsilon} - s| < \eta$ and

p	$\max \lvert u^*_X - u^*_{[0,1]} \rvert$
1	6
2	2
3	0.4
4	0.1
5	$0.2\ 10^{-1}$
6	$0.6\ 10^{-2}$
7	$0.2\ 10^{-2}$
8	$0.4\ 10^{-3}$
9	$0.1\ 10^{-3}$
10	$0.2\ 10^{-4}$
11	$0.6\ 10^{-5}$
12	$0.1\ 10^{-5}$
13	$0.4\ 10^{-6}$
14	$0.1\ 10^{-6}$
15	$0.2\ 10^{-7}$

Table 1.1: Uniform convergence of u^*_X towards $u^*_{[0,1]}$ on $[0,1]$.

$-f(\bar{x}_{a,\epsilon}) < -f(s) + \epsilon'$. Since $0 \leq a|s - \bar{x}_{a,\epsilon}| \leq f(s) - f(\bar{x}_{a,\epsilon}) + \epsilon$, we obtain $|f(s) - f(\bar{x}_{a,\epsilon})| \leq \epsilon + \epsilon'$ and $0 \leq a|s - \bar{x}_{a,\epsilon}| \leq \epsilon + \epsilon'$. Consequently we deduce

$$|f(\bar{x}_{a,\epsilon}) + a|s - \bar{x}_{a,\epsilon}| - f(s) \leq 2(\epsilon + \epsilon').$$

Then we use inequalities (1.1) to end the proof. □

1.1.3 Numerical errors

The uniform convergence of $u^*_X(s)$ towards $u^*_{[0,1]}(s)$ is illustrated by Table 1.1. We estimated the function $u_{[0,1]}(x) = x^2$ at $x_i = i/2^p$ for $i = 1, \ldots, 2^p$. The computation was performed on Maple V with 10 digits accuracy.

Apart from round-off errors, there are two types of numerical errors related to the convergence of $u^*_{[-a,a]}$ and of u^*_X.

When $H^*_{[-a,a]}(s_0) \cap [-a,a]$ is empty, $u^*_X(s_0)$ does not converge to $u^*_{[-a,a]}(s_0)$. We need to use the convergence of $u^*_{[-a,a]}$ to u^* to find a large enough interval to contain a point in $H^*_{[-a,a]}(s_0)$. Only then can we obtain the convergence of $u^*_X(s_0)$

to $u^*_{[-a,a]}(s_0)$. In fact, Hiriart-Urruty [6] proved:

$$\partial u^*(s) \cap [-a,a] \neq \emptyset \Leftrightarrow u^*_{[-a,a]}(s) = u^*(s).$$

Since we compute $\partial u^*_X(s_0) = \operatorname{co} H^*_X(s_0)$ which converges to $\partial u^*(s_0)$, we can increase a until $\partial u^*(s) \cap [-a,a]$ is non-empty.

Even if we assume $u^*_{[-a,a]}(s_0) = u^*(s_0)$, numerical problems may arise when the graph of u has a vertical tangent at $\bar{x} \in [-a,a]$. Figures 1.12 and 1.15 show that $H^*_X(s_0)$ converges to $H^*_{[-a,a]}(s_0)$ without attaining the limit. The convergence of $u^*_X(s_0)$ ensures that this type of error decreases as n goes to infinity.

1.2 The Discrete Legendre Transform: numerical computation

In this section we are mainly interested with the computation time of the Discrete Legendre Transform (DLT). We present two algorithms which are faster than a direct computation.

In a preliminary step, we note that the d-dimensional Legendre–Fenchel transform can be factorized with 1-dimensional transforms. Indeed, the DLT takes n points in $X \subset \mathbb{R}^d$ and determines for each slope s in a set of m slopes $S \subset \mathbb{R}^d$, the point that is maximal in the direction $(s,-1)$. In other words, it computes:

$$u^*_X(s) = \max_{x \in X} \langle (x, u(x)), (s,-1) \rangle,$$

for all s in S.

We always assume the set S to be *ordered* along all its coordinates. As for X, we distinguish the case where it is not ordered (called the general case) from the case where it is ordered along all its coordinates (called the particular case).

When both $X = X_1 \times \cdots \times X_d$ and $S = S_1 \times \cdots \times S_d$ have a grid-like structure, we denote $x = (x_1, \ldots, x_d) \in X$ and $s = (s_1, \ldots, s_d) \in S$. The partial DLT computed with respect to the ith variable s_i on X_i, for all parameter values: $(x_1, \ldots, x_{i-1}, s_{i+1}, \ldots, s_d)$ in $X_1 \times \cdots \times X_{i-1} \times S_{i+1} \times \cdots \times S_d$ is denoted

$\tilde{u}^*_{X_i}(x_1,\dots,x_{i-1};s_i;s_{i+1},\dots,s_d)$. The d-dimensional DLT reduces to the following 1-dimensional DLT:

$$\tilde{u}^*_{X_d}(x_1,\dots,x_{d-1};s_d) = \max_{x_d\in X_d}[s_d x_d - u(x_1,\dots,x_d)],$$
$$\vdots$$
$$\tilde{u}^*_{X_i}(x_1,\dots,x_{i-1};s_i;s_{i+1},\dots,s_d) =$$
$$\max_{x_i\in X_i}[s_i x_i - \tilde{u}^*_{X_{i+1}}(x_1,\dots,x_i;s_{i+1};s_{i+2},\dots,s_d)],$$
$$\vdots$$
$$u^*_X(s) = \tilde{u}^*_{X_1}(s_1;s_2,\dots,s_d) = \max_{x_1\in X_1}[s_1x_1 - \tilde{u}^*_{X_2}(x_1;s_2;s_3,\dots,s_d)].$$

We show that the 1-dimensional FLT takes $O((n+m)\log_2(n+m))$ time in section 1.2.1, and that the 1-dimensional LLT requires $O(n\log_2 h + m)$ in section 1.2.2, where h is the number of vertices of the convex hull of X. Hence, computing the d-dimensional DLT with the FLT involves

$$O(n_1\dots n_{d-1}[(n_d+m_d)\log_2(n_d+m_d)]$$
$$\vdots$$
$$+n_1\dots n_{i-1}m_{i+1}\dots m_d[(n_i+m_i)\log_2(n_i+m_i)]$$
$$\vdots$$
$$+m_2\dots m_d[(n_1+m_1)\log_2(n_1+m_1)])$$

time, where $n_i = |X_i|$ and $m_i = S_i$. The LLT algorithm takes

$$O(n_1\dots n_{d-1}[n_d\log_2 h_d + m_d]$$
$$\vdots$$
$$+n_1\dots n_{i-1}m_{i+1}\dots m_d[n_i\log_2 h_i + m_i]$$
$$\vdots$$
$$+m_2\dots m_d[n_1\log_2 h_1 + m_1])$$

time, where h_i is the number of $\operatorname{co} X_i$. If we assume $n_i = m_i = n_1$ for $i=1,\dots,n_1$, we obtain a $O(n\log_2 n)$ time complexity for the FLT, and $O(n\log_2\tilde{h})$ for the LLT, with $\tilde{h} = h_1\dots h_d$ ($\tilde{h}$ is not equal to the number of vertices of $\operatorname{co} X$).

When all sets X_i are ordered, the complexity of the FLT algorithm remains the same, while the LLT algorithm takes

$$\begin{aligned} O(n_1 \dots n_{d-1}[n_d + m_d] \\ \vdots \\ +n_1 \dots n_{i-1} m_{i+1} \dots m_d[n_i + m_i] \\ \vdots \\ +m_2 \dots m_d[n_1 + m_1]) \end{aligned}$$

time. When $n_i = m_i = n_1$ the LLT takes $O(n)$ time.

Eventually, we reduced the computation time from $O(n^2)$ (by a straightforward computation, see page 25) to $O(n)$, when X is ordered. Since we aim at approximating the Legendre–Fenchel transform, we can choose X and S such as to obtain a *linear-time* algorithm.

1.2.1 The FLT algorithm

We present the 1-dimensional FLT algorithm. Since sorting n points requires $O(n \log_2 n)$ —which is not more than our algorithm— we assume that the set X is ordered.

Brenier [1] gave the basis of a recursive algorithm to compute the discrete Legendre–Fenchel transform on the interval [0,1]. To obtain an iterative algorithm, we introduce a parameter τ. In addition to considering a general interval, we clearly separate primal and dual spaces by computing the Legendre–Fenchel transform on

$$X = \{a + i\frac{b-a}{n} \ : \ i = 1, 2, \dots, n\},$$

for the slopes in

$$S = \{a^* + j\frac{b^* - a^*}{m} \ : \ i = 1, 2, \dots, m\}.$$

To emphasize the number of points in X and S, we shall denote $X_n = X$ and $S_m = S$ in the present section.

We introduce the parameter τ as follows:

$$
\begin{aligned}
u_X^*(s,\tau) &= \max_{x\in X}[sx-u(x-\tau)],\\
H_X^*(s,\tau) &= \operatorname*{Argmax}_{x\in X}[sx-u(x-\tau)] = \{x\in X \ : \ u_X^*(s,\tau)=sx-u(x-\tau)\},\\
h_X^*(s,\tau) &\in H_X^*(s,\tau) \text{ is a selection in } H_X^*(s,\tau).
\end{aligned}
$$

We take $\bar{n}=2^p$ and $\bar{m}=2^q$ where p and q are two positive integers.

The FLT algorithm aims at computing $u_{\bar{n}}^*(s,0)$ and $H_{\bar{n}}^*(s,0)$ for $s\in S_{\bar{m}}$, knowing the four real numbers a,b,a^*,b^*, the two positive integers p,q and the values of the function u at points in $X_{\bar{n}}$.

We name n and m two integers satisfying: $n\in\{2^0,2^1,\dots 2^p\}$ and $m\in\{2^0,2^1,\dots 2^q\}$.

Let us look at the operations necessary to go from step n to step $2n$. We write:

$$
\begin{aligned}
X_{2n} &= X_n \cup \left(X_n - \frac{b-a}{2n}\right),\\
\text{and } u_{X_{2n}}^*(s,\tau) &= \max\left\{\max_{x\in X_n}[xs-u(x-\tau)], \max_{x\in X_n-\frac{b-a}{2n}}[xs-u(x-\tau)]\right\}.
\end{aligned}
$$

Using the change of variable $x'=x+(b-a)/(2n)$, we find:

$$
\begin{aligned}
u_{2n}^*(s,\tau) &= \max\left\{u_{X_n}^*(s,\tau), u_{X_n}^*(s,\tau+\frac{b-a}{2n})-s\frac{b-a}{2n}\right\},\\
H_{2n}^*(s,\tau) &= \begin{cases} H_{X_n}^*(s,\tau), \text{ if } u_{2n}^*(s,\tau)=u_{X_n}^*(s,\tau),\\ H_{X_n}^*(s,\tau+(b-a)/(2n))-s(b-a)/(2n), \text{ otherwise.}\end{cases}
\end{aligned}
\tag{1.2}
$$

The following lemma is the basis of the FLT algorithm.

Lemma 1.1. *The set-valued function $H_{X_n}^*(.,\tau): S_m\to S_m$ is monotone.*

Proof. Proposition (1.1)-iii) implies the lemma. Nevertheless we give its simple proof. For all $s,s'\in\mathbb{R}$, we have:

$$
\begin{aligned}
u_{X_n}^*(s,\tau) &= h_{X_n}^*(s,\tau)s-u(h_{X_n}^*(s,\tau)-\tau) \geq h_{X_n}^*(s',\tau)s-u(h_{X_n}^*(s',\tau)-\tau),\\
u_{X_n}^*(s',\tau) &= h_{X_n}^*(s',\tau)s'-u(h_{X_n}^*(s',\tau)-\tau) \geq h_{X_n}^*(s,\tau)s'-u(h_{X_n}^*(s,\tau)-\tau).
\end{aligned}
$$

Adding the two lines, we get:

$$(h^*_{X_n}(s,\tau) - h^*_{X_n}(s',\tau))(s-s') \geq 0. \quad \square$$

Hence, we deduce the following "optimized" formulas, for all s in $\mathbb{R}$:

$$\text{(1.3)} \qquad \begin{aligned} u^*_{X_n}(s,\tau) &= \max_{\substack{x\in X_n \\ H^*_{X_n}(s-(b-a)/(2n),\tau)\leq x\leq H^*_{X_n}(s+(b-a)/(2n),\tau)}} [xs - u(x-\tau)], \\ H^*_{X_n}(s,\tau) &= \operatorname*{Argmax}_{\substack{x\in X_n \\ H^*_{X_n}(s-(b-a)/(2n),\tau)\leq x\leq H^*_{X_n}(s+(b-a)/(2n),\tau)}} [xs - u(x-\tau)]. \end{aligned}$$

Looking for the maximum on a smaller set allows us to compute *faster* the Discrete Legendre Transform. In the following two sections we detail the algorithm and we compute its complexity.

The algorithm

We compute all values of the parameter τ as follows: knowing $u^*_{X_n}(s,\tau)$ and $u^*_{X_n}(s,\tau+(b-a)/2n)$ at step $n=2^i$, we compute $u^*_{2n}(s,\tau)$ with formula (1.2). We outline the computation of τ with a tree branch:

$$\left.\begin{array}{c} \tau \\ \\ \tau + \frac{b-a}{2n} \end{array}\right\} \longrightarrow \tau,$$

i.e., from τ and $\tau+(b-a)/2n$, we compute the updated τ. To clarify our explanation, we introduce the following notation:

$$\left.\begin{array}{c} f^i_k = \tau \\ \\ f^i_{k+1} = \tau + \frac{b-a}{2n} \end{array}\right\} \longrightarrow f^{i+1}_k = \tau.$$

So the sequence $(f^i)_{k=1,\ldots,2^i}$ stores the ith level of the tree. In order to compute the whole tree, we only need a, b and $\bar{n} = 2^p$.

Remark 1.7. The *order* of the finite sequence $(f^i_k)_{k,i}$ is obviously needed to apply the algorithm. For example we know that:

$$\{f^0_k\}_{k=1,\ldots,2^p} = X_{2^p} - \frac{b-a}{2^p},$$

yet we cannot apply the algorithm without knowing how the elements of the sequence $(f^i_k)_{k,i}$ are ordered.

For example, we take $\bar{n} = 8$ and compute:

$$\left.\begin{array}{l} f_1^{p-3} = 0 \\ f_2^{p-3} = \frac{b-a}{\bar{n}/4} \end{array}\right\} f_1^{p-2} = 0$$

$$\left.\begin{array}{l} f_3^{p-3} = \frac{b-a}{\bar{n}/2} \\ f_4^{p-3} = \frac{b-a}{\bar{n}/2} + \frac{b-a}{\bar{n}/4} \end{array}\right\} f_2^{p-2} = \frac{b-a}{\bar{n}/2}$$

$$\left.\begin{array}{l} f_5^{p-3} = \frac{b-a}{\bar{n}} \\ f_6^{p-3} = \frac{b-a}{\bar{n}} + \frac{b-a}{\bar{n}/4} \end{array}\right\} f_3^{p-2} = \frac{b-a}{\bar{n}}$$

$$\left.\begin{array}{l} f_7^{p-3} = \frac{b-a}{\bar{n}} + \frac{b-a}{\bar{n}/2} \\ f_8^{p-3} = \frac{b-a}{\bar{n}} + \frac{b-a}{\bar{n}/2} + \frac{b-a}{\bar{n}/4} \end{array}\right\} f_4^{p-2} = \frac{b-a}{\bar{n}} + \frac{b-a}{\bar{n}/2}$$

$$\left.\begin{array}{l} f_1^{p-2} = 0 \\ f_2^{p-2} = \frac{b-a}{\bar{n}/2} \end{array}\right\} f_1^{p-1} = 0 \qquad \left.\begin{array}{l} f_3^{p-2} = \frac{b-a}{\bar{n}} \\ f_4^{p-2} = \frac{b-a}{\bar{n}} + \frac{b-a}{\bar{n}/2} \end{array}\right\} f_2^{p-1} = \frac{b-a}{\bar{n}}$$

$$\left.\begin{array}{l} f_1^{p-1} = 0 \\ f_2^{p-1} = \frac{b-a}{\bar{n}} \end{array}\right\} f_1^{p} = 0.$$

For $[a, b] = [0, 1]$, the first three values of $\bar{n}$ give:

$\bar{n} = 2$	f_1^0				f_2^0				
	0				$\frac{1}{2}$				1

$\bar{n} = 4$	f_1^0		f_3^0		f_2^0		f_4^0		
	0		$\frac{1}{4}$		$\frac{1}{2}$		$\frac{3}{4}$		1

$\bar{n} = 8$	f_1^0	f_5^0	f_3^0	f_7^0	f_2^0	f_6^0	f_4^0	f_8^0	
	0	$\frac{1}{8}$	$\frac{1}{4}$	$\frac{3}{8}$	$\frac{1}{2}$	$\frac{5}{8}$	$\frac{3}{4}$	$\frac{7}{8}$	1.

For $\bar{n} = 8$ the whole tree is:

$n = 1$	f_1^0	f_5^0	f_3^0	f_7^0	f_2^0	f_6^0	f_4^0	f_8^0	
	0	$\frac{1}{8}$	$\frac{1}{4}$	$\frac{3}{8}$	$\frac{1}{2}$	$\frac{5}{8}$	$\frac{3}{4}$	$\frac{7}{8}$	1

$n = 2$	f_1^1	f_3^1	f_2^1	f_4^1					
	0	$\frac{1}{8}$	$\frac{1}{4}$	$\frac{3}{8}$					1

$n = 4$	f_1^2	f_2^2							
	0	$\frac{1}{8}$							1

$n = 8$	f_1^3								
	0								1.

We are now ready to describe the FLT algorithm. We use a Pascal-like syntax.

1. **Input** $p, q, a, b, a^*, b^*, (u(x_i))_{i=1,\dots,\bar{n}}$.

2. **Compute** *the whole tree* $\big((f_k^i)_{k=1,\dots,2^{p-i}}\big)_{i=0,\dots,p}$.

3. **Initialize** $i := 0, n := 1, m := 1, r := \min(p,q)$;

$$\begin{cases} u_1^*(s,\tau) = sb - u(b-\tau) & \textit{for } s = b^*, \\ H_1^*(s,\tau) = \{b\} & \textit{and } \tau \in (f_k^0)_{k=1,\dots,2^p}. \end{cases}$$

4. **For** i=1 **to** r **do begin**

5. *Use Formula* (1.3) *to compute* $u_{X_n}^*(s,\tau)$ *and* $H_{X_n}^*(s,\tau)$, *for* $s \in S_{2m}$ *and* $\tau \in (f_k^{i-1})_{k=1,\dots,2^{p-i-1}}$.

6. *Use Formula* (1.2) *to compute* $u_{2n}^*(s,\tau)$ *and* $H_{2n}^*(s,\tau)$, *for* $s \in S_{2m}$ and $\tau \in (f_k^i)_{k=1,\dots,2^{p-i}}$.

7. Assign $n := 2n$ and $m := 2m$.

8. **End.**

9. **If** $p < q$, **then for** $i = r+1$ **to** q **do** Apply formula (1.3)

10. **If** $q < p$, **then for** $l = r+1$ **to** p **do** Apply formula (1.2)

11. **Display** *the results:* $u_{\bar{n}}^*(s,0)$ *and* $H_{\bar{n}}^*(s,0)$ *for* $s \in S_{\bar{m}}$.

If $p = q$, the steps 9 and 10 are not performed, otherwise the remaining points are computed by using only one of the two formulas.

Complexity of the FLT algorithm

We include and complete complexity computations made in [1]. In addition, we make some analogies with previous FFT complexity results [4].

To compute

$$u_{\bar{n}}^*(s,0) = \max_{x \in X_{\bar{n}}}[xs - u(x)],$$

for all s in $X_{\bar{n}}$ with a direct method, we compare the values $sx - u(x)$, x in $X_{\bar{n}}$ at every s in $S_{\bar{m}}$. Hence, we need $\theta(\bar{n}\bar{m})$ elementary operations.

For the sake of simplicity, let us we assume $\bar{n} = \bar{m}$. A straightforward computation uses $\theta(\bar{n}^2)$ elementary operations. Yet, only $\theta(\bar{n}\log_2 \bar{n})$ operations are needed if we use formula (1.3), as the following argument shows.

First, we consider how many elementary operations are needed for going from step n to step $2n$.

We use Formula (1.3) to compute $u^*_{X_n}(s,\tau)$ for all s in $S_{2m} \setminus S_m$. Since the mapping $h^*_{X_n}(.,\tau)$ is non-decreasing and takes values in X_n, we look for the maximum at, at worst, n points in

$$[h^*_{2n}(a + \frac{b-a}{2n}, \tau), h^*_{2n}(a + (2n-1)\frac{b-a}{2n}, \tau)].$$

Consequently, we compute $u^*_{X_n}(s,\tau)$ for all s in $S_{2m} \setminus S_m$ with $O(n)$ operations.

Since the set $(f^i_k)_{k=1,\dots,2^p}$ has $\bar{n}/n = 2^{p-i}$ elements, we need $O(n \times \bar{n}/n)$ operations to compute $u^*_{X_n}(s,\tau)$ for $s \in S_{2m}$ and $\tau \in (f^i_k)_{k=1,\dots,\bar{n}/n}$.

After p applications of our process, we obtain $u^*_{\bar{n}}(s,0)$ for all s in $S_{\bar{n}}$ in $O(\bar{n}\log_2 \bar{n})$ time.

Remark 1.8. We did not count the number of operations due to formula (1.2) because it is very small against the one coming from formula (1.3).

When $\bar{n} \neq \bar{m}$, we name $\bar{R} = \min(\bar{n}, \bar{m})$ and we easily obtain an $O(\bar{R}\log_2 \bar{R} + |\bar{m} - \bar{n}|\bar{R})$ complexity. The second term comes from performing steps 9 and 10 in the algorithm.

Now, if we fix $\bar{m}$ and let $\bar{n}$ tend to infinity, we obtain a linear cost: $O(\bar{n})$. In this case, a straightforward computation of the maximum, $u^*_{\bar{n}}(s,0)$, gives the same cost. Thus, the FLT algorithm is only worth applying when we want to compute a numerical approximation of u^* on the whole of $[a^*, b^*]$.

Remark 1.9. To simplify our study we assumed that $X_{\bar{n}}$ and $S_{\bar{m}}$ contained equidistant points. For the more general case we only need two functions:

$$\begin{array}{rcl} \varphi_1 : \{1,\dots,\bar{n}\} & \longrightarrow & X_{\bar{n}} \\ i & \longmapsto & x_i \end{array} \quad \text{and} \quad \begin{array}{rcl} \varphi_2 : X_{\bar{n}} & \longrightarrow & \{1,\dots,\bar{n}\} \\ x_i & \longmapsto & i \end{array}.$$

For example, letting

$$\varphi_1(x_i) = a + i\frac{b-a}{\bar{n}} \text{ and } \varphi_2(i) = \frac{x_i - a}{b-a} \times \bar{n},$$

reduces to the case of equidistant points. These functions must be quickly estimable, to avoid slowing down the algorithm.

Remark 1.10. As Brenier noted in [1], there is an analogy between the complexity of the FLT algorithm and the complexity of the Fast Fourier Transform (FFT) [4]. The FFT allows a faster computation of

$$\sum_{j=0}^{n-1} u_j e^{2i\pi jk/n}, \text{ for } k = 0, \ldots, n-1 \tag{1.4}$$

by using the special form of the matrix associated with that transformation. Taking a Fourier transform with $\bar{n} = 2^p$ points, we obtain a $O(\bar{n} \log_2 \bar{n})$ complexity. The FLT algorithm has *the same complexity.* If we write the DLT as

$$\max_{j=1,\ldots,n} [x_j s_k - u(x_j)], \text{ for } k = 0, \ldots, n-1$$

and replace the maximum by the summation and the summation by the product, we obtain a formula close to (1.4).

Numerical experiments

At the end of this chapter, we give examples of DLT computations which illustrate the convergence properties and which exhibit some numerical problems. In addition, we compare computation times of the FLT algorithm with the direct computation algorithm. We computed the convex hull of:

$$u(x) = \begin{cases} x\ln(x) & \text{if } x > 0, \\ +\infty & \text{otherwise,} \end{cases}$$

by applying twice the FLT and a straight computation algorithm, and summarized the results in Table 1.2.

1.2.2 The LLT algorithm

As for the FLT algorithm, we only need to present the 1-dimensional case. To begin with we carefully study a recursive implementation of the FLT algorithm to identify which part can be improved. In fact, that algorithm can be viewed as a Divide-and-Conquer paradigm (we use the terminology and notations of [5]).

p	FLT algorithm	Straight computation
7	1s	1s
8	1s	2s
9	3s	7s
10	8s	24s
11	18s	1min 35s
12	25s	6min 19s
13	1min 2s	23min 8s
14	1min50s	1h30min

Table 1.2: Comparison: the FLT algorithm vs straight computation.

For expository purpose we present the case where both $n = |X|$ and $m = |S|$ are even, and m is greater or equal to n. The other cases follow trivially.

A recursive version of the FLT algorithm may be described as follows:

1. **Divide step**

   Divide the set $X = \{x_i\}_{i=1,\dots,n}$ and the set $S = \{s_j\}_{j=1,\dots,m}$ in two smaller sets of roughly equal sizes: $X^o = \{x_1, x_3, \dots, x_{n-1}\}$, $X^e = \{x_2, x_4, \dots, x_n\}$, $S^o = \{s_1, s_3, \dots, s_{m-1}\}$ and $S^e = \{s_2, s_4, \dots, s_m\}$.

2. **Conquer step**

   (a) Compute recursively:

   $$u^*_{X^o}(s) = \max_{x \in X^o}[sx - u(x)] \text{ for } s \in S^o,$$
   $$u^*_{X^e}(s) = \max_{x \in X^e}[sx - u(x)] \text{ for } s \in S^o.$$

   (b) Next compute: $u^*_{X^o}(s)$ and $u^*_{X^e}(s)$ for $s \in S^e$.

3. **Merge step**

   Merge $u^*_{X^o}(s)$ with $u^*_{X^e}(s)$ to obtain:

   $$u^*_X(s) = \max_{x \in X^o \cup X^e}[sx - u(x)] \text{ for } s \in S = S^o \cup S^e.$$

Step 2b is the key of the algorithm. Since any selection $h^*_X(s) \in H^*_X(s)$ is a non-decreasing function, we can perform step 2b in $O(n + m)$ time (and at best in $\Omega(m)$ time) by using the formula:

$$u^*(s_j) = \max_{\substack{x_i \\ h^*_X(s_{j-1}) \le x_i \le h^*_X(s_{j+1})}} [x_i s_j - u(x_i)].$$

We can achieve step 1 in $O(1)$ time (since we do not have to explicitly copy the selected subsets), and step 3 in $\Theta(m)$ time. In conclusion, the complexity of the FLT algorithm is bounded above[2] by:

$$\overline{T}(n,m) = 2\overline{T}(\frac{n}{2}, \frac{m}{2}) + O(n+m) = O((n+m)\log_2(n+m)),$$

and below by:

$$\underline{T}(n,m) = 2\underline{T}(\frac{n}{2}, \frac{m}{2}) + \Omega(m) = \Omega(m\log_2(n+m)).$$

If we choose $m = n-1$ and

$$s_i = c_i = \frac{u(x_{i+1}) - u(x_i)}{x_{i+1} - x_i}, \tag{1.5}$$

for $i = 1, \ldots, m$; after two applications of the FLT algorithm we obtain the (lower) convex hull of the set of points $\{x_i, u(x_i)\}_{i=1,\ldots,n}$ in the same complexity as the incremental FLT algorithm: $\Theta(n\log_2 n)$.

At first sight the FLT algorithm does not seem to need the input data to be pre-sorted along the x-axis. However to use Lemma 1.1, we need the sequence $(x_i)_i$ to be increasing. Indeed, knowing two indices i_1 and i_2, we want to generate the set $\{x_i \,:\, x_{i_1} \le x_i \le x_{i_2}\}$ without looking at the whole sequence.

Consequently first we have to sort the sequence $(x_i)_{i=1,\ldots,n}$ and only then can we apply the FLT algorithm. Since sorting requires $\Theta(n\log_2 n)$ time, the FLT algorithm enjoys the same complexity when applied to the general convex hull problem (when the input data are not assumed to be pre-sorted along the x-axis).

Noticing that sorting is as hard as finding the convex hull [16] (both calculations have the same complexity), we may apply the Ultimate Planar Convex Hull Algorithm [10] to do both sorting and computing the convex hull instead of

[2] Since $(\log_2 n + \log_2 m)/2 \le \max(\log_2 n, \log_2 m) \le \log_2(n+m) \le \log_2 n + \log_2 m$ with $n, m \ge 2$, we have: $O(\log_2 n + \log_2 m) = O(\max(\log_2 n, \log_2 m)) = O(\log_2(n+m))$.

only sorting. That would reduce the computation time greatly when there are much fewer vertices than input points, but the worst case time complexity would be the same: $O(n \log_2 h)$ with h the number of vertices of the convex hull.

We note that there is a transformation in $O(n)$ operations that changes the convex hull problem in computing the discrete Legendre–Fenchel transform. Since we know that the former requires $\Theta(n \log_2 n)$ operations [5], we deduce that the later has the same lower bound (this is a straightforward application of Proposition 1, p29, of [16]). We summarize the links between the computation of the convex hull and the DLT on Figure 1.2.2. Eventually a pre-computation can improve the FLT algorithm which would become *optimal* with respect to both n and h instead of being optimal only with respect to n.

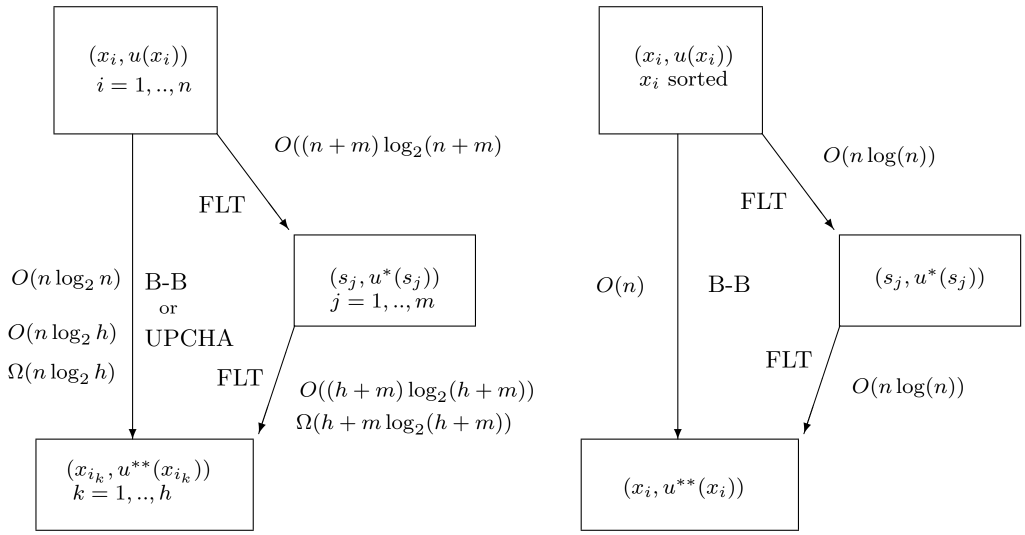
There is an interesting particular case when the sequence $(x_i)_i$ is non-decreasing. In this case, we can compute the convex hull in *linear-time* by using the Divide-and-Conquer or the Beneath-Beyond algorithms [5] (others may be used, see Part 4.14 in [16]).

The basic motivation of our approach is to find an algorithm to compute the discrete Legendre–Fenchel transform *faster* than the FLT algorithm *when the sequence* $(x_i)_i$ *is non-decreasing*. This situation is illustrated with Figure 1.2.2.

We show in section 1.2.2 that the LLT algorithm runs in $\Theta(n + m)$ time when the sequence $(x_i)_i$ is non-decreasing (this is a trivial lower bound since we obviously need to read all our input data at least once). Thus, when we choose our slopes as in (1.5), we can compute the discrete Legendre–Fenchel transform in $\Theta(n)$ time and the *LLT is optimal*.

To conclude, in the general case the LLT algorithm and the FLT algorithm have the same worst-case time complexity. However, when the input data is sorted along an axis, the LLT algorithm has a better worst-case time complexity and is, indeed, optimal.

In addition to the worst-case analysis, we can easily give an average case analysis when the sequence $(x_i)_i$ is not assumed increasing.



(a) The general case (b) The particular case

Figure 1.1: Computation time of the FLT algorithm.

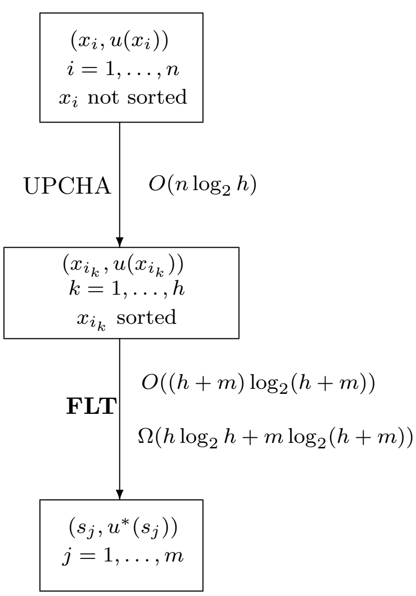


Figure 1.2: Improved computation time of the FLT algorithm.

For a positive number p with $p < 1$, we consider a distribution whose expected number of extreme points in a sample of size n is $O(n^p)$. This set of distributions includes uniform distributions in a convex polygon, uniform distributions on a circle and normal distributions on the plane. The convex hull of a sample of n points may be computed with $O(n)$ operations (Theorem 4.5 in [16]). If we add the complexity of the LLT algorithm, the DLT is obtained with an average time complexity of $O(n + m)$.

Consequently, computing the discrete Legendre Transform by first preprocessing the points with a convex hull algorithm, next applying the LLT algorithm has a *linear expected time*.

In addition, if one does not need great accuracy, faster computation can be achieved by using approximate convex hull algorithms (see Part 4.1.2 of [16]).

In fact, all the algorithms built for the planar convex hull problem can be straightforwardly applied to our framework. For example if the data points are the n vertices of a simple polygon, the convex hull can be constructed in $\Theta(n)$ operations (Theorem 4.12 in [16]); thus the LLT algorithm runs in linear-time in this case.

We now give the theoretical basis of the LLT algorithm, followed by a full description of the algorithm. We prove complexity results and compare them with numerical experiments.

Theoretical foundation

The reader should not be confused by talking about planar version of the LLT algorithm, which refers to the geometrical point of view (our data $(x_i, u(x_i))$ belongs to the plane) and the one dimensional version of the LLT algorithm which refers to the functional point of view (u is a univariate function). Both phrases refer to the basic version of the LLT in the same one-dimensional setting.

We take some input data of the following form: $P_i = (x_i, u(x_i))$ is a point in the plane, where $(x_i)_{i=1,\dots,n}$ are real numbers and u is a real-valued function of the real variable. We do not assume any property on u (although it needs to be upper semi-continuous to ensure the convergence of the discrete Legendre–Fenchel transform to u^*). To simplify the presentation and point out the discrete setting of this section, we will sometimes use the notation $y_i = u(x_i)$.

We consider two different cases.

- First we do not assume any additional property, we name this the general case. We do some preprocessing by applying the Ultimate Planar Convex Hull algorithm [10] to obtain the increasing sequence of vertices belonging to the convex hull in $O(n \log_2 h)$ time. We consider that sequence as input data to the LLT algorithm.

- Secondly we assume that the sequence $(x_i)_{i=1,\ldots,n}$ is already sorted. The preprocessing step in this case consists of applying the Beneath-Beyond algorithm [5] to build the sequence of vertices of the convex hull in $O(n)$ time.

Eventually, the only difference lies in the preprocessing step. To describe the main part of the LLT algorithm, we assume that, after a pre-processing step, the sequence $(x_i)_{i=1,\ldots,n}$ is increasing such that the points $(P_i)_{i=1,\ldots,n}$ are vertices of the hull and no three points are collinear. We note that this is equivalent to taking the points P_i on the graph of a convex function, so we may assume that u is convex (if it is not, we apply the algorithm to its convex hull computed in the pre-processing step).

The only data needed in the space of slopes is an increasing sequence of slopes $(s_j)_{j=1,\ldots,m}$. Now, using the convexity property of u, we build a new sequence:

$$c_i = \frac{u(x_{i+1}) - u(x_i)}{x_{i+1} - x_i},$$

for $i = 1, \ldots, n-1$. We recall the set-valued mapping:

$$H_X^*(s) = \operatorname*{Argmax}_{i=1,\ldots,n}(sx_i - u(x_i)),$$

which gives all the points of the x_i sequence where the maximum is attained.

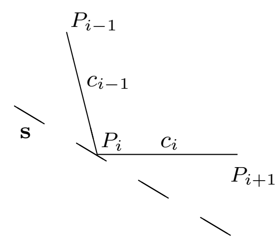


Figure 1.3: The line with slope s goes through P_i and no other point P_j, $i \neq j$.

We claim that computing

$$u_X^*(s_j) = \max_{i=1,\dots,n} [s_j x_i - u(x_i)]$$

for all $j = 1, \dots, m$, amounts to merging the two sequences $(s_j)_{j=1,\dots,m}$ and $(c_i)_{i=1,\dots,m-1}$.

Lemma 1.2.

$$\textit{If } c_{i-1} < s < c_i,\ H_X^*(s) = \{x_i\}.$$

$$\textit{If } c_i = s,\ H_X^*(s) = \{x_i, x_{i+1}\}.$$

Proof. We suppose $c_{i-1} < s < c_i$. Since the sequence $(c_k)_{k=1,\dots,n-1}$ is increasing, we obtain for $k = 2, \dots, i$:

$$\frac{y_k - y_{k-1}}{x_k - x_{k-1}} < s,$$

which implies $sx_k - y_k > sx_{k-1} - y_{k-1}$. So we obtain the following inequalities:

$$sx_i - y_i > sx_{i-1} - y_{i-1} > \cdots > sx_1 - y_1.$$

Using $s < c_i$ gives:

$$sx_n - y_n < sx_{n-1} - y_{n-1} < \cdots < sx_i - y_i.$$

We illustrate this case with Figure 1.3. Consequently $sx_i - y_i$ is the strict maximum of the sequence $(sx_k - y_k)_k$, which proves the first part of the lemma.

For the second part, we use the same arguments as above to deduce:

$$sx_1 - y_1 < \cdots < sx_{i-1} - y_{i-1} < sx_i - y_i = sx_{i+1} - y_{i+1} < \cdots < sx_n - y_n,$$

which implies the last part of the lemma. Figure 1.4 illustrates this case. □

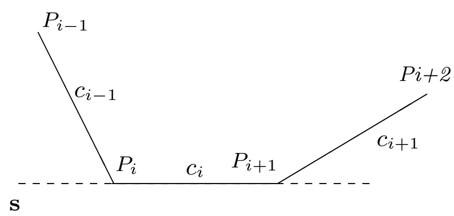


Figure 1.4: The line with slope s goes through P_i and P_{i+1}.

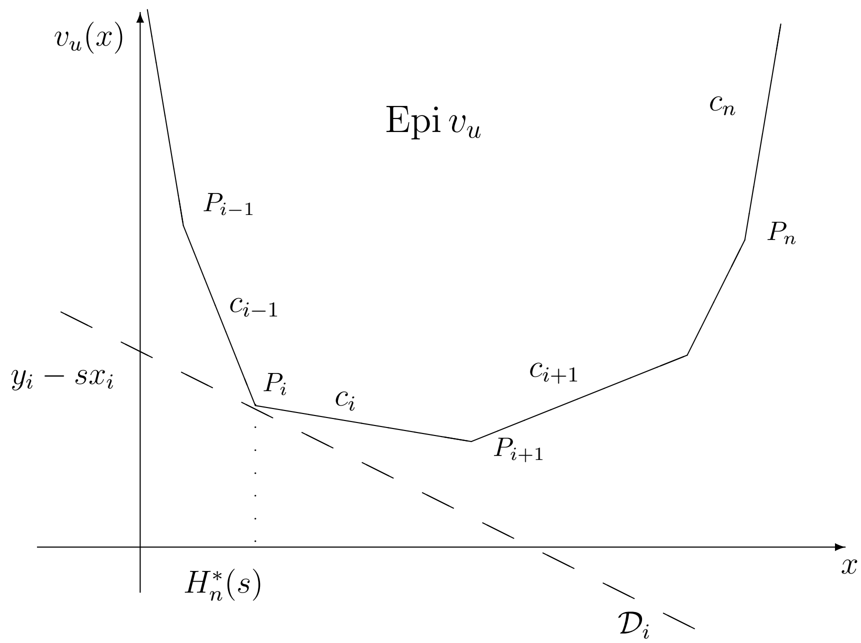


Figure 1.5: Geometric interpretation of the LLT algorithm.

Remark 1.11 (Geometric interpretation). The lemma strongly relies on the convexity assumption: it is a consequence of the monotone property of the subdifferential.

We define v_u as the piecewise affine function going through each point P_i, and extend it linearly outside of $[x_1, x_n]$. Figure 1.5 shows its graph.

The function v_u is convex and its subdifferential is:

$$\partial v_u(x) = \begin{cases} \{c_i\} & \text{if } x \in (x_i, x_{i+1}), \\ [c_i, c_{i+1}] & \text{if } x = x_{i+1}, \\ \{c_1\} & \text{if } x \in (-\infty, x_1), \\ \{c_n\} & \text{if } x \in (x_n, +\infty). \end{cases}$$

The epigraph of v_u intersects its support line with slope s, $\mathcal{D}$, at

$$\operatorname{co} H_X^*(s) \times v_u(\operatorname{co} H_X^*(s)).$$

Since the line $\mathcal{D}$ goes through a point P_i, its equation can be written $y = s(x - x_i) + y_i$. So $\mathcal{D}$ cuts the y-axis at $(0, y_i - sx_i)$. Computing the Legendre–Fenchel transform amounts to finding the point P_i where $y_i - sx_i$ is minimum.

The LLT algorithm

We give here an incremental implementation of the LLT algorithm. Our input data consists of: $y_i = u(x_i)$, $P_i = (x_i, y_i)$ and s_j for $i = 1, \ldots, n$ and $j = 1, \ldots, m$.

Step 1 The Ultimate Planar Convex Hull algorithm or the Beneath-Beyond algorithm are used in a pre-processing step to build the convex hull of $(P_i)_i$. We name the resulting sequence so that $(P_i)_{i=1,\ldots,h}$ is the sequence of vertices of the convex hull.

Step 2 We use Lemma 1 to **compute** $H_X^*(s_j)$ for all $j = 1, \ldots, m$ with the following algorithm:

1. $i := 1; j := 1;$
2. While ($s_j < c_{n-1}$ and $i < n$ and $j \leq m$) do
   (a) While $s_j > c_i$ do $i := i + 1$;
   (b) If $s_j = c_i$ then $H_X^*(s_j) := \{x_i, x_{i+1}\}; i := i + 1$; else $H_X^*(s_j) := \{x_i\}$
   (c) $j := j + 1$;
3. for $k = j$ to m do $H_X^*(s_j) := \{x_n\}$.

If one prefers a parallelizable algorithm, a Divide-and-Conquer paradigm can be used to merge both sequences $(c_i)_{i=1,\ldots,n}$ and $(s_j)_{j=1,\ldots,m}$.

Complexity of the planar LLT algorithm

In the general case (the points P_i are not assumed to be the vertices of the convex hull) we denote by h the number of vertices of the hull.

Proposition 1.6. *Step 1 takes $O(n \log_2 h)$ time in the general case, and $O(n)$ time otherwise. Step 2 takes $O(h+m)$ time .*

Proof. The complexity of step 1 is proved in [5, 10]. Merging two ordered sequences is well-known to take $O(h+m)$ time. □

Remark 1.12. Even if in the case

$$s_1 < \cdots < s_m < c_1 < \cdots < c_n,$$

we have a $\Omega(m)$ complexity, the most accurate numerical results are obtained when:

$$c_1 < s_1 < c_2 < s_2 < \cdots < s_{m-1} < c_n < s_m.$$

Then the LLT algorithm takes $\Omega(n+m)$ time.

Remark 1.13. In the second case (the x_i are already sorted), if we fix m we compute the DLT in $O(h)$ time. This is the best known and possible result since we have to read our data at least once. In Section 1.2.1, we saw that the FLT algorithm shares the same complexity. In fact it is the same as doing a straightforward computation of $\max_i[sx_i - y_i]$. However in the convex case we do not have to look at all the input data. In this case, a Divide-and-Conquer paradigm gives the result in $O(\log_2 h)$ time (this is equivalent to inserting a real number in an already sorted real sequence).

Remark 1.14. The main point of any algorithm which computes the discrete Legendre–Fenchel transform is to merge two sequences $(c_i)_i$ and $(s_j)_j$. By preprocessing both sequences, we can assume they are both increasing. As for the multiplicative constant in $O(n+m)$, our algorithm has the best possible one when $n = m$. In another setting, Knuth [11] looked for the algorithm with the best possible constant with respect to $n - m$.

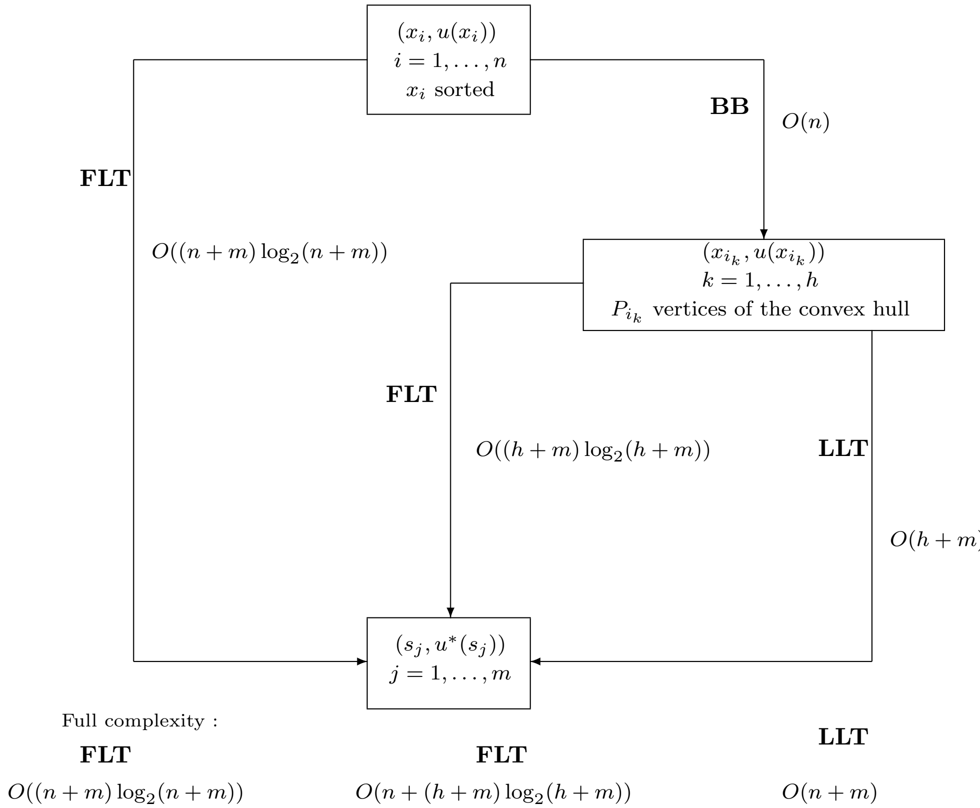
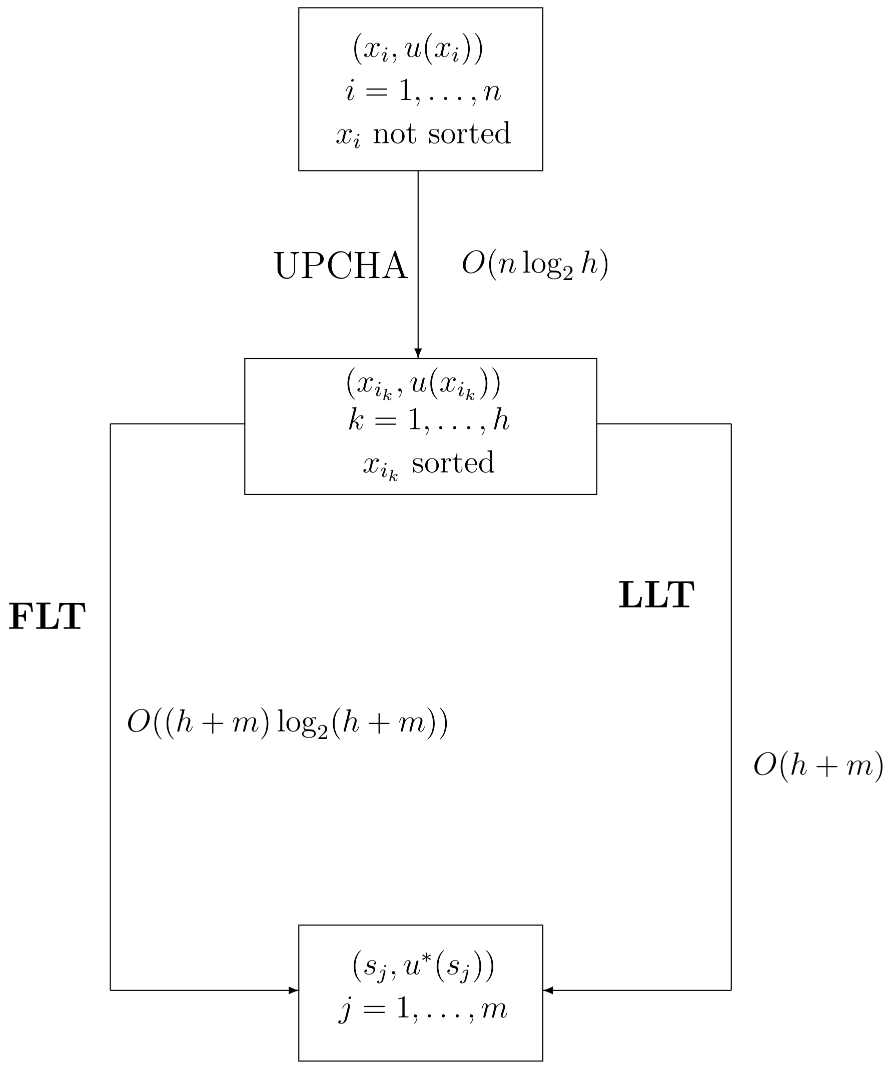


Figure 1.6: Comparison FLT vs LLT with input data sorted along the x-axis.

Remark 1.15. If we assume the $(x_i, u(x_i))_i$ are already vertices of the convex hull, we still have a $O(n+m)$ complexity. In other words, computing the convex hull does not take more time than computing the DLT.

The LLT algorithm runs clearly faster than the FLT algorithm. First, we consider the particular case when the sequence $(x_i)_i$ is increasing. We describe the three possibilities in Figure 1.6. The LLT algorithm with a linear complexity is far better than the FLT algorithm applied with or without pre-computing the convex hull. Next we illustrate the general case in Figure 1.7. The LLT algorithm runs in $O(n\log_2 h + m)$ time vs $O((n+m)\log_2 h + (m+h)\log_2 m)$ for the FLT algorithm.

In conclusion the LLT algorithm runs faster. However the FLT algorithm permits to compute the convex hull with an optimal worst-case time complexity, whereas the LLT algorithm cannot. In fact, the FLT algorithm may be used for



Full complexity :

FLT	**LLT**
$O((n+m)\log_2 h + (m+h)\log_2 m)$	$O(n \log_2 h + m)$

Figure 1.7: Comparison FLT vs LLT in the general case.

two various purposes —computing the DLT or the convex hull— while the LLT algorithm can only compute the DLT. Since we aim at computing the DLT in the plane, the planar LLT algorithm has the best worst-case time complexity with respect to n, h and m.

Numerical experiments

We present here numerical experiments made with the package Maple V release 3 with 10 digits accuracy. We implemented the LLT algorithm and recorded the average CPU time (in seconds) taken by the algorithm for several values of n and m.

As input data we took the convex function $u(x) = x^2/2 + x\ln(x) - x$ with $x_i = 10i/n$ and $s_j = -5 + 10j/m$.

Figure 1.8 presents our results. We took $n = m$ and drew the least-squares line. Figure 1.9 shows the entire graph when $n = 4, \dots, 30$ and $m = 4, \dots, 30$. The equation of the least-squares plane is:

$$(x, y) \mapsto 0.00033\, x + 0.0014\, y + 0.04.$$

The maximum relative error between the computation time and the least-square plane is only .14. Hence the computation time is clearly linear.

Beyond the plane

Remark 1.16. The decomposition

$$\max_{(x_1,x_2)\in\mathbb{R}^2}[\langle s, x\rangle - u(x)] = \max_{x_1\in\mathbb{R}}[s_1x_1 + \max_{x_2\in\mathbb{R}}[s_2x_2 - u(x_1, x_2)]]. \tag{1.6}$$

is not symmetric. If we factorize

$$u^*(s_1, s_2) = \max_{x_2}[s_2x_2 + \max_{x_1}[s_1x_1 - u(x_1, x_2)]], \tag{1.7}$$

we obtain a $O(n_1n_2 + m_1m_2 + m_1n_2)$ complexity for the particular case. Indeed, the order of the decomposition has a clear effect on the complexity. If $n_1m_2 > m_1n_2$ we should use formula (1.7), otherwise formula (1.6) gives faster computations.

Table 1.3 illustrates this case. We computed the same discrete Legendre transform by using both formulas. The first four columns show the size of the

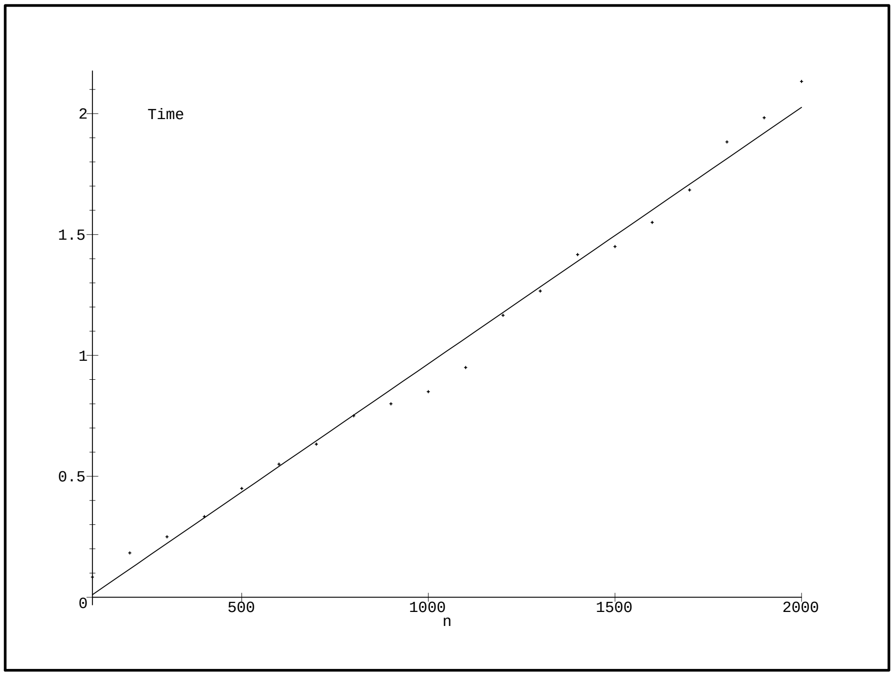


Figure 1.8: Linear computation time of the LLT algorithm when $n = m$.

two meshes, the fifth shows the computation time and the last column displays an approximation of the theoretical number of elementary operations.

We note that the algorithm is sensitive to $\tilde{h}_1$ and h_2, the vertices of the computed convex hulls. Consequently, factorizing in one way or the other may greatly affects the computation time when there are few vertices on the hull in one direction and many in the other.

The numerical results clearly confirm our theoretical study. Besides one can easily find the fastest way to do the computation by looking at the formula for the resulting time complexity.

Remark 1.17. When applying the LLT algorithm in two or higher dimensions, we can choose X without a grid-like structure but S has to have a grid-like structure. Indeed

$$\max_{x_2 \in X_2} [s_2 x_2 - u(x_1, x_2)]$$

already depends on X_1, so assuming x_2 depends on X_1 is not an additional

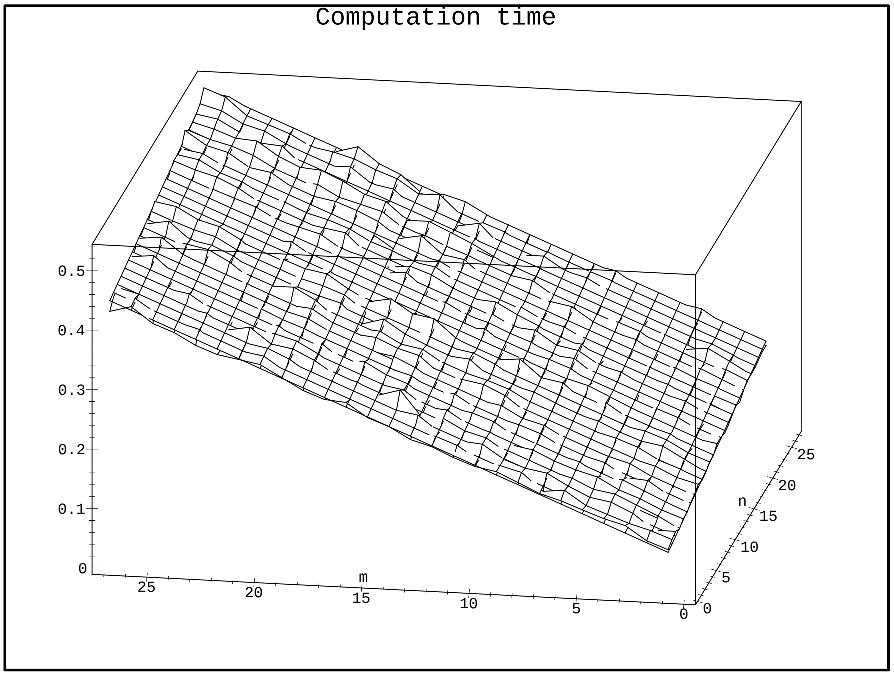


Figure 1.9: Linear computation time of the LLT algorithm.

constraint. However considering that s_2 depends on S_1 is an additional constraint since we would have to compute the maximum for all s_1 in S_1.

To sum up our argument, we can consider a general mesh for the primal points, which allows to concentrate on singular values, but the slopes domain *must* be a boxed set.

Remark 1.18. In the multi-dimensional setting, one could think of applying twice the LLT algorithm to compute the convex hull. Indeed, the multi-dimensional LLT algorithm uses only a planar convex hull algorithm. However this is not so straightforward. For $d = 3$, if we could easily choose $s \in S \subset \mathbb{R}^3$ such that applying twice the LLT algorithm gives $(x, u^{**}(x))$ for $x \in X$. Then the convex hull would be obtained in $O(n \log_2 n)$ time, which is not possible. Indeed the worst-case lower bound is $\Omega(n^2)$ (the Beneath-Beyond algorithm is optimal in that case [5]).

Remark 1.19. If $u(x_1, x_2) = u_1(x_1) + u_2(x_2)$ and u_1, u_2 are convex, no convex hull

Table 1.3: Comparison of time computation with respect to the order of computation.

n1	n2	m1	m2	Time in s.	n1*n2+m1*m2+n1*m2
10	20	10	10	0.5	400
20	10	10	10	0.7	500
30	10	10	20	1.9	1100
30	10	20	10	1.3	800
10	30	10	20	1.0	700
10	30	20	10	0.8	600
100	10	10	100	27.2	12000
10	100	100	10	2.6	2100

need to be computed to apply the LLT algorithm. Indeed for any $x_1 \in X_1$ the set

$$\{(x_2, u(x_1, x_2)) \ : \ x_2 \in X_2\}$$

is convex (because u_2 is convex). Since u_1 is convex the set

$$\{(x_1, -\max_{x_2 \in X_2}[s_2 x_2 - u(x_1, x_2)]) \ : \ x_1 \in X_1\}$$

is also convex.

Figure 1.10 shows that the running time of the LLT algorithm grows up linearly with respect to the number of points, when the input data is already sorted along each axis. We took $n_1 = n_2 = m_1 = m_2$, $u(x, y) = (x^2 + y^2)/2$ on $(-10, 10] \times (-10, 10]$, and a uniform partition on $(-10, 10] \times (-10, 10]$.

Conclusion

First computing the convex hull, next the DLT clearly improves the computation time. Not only do we obtain a linear-time complexity when our input data are sorted along each axis, but also can we use the best convex hull algorithm for our particular input data.

In the planar case, both the LLT algorithm and the FLT algorithm are worst-case time optimal in the general case, although the LLT algorithm is much faster as Figure 1.8 and 1.6 show.

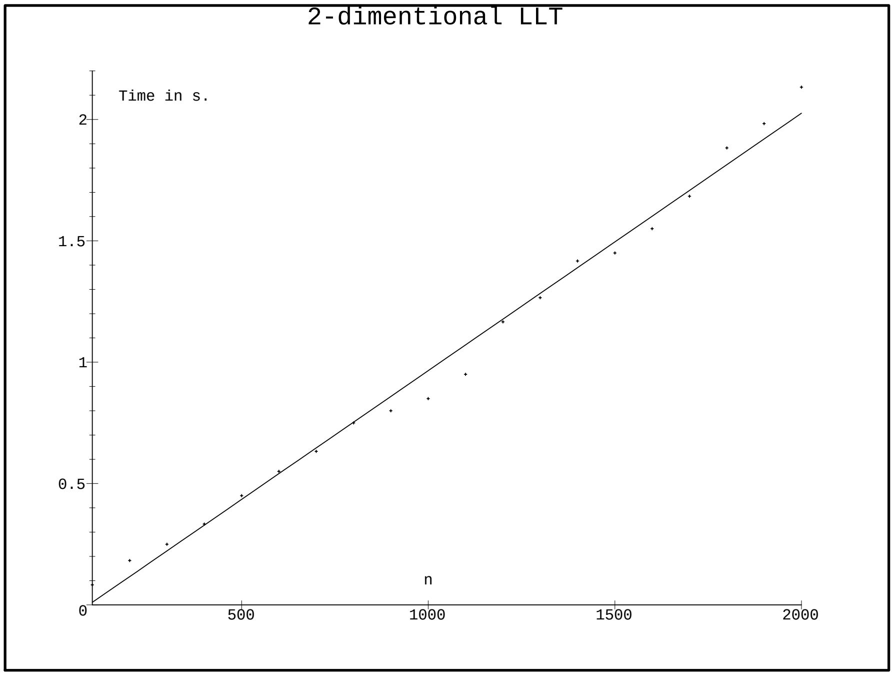


Figure 1.10: Linear computation time for n^2 input data points.

In higher dimensions, we only need to compute several planar discrete Legendre–Fenchel transforms. The order in which we compute them greatly affects the complexity; a clever choice can speed up all computations as Table 1.3 shows.

1.3 Applications

We can compute accurate numerical approximations of the Legendre–Fenchel transform and of all computations involving it. For example the inf-convolution or epigraphic sum:

$$f \Box g(x) = \inf_{y \in \mathbb{R}} [f(y) + g(x - y)]$$

of two convex functions f and g can be reduced to several Legendre–Fenchel computations. We suppose f and g are underestimated by an affine function, we obtain:

$$(f \Box g)^* = f^* + g^*.$$

When $f \Box g$ is lower semi-continuous (this is always true in the one-dimensional case), we can write:

$$f \Box g = (f^* + g^*)^*. \tag{1.8}$$

Corrias [3] deduced numerical solutions of some Hamilton–Jacobi equations involving inf-convolutions. Figure 1.18 is an example of such a computation. In fact the set-valued function

$$x \mapsto \operatorname*{Argmin}_y [f(y) + g(x - y)]$$

is monotone, so Corrias built an algorithm in $O(|X| \log_2 |X|)$ with the same argument we used for the FLT algorithm. However using formula (1.8) and the LLT algorithm, we obtain a linear-time algorithm.

The deconvolution or epigraphic star-difference [7] of a lower semi-continuous convex function f by another lower semi-continuous convex function g can be written under the technical hypothesis:

$$\text{there are } x_0, r_0 \text{ such that for all } x \text{ in } \mathbb{R}\ ,\ f(x) \leq g(x - x_0) + r_0\ ;$$

as:

$$f \Diamond g(x) = \sup_{y \in \mathbb{R}} [f(y) - g(y - x)] = (f^* - g^*)^*.$$

Figure 1.20 illustrates a deconvolution computation.

Others applications are being considered, we put in Section 1.4 numerous graphical examples. In particular Figure 1.21 comes from a chemistry problem. In the future, we plan to apply the DLT in multi-fractal analysis [12].

1.4 Graphical illustrations of the DLT

When there is no explicit formula for the conjugate we can still compute a numerical approximation as shown in Figure 1.11 produced with the Maple numerical package. The Lambert function W is defined as the inverse function of $x \mapsto x\exp(x)$ on $]0,+\infty[$ (see [2]). We took:

$$u(x) = x\log(x) + \frac{x^2}{2} - x,$$
$$u^*(s) = \frac{1}{2}[W(e^s)]^2 + W(e^s).$$

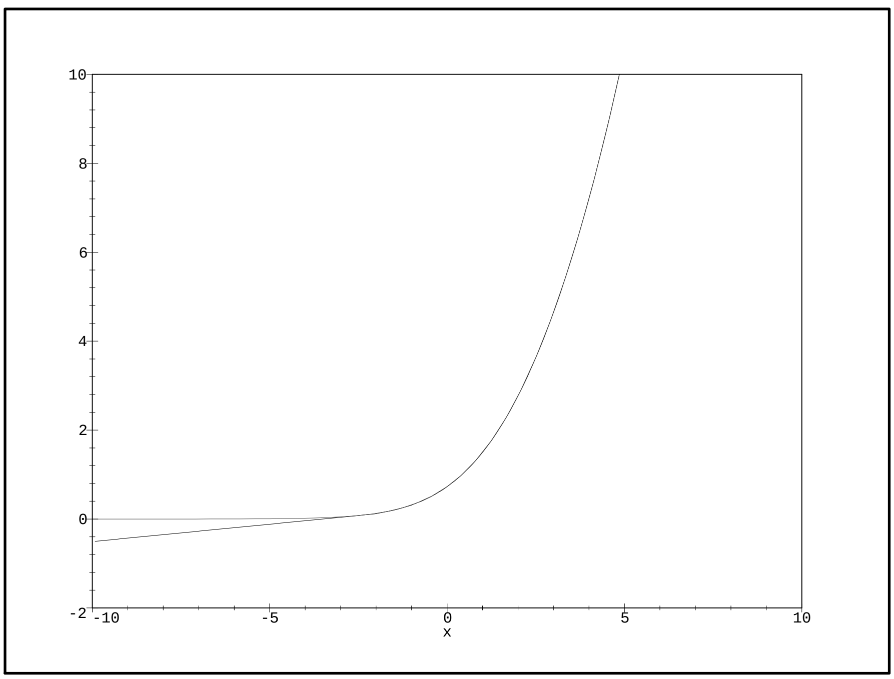


Figure 1.11: Application of Legendre's formula when u^* cannot be explicitly written with standard functions.

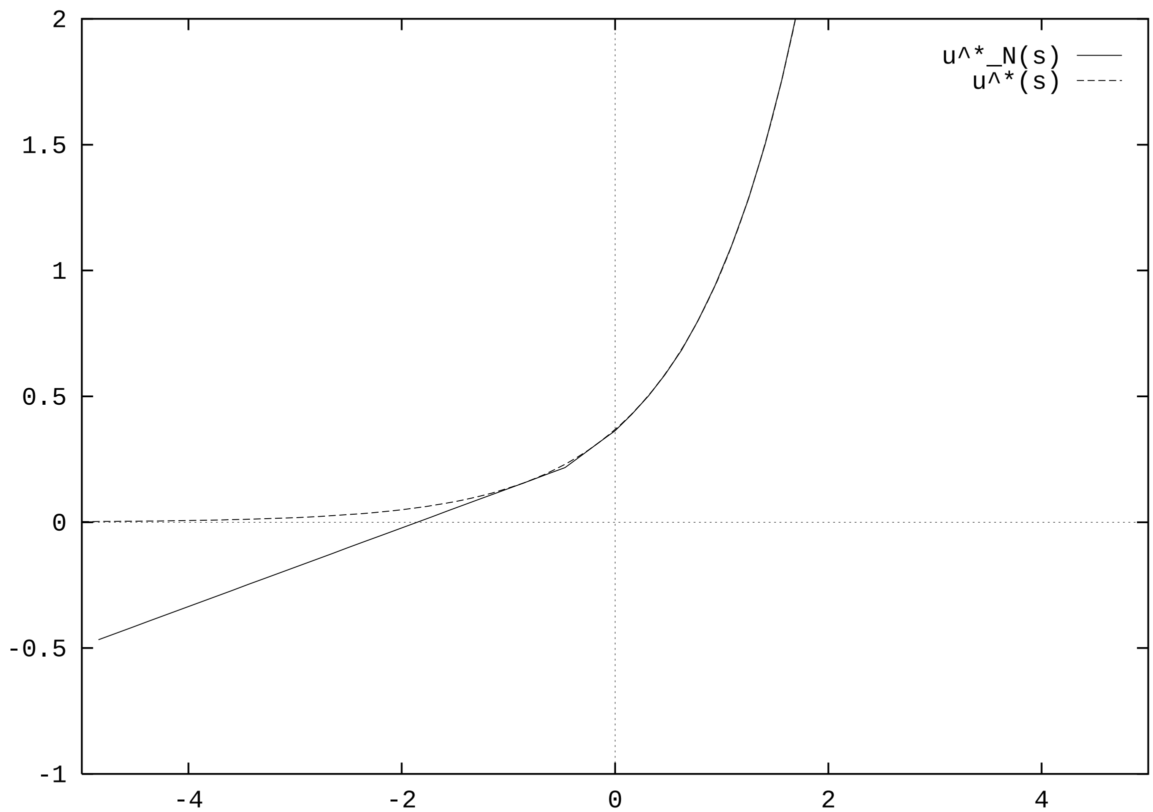


Figure 1.12: Case u is an extended real-valued function

$$u(x) = \begin{cases} x\log(x) & \text{if } x > 0, \\ +\infty & \text{otherwise.} \end{cases}$$

$$u^*(s) = e^{s-1}$$

To obtain the desired convergence, we must take greater values of N. The problem here comes from the vertical tangent at the origin which prevents the supremum in the computation of the conjugate u^* from being attained.

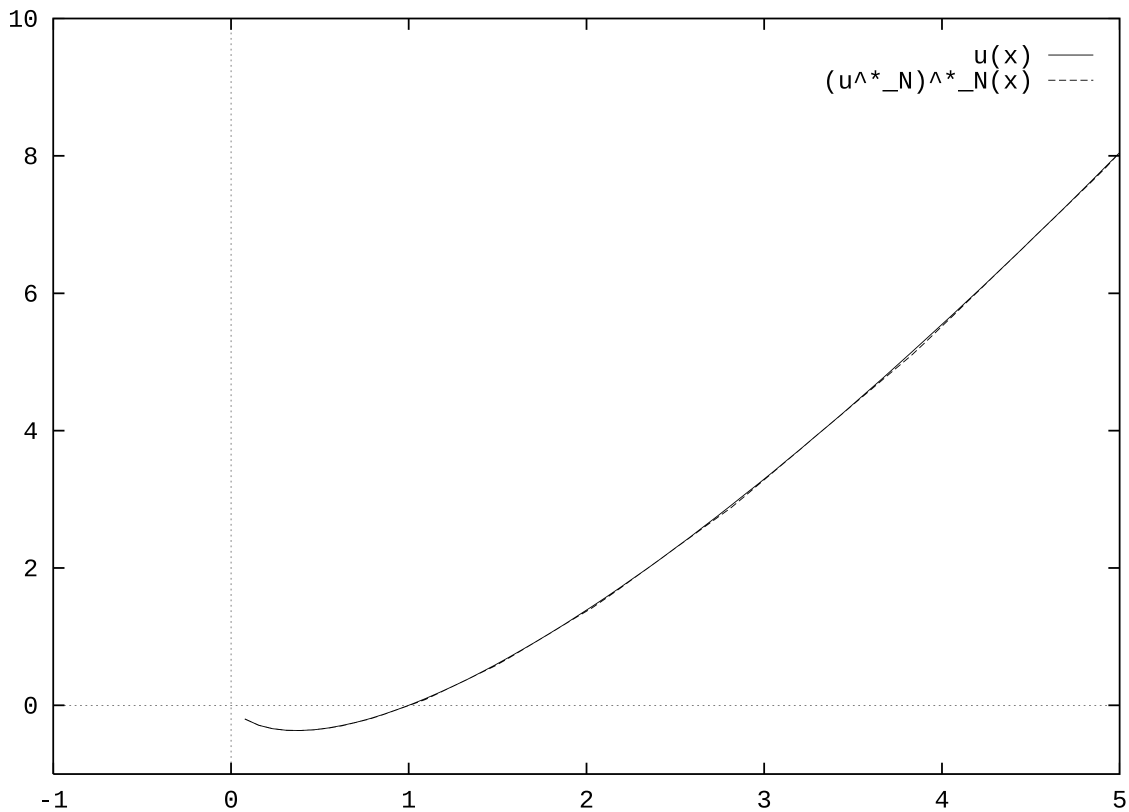


Figure 1.13: Case u is an extended real-valued function.

$$u(x) = \begin{cases} x\log(x) & \text{if } x \geq 0, \\ +\infty & \text{otherwise;} \end{cases}$$

$$u^{*}_{X}{}^{*}_{X}(x) = \max_{s \in S}[xs - u^{*}_{X}(s)],$$

$$u^{**} = u.$$

We obtain a very accurate numerical estimate of u^{**}.

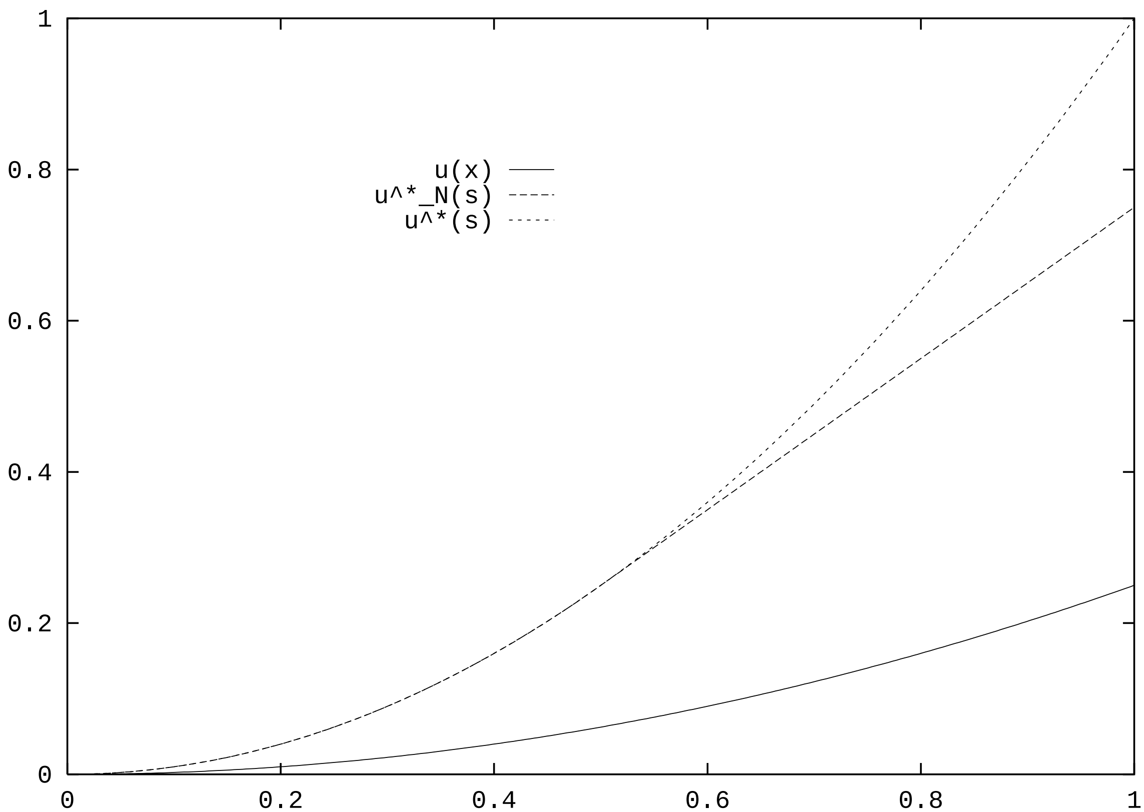


Figure 1.14: Gap between u^* and u^*_X

$$u(x) = \frac{x^2}{4},$$
$$u^*(x) = x^2.$$

The supremum is not always reached in the interval $[a, b]$: that creates the difference between the graph of the conjugate and the approximation computed. The key is to take larger intervals to obtain the convergence.

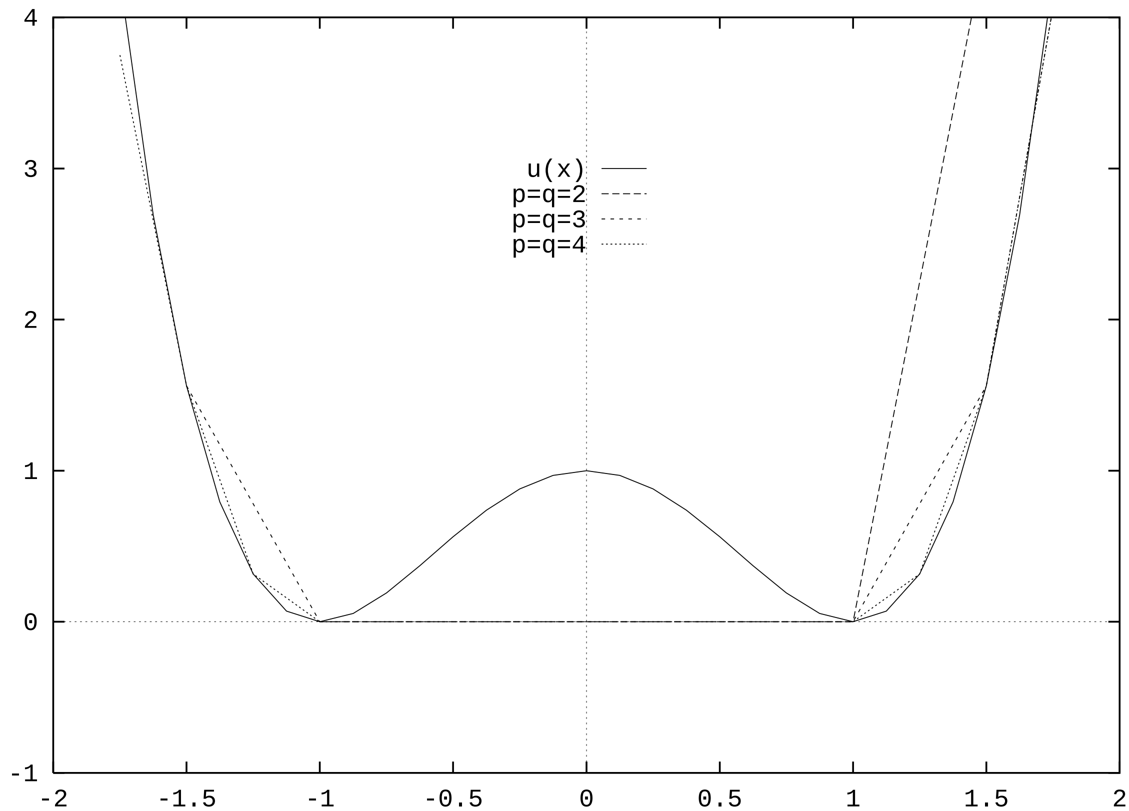


Figure 1.15: Convergence of $u^{*}_{X}{}^{*}_{X}$ towards u^{**} when p goes to infinity

$$u(x) = (x^2-1)^2,$$

$$u^{**}(x) = \begin{cases} (x^2-1)^2 & \text{if } |x| \geq 1, \\ 0 & \text{if } |x| \leq 1. \end{cases}$$

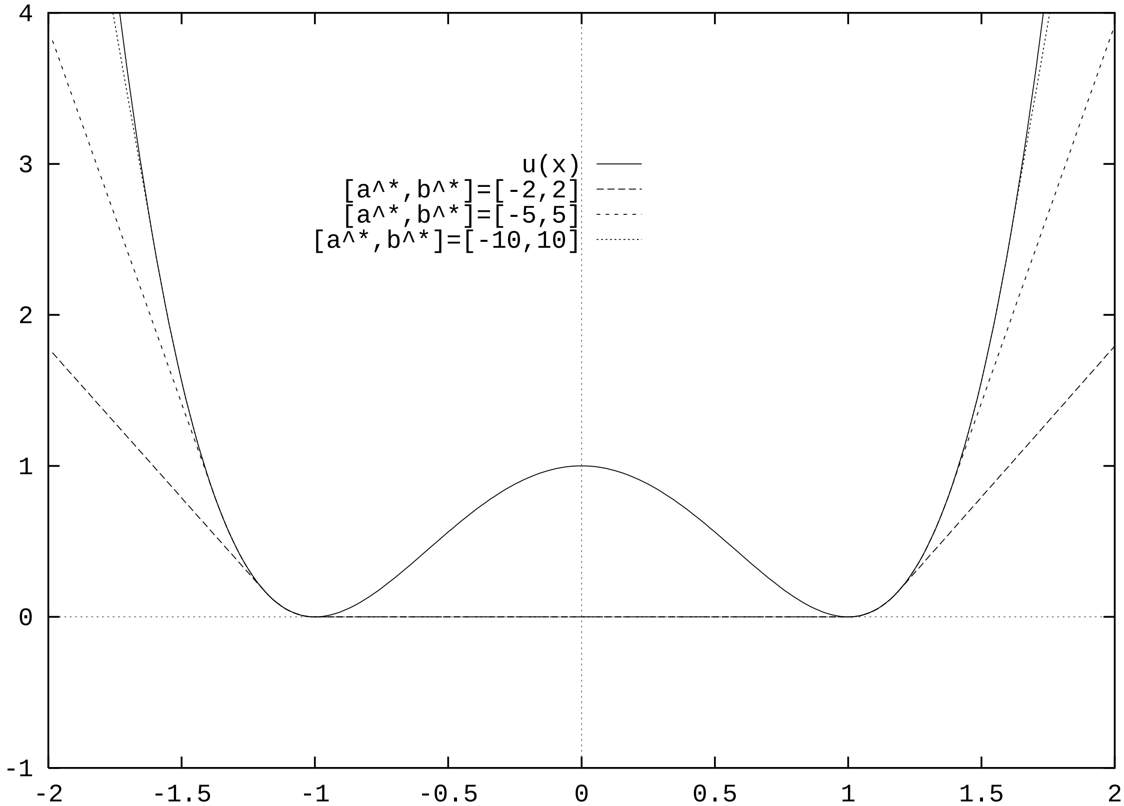


Figure 1.16: Convergence of u^{**}_{XX} towards u^{**}.

$$u(x) = (x^2 - 1)^2,$$

$$u^{**}(x) = \begin{cases} (x^2-1)^2 & \text{if } |x| \geq 1, \\ 0 & \text{if } |x| \leq 1. \end{cases}$$

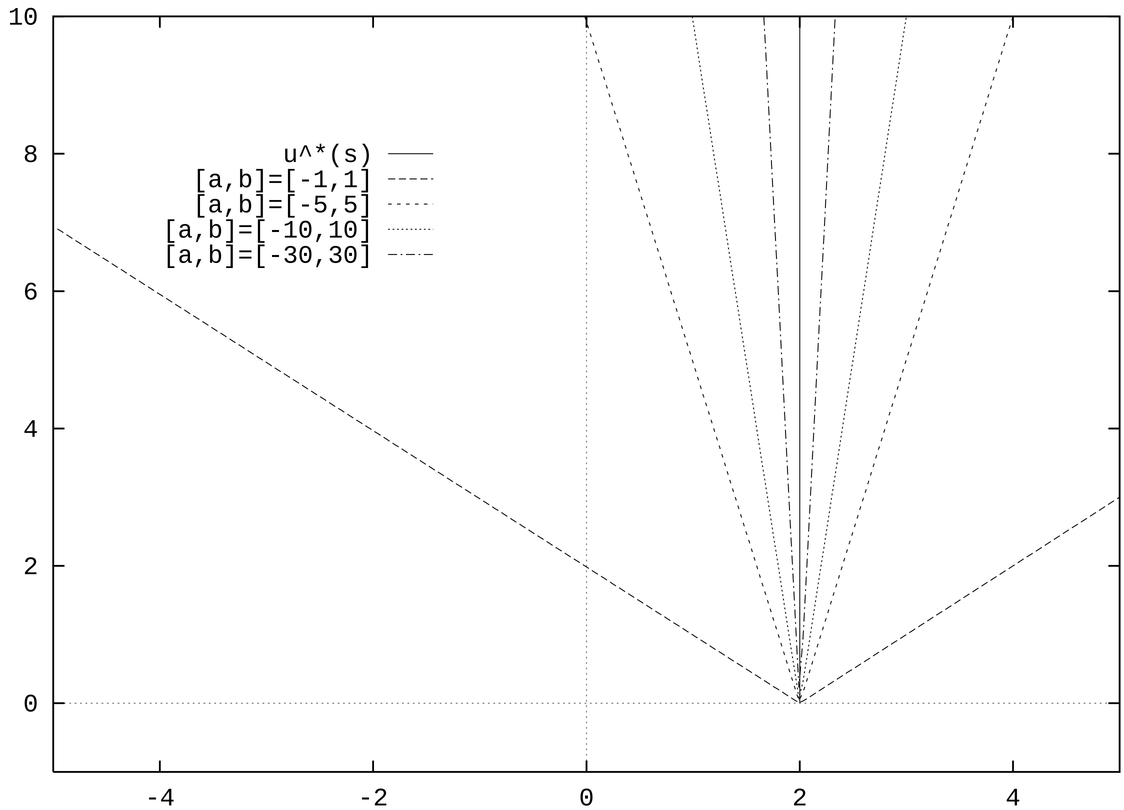


Figure 1.17: Convergence of u^*_X towards u^*.

$$u(x) = 2x,$$
$$u^*(s) = I_{\{2\}}(s).$$

This simple example shows that we can even approximate indicator functions. The graph of the approximate converges towards a vertical line.

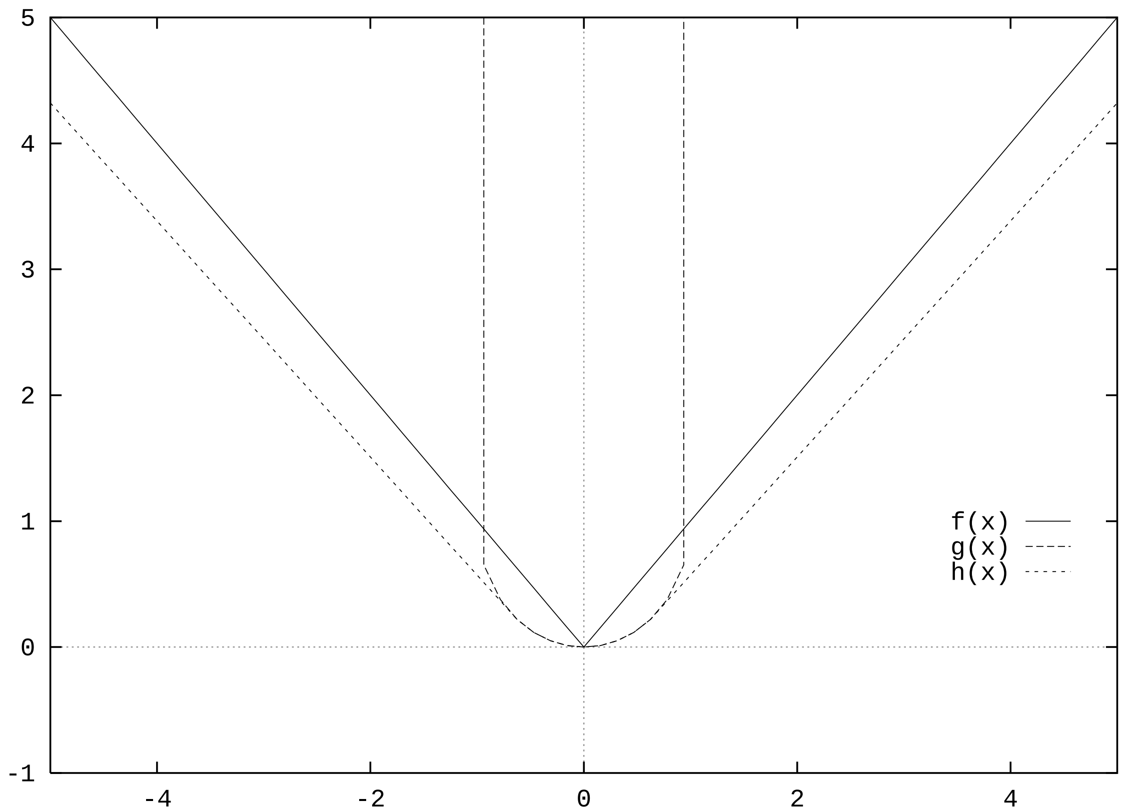


Figure 1.18: Inf-convolution computation

$$f(x) = |x|,$$
$$g(x) = \begin{cases} 1 - \sqrt{1 - x^2} & \text{if } x \in [-1, 1], \\ +\infty & \text{otherwise,} \end{cases} \qquad h(x) = (f \Box g)(x).$$

The function g is the so-called "Ball Paint function" (see Chap. I, page 12 in [7]). It is a regularization kernel. In this example, it smoothes the discontinuity at the origin.

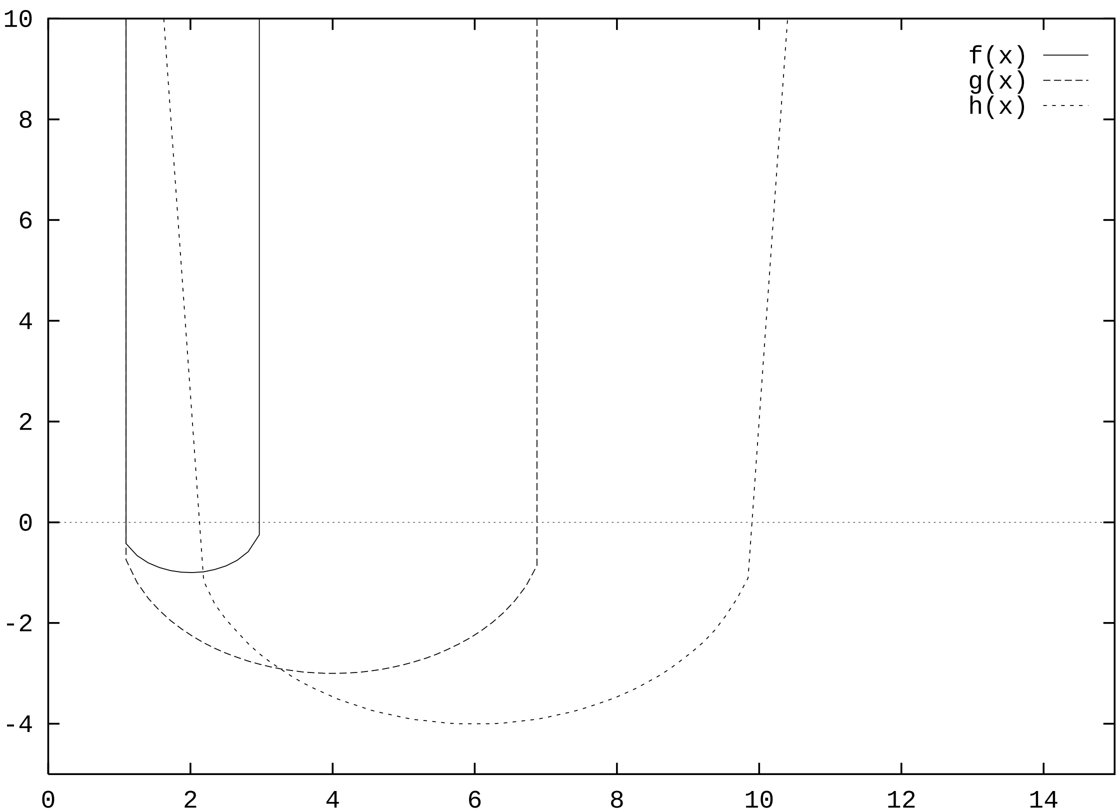


Figure 1.19: Inf-convolution computation

$$f_{a,c}(x) = \begin{cases} -\sqrt{a^2 - (x-c)^2} & \text{if } |x-c| \le a, \\ \infty & \text{otherwise;} \end{cases}$$

$$f_{1,2} \Box f_{3,4} = f_{4,6},$$

$$f = f_{1,2} \qquad g = f_{3,4} \qquad h = f_{4,6}.$$

This is an example of an inf-convolution. This family of "Ball Paint functions" is stable under the inf-convolution operation and we obtain good numerical results.

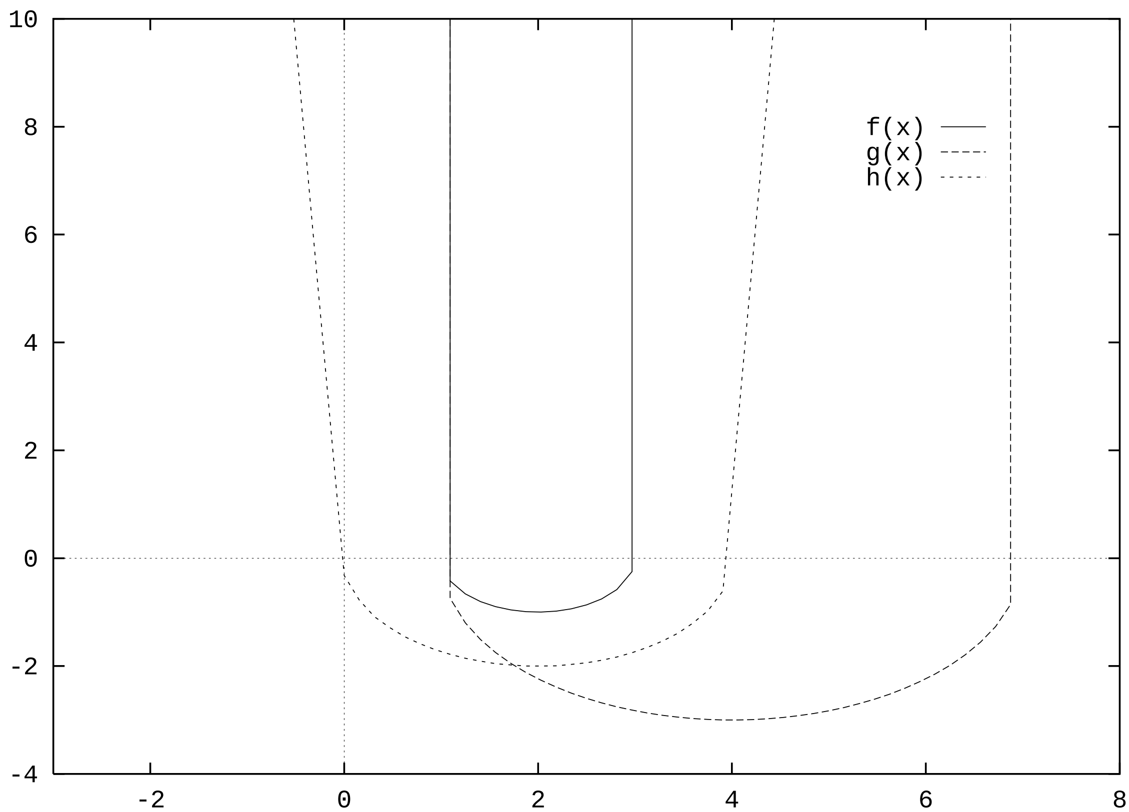


Figure 1.20: Deconvolution computation

$$f_{a,c}(x) = \begin{cases} -\sqrt{a^2 - (x-c)^2} & \text{if } |x-c| \leq a, \\ \infty & \text{otherwise,} \end{cases}$$

$$f_{3,4} \diamond f_{1,2} = f_{2,2},$$

$$f = f_{1,2} \qquad g = f_{3,4} \qquad h = f_{2,2}.$$

Here we show an application of the FLT algorithm to compute a deconvolution.

In the next example, taken from [9], we want to find the composition at equilibrium of two liquid components by minimizing the Gibbs free energy. This amounts to computing the biconjugate of a function u at a given point b. Although the FLT algorithm seems ill-suited for that purpose (it works best to compute the biconjugate on a whole interval), it is interesting to try it on this example for several reasons. First, the function u has a very bad numerical behavior with two vertical tangents and a small range. Then one may want to know the composition for several values or even on a whole interval.

We obtain good numerical results for computing $u^{**}(b)$, but the FLT algorithm does not give the phases of b, *i.e.*, the points x_1 and x_2 belonging to both the graph of u and u^{**} for which $u'(x_1) = u'(x_2) = (u^{**})'(x_1) = (u^{**})'(x_2)$. We can detect the first point x_1 by looking at points which share the same tangent as b but a bad numerical behavior prevents us from detecting the second one. All the computational results taken from [9] are made with a 10^{-5} precision, Table 1.5 gives the numerical results.

This example shows the limit of the FLT algorithm: it allows to compute the whole conjugate or biconjugate but it is ill-suited for computing these functions at a finite number of points.

Table 1.4: Numerical data for the function u

$g_{1,2}$	.30794
$g_{2,1}$	.15904
$m_{1,2}$	.92535
$m_{2,1}$	.74601

Table 1.5: Numerical results

$u^{**}(1/2)$ computed in [9]	$-2.0198\ 10^{-2}$
$u^{**}_{XX}(1/2)$	$-2.0209\ 10^{-2}$
error	$1.1\ 10^{-5}$
x_1 computed in [9]	$4.557\ 10^{-3}$
x_1 computed with the FLT	$4.562\ 10^{-3}$
error	$5\ 10^{-6}$

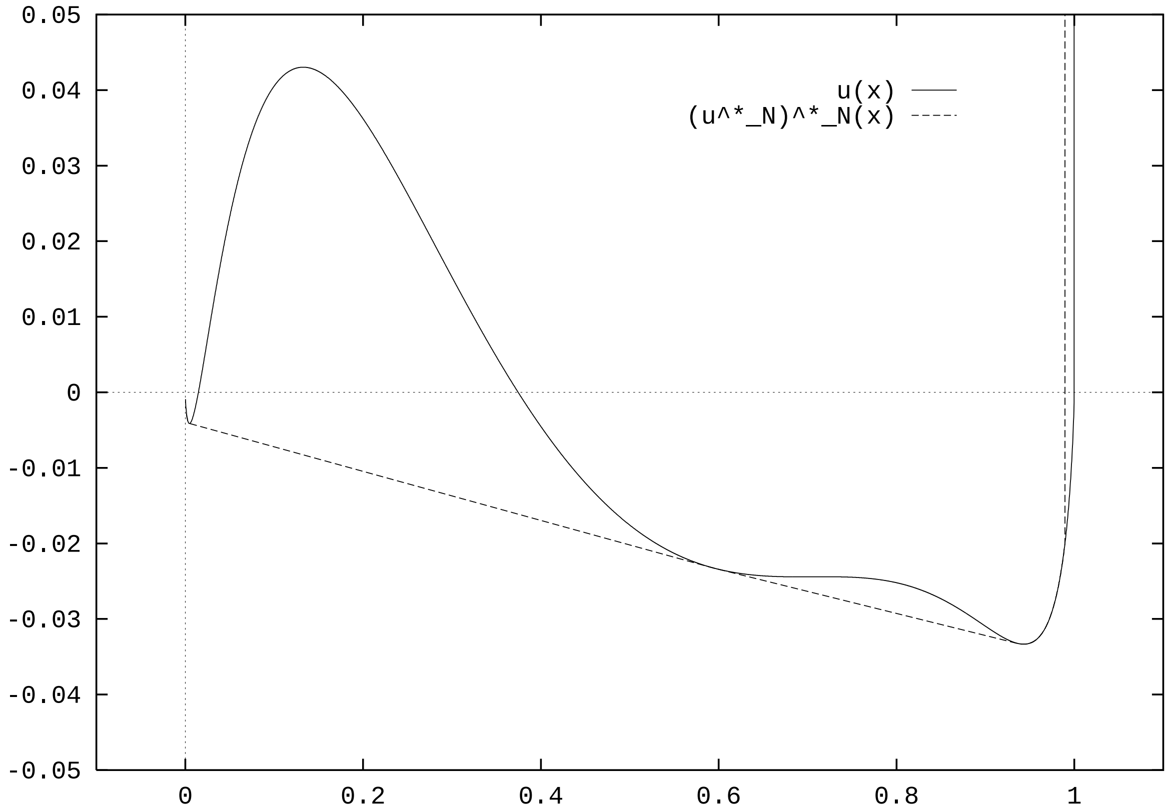


Figure 1.21: Example of biconjugate calculus found in Chemistry

$$u(x) := \frac{m_{1,2}}{\frac{g_{1,2}}{1-x} + \frac{1}{x}} + \frac{m_{2,1}}{\frac{g_{2,1}}{x} + \frac{1}{1-x}} + x\ln(x) + (1-x)\ln(1-x)$$

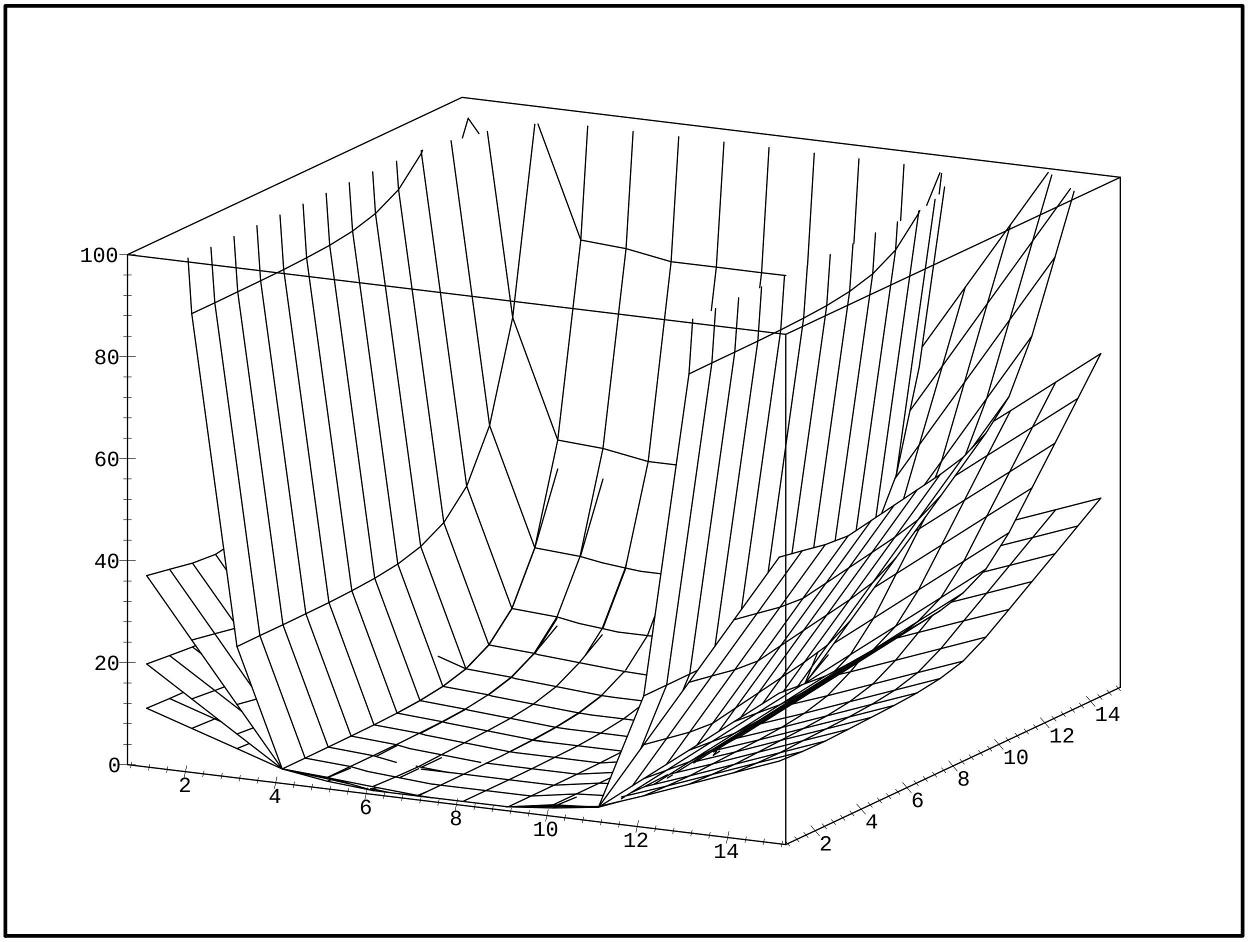


Figure 1.22: Two dimensional biconjugate computation

$$u(x, y) = (x^2 - 4)^2 + e^y$$

In this two-dimensional example, we see that the computed surfaces wrap around the graph of u (the upper surface).

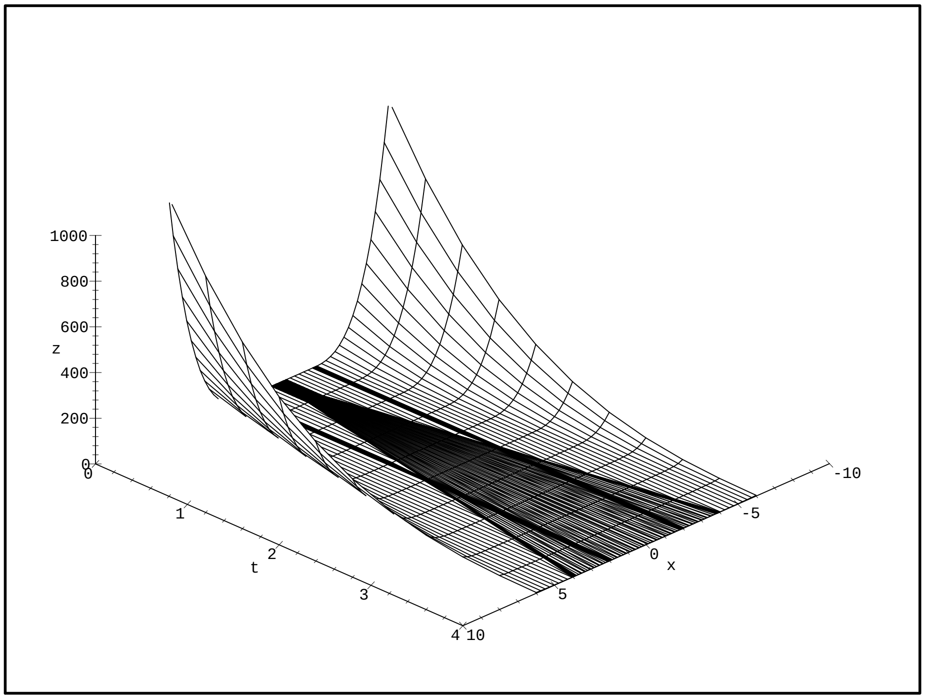


Figure 1.23: Solution of a Hamilton–Jacobi equation

We define

$$\theta(x) = 1 - \sqrt{1 - x^2},$$
$$f(x) = \begin{cases} (x^2-1)^2 & \text{if } |x| > 1, \\ 0 & \text{otherwise.} \end{cases}$$

In view of Theorem 12, page 15 in [15], the function

$$F(x,t) = \begin{cases} (f \square t\theta(\frac{\cdot}{t}))(x) & \text{if } t > 0, \\ f(x) & \text{if } t = 0, \\ +\infty & \text{otherwise,} \end{cases}$$

satisfies the following Hamilton–Jacobi equation:

$$\begin{cases} \frac{\partial F}{\partial t} + \theta^*(\frac{\partial F}{\partial x}) = 0, \\ \lim_{t \to 0^+} F(.,t) = f. \end{cases}$$

We computed the function $(x,t) \mapsto F(x,t)$ with the LLT algorithm, and drew it in Figure 1.23. We clearly see that at any given point x_0, $F(x_0,t)$ goes to 0 when t goes to infinity.

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Chapter 2

Second order expansion of the closed convex hull of a function

Introduction

How smooth is the (closed) convex hull of a function? We consider a function $E : \mathbb{R}^n \to \mathbb{R}$ and denote $\bar{\text{co}}E$ its closed convex hull. We want to know what smoothness is inherited by $\bar{\text{co}}E$.

Applications arising in three distinct fields clearly motivate that question.

- The problem of thermodynamic phase equilibrium [27, 33, 34] (when different fluids are mixed, one wishes to know how each fluid is distributed in each of the phase present at equilibrium) amounts to computing the convex hull of a function describing the Helmholtz free energy [48]. Since the resulting function E happens to be smooth and coercive, $\bar{\text{co}}E$ is continuously differentiable, and $\nabla\bar{\text{co}}E$ is locally Lipschitz [21, 42].

- New second-order objects were defined to study viscosity solutions of certain Hamilton-Jacobi equations [1]. They led to an interesting relation between second-order information of E and $\bar{\text{co}}E$.

- Finally, $\bar{\text{co}}E$ is an important tool when one wants to study the global minimum of E. In fact, a global minimum $\bar{x}$ of E is characterized by:

$$\nabla E(\bar{x}) = 0 \text{ and } E(\bar{x}) = \bar{co}E(\bar{x}),$$

(see [26]).

Consequently, numerous authors have studied the (closed) convex hull both numerically and theoretically. On one hand, several algorithm have been developed for "continuous" convex hull [7, 34] and for discrete convex hulls (the Divide-and-Conquer and Beneath-Beyond algorithms [15, 47], the Ultimate Planar Convex Hull Algorithm [35], the Fast Legendre Transform algorithm [14, 43, 44, 46], Quickhull [3, 47], ...). On the other hand, first-order smoothness of $\bar{\text{co}}E$ is well known [4, 21, 49]. Local Lipschitz regularity of the gradient is proved in [21] under coercivity assumption, and extended to the broader class of *epi-pointed* functions (as defined in [4]) in [42].

Our aim here is *to study the second-order regularity of* $\bar{\text{co}}E$. Very little is known about it, except that either additional assumptions or a generalized second-order derivative are needed to obtain new results. Indeed, if $E(x) = (x^2 - 1)^2$, E is infinitely differentiable, everywhere defined, and 1-coercive. Yet at $x = 1$, $\bar{\text{co}}E$ is not twice differentiable.

Several extensions of usual second-order derivatives have appeared in the literature [1, 24, 52], but none appears to give a satisfactory answer to our problem.

However, when $\bar{\text{co}}E$ is a univariate function, it has a de la Vallée–Poussin directional second-order derivative at any point x in any direction d:

$$D^2\bar{\text{co}}E(x;d) = \lim_{t\to 0^+} \frac{2}{t}\left[\frac{\bar{\text{co}}E(x+td) - \bar{\text{co}}E(x)}{t} - \langle \nabla\bar{\text{co}}E(x), d\rangle\right], \tag{2.1}$$

that is, $\bar{\text{co}}E$ has a second-order approximation around x in the direction d:

$$\bar{\text{co}}E(x+td) = \bar{\text{co}}E(x) + t\langle \nabla\bar{\text{co}}E(x), d\rangle + \frac{t^2}{2}D^2\bar{\text{co}}E(x;d) + o(t^2),$$

with $o(t^2)/t^2 \to 0$ when $t \to 0^+$.

Jessen (see pages 8–9 in Busemann's book [8]) and in a broader setting Borwein and Noll [5] showed that for convex functions the de la Vallée–Poussin directional second-order derivative exists if and only if the Dini directional second-order derivative:

$$\bar{\text{co}}E''(x;d) = \lim_{t\to 0^+} \frac{\langle \nabla\bar{\text{co}}E(x+td), d\rangle - \langle \nabla\bar{\text{co}}E(x), d\rangle}{t}$$

exists; in that case they are equal. In Section 2.3 we sum up results on directional second-order derivatives, and prove that $D^2\bar{\text{co}}E(x;d)$ exists and is either 0 or $E''(x)d^2$, where E'' is the usual second-order derivative.

The one-dimensional case provides a better understanding of the second-order behavior of the (closed) convex hull. Even though it is simpler and can be studied by elementary techniques (see [6]), there are applications involving only univariate functions [33, 38, 39, 40, 41]. In addition, since the convex hull of a separable function is separable [37], its directional second-order derivatives exist. In other words, for $E(x_1,\dots,x_n) = E_1(x_1) + \cdots + E_n(x_n)$, with $E_i : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$, the convex hull can be written: $\bar{\text{co}}E(x_1,\dots,x_n) = \bar{\text{co}}E_1(x_1) + \cdots + \bar{\text{co}}E_n(x_n)$, so all one-dimensional results apply.

In higher dimensions or when E is not separable, we tried several approaches and obtain partial results which emphasize the difficulties encountered.

First in Section 2.4, we show that the second-order directional derivative exists for some directions d, and is either $\langle \nabla^2 E(x)d, d\rangle$ or 0. We mention problems arising in higher dimensions and we give upper bounds for the upper second order directional derivative.

Next, in Section 2.5 we study phase simplices. We prove that minimal phase simplices are non-degenerate, and we characterize the uniqueness of phase decomposition with maximal phase simplices. That self-contained section is very geometric.

Section 2.6 aims at studying the set-valued function which maps a point to all of its phases. Even though it is upper semi-continuous, compact-valued, and locally bounded, we build an example for which no continuous selection exists. We end remarks on the phase set-valued function with a note on epi-derivatives. Under our hypotheses, existence of a second-order directional derivative amounts to twice epi-differentiability.

Finally, in Section 2.7 we apply recent results on the lower de la Vallée–Poussin directional second-order derivative of a marginal function [11]. In all that section, the convex hull is viewed as a marginal function.

2.1 First-order properties of the convex hull

Let $E : \mathbb{R}^n \to (-\infty, +\infty]$ be any function. We define the domain of E as $\mathrm{Dom}(E) = \{x \in \mathbb{R}^n \ : \ E(x) < \infty\}$. We assume throughout that E satisfies:

(2.2) the function $E : \mathbb{R}^n \to (-\infty, +\infty]$ is lower semi-continuous (lsc), there is an affine mapping minorizing E, and $\mathrm{Dom}(E)$ is nonempty.

We define the convex hull of E by:

$$x \in \mathbb{R}^n \mapsto \mathrm{co}\, E(x) = \inf\{r \in \mathbb{R} \ : \ (x, r) \in \mathrm{co}\, \mathrm{Epi}\, E\},$$

where $\mathrm{Epi}\, E = \{(x, r) \in \mathbb{R}^n \times \mathbb{R} \ : \ E(x) \leq r\}$ is the epigraph of E. Statements (i)–(ii) below recall several way of computing $\mathrm{co}\, E(x)$ (see [25, 49]):

(i) $\quad \mathrm{co}\, E(x) = \sup\{g(x) \ : \ g \text{ convex}, \ g \leq E\},$

(ii) $\quad \mathrm{co}\, E(x) = \inf\{\sum_{i=1}^{p} \lambda_i E(x_i) \ : \ \lambda \in \Delta_p \text{ and } \sum_{i=1}^{p} \lambda_i x_i = x\},$

where $\Delta_p = \{\lambda = (\lambda_1, \ldots, \lambda_p) \in \mathbb{R}^p \ : \ \sum_{i=1}^{p} \lambda_i = 1 \text{ and } \lambda_i \geq 0\}$.

Instead of the convex hull, if we take the closed convex hull of $\mathrm{Epi}\, E$, we obtain the closed convex hull of E. Thus it is defined by:

$$x \in \mathbb{R}^n \mapsto \bar{\mathrm{co}} E(x) = \inf\{r \in \mathbb{R} \ : \ (x, r) \in \bar{\mathrm{co}}\, \mathrm{Epi}\, E\}.$$

As for (i)–(ii), there are ways of computing the closed convex hull. We have for all x in $\mathbb{R}^n$:

(iii) $\quad \bar{\mathrm{co}} E(x) = \sup\{g \ : \ g \text{ closed convex}, \ g \leq E\},$

(iv) $\quad \bar{\mathrm{co}} E(x) = \sup\{\langle a, x\rangle + b \ : \ \langle a, .\rangle + b \leq E\},$

(iii) $\quad \bar{\mathrm{co}} E = E^{**},$

where $E^{**} = (E^*)^*$ is the Legendre–Fenchel biconjugate of E.

To relate the first-order smoothness of $\bar{\mathrm{co}} E$ to the smoothness of E, we need the concept of epi-pointedness.

Definition 2.1 (Benoist and Hiriart–Urruty [4]).
The function E is *epi-pointed* if there is $s \in \mathbb{R}^n, \sigma > 0, r \in \mathbb{R}$ which satisfy:

$$E \geq \sigma\|.\| + \langle s, .\rangle - r,$$

where $\langle ., .\rangle$ stands for the usual scalar product on $\mathbb{R}^n$ and $\|.\|$ is its associated norm.

In fact the epi-pointedness of E is equivalent to (see Proposition 4.5 in [4]):

(2.3) $E : \mathbb{R}^n \to (-\infty, \infty]$ is minorized by $n+1$ affine functions $\langle s_i, .\rangle - r_i$ with affinely independent slopes s_i.

Remark 2.1. Usually one assumes instead that the function E is a 1-*coercive* function, that is,

$$\lim_{\|x\|\to\infty} \frac{E(x)}{\|x\|} = +\infty.$$

Clearly, if E is 1-coercive, it is epi-pointed. In addition, the closed convex hull and the convex hull of a 1-coercive function are equal.

To state the main result of this section, we use the *asymptotic function* E_∞ (also named the recession function, see Chap. IV, Section 3.2 in [25]). The function E_∞ is geometrically defined by:

$$\mathrm{Epi}(E_\infty) = (\mathrm{Epi}\, E)_\infty,$$

where the asymptotic set of a nonempty closed set S is defined by:

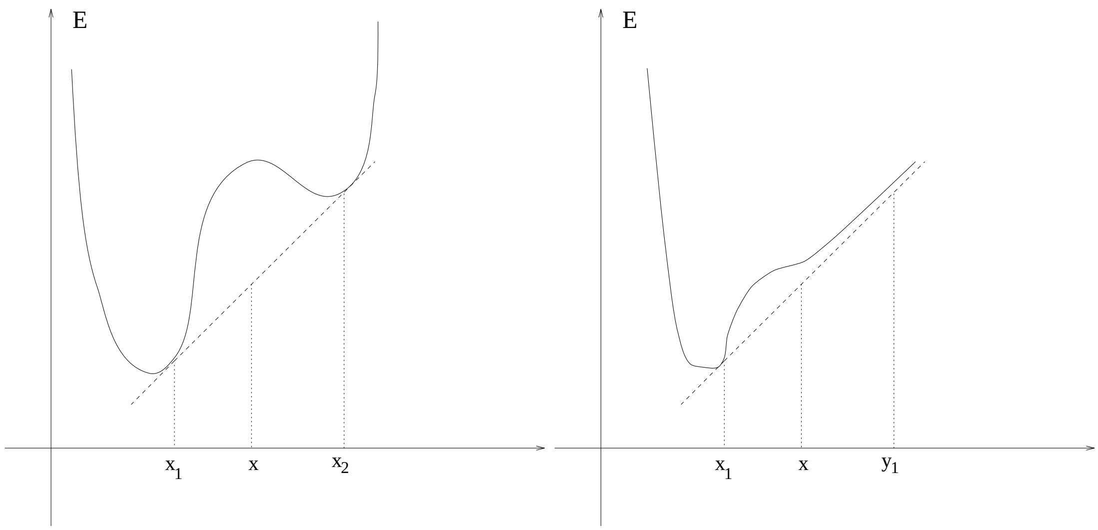
$$S_\infty = \{d \in \mathbb{R}^n; \exists\{x_k\}_k \subset S, \exists\{t_k\}_k \subset \mathbb{R}^+ \text{ with } t_k \to 0, \text{ such that } d = \lim t_k d_k\}.$$

The next Theorem is the starting point of our analysis.

Theorem 2.1 (Benoist and Hiriart–Urruty [4]).
We suppose $E : \mathbb{R}^n \to (-\infty, +\infty]$ is epi-pointed and satisfies (2.2). Then for all x in $\mathrm{Dom}(\bar{co}E)$, the following holds:

(i) There are points $x_1, \ldots, x_p$ in $\mathrm{Dom}\, E$, real numbers $\alpha_1, \ldots, \alpha_p$ in $\mathbb{R}^+ \cap \Delta_p$, and possibly points $y_1, \ldots, y_q$ in $\mathrm{Dom}\, E_\infty \setminus \{0\}$ such that:

$$(2.4)\qquad x = \sum_{i=1}^{p} \alpha_i x_i + \sum_{j=1}^{q} y_j \text{ and } \bar{co}E(x) = \sum_{i=1}^{p} \alpha_i E(x_i) + \sum_{j=1}^{q} E_\infty(y_j).$$



(a) E is 1-coercive (b) E is not 1-coercive but is epi-pointed

Figure 2.1: Phases of x

Equalities (2.4) *is called a phase decomposition of* x*, and* $x_1, \ldots, x_p$ *are the phases (or phase point) of* x*. We may choose a decomposition of the above type with* $0 \le q \le n$ *and* $p + q \le n + 1$*. If, in addition,* E *is a* 1*-coercive function, we may choose a phase decomposition with* $q = 0$.

(ii) For any phase decomposition (2.4)*, we have:*

$$\partial \bar{\text{co}} E(x) = [\bigcap_{i=1}^{p} \partial E(x_i)] \cap [\bigcap_{j=1}^{q} \partial E_\infty(y_j)].$$

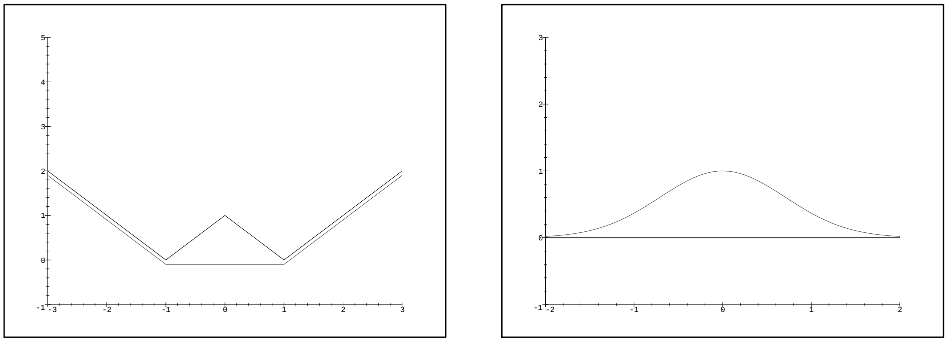
Moreover, the closed convex hull $\bar{\text{co}}E$ *is affine on*

$$\text{co}\{x_1, \ldots, x_p\} + \mathbb{R}^+ y_1 + \cdots + \mathbb{R}^+ y_q.$$

As usual, ∂ stands for the subdifferential in the sense of convex analysis.

Figures 2.1 illustrates Property (i). The points $(x_1, E(x_1))$, $(x_2, E(x_2))$, and $(y_1, \bar{\text{co}}E(y_1))$ are in the supporting hyperplane going through $(x, \bar{\text{co}}E(x))$.

A consequence of Theorem 2.1 is that a univariate function is always affine on a neighborhood of points where $\bar{\text{co}}E$ does not stick to E.



(a) The function $E(x) = ||x| - 1|$ is epi-pointed and affine on a neighborhood of $x_0 = 0$ (b) The function $E(x) = exp(-x^2)$ is not epi-pointed

Figure 2.2: Both univariate functions satisfy $E(x_0) > \bar{\text{co}}E(x_0)$ at $x_0 = 0$. Hence they are affine on a neighborhood of x_0 (Corollary 2.1)

Corollary 2.1. *Consider a univariate function $E : \mathbb{R} \to \mathbb{R}$. If there is x_0 such that $\bar{\text{co}}E(x_0) < E(x_0)$ then either:*

- *the function E is epi-pointed and $\bar{\text{co}}E$ is affine on a neighborhood of x_0,*
- *or the function E is not epi-pointed and $\bar{\text{co}}E$ is an affine function on $\mathbb{R}$.*

Proof. First, we assume $\bar{\text{co}}E$ is not differentiable at x_0. Its subdifferential at x_0 is denoted $\partial\bar{\text{co}}E(x_0) = [s^-, s^+]$ with $s^- < s^+$. Thus E is minorized by two affine functions: $x \mapsto s^-(x - x_0) + \bar{\text{co}}E(x_0)$ and $x \mapsto s^+(x - x_0) + \bar{\text{co}}E(x_0)$. According to Property (2.3), E is epi-pointed. So we apply Theorem 2.1: there are x_1 and either, x_2 or y_1, that build the set $\text{co}\{x_1, x_2\} + \mathbb{R}^+ y_1$ on which $\bar{\text{co}}E$ is affine. Since x_0 belongs to the interior of this set, $\bar{\text{co}}E$ is affine on a neighborhood of x_0.

Now, we suppose $\bar{\text{co}}E$ is differentiable at x_0. We take x any point in a neighborhood of x_0. If $\partial\bar{\text{co}}E(x)$ is not equal to $\{(\bar{\text{co}}E)'(x_0)\}$, we use the same argument again: there are two affine functions with different slopes that minorize E. We deduce again that $\bar{\text{co}}E$ is affine on a neighborhood of x_0.

The only remaining case is when $\bar{\text{co}}E$ is differentiable everywhere with a constant derivative. The function $\bar{\text{co}}E$ is then clearly affine. □

We illustrate both cases with Figures 2.2.

Example 2.1. The function $E(x) = ||x| - 1|$ at $x_0 = 0$ illustrates the first case.

For the second case, consider $E(x) = exp(-x^2)$.

We can clearly deduce the first-order smoothness of $\bar{\text{co}}E$ from Theorem 2.1 page 67. Indeed, when it applies and either of the following assumptions are satisfied:

- the function E is Fréchet differentiable and everywhere finite;
- the set $\partial E(x)$ is empty for all x in $\text{Bd}(\text{Dom}\, E)$ —the boundary of $\text{Dom}\, E$— and E is Gâteau differentiable on the interior of its domain;

then $\bar{\text{co}}E$ is continuously differentiable on $\text{int}(\text{Dom}\, E)$. In addition, for all phase x_i of x, we have:

$$\nabla \bar{\text{co}}E(x) = \nabla E(x_i).$$

In the particular case E is a univariate function, we do not need the epi-pointedness hypothesis for $\bar{\text{co}}E$ to be differentiable.

Corollary 2.2 (Hiriart–Urruty). *Assume $E : \mathbb{R} \to \mathbb{R}$ is differentiable and there is an affine mapping minorizing E. Then $\bar{\text{co}}E$ is differentiable on $\mathbb{R}$.*

Proof. We proceed with an argument by contradiction: we suppose $\bar{\text{co}}E$ is not differentiable at x_0. Since $\bar{\text{co}}E$ is convex, the following limits exist:

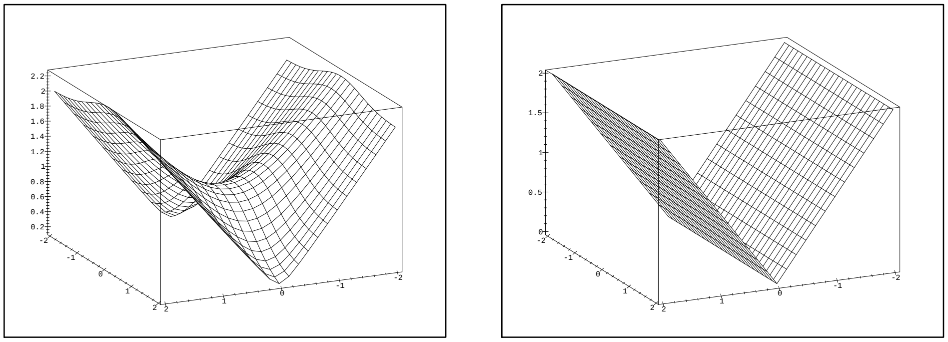
$$s_1 = \lim_{t \to 0^+} \frac{\bar{\text{co}}E(x_0 - t) - \bar{\text{co}}E(x_0)}{t} \text{ and } s_2 = \lim_{t \to 0^+} \frac{\bar{\text{co}}E(x_0 + t) - \bar{\text{co}}E(x_0)}{t}.$$

If $s_1 = s_2$, $\bar{\text{co}}E$ would be differentiable which contradicts our assumption. So $s_1 < s_2$ and $\partial \bar{\text{co}}E(x_0) = [s_1, s_2]$.

If $E(x_0) > \bar{\text{co}}E(x_0)$, the function $\bar{\text{co}}E$ would be affine on a neighborhood of x_0 (Corollary 2.1 page 69) which contradicts the fact it is not differentiable at x_0.

We deduce that $E(x_0) = \bar{\text{co}}E(x_0)$. Both affine functions $x \mapsto s_i(x - x_0) + E(x_0)$ (for $i = 1, 2$) underestimate E. We apply Property (2.3) to obtain the epi-pointedness of E. Consequently Theorem 2.1 page 67 gives the following contradiction which ends the proof:

$$[s_1, s_2] = \{\nabla E(x_0)\} \cap \partial E_\infty(y_j). \quad \square$$



(a) The function E is not epi-pointed (b) Its convex hull shares no common point with E

Figure 2.3: Theorem 2.1 does not apply to E

In our study we always assume E is differentiable and epi-pointed. Unless stated otherwise, we suppose $\operatorname{Dom} E = \mathbb{R}^n$ and E is twice differentiable everywhere. These hypotheses can usually be weakened to:

- E is twice differentiable on the interior of its domain,
- and ∂E is empty at points in $\operatorname{Dom}(E) \cap \operatorname{Bd}(\operatorname{Dom}(E))$ (the main idea is to avoid that any phase belongs to the border of $\operatorname{Dom} E$).

Remark 2.2 (Example 4.1 in [4]). Corollary 2.2 page 70 does not generalize to higher dimensions. For example it does not hold for the C^∞ function $E(x, y) = \sqrt{x^2 + \exp(-y^2)}$ whose convex hull, $\bar{co}E(x, y) = |x|$, is not differentiable at the origin. For that function, no point has a phase since the function E is never equal to $\bar{co}E$. See Figures 2.3

2.2 Beyond first-order differentiability

When E is differentiable and epi-pointed, $\bar{\text{co}}E$ is continuously differentiable, convex and epi-pointed. In this section we suppose ∇E is *locally α-hölder continuous* on $\mathbb{R}^n$, that is, for all x_0 in $\mathbb{R}^n$ there is a ball $B(x_0, r)$ of radius r centered at x_0, and a positive number K such that:

$$\forall x, y \in B(x_0, r) \qquad \|\nabla g(x) - \nabla g(y)\| \leq K \|x - y\|^\alpha.$$

We name $C^{1,\alpha}(\Omega)$ the set of continuously differentiable functions with α-hölder continuous gradient on Ω.

When E is 1-coercive and α-hölder continuous, Rabier and Griewank [21] proved that $\nabla \bar{\text{co}} E$ is also α-hölder continuous. A slight modification of their proof permits us to obtain the following more general result.

Theorem 2.2. *Let E satisfies (2.2) of page 66. If the following assumptions hold:*

(i) for all x in $\text{Bd}(\text{Dom}\, E) \cap \text{Dom}\, E$, $\partial E(x)$ is empty;

(ii) the function E is epi-pointed;

(iii) the gradient ∇E is α-hölder continuous on
$$\text{Dom}(E)^* = \{x \in \text{Dom}(E) \ : \ \partial E(x) \text{ is not empty}\}.$$

Then $\bar{\text{co}} E$ is continuously differentiable, and $\nabla \bar{\text{co}} E$ is α-hölder continuous on $\text{co}(\text{int}\,\text{Dom}\, E)$.

Proof. We only sketch here the main steps of the full proof which can be found in [42].

First, Assumption (ii) implies that there are $s \in \mathbb{R}^n$, $\sigma > 0$ and $r \in \mathbb{R}$ such that $E \geq \sigma\|.\| + \langle s, . \rangle - r$. So the function $g = E - \langle s, . \rangle$ satisfies the following properties:

- the set $\text{Dom}\, g$ is nonempty, and g is a lower semi-continuous function underestimated by an affine mapping. In other words g satisfies Assumption (2.2).
- g is epi-pointed ($g \geq \sigma\|.\| - r$).
- g satisfies Assumption (i) ($\text{Dom}\, g = \text{Dom}\, E$ and $\text{Dom}(g)^* = \text{Dom}(E)^*$).
- g is in $C^{1,\alpha}(\text{Dom}(g)^*)$, in fact $\|\nabla g(x) - \nabla g(y)\| = \|\nabla E(x) - \nabla E(y)\|$.

Finally $\bar{\text{co}} E = \bar{\text{co}} g + \langle s, r \rangle$, so we only need to prove the result for g. Due to Theorem 2.1 page 67, the function g is continuously differentiable on $\text{Dom}(g)^*$.

All in all, we only need to prove that $\nabla \bar{\text{co}} g$ is locally α-hölder continuous. This is done by slightly modifying the proof of Theorem 4.2 in [21]. □

2.3 Directional second-order differentiability in one dimension

In all this section E is a univariate function. We start by writing the main result.

Theorem 2.3. *We assume E satisfies (2.2) of page 66, as well as hypotheses (i) and (ii) of Theorem 2.2 page 72. If E is twice differentiable on* $\mathrm{Dom}(E)^*$ *then* $\bar{\mathrm{co}}E$ *is $C^{1,1}$, twice directionally differentiable at any point x_0 in* $\mathrm{int}(\mathrm{Dom}\,\bar{\mathrm{co}}E)$, *and $D^2\bar{\mathrm{co}}E(x_0;d)$ belongs to $\{0, E^{''}(x_0)d^2\}$.*

To prove Theorem 2.3, we summarize basic results on second-order directional derivatives in the next subsection.

2.3.1 Second-Order directional derivatives

For a function $f : \mathbb{R} \to \mathbb{R}$, we define —when the limits exist— its *right-hand side derivative*:

$$f_r^{'}(x) = \lim_{h\to 0^+} \frac{f(x+h) - f(x)}{h},$$

and its *second-order (right-hand side) directional derivatives*:

$$\begin{aligned} D^2 f_r(x) &= D^2 f(x;1) &= \lim_{t\to 0^+} \frac{2}{t}\left[\frac{f(x+t)-f(x)}{t} - f'(x)\right], \\ f_r^{''}(x) &= f^{''}(x;1) &= \lim_{t\to 0^+} \frac{f'(x+t)-f'(x)}{t}. \end{aligned}$$

Left hand-side derivatives are defined similarly.

We begin with several remarks.

Remark 2.3. If we consider the function f defined by $f(x) = x^3\sin(1/x)$ if $x \neq 0$ and $f(0) = 0$, it is differentiable at $x = 0$ with $f^{'}(0) = 0$. In addition, f has a second-order de la Vallée–Poussin directional derivative at $x = 0$: $D^2 f_r(0) = 0$. However a quick computation gives:

$$\frac{f^{'}(0+h) - f^{'}(0)}{h} = h\sin(\frac{1}{h}) - \cos(\frac{1}{h}).$$

So f does not have a second-order Dini directional derivative at $x = 0$. In other word, f has a second-order development at 0:

$$f(0+h) = f(0) + hf^{'}(0) + \frac{h^2}{2} D^2 f_r(0) + o(h^2),$$

but $f^{'}$ is not directionally differentiable at 0.

The following lemma clarifies how both second-order directional derivatives are linked together.

Lemma 2.1 (Chapter I, Theorem 5.2.1 in [25]). *(i) Let $f : \mathbb{R} \to \mathbb{R}$ admit a right hand-side first-order derivative at x_0. If $f_r^{''}(x_0)$ exists, $D^2 f_r(x_0)$ exists and $D^2 f_r(x_0) = f_r^{''}(x_0)$. The converse is not always true.*

(ii) If $f : \mathbb{R} \to \mathbb{R}$ is convex, the converse is true.

We end this section with a remark on relations between second-order information of E and $\bar{\text{co}}E$ at phase points.

Remark 2.4. If the function $E : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ is twice differentiable, its second-order derivative $E^{''}$ is nonnegative at each phase x_i of x. Indeed at such x_i, we have $E(x_i) = \bar{\text{co}}E(x_i)$ and $E^{'}(x_i) = (\bar{\text{co}}E)^{'}(x_i)$. Since $\bar{\text{co}}E \leq E$ and $\bar{\text{co}}E$ is convex, we deduce:

$$0 \leq \frac{\bar{\text{co}}E(x_i + \lambda d) - \bar{\text{co}}E(x_i) - \lambda(\bar{\text{co}}E)^{'}(x_i)d}{\lambda^2/2} \leq \frac{E(x_i + \lambda d) - E(x_i) - \lambda E^{'}(x_i)d}{\lambda^2/2}.$$

It follows that for all d:

$$0 \leq \underline{D}^2 \bar{\text{co}}E(x_i; d) \leq \overline{D}^2 \bar{\text{co}}E(x_i; d) \leq E^{''}(x_i)d^2,$$

where $\underline{D}^2 \bar{\text{co}}E(x_i; d)$ (resp. $\overline{D}^2 \bar{\text{co}}E(x_i; d)$) is the lower (resp. upper) second-order de la Vallée–Poussin directional derivative obtained by substituting lim with lim inf (resp. lim sup) in (2.1). Similarly we will name $\underline{\bar{\text{co}}E}^{''}(x_i; d)$ (resp. $\overline{\bar{\text{co}}E}^{''}(x_i; d)$) the lower (resp. upper) second-order Dini directional derivative.

2.3.2 Preliminaries lemmas

We begin with a remark that will be generalized to higher dimensions with Lemma 2.6 page 83.

Remark 2.5. When $\bar{\text{co}}E$ has a positive second-order derivative at x_0, x_0 is a single-phase point, that is $p = 1$ in (2.4). Indeed, if $\bar{\text{co}}E(x_0) \neq E(x_0)$, $\bar{\text{co}}E$ would be affine on a nonempty neighborhood of x_0 (Corollary 2.1 page 69). Thus $(\bar{\text{co}}E)^{''}(x_0) > 0$ could not hold.

Since $\bar{\text{co}}E$ is convex, all lower and upper second-order directional derivatives are nonnegatives. The next lemma states the main inequalities between second-order directional derivatives.

Lemma 2.2. *Suppose $f : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ is convex, continuously differentiable and verifies Assumption (2.2) of page 66. Then the following inequalities hold:*

$$\underline{f}_r^{''}(x_0) \leq \underline{D}^2 f_r(x_0) \leq \overline{D}^2 f_r(x_0) \leq \overline{f}_r^{''}(x_0). \tag{2.5}$$

Proof. The proof is very geometric and very close to Busemann's Proof of Lemma 2.1 (see pages 8–9 in [8]). We illustrate it with Figures 2.4. First we set our notations.

Preliminary step. Let τ_f be the graph of the convex $C^{1,1}$ function f. For x_0 in $\text{int}(\text{Dom}\, f)$, we name $y_0 = f(x_0)$ and $k = f(x_0 + h) - f(x_0)$ (with $h > 0$). We will use the notations:

$$p_0 = \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} \text{ and } p_h = \begin{pmatrix} x_0 + h \\ y_0 + k \end{pmatrix}.$$

We name τ_h the circle going through p_0 and p_h, and tangent to τ_f at p_0. We denote a_h its center and r_h its radius (we allow r_h to take the value: $+\infty$). The line δ_h is defined as the perpendicular at the tangent to τ_f at p_h; Q_h is the intersection point of δ_h with δ_0; and R_h is the distance between p_0 and Q_h (R_h can be infinite).

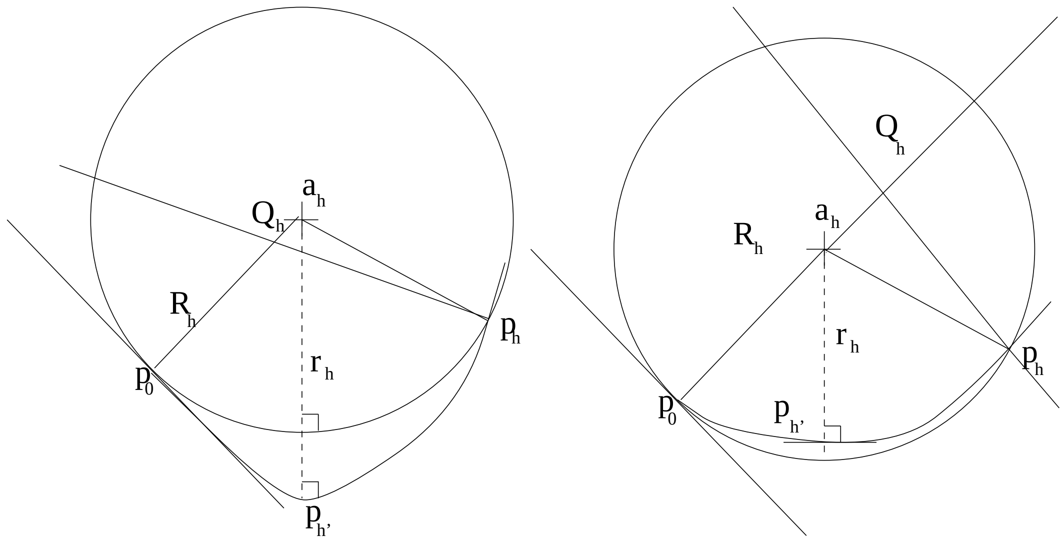
First step: We show that there is h' in $(0, h)$, s.t. $R_{h'} = r_h$.

We name $\mathcal{A}$ the graph of f generated when x belongs to $[x_0, x_0 + h]$. Since f is continuous, $\mathcal{A}$ is a compact set of $\mathbb{R}^2$ and the function:

$$\phi : h^{'} \mapsto (x_0 + h^{'} - x_{a_h})^2 + (f(x_0 + h^{'}) - y_{a_h})^2$$

is continuous on $\mathcal{A}$ (indeed, for h small enough and $0 < h^{'} < h$, $x_0 + h^{'}$ belongs to $\text{int}(\text{Dom}\, f)$), the function φ attains its maximum and its minimum over $\mathcal{A}$.

If both extrema are in $\{x_0, x_0 + h\}$, we have $\phi(h^{'}) = \phi(x_0)$ for all $h^{'}$, and step 1 is proved. Hence we can assume there is at least one extremum in $(0, h)$.



(a) Case $p_{h'}$ is out of the circle (b) Case $p_{h'}$ is in the circle

Figure 2.4: Geometrical interpretation

As the function ϕ is differentiable, there is $\bar{h}'$ in $(0,h)$ for which $\phi'(\bar{h}') = 0$. In other words, we have:

$$2(x_0 + \bar{h}' - x_{a_h}) + 2f'(x_0 + \bar{h}')(f(x_0 + \bar{h}') - y_{a_h}) = 0.$$

Consequently, we obtain:

$$f'(x_0 + \bar{h}')(y_{a_h} - y_{\bar{h}'}) = x_0 + \bar{h}' - x_{a_h}. \tag{2.6}$$

Since $f'(x_0 + \bar{h}')(y - y_{\bar{h}'}) = x_0 + \bar{h}' - x$ is the equation of $\delta_{\bar{h}'}$ (the normal to τ_f at $p_{\bar{h}'}$), Formula (2.6) means that a_h belongs to $\delta_{\bar{h}'}$. It follows that $Q_{\bar{h}'} = a_h$. Hence $R_{\bar{h}'} = r_h$.

Step 1 implies that the following stream of inequality holds:

$$0 \le \liminf_{h \to 0^+} R_h \le \liminf_{h \to 0^+} r_h \le \limsup_{h \to 0^+} r_h \le \limsup_{h \to 0^+} R_h. \tag{2.7}$$

Indeed, we consider a sequence h_n s.t. $\liminf r_h = \lim r_{h_n}$. Due to step 1, we can build a new sequence $\bar{h}'_n$ such that $R_{\bar{h}'_n} = r_{h_n}$. We deduce:

$$\liminf r_h = \lim r_{h_n} = \lim R_{\bar{h}'_n} \ge \liminf R_h.$$

The remaining inequality is proved similarly.

Last step: we prove (2.5) by substituting R_h and r_h in (2.7).

From the equation of δ_0: $f'(x_0)(y-y_0) = x_0 - x$, we deduce

$$\begin{aligned} x_{a_h} &= x_0 - \frac{f'(x_0)}{2}\frac{h^2+k^2}{k-hf'(x_0)}, \\ y_{a_h} &= y_0 + \frac{1}{2}\frac{h^2+k^2}{k-hf'(x_0)}. \end{aligned}$$

(a_h is the intersection between δ_0 and the perpendicular bisector of $[p_0, p_h]$). Whence we obtain

$$\begin{aligned} r_h^2 &= \frac{1+(f'(x_0))^2}{4}\left(\frac{h^2+k^2}{k-hf'(x_0)}\right)^2, \\ &= (1+(f'(x_0))^2)\left(\frac{1+((f(x_0+h)-f(x_0))/h)^2}{\frac{2}{h}((f(x_0+h)-f(x_0))/h-f'(x_0))}\right)^2. \end{aligned}$$

Now from the equation of δ_h ($f'(x_0+h)(y-y_h) = x_h - x$), we find the coordinates of Q_h:

$$\begin{aligned} x_{Q_h} &= x_0 - f'(x_0)\frac{f'(x_0+h)k+h}{f'(x_0+h)-f'(x_0)}, \\ y_{Q_h} &= y_0 + \frac{f'(x_0+h)k+h}{f'(x_0+h)-f'(x_0)}. \end{aligned}$$

We deduce the distance between p_0 and Q_h:

$$R_h^2 = (1+(f'(x_0))^2)\left(\frac{f'(x_0+h)(f(x_0+h)-f(x_0))/h+1}{(f'(x_0+h)-f'(x_0))/h}\right)^2.$$

To conclude we substitute

$$\liminf r_h = \frac{(1+(f'(x_0))^2)^{\frac{3}{2}}}{\limsup \frac{2}{h}((f(x_0+h)-f(x_0))/h-f'(x_0))}$$

and

$$\liminf R_h = \frac{(1+(f'(x_0))^2)^{\frac{3}{2}}}{\limsup (f'(x_0+h)-f'(x_0))/h}$$

in Inequalities (2.7) to find

$$\overline{D}^2 f_r(x_0) \leq f_r''(x_0).$$

The inequality for lower second-order derivatives is proved similarly. We end the proof by noting that when $r_h = \infty$, we have $R_h = \infty$ and $\mathcal{A} = [p_0, p_h]$. Hence Inequalities (2.5) still holds. □

Remark 2.6. As J. Borwein remarked, the whole proof reduces to a mean-value argument. Indeed, the continuous function $\phi(h')$ is differentiable on $(0, h)$, and $\phi(0) = \phi(h) = r_h$. Applying Rolle's Theorem, there exists $\bar{h}'$ in $(0, h)$ satisfying $\phi'(\bar{h}') = 0$. That last equation may be rewritten as

$$\frac{f(x_0+h) - f(x_0) - hf'(x_0)}{h^2/2} \frac{1 + f'(x_0+\bar{h}')\frac{f(x_0+\bar{h}')-f(x_0)}{\bar{h}'}}{1 + \left(\frac{f(x_0+h)-f(x_0)}{h}\right)^2} = \frac{f'(x_0+\bar{h}') - f'(x_0)}{\bar{h}'}.$$

Inequalities (2.5) follow.

2.3.3 Main result in the one dimensional case

We are now ready to prove the second part of Theorem 2.3 page 73 (we already know that $\bar{\text{co}}E$ is $C^{1,1}$). First we show that $\bar{\text{co}}E$ is twice directionally differentiable. Next we compute its second-order directional derivative.

Lemma 2.3. *When the hypotheses of Theorem 2.3 hold,* $\bar{\text{co}}E$ *is twice directionally differentiable at any point* x_0 *in* $\text{int}(\text{Dom}(\bar{\text{co}}E))$.

Proof. We take x_0 in $\text{int}(\text{Dom}\,\bar{\text{co}}E)$. To simplify our notations, we name: $\bar{l} = \overline{\bar{\text{co}}E}''_r(x_0)$, $\underline{l} = \underline{\bar{\text{co}}E}''_r(x_0)$, $\overline{L} = \overline{D}^2\bar{\text{co}}E_r(x_0)$, and $\underline{L} = \underline{D}^2\bar{\text{co}}E_r(x_0)$. Lemma 2.5 now reads: $0 \le \underline{l} \le \underline{L} \le \overline{L} \le \bar{l}$.

If $\bar{\text{co}}E(x_0) < E(x_0)$, $\bar{\text{co}}E$ is affine on a neighborhood of x_0 (Corollary 2.1 page 69) and we are done. So we can assume $\bar{\text{co}}E(x_0) = E(x_0)$ (x_0 is its own phase).

Since $\bar{\text{co}}E \le E$ and $\bar{\text{co}}E'(x_0) = E'(x_0)$, we have:

$$\overline{L} \le E''(x_0). \tag{2.8}$$

Using an argument by contradiction we are going to prove that $\underline{L} = \overline{L}$. Lemma 2.1 page 74 will then end the proof.

We suppose $\underline{L} < \overline{L}$ and consider $(\alpha_k)_k$, a sequence of positive real numbers decreasing to 0. We build two new sequences $(\gamma_n)_n$ and $(\beta_n)_n$ as follows:

- when $\bar{\text{co}}E(x_0+\alpha_k) < E(x_0+\alpha_k)$, we set $\gamma_n = \alpha_k$;
- otherwise $\bar{\text{co}}E(x_0+\alpha_k) = E(x_0+\alpha_k)$ and we define $\beta_n = \alpha_k$.

We clearly have $\{\alpha_n\}_n = \{\beta_n\}_n \cup \{\gamma_n\}_n$.

Since $\bar{\text{co}}E(x_0+\beta_n) = E(x_0+\beta_n)$, that is, $x_0+\beta_n$ is its own phase, we have $\bar{\text{co}}E^{'}(x_0+\beta_n) = E^{'}(x_0+\beta_n)$. We deduce:

$$\frac{\bar{\text{co}}E^{'}(x_0+\beta_n) - \bar{\text{co}}E^{'}(x_0)}{\beta_n} = \frac{E^{'}(x_0+\beta_n) - E^{'}(x_0)}{\beta_n} \to E^{''}(x_0).$$

Eventually it only remains to show that $(\bar{\text{co}}E'(x_0+\gamma_n) - \bar{\text{co}}E'(x_0))/\gamma_n$ converges.

Due to Theorem 2.1 of 67, there is a largest interval containing $x_0+\gamma_n$ on which $\bar{\text{co}}E$ is affine. We name it $[c_{n+1}, c_n]$.

If $c_{n+1} \leq x_0$, $\bar{\text{co}}E^{'}$ is constant on the nonempty interval $[x_0, c_n]$, so for all t in $(0, \gamma_n)$ we have:

$$\frac{\bar{\text{co}}E^{'}(x_0+t) - \bar{\text{co}}E^{'}(x_0)}{t} = 0.$$

Consequently $\underline{l} = \bar{l} = \underline{L} = \overline{L} = 0$. We obtain a contradiction with $\underline{L} < \overline{L}$.

Thus $c_{n+1} > x_0$. We can build a sequence $c_n > x_0$ converging to x_0. Now we define $\xi_n = c_n - x_0$. Due to $x_0+\gamma_n < c_n = x_0+\xi_n$, we have $0 < \gamma_n < \xi_n$.

Since $\bar{\text{co}}E^{'}$ is monotone, $\bar{\text{co}}E^{'}(x_0+\gamma_n) - \bar{\text{co}}E^{'}(x_0) \geq 0$. So we can write:

$$\begin{aligned}\frac{\bar{\text{co}}E^{'}(x_0+c_n) - \bar{\text{co}}E^{'}(x_0)}{\gamma_n} &= \frac{E^{'}(x_0+\xi_n) - E^{'}(x_0)}{\gamma_n} \\ &\geq \frac{E^{'}(x_0+\xi_n) - E^{'}(x_0)}{\xi_n} \xrightarrow[n\to+\infty]{} E^{''}(x_0).\end{aligned}$$

It follows that $\underline{l} \geq E^{''}(x_0)$. We apply Lemma 2.5 with inequality (2.8) to obtain the following contradiction:

$$E^{''}(x_0) \leq \underline{l} \leq \underline{L} < \overline{L} \leq E^{''}(x_0).$$

We conclude that $\underline{L}$ must be equal to $\overline{L}$: $\bar{\text{co}}E$ has a second-order de la Vallée–Poussin directional derivative. Since it is convex, it also has a second-order Dini directional derivative (Lemma 2.1 page 74). □

We end the proof of Theorem 2.3 by computing the set of possible values for the second-order directional derivatives of $\bar{\text{co}}E$.

Lemma 2.4. *The second-order right-hand side derivatives of* $\bar{\text{co}}E$ *satisfy:*

$$\bar{\text{co}}E_r^{''}(x_0) = D^2\bar{\text{co}}E_r(x_0) \in \{0, E^{''}(x_0)\}.$$

Proof. We already know: $0 \leq \bar{\text{co}}E_r^{''}(x_0) \leq E^{''}(x_0)$. Now we assume $\bar{\text{co}}E_r^{''}(x_0) > 0$ and take $(\alpha_k)_k$ a sequence of positive real numbers decreasing to 0. We build $(\beta_n)_n$, $(\gamma_n)_n$, and $(c_n)_n$ as in the preceding proof.

We only need to show that $(\bar{\text{co}}E'(x_0+\gamma_n)-\bar{\text{co}}E'(x_0))/\gamma_n$ converges to $\bar{\text{co}}E_r'(x_0)$ when n goes to infinity. We cannot have $c_{n+1} \leq x_0$ since the same argument as before would imply $\bar{\text{co}}E_r'(x_0) = 0$. So we can build the sequence $(c_n)_n$ to obtain $\underline{l} \geq E''(x_0)$. All in all, we obtain:

$$\frac{\bar{\text{co}}E^{'}(x_0 + \alpha_n) - \bar{\text{co}}E^{'}(x_0)}{\alpha_n} \to \bar{\text{co}}E_r^{''}(x_0) \geq E^{''}(x_0). \quad \square$$

Since convexity implies a kind of smoothness on a function, one may wonder whether there are convex $C^{1,1}$ functions which do not admit second-order directional derivative. The next example answers positively to that question.

Example 2.2. We build a $C^{1,1}$ convex function f which is not twice directionally differentiable. We recursively build a sequence of squares:

$$[\frac{1}{2}, 1]^2, [\frac{1}{4}, \frac{1}{2}]^2, [\frac{1}{8}, \frac{1}{4}]^2, \dots, [\frac{1}{2^{n+1}}, \frac{1}{2^n}]^2, \dots$$

on the unit square. On each set $S_n = [\frac{1}{2^{n+1}}, \frac{1}{2^n}]^2$, we define $A_n = (1/2^n, 1/2^n)$, $B_n = ((1/2^{n+1} + 1/2^n)/2, 1/2^{n+1})$, and $C_n = (1/2^{n+1}, 1/2^{n+1})$.

The piecewise affine function g going through the point A_n, B_n and C_n for all n (see Figure 2.5 page 81) is monotone and locally Lipschitz. We set $g(0) = 0$. We consider $\lambda_k = \frac{1}{2^k}$. Then:

$$\frac{g(\lambda_k) - g(0)}{\lambda_k} = 1 = \bar{l}.$$

For $t_k = (1/2^{k+1} + 1/2^k)/2$ we obtain:

$$\frac{g(t_k) - g(0)}{t_k} = \frac{2}{3} = \underline{l}.$$

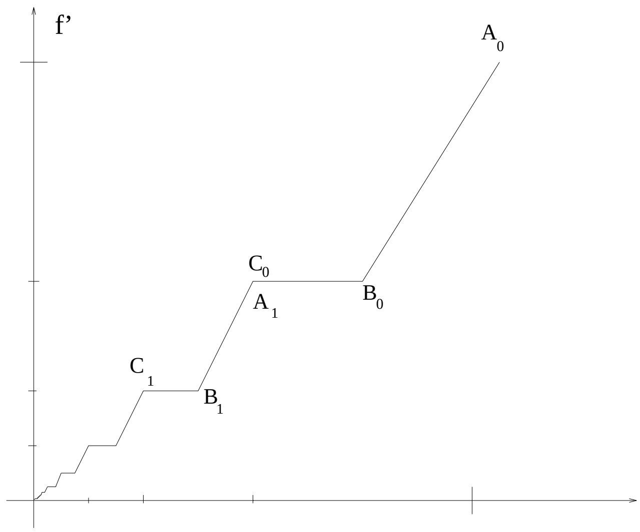


Figure 2.5: The derivative $f^{'}$ is monotone, locally Lipschitz and not directionally differentiable at the origin.

All in all, $\underline{l} < \bar{l}$. So the function f defined by $f(t) = \int_0^t g(s)ds$ is convex $C^{1,1}$. Yet it is not twice directionally differentiable at 0.

2.4 From one to several dimensions

We assume that the function $E : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ satisfies the following assumptions:

$$
\begin{array}{ll}
 & \bullet E \text{ has a nonempty domain } \operatorname{Dom}(E) = \{x \in \mathbb{R}^n \ : \ E(x) < \infty\}; \\
 & \bullet E \text{ is lower semi-continuous;} \\
 & \bullet E \text{ is epi-pointed;} \\
(2.9) & \bullet E \text{ is twice differentiable on } \operatorname{Dom}(E)^*; \\
 & \bullet \text{ there is an affine function minorizing } E; \\
 & \bullet E \text{ satisfies: } \forall x \in Bd(\operatorname{Dom} E) \cap \operatorname{Dom} E \ , \ \partial E(x) = \emptyset.
\end{array}
$$

In higher dimensions we can straightforwardly obtain the following relations between a point x_0 and its associated phase points x_i.

Lemma 2.5. *Let E satisfies hypothesis (2.9). The following hold.*

(i) The Hessian $\nabla^2 E(x_i)$ *is positive semi-definite at any phase* x_i *of* x*; moreover for any direction* d *in* $\mathbb{R}^n$*:*

$$0 \leq \overline{D}^2 \bar{\text{co}} E(x_i; d) \leq \langle \nabla^2 E(x_i) d, d \rangle.$$

(ii) If E *is 1-coercive, we have for all* d *and any phase decomposition* $x = \sum \lambda_i x_i$*:*

$$0 \leq \overline{D}^2 \bar{\text{co}} E(x; d) \leq \sum_i \lambda_i \overline{D}^2 \bar{\text{co}} E(x_i; d) \leq \sum_i \lambda_i \langle \nabla^2 E(x_i) d, d \rangle.$$

Proof. Part (i) of the Lemma comes from an easy manipulation of the Inequality: $\bar{\text{co}} E(x_i + \lambda d) \leq E(x_i + \lambda d)$ along with both equalities: $\bar{\text{co}} E(x_i) = E(x_i)$ and $\nabla \bar{\text{co}} E(x_i) = \nabla E(x_i)$.

We now turn to Part (ii). The convexity of $\bar{\text{co}} E$ implies:

$$\bar{\text{co}} E(x + td) \leq \bar{\text{co}} E(\sum_i \lambda_i (x_i + td)) \leq \sum_i \lambda_i \bar{\text{co}} E(x_i + td).$$

Since $\bar{\text{co}} E(x) = \sum \lambda_i \bar{\text{co}} E(x_i)$ and $\nabla \bar{\text{co}} E(x) = \sum \lambda_i \nabla \bar{\text{co}} E(x_i)$, we obtain:

$$\limsup_{t \to 0_+} \frac{\bar{\text{co}} E(x + td) - \bar{\text{co}} E(x) - t \langle \nabla \bar{\text{co}} E(x), d \rangle}{t^2/2} \leq$$
$$\sum_i \lambda_i \limsup_{t \to 0_+} \frac{\bar{\text{co}} E(x_i + td) - \bar{\text{co}} E(x_i) - t \langle \nabla \bar{\text{co}} E(x_i), d \rangle}{t^2/2},$$
$$= \sum_i \lambda_i D^2 \bar{\text{co}} E(x_i; d).$$

We put $\bar{\text{co}} E(x_i) = E(x_i)$ and $\nabla \bar{\text{co}} E(x_i) = \nabla E(x_i)$ in the above inequality to obtain the remaining part of (ii). □

Inequalities (2.5) and Lemma 2.1 still hold in higher dimensions as the following Corollary states.

Corollary 2.3. *Let* $g : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ *admits a right hand-side first-order derivative at* x_0*. The following properties hold:*

(i) If $g''(x_0; d)$ *exists,* $D^2 g(x_0; d)$ *exists and* $D^2 g(x_0; d) = g''(x_0; d)$*. The converse is not always true.*

(ii) If g is convex, the converse is true.

(iii) If g is a convex C^1 function and satisfies (2.2) page 66, then for all direction d:

$$\underline{g}''(x_0; d) \leq \underline{D}^2 g(x_0; d) \leq \overline{D}^2 g(x_0; d) \leq \overline{g}''(x_0; d). \tag{2.10}$$

Proof. We define $\varphi : t \mapsto f(x_0 + td)$. We compute $\varphi_r''(0) = f''(x_0; d)$ and $D^2\varphi_r(0) = D^2 f(x_0; d)$. Eventually Lemma 2.1 applied to φ gives inequalities (2.5). □

The analogue of Remark 2.5 page 74 can now be proved. It shows some difficulties due to the multidimensional setting: when $\bar{\text{co}}E(x_0) < E(x_0)$, $\bar{\text{co}}E$ is not always affine on a neighborhood of x_0: Corollary 2.1 page 69 does not hold for multivariate functions E.

Lemma 2.6. *Let E satisfies (2.9) page 81.*

(i) If E is a univariate function and $(\bar{\text{co}}E)_r''(x_0)$ is positive then $\bar{\text{co}}E(x_0) = E(x_0)$.

(ii) When E is defined on $\mathbb{R}^n$, we define $S(x_0)$ by $S(x_0) = \text{co}\{x_i\}$, $\mathcal{A}(x_0)$ as the smallest affine subspace containing $S(x_0)$ ($\mathcal{A}(x_0)$ is the affine hull of $S(x_0)$), and $\mathcal{V}(x_0)$ as the linear subspace associated with $\mathcal{A}(x_0)$.

If $\bar{\text{co}}E$ is twice directionnally differentiable at x_0 and there is a direction d in $\mathcal{V}(x_0)$ s.t. $D^2\bar{\text{co}}E(x_0; d)$ is positive then $\bar{\text{co}}E(x_0) = E(x_0)$.

Proof. Part (i) is clear, so we turn to Part (ii). We use an argument by contradiction. We suppose $\bar{\text{co}}E(x_0) < E(x_0)$. Then we can take a direction d in $\mathcal{V}(x_0)$. For λ small enough, $x_0 + \lambda d$ belongs to $A(x_0)$. Since $\bar{\text{co}}E$ is affine on $\mathcal{A}(x_0)$, it is twice directionally differentiable with $D^2\bar{\text{co}}E(x_0; d) = 0$. That contradiction ends the proof. □

Remark 2.7. The direction d must be in $\mathcal{V}(x_0)$ for (ii) to hold. Indeed we consider the function $E(x) = (x^2 - 1)^2 + y^2$ at $x_0 = (0, 0)$ in the direction $d = (0, 1)$. We compute: $S(x_0) = [-1, 1] \times \{0\}$, $\mathcal{A}(x_0) = \mathbb{R} \times \{0\} = \mathcal{V}(x_0)$, and $\bar{\text{co}}E''(x_0; d) = 2 > 0$. So d does not belong to $\mathcal{V}(x_0)$. We have: $1 = E(0,0) > \bar{\text{co}}E(0,0) = 0$. In conclusion, Property (ii) does not always hold for directions not in $\mathcal{V}(x_0)$.

For now on, we suppose:

(2.11) E satisfies Property (2.9) page 81 and is 1-coercive.

We recall that when (2.11) holds, the convex hull co$E$ is lower semi-continuous. So it is equal to the closed convex hull $\bar{\text{co}}E$ (we will continue to use the notation $\bar{\text{co}}E$).

Keeping in mind the definitions of $S(x)$, $\mathcal{A}(x)$ and, $\mathcal{V}(x)$, we define:

- the set of directions going out of $S(x)$ (outer directions):

$$\mathcal{V}^o(x) = \{d \in \mathcal{V}(x); \exists \bar{\lambda} > 0 \ \forall \lambda \in (0, \bar{\lambda}) \ x + \lambda d \notin \text{ri}S(x)\};$$

- the set of directions going in $S(x)$ (inner directions):

$$\mathcal{V}^i(x) = \{d \in \mathcal{V}(x); \exists \bar{\lambda} > 0 \ \forall \lambda \in (0, \bar{\lambda}) \ x + \lambda d \in \text{ri}S(x)\};$$

- the set of directions along which $\bar{\text{co}}E$ sticks to E:

$$\mathcal{V}^=(x) = \{d \in \mathcal{V}(x); \exists \bar{\lambda} > 0 \ \forall \lambda \in (0, \bar{\lambda}) \ \bar{\text{co}}E(x + \lambda d) = E(x + \lambda d)\};$$

- the set of directions along which there is a gap between $\bar{\text{co}}E$ and E:

$$\mathcal{V}^{\neq}(x) = \{d \in \mathcal{V}(x); \exists \bar{\lambda} > 0 \ \forall \lambda \in (0, \bar{\lambda}) \ \bar{\text{co}}E(x + \lambda d) < E(x + \lambda d)\}.$$

We name ri$S(x)$ the relative interior of $S(x)$.

We can compute the second-order directional derivatives of $\bar{\text{co}}E$ for directions d in $\mathcal{V}^i(x)$ or in $\mathcal{V}^=(x)$.

Lemma 2.7. *(i) For all d in $\mathcal{V}^i(x)$, $\bar{\text{co}}E''(x; d) = 0$ and $\bar{\text{co}}E''(x_i; d) = 0$ (the closed convex hull is affine along such directions).*

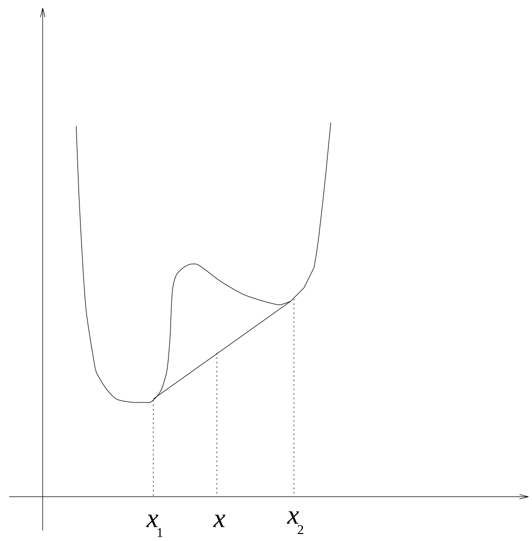


Figure 2.6: Any direction d starting from x belongs to $\mathcal{V}^{\neq}(x)$ and to $\mathcal{V}^{i}(x)$.

(ii) For all d in $\mathcal{V}^{=}(x)$, $\bar{\text{co}}E''(x;d) = \langle \nabla^2 E(x)d, d\rangle$ (the closed convex hull sticks to E along such directions).

(iii) Only in one dimension does the following inclusion holds:

$$\mathcal{V}^{\neq}(x) \subsetneq \mathcal{V}^{i}(x).$$

Proof. Since $\bar{\text{co}}E$ is affine on $S(x)$, Part (i) holds. Part (ii) is a straight consequence of the definition of $\mathcal{V}^{=}(x)$. It only remains to prove (iii). The inclusion is a straight consequence of Theorem 2.1 page 67, it is illustrated by Figure 2.6.

We now give a counter-example for the inclusion (iii) when E is defined on the plane. We take $E(x,y) = (x^2-1)^2 + y^2$, $(\bar{x},\bar{y}) = (0,0)$ and $d = (0,1)$. Then d is in $\mathcal{V}^{\neq}(x) = \mathbb{R}\times\mathbb{R}^*$ but not in $\mathcal{V}^{i}(x) = \mathbb{R}\times\{0\}$. □

Remark 2.8. If $S(x) \neq \{x\}$, there is a point x_i in $S(x)$. Then the direction $d = x - x_i$ is in $\mathcal{V}^{i}(x)$ and we have $\bar{\text{co}}E''(x;d) = \bar{\text{co}}E''(x_i;d) = 0$. Hence if $\bar{\text{co}}E$ is twice differentiable at x (resp. x_i), d is an eigenvector of $\nabla^2\bar{\text{co}}E(x)$ (resp. $\nabla^2\bar{\text{co}}E(x_i)$) associated with the null eigenvalue.

2.5 A geometric approach using phase simplices

In this section, we study the geometry of the phases x_i of a point x. Our terminology follows closely that of [48].

Before stating the main results, we need to define what we call a minimal phase simplex.

We assume E satisfies the Assumption (2.9) of page 81. We consider a phase decomposition (2.4) of x with $\alpha_i > 0$ and $x_i \neq x_j$ when $i \neq j$. The *phase number function* $\phi : \mathrm{Dom}(\bar{\mathrm{co}}E) \to \{1, \dots, n+1\}$ (page 355 in [48]) maps x to the smallest number of phases p in a phase decomposition of x.

We say that a phase decomposition of x is *minimal* when it has $\phi(x)$ phases.

The phase number function enjoys some smoothness when E is 1-coercive as the following Lemma states. If E is only epi-pointed, we do not know whether ϕ is still smooth.

Lemma 2.8 (Theorem 2.2 in [48]). *When E satisfies (2.11), ϕ is lower semi-continuous.*

Now we recall the definition of a phase simplex.

We say that the points $x_0, \dots, x_p$ forms a *p-simplex* when either of the following holds:

- The points $x_0, \dots, x_p$ are affinely independent.
- The vectors $x_1 - x_0, \dots, x_p - x_0$ are linearly independent.

Now we define the *phase simplex* $\sum(x)$ associated with a phase decomposition (2.4) by $\sum(x) = \mathrm{co}\{x_1, \dots, x_p\}$. We call *minimal phase simplex*, any phase simplex associated with a minimal phase decomposition. The next Proposition justifies our terminology.

Proposition 2.1. *We assume E satisfies (2.11) and x is in* $\mathrm{Dom}(\bar{\mathrm{co}}E)$. *If $x_1, \dots, x_p$ are phases associated with a minimal phase decomposition, the phase simplex $\sum(x) = \mathrm{co}\{x_1, \dots, x_p\}$ is a $(p-1)$-simplex.*

Proof. We assume that $\sum(x)$ is not a $(p-1)$-simplex, we are going to prove that it cannot be a minimal phase simplex.

Step 1. We write x as a convex combination of $p-1$ phases.

Since the points x_i are not affinely independent, there are $\delta_1, \dots, \delta_p$ not all null which verifies: $\sum_{i=1}^p \delta_i = 0$ and $\sum_{i=1}^p \delta_i x_i = 0$.

There is at least one positive δ_i, thus we can define:

$$t^* = \frac{\alpha_{i_0}}{\delta_{i_0}} = \min\{\frac{\alpha_j}{\delta_j} \ : \ j \in \{i \ : \ \delta_i > 0\}\}.$$

We set $\alpha_i^{'} = \alpha_i - t^* \delta_i$. We are going to prove that the numbers $\alpha_1', \dots, \alpha_p'$ form a convex combination of x.

Indeed $\sum_{i=1}^p \alpha_i^{'} = \sum_{i=1}^p \alpha_i - t^* \sum_{i=1}^p \delta_i = 1$, and $\sum_{i=1}^p \alpha_i^{'} x_i = \sum_{i=1}^p \alpha_i x_i - t^* \sum_{i=1}^p \delta_i x_i = x$. Moreover $\alpha_i^{'} \geq 0$ for all i (for i with $\delta_i \leq 0$, we clearly have $\alpha_i^{'} \geq 0$; and when $\delta_i > 0$, we have $t^* \leq \alpha_i / \delta_i$, hence $\alpha_i^{'} \geq 0$).

To obtain Step 1, we just check that $\alpha_{i_0}^{'} = \alpha_{i_0} - t^* \delta_{i_0} = \alpha_{i_0} - \frac{\alpha_{i_0}}{\delta_{i_0}} \delta_{i_0} = 0$.

Final Step. We prove that the infimum defining $\bar{\text{co}}E$ is attained at these $p-1$ phases.

Since $\bar{\text{co}}E$ is affine on $\sum(x)$, we write $\bar{\text{co}}E(y) = \langle a, y \rangle + b$, for all y in $\sum(x)$. Using the fact that the phase points x_i are themselves single phase points, we deduce:

$$\sum_{i=1}^p \alpha_i^{'} E(x_i) = \sum_{i=1}^p \alpha_i^{'} \bar{\text{co}}E(x_i) = \sum_{i=1}^p \alpha_i^{'} (\langle a, x_i \rangle + b) = \langle a, x \rangle + b = \bar{\text{co}}E(x).$$

Since $\alpha_{i_0}^{'} = 0$, we clearly have $\phi(x) < p$. □

Remark 2.9. The converse is false: a $(p-1)$-simplex which is a phase simplex is not always associated with a minimal phase decomposition as Figure 2.7 shows.

In [48], the authors distinguish several simplices: simplex of phase bifurcation and maximal phase simplex. Since we do not use their generic assumption, we do not have uniqueness of the phases. However uniqueness holds when there is only one maximal phase simplex. First we define what is a maximal phase simplex.

Definition 2.2 (page 370 in [48])**.** We say that a phase simplex $\sum(x)$ is *maximal* if it is not *the face* of a larger phase simplex.

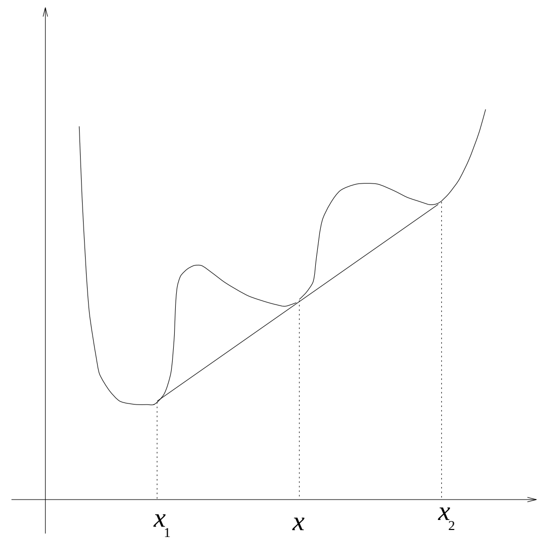


Figure 2.7: $\sum(x) = [x_1, x_2]$ is a 1-simplex but not a minimal phase simplex ($\phi(x) = 1 < 2$).

We recall the definition of a *face* (Definition 2.3.6, Chap. III in [25]). A nonempty convex subset $F \subset \sum(x)$ is a *face* of $\sum(x)$ if

$$\left.\begin{array}{c}(y_1, y_2) \in \sum(x) \times \sum(x) \text{ and} \\ \exists \alpha \in (0,1) \ : \ \alpha y_1 + (1 - \alpha y_2) \in F\end{array}\right\} \Rightarrow [y_1, y_2] \subset F.$$

Next we state without proof a simple lemma.

Lemma 2.9. *If $\sum(x) = \mathrm{co}(x_1, \ldots, x_p)$ is a $(p-1)$-simplex, its extreme points are $\{x_1, \ldots, x_p\}$.*

We recall that a point y is an *extreme point* of the convex set $\sum(x)$ if there are no two different points y_1 and y_2 in $\sum(x)$ such that $y = 1/2(y_1 + y_2)$ (Definition 2.3.1, Chap. III in [25]). The set of extreme points of $\sum(x)$ is denoted $\mathrm{ext} \sum(x)$.

Finally we state our uniqueness result.

Proposition 2.2. *The followings are equivalent:*

(i) x has a unique maximal phase simplex.

(ii) x has a unique phase decomposition (up to the order of the x_i).

Proof. We prove each implication separately.

- We assume $\sum = \sum(x) = \text{co}\{x_1, \ldots, x_p\}$ is a unique maximal phase simplex and we consider another phase simplex $\sum' = \sum'(x) = \text{co}\{x'_1, \ldots, x'_{p'}\}$. We are going to prove that each x'_i belongs to $\{x_1, \ldots, x_p\}$.

  We name $\sum''$ a maximal phase simplex containing $\sum'$ as a face. If x'_i does not belong to $\{x_1, \ldots, x_p\}$, $\sum'$ cannot be a face of $\sum$. So $\sum''$ is a maximal phase simplex not equal to $\sum$. That contradiction proves Part (i).

- Rabier and Griewank ([48] page 373) proved that when x has a unique phase decomposition, it has a unique phase simplex. □

2.6 An analytic approach using set-valued functions

We study the set-valued function $\overset{\cup}{P}$ which associates all phases to a given point x. We begin with a short discussion about what we can hope from such a set-valued function. Unfortunately, we build a example for which $\bar{\text{co}}E$ has second-order directional derivatives and $\overset{\cup}{P}$ has not even a continuous selection. So we cannot deduce regularity results on $\bar{\text{co}}E$ from $\overset{\cup}{P}$.

We close this section with another non fruitful approach: to use second-order epi-derivative. We show that existence of such a derivative is equivalent to the existence of second-order directional derivative.

2.6.1 Position of the problem

To study the first-order expansion of $\nabla\bar{\text{co}}E$, we suppose we can define on a neighborhood of a phase x_i of x, a function φ_i which maps any point y to one of its phase y_i. If φ_i is differentiable at x, we have:

$$\frac{\nabla\bar{\text{co}}E(x+td) - \nabla\bar{\text{co}}E(x)}{t} = \frac{\nabla E(\varphi_i(x+td)) - \nabla E(\varphi_i(x))}{t} \xrightarrow[t\to 0_+]{} \nabla^2 E(\varphi_i(x)).\varphi'_i(x)d.$$

Hence $\bar{\text{co}}E$ would be twice differentiable at x.

We can restrict our search to locally Lipschitz selections φ_i by using the following results on the generalized Jacobian in Clarke's sense. Clarke [9] defined

$\partial F(x)$ the generalized Jacobian of a function $F : \mathbb{R}^n \to \mathbb{R}^n$ at a point x as:

$$\partial F(x) = \text{co}\{\lim_{x^n \to x} JF(x^n);\ \text{for } x^n \notin \Omega_F\},$$

with $JF(x^n)$ the usual Jacobian matrix and Ω_F the set of points at which F fails to be differentiable.

Lemma 2.10 (Jacobian chain rule page 75 in [9])**.** *Let $H = G \circ F$, where $F : \mathbb{R}^n \to \mathbb{R}^n$ is Lipschitz near x and $G : \mathbb{R}^n \to \mathbb{R}^n$ is C^1 on a neighborhood of $F(x)$. Then for any direction d in $\mathbb{R}^n$, one has:*

$$\partial(G \circ F)(x).d = \nabla G(F(x)).\partial F(x).d.$$

Consequently if there is a locally Lipschitz selection φ, the Jacobian chain rule and the equation: $\nabla \bar{\text{co}} E(x) = \nabla E(\varphi(x))$ would imply:

$$\partial(\nabla \bar{\text{co}} E)(x).d = \nabla^2 E(\varphi(x)).\partial\varphi(x).d.$$

Unfortunately we can find examples —such as Figure 2.8 page 91— where no continuous function φ_i exists (at least under assumption (2.11)). To help understanding what are the properties of the phase points we are going to study $\overset{\cup}{P}(x)$: the set of all phases x_i of x. It turns out that $\overset{\cup}{P}(x)$ is an upper semi-continuous nonempty compact-valued set-valued map. We are also interested by its convex hull: $\overset{\cup}{S}$: $x \mapsto \text{co}\ \overset{\cup}{P}(x)$ because it has all properties of $\overset{\cup}{P}$ and in addition it is convex-valued.

We use definitions and properties on set-valued mapping as one can find in [2, 36]. We name set-valued function (also named multi-function, set-valued mapping or correspondence) a function which takes values in the subsets of $\mathbb{R}^n$.

We keep in mind the following characterization of a phase decomposition.

Lemma 2.11 (Rabier and Griewank, Remark 2.1 in [48])**.** *we assume E satisfies (2.11). If $\lambda_1, \ldots, \lambda_p$ and $x_1, \ldots, x_p$ satisfies: $\sum_{i=1}^p \lambda_i x_i = x$ with λ in Δ_p and $\lambda_i > 0$, then the followings are equivalent:*

(i) $\bar{\text{co}} E(x) = \sum_{i=1}^p \lambda_i E(x_i)$.

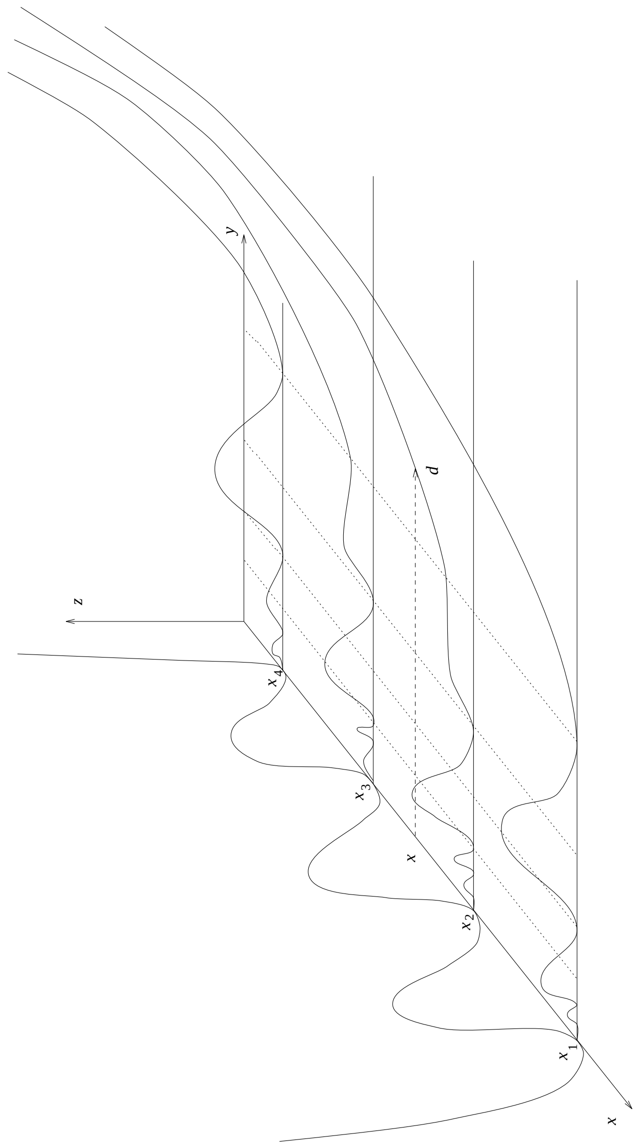


Figure 2.8: There is no continuous phase selection at x: we cannot find a continuous curve on both the graph of E and the plane $z = 0$. Yet $\bar{\text{co}}E$ is C^2 on a neighborhood of x.

(ii) The affine hyperplane tangent to the graph of E at $(x_i, E(x_i))$ is under this graph, that is, for all $i, j = 1, \dots, p$:

$$\begin{aligned}&\nabla E(x_i) = \nabla E(x_j),\\ &E(x_i) - \langle \nabla E(x_i), x_i\rangle = E(x_j) - \langle \nabla E(x_j), x_j\rangle,\\ &E(.) \geq \langle \nabla E(x_i), . - x_i\rangle + E(x_i).\end{aligned} \tag{2.12}$$

We are going to study the set-valued mappings: $\overset{\cup}{P}$: $\operatorname{Dom} \bar{\text{co}}E \subset \mathbb{R}^n \rightrightarrows \mathbb{R}^n$ and $\overset{\cup}{S}$: $\operatorname{Dom} \bar{\text{co}}E \subset \mathbb{R}^n \rightrightarrows \mathbb{R}^n$ defined by:

$$\begin{aligned}\overset{\cup}{P}(x) &= \{x_i \in \mathbb{R}^n \;:\; \nabla \bar{\text{co}}E(x_i) = \nabla \bar{\text{co}}E(x) \text{ and } \partial E(x_i) \neq \emptyset\},\\ \overset{\cup}{S}(x) &= \{x_i \in \mathbb{R}^n \;:\; \nabla \bar{\text{co}}E(x_i) = \nabla \bar{\text{co}}E(x)\}.\end{aligned}$$

The set $\overset{\cup}{P}(x)$ contains all the phases of x while $\overset{\cup}{S}(x)$ is the convex hull of all phase simplices of x as the following Proposition shows. Note that we consider *any phase decomposition*, even phase decompositions (2.4) with $\lambda_i = 0$.

To prove the next Proposition, we need the following Lemma.

Lemma 2.12. *If g is a C^1 convex function, the following implication holds:*

$$\nabla g(x) = \nabla g(y) \Rightarrow \; g \textit{ is affine on the interval } [x, y].$$

Proof. If $g : \mathbb{R} \to \mathbb{R}$ is a univariate function, g' is a continuous non decreasing function with $g'(x) = g'(y)$. So g is affine on $[x, y]$ and the Proposition holds.

Otherwise, we define $d = y - x$ and $\varphi(t) = g(x + td)$. The function φ is convex, C^1 with $\varphi'(0) = \varphi'(1)$. Since φ is univariate, $\varphi(t) = t\varphi'(0) + \varphi(0)$, that is, $g(x + td) = t\langle \nabla g(x), d\rangle + g(x)$. We just proved that g is affine on $[x, y]$. □

We can now compute the sets $\overset{\cup}{S}(x)$ and $\overset{\cup}{P}(x)$.

Proposition 2.3. *The followings hold.*

$$\overset{\cup}{S}(x) = \cup\{\textstyle\sum(x); \sum(x) \textit{ is a phase simplex of } x\}, \tag{2.13}$$

$$= \text{co}\, \overset{\cup}{P}(x), \tag{2.14}$$

$$\overset{\cup}{P}(x) = \{x_i \in \mathbb{R}^n; \nabla \bar{\text{co}}E(x) \in \partial E(x_i)\} \tag{2.15}$$

$$= \{x_i \in \mathbb{R}^n; E(x_i) = \bar{\text{co}}E(x) + \langle \nabla \bar{\text{co}}E(x), x_i - x\rangle\}. \tag{2.16}$$

If $x = \sum_i \lambda_i x_i$ *with* λ *in* Δ_p*, the following relation holds:*

$$x_1, \dots, x_p \in \overset{\cup}{P}(x) \Leftrightarrow \overline{\text{co}}E(x) = \sum_i \lambda_i E(x_i). \tag{2.17}$$

Remark 2.10. One may think that $\overset{\cup}{S}(x)$ is polyhedral. Although it is true when x enjoys a unique phase decomposition, $\overset{\cup}{S}(x)$ is no longer polyhedral when uniqueness does not hold. For example we take $E(x,y) = (x^2+y^2-1)^2$. The graph of E is the rotation of the graph of $x \mapsto (x^2-1)^2$ around the vertical axis. Consequently $\overset{\cup}{S}(x)$ is the closed unit ball in $\mathbb{R}^2$, and $\overset{\cup}{P}(x)$ is the unit circle. Hence $\overset{\cup}{S}(x)$ is not polyhedral neither $\overset{\cup}{P}(x)$ is finite, nor even countable.

Proof. Since $\overline{\text{co}}E$ is affine on any phase simplex $\sum(x)$ and x is in $\sum(x)$, the gradient $\nabla\overline{\text{co}}E$ is equal to $\nabla\overline{\text{co}}E(x)$ on the union of all phase simplices of x. Hence this last set is in $\overset{\cup}{S}(x)$.

Conversely we take y in $\overset{\cup}{S}(x)$. Due to Lemma 2.12 page 92, $\overline{\text{co}}E$ is affine on $[x,y]$, so we can write:

$$\forall z \in [x,y], \overline{\text{co}}E(z) = \langle \nabla\overline{\text{co}}E(y), z-y\rangle + \overline{\text{co}}E(y). \tag{2.18}$$

Now we consider a phase decomposition $y = \sum_i \lambda_i y_i$ of y, and a phase decomposition $x = \sum_i \alpha_i x_i$ of x. Using (2.18), we see that relations (2.12) hold for $\sum = \{x_1, \dots, x_p, y_1, \dots, y_r\}$. Using Lemma 2.11, we deduce that $\text{co}\sum$ is a phase simplex of x. Consequently y is in the union of all phase simplices of x: we just proved (2.13).

We clearly have $\overset{\cup}{P}(x) \subset \overset{\cup}{S}(x)$. Now we take y in $S(x)$ and consider a phase decomposition $y = \sum_i \lambda_i y_i$ of y. We have $\partial\overline{\text{co}}E(y_i) \neq \emptyset$ and $\nabla\overline{\text{co}}E(y_i) = \nabla\overline{\text{co}}E(y) = \nabla\overline{\text{co}}E(x)$. Hence y is in $\text{co}\,\overset{\cup}{P}(x)$. We proved (2.14).

Similar arguments show that (2.15) holds.

We now turn to (2.16). If $E(x_{i_0}) = \overline{\text{co}}E(x) + \langle\nabla\overline{\text{co}}E(x), x_{i_0} - x\rangle$ holds for x_{i_0}, we have $E(x_{i_0}) \geq \overline{\text{co}}E(x_{i_0}) \geq \overline{\text{co}}E(x) + \langle\nabla\overline{\text{co}}E(x), x_{i_0} - x\rangle = E(x_{i_0})$. So x_{i_0} is clearly in $\overset{\cup}{P}(x)$.

Conversely we take x_i in $\overset{\cup}{P}(x)$ and define the plane $\mathcal{P}$ by:

$$(u, v) \in \mathcal{P} \Leftrightarrow v = E(x_i) + \langle \nabla \bar{\text{co}} E(x), u - x_i \rangle.$$

Since $E(x_i) - \langle \nabla E(x_i), x_i \rangle = \bar{\text{co}} E(x) - \langle \nabla \bar{\text{co}} E(x), x \rangle$, the point $(x, \bar{\text{co}} E(x))$ belongs to $\mathcal{P}$. Hence (2.16) is true.

Last we prove the equivalence (2.17). We suppose $x = \sum_i \lambda_i x_i$ with λ in Δ_p and $x_1, \ldots, x_p \in \overset{\cup}{P}(x)$. Since $\bar{\text{co}} E$ is affine on $\text{co}\{x_1, \ldots, x_p\}$ and $E(x_i) + \langle \nabla \bar{\text{co}} E(x), . - x_i \rangle \leq \bar{\text{co}} E \leq E$, we have: $\bar{\text{co}} E(x) = \sum_i \lambda_i \bar{\text{co}} E(x_i)$ and $E(x_i) \leq \bar{\text{co}} E(x_i) \leq E(x_i)$.

The converse implication is obvious. $\square$

We are now ready to study the smoothness of $\overset{\cup}{P}$ and $\overset{\cup}{S}$.

Proposition 2.4. *If E satisfies Assumption (2.11) page 84, $\overset{\cup}{P}(x)$ and $\overset{\cup}{S}(x)$ are nonempty compact sets of $\mathbb{R}^n$. Both set-valued functions map compact sets on compact sets.*

Proof. The closedness of $\overset{\cup}{S}(x)$ and $\overset{\cup}{P}(x)$ follows from the continuity of ∇E and $\nabla \bar{\text{co}} E$. The only non trivial fact is the "local boundedness property".

Let B be a compact subset of $\mathbb{R}^n$, we are going to prove that $\overset{\cup}{P}(B)$ is bounded by using an argument by contradiction.

Suppose there is a sequence x_1^k in $\overset{\cup}{P}(B)$ s.t. $|x_1^k| \to \infty$ when $k \to \infty$. We call x^k the sequence of points s.t. x_1^k belongs to $\overset{\cup}{P}(x^k)$. Since $\nabla \bar{\text{co}} E(x^k)$ is in $\partial E(x_1^k)$, we can write:

$$E \geq \bar{\text{co}} E \geq E(x_1^k) + \langle \nabla \bar{\text{co}} E(x^k), . - x_1^k \rangle.$$

It follows that $E(x_1^k) = \bar{\text{co}} E(x_1^k)$, and $\nabla E(x_1^k) = \nabla \bar{\text{co}} E(x_1^k)$. We use Lemma 2.12 to deduce:

$$E(x_1^k) = \bar{\text{co}} E(x_1^k) = \bar{\text{co}} E(x^k) + \langle \nabla \bar{\text{co}} E(x^k), x_1^k - x^k \rangle.$$

Consequently there are C_0 and C_1 in $\mathbb{R}$ s.t.

$$\frac{E(x_1^k)}{|x_1^k|} \leq \frac{C_0}{|x_1^k|} + C_1.$$

Taking the limit when k goes to infinity, we find that E cannot be 1-coercive.

Since $\overset{\cup}{S}(x) = \text{co}\, \overset{\cup}{P}(x)$, $\overset{\cup}{S}$ is locally bounded too. □

Before stating the smoothness of $\overset{\cup}{S}$ and $\overset{\cup}{P}$, we recall some definitions about continuity of set-valued mappings [2, 36].

Definition 2.3. Let $A : \mathbb{R}^n \rightrightarrows \mathbb{R}^n$ be a set-valued mapping.

- A is *upper semi-continuous* (usc) if for all x in $\mathbb{R}^n$, for all sequence x^k converging to x and for all open set O s.t. $A(x) \subset O$, there is $\bar{k}$ s.t. for $k \geq \bar{k}$, $A(x^k) \subset O$.

- A is *lower semi-continuous* (lsc) if for all x in $\mathbb{R}^n$, for all sequence x^k converging to x and for all open set O s.t. $A(x) \cap O \neq \emptyset$, there is $\bar{k}$ s.t. for $k \geq \bar{k}$, $A(x^k) \cap O \neq \emptyset$.

The next Proposition states the smoothness of $\overset{\cup}{S}$ and $\overset{\cup}{P}$.

Proposition 2.5. *If E satisfies* (2.11)*, $\overset{\cup}{S}$ and $\overset{\cup}{P}$ are upper semi-continuous.*

Proof. Since both set-valued functions are closed and locally bounded, they are usc. Netherveless we choose to include the full proof of this result.

We first prove with an argument by contradiction that $\overset{\cup}{S}$ is usc.

Let x^k be a sequence converging to x and let O be an open set containing $\overset{\cup}{S}(x)$. We take x_i^k in $\overset{\cup}{S}(x^k)$, we need to find a point y_i^k in $\overset{\cup}{S}(x)$ as close as we want to x_i^k. We choose $y_i^k = \text{Proj}_{\overset{\cup}{S}(x)}(x_i^k)$: the projection of x_i^k on the closed convex set $\overset{\cup}{S}(x)$.

We take $\delta > 0$ and use an argument by contradiction. If for all $\bar{k}$, there is an integer $k \geq \bar{k}$ s.t. $|x_i^k - y_i^k| > \delta$, we can build a subsequence $x_i^{k_p}$ in $\overset{\cup}{S}(x^{k_p})$ verifying that inequality.

Now using the boundedness property of $\overset{\cup}{S}$ we can extract a converging subsequence; so we can suppose that $x_i^{k_p}$ converges towards x_i. Using the continuity of the projection on a closed convex set, we find:

$$\|x_i - \text{Proj}_{\overset{\cup}{S}(x)}(x_i)\| > \delta.$$

But this is impossible since the limit x_i is obviously in $\overset{\cup}{S}(x)$ (by continuity of $\nabla \bar{\text{co}} E$). Consequently, $\overset{\cup}{S}$ is upper semi-continuous.

Since E and $\bar{\text{co}} E$ are smooth, Graph $\overset{\cup}{P} = \{(x, x_i) \; : \; x_i \in \overset{\cup}{P}(x)\}$ is closed. We apply the next Lemma to obtain the usc of $\overset{\cup}{P}$. □

Lemma 2.13 (Chap. 1, Theorem 1 in [2])**.** *Let F and G be two set-valued functions such that, for all x in $\mathbb{R}^n$, $F(x) \cap G(x) \neq \emptyset$. We suppose F is upper semi-continuous at x_0, $F(x_0)$ is compact, and the graph of G is closed. Then the set-valued function $F \cap G : x \mapsto F(x) \cap G(x)$ is upper semi-continuous at x_0.*

We name *selection* of a set-valued function F, any function $f : \text{Dom}\, F \subset \mathbb{R}^n \to \mathbb{R}^n$ such that for all x, $f(x)$ is in $F(x)$.

We are interested by continuous selections φ_i of $\overset{\cup}{P}$ such that for any x in $\mathbb{R}^n$ and any x_i in $\overset{\cup}{P}(x)$ there is a neighborhood U of x on which φ_i is defined, and $\varphi_i(x) = x_i$. Unfortunately $\overset{\cup}{S}$ is lower semi-continuous as soon as there is such a selection (see Example 8.4.10 in [36] or Chap. 1, Part 10, Proposition 1 in [2]). The following example shows $\overset{\cup}{S}$ is not lsc even when E is a univariate polynomial.

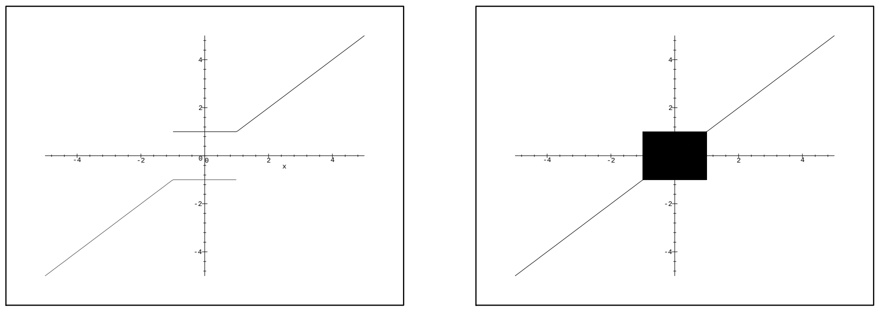
Example 2.3. Take $E(x) = (x^2 - 1)^2$, $O = (-2, 0)$, $x = 1$ and $x^k = 1 + 1/k$. We easily compute $\overset{\cup}{S}(x^k) = \{1 + 1/k\}$ and $\overset{\cup}{S}(x) = [-1, 1]$. But for all k we have $\overset{\cup}{S}(x^k) \cap O = \emptyset$. Consequently $\overset{\cup}{S}$ is not lsc (see Figure 2.9).

Hence we cannot apply directly Michael's selection Theorem (Chap. 1, Theorem 1 in [2]) to find a continuous selection of $\overset{\cup}{S}$.

By the way, we note that there is an obvious explicit C^∞ selection of $\overset{\cup}{S}$: the identity. However it does not give any useful information about the existence of a second-order expansion. In fact we seek a selection of $\overset{\cup}{P}$ as the following example shows.

Example 2.4. Consider $E(x) = (x^2 - 1)^2$, we have $x \in \overset{\cup}{S}(x)$ for all x but it does not give us much information. We take $x = 1$ and $d = -1$. The function

$$\varphi_1 : y \in (-1, \infty) \mapsto \begin{cases} y \text{ if } y \geq 1, \\ 1 \text{ otherwise;} \end{cases}$$



(a) $\overset{\cup}{P}$ (b) $\overset{\cup}{S}$

Figure 2.9: Both $\overset{\cup}{S}$ and $\overset{\cup}{P}$ are not lsc at $x = 1$. Yet there is a smooth selection of $\overset{\cup}{P}$ defined on a neighborhood of 1.

is a directionally differentiable continuous selection of $\overset{\cup}{P}$. Consequently $\bar{\text{co}}E$ is directionally differentiable with:

$$(\bar{\text{co}}E)''(1, -1) = E^{''}(\varphi_1(1)).\varphi_1{}'(1).$$

What smoothness can be hoped for $\overset{\cup}{P}$? Since it is not lsc, it cannot satisfy the locally continuous selectionnable property:

For all $x_i \in \overset{\cup}{P}(x)$, *there is* V *a neighborhood of* x *and a continuous function* $\varphi : V \to \mathbb{R}^n$ *s.t.* $\varphi(x) = x_i$ *and for all* $y \in V$, $\varphi(y) \in \overset{\cup}{P}(y)$.

Indeed it implies the lower semi-continuity of $\overset{\cup}{P}$ (see [47]).

Note that a weaker property like:

There is x_i *in* $\overset{\cup}{P}(x)$, V *a neighborhood of* x *and a continuous function* $\varphi : V \to \mathbb{R}^n$ *s.t.* $\varphi(x) = x_i$ *and for all* $y \in V$, $\varphi(y) \in \overset{\cup}{P}(y)$.

would be enough to claim the existence of second-order directional derivatives of $\bar{\text{co}}E$. Unfortunately Figure 2.8 page 91 shows it is not always true under Hypothesis (2.11).

We close this section with a quick study of epi-derivative applied to our convex hull problem. In fact the function $\bar{\text{co}}E$ is too smooth: the second-order epi-derivatives exists if and only if the classical second-order directional derivative exists.

2.6.2 The second-order epi-derivative approach

The key idea of second-order epi-derivative is to consider the function:

$$\Delta_t(d) = \frac{f(x+td) - f(x) - t\langle \nabla f(x), d\rangle}{\frac{1}{2}t^2},$$

for $t > 0$, and to study whether its epigraph set-converges [51].

Our function f would be twice epi-differentiable at a point x if $\Delta_t(d)$ epi-converges for all d to a limit $f''_x(d)$ with $f''_x(0) > -\infty$ (see [52]). When it happens $d \mapsto f''_x(d)$ is convex, lsc, positively homogeneous of degree two.

Like with classical derivatives there is a strong link between the existence of a second-order expansion of f and existence of a derivative of ∇f. We directly state the result for $\bar{\text{co}}E$.

Lemma 2.14. *Under assumption* (2.11) *the followings are equivalent:*

(i) The function $\bar{\text{co}}E$ *is twice epi-differentiable at* x.

(ii) Its gradient $\nabla\bar{\text{co}}E$ *is proto-differentiable at* x.

In our setting (ii) means that the set:

$$\{(d, \frac{\nabla\bar{\text{co}}E(x+td) - \nabla\bar{\text{co}}E(x)}{t}); d \in \mathbb{R}^n\} \tag{2.19}$$

set-converges when t decreases to 0 with $t > 0$.

If we define the quotient:

$$Q_t = \frac{\nabla\bar{\text{co}}E(x+td) - \nabla\bar{\text{co}}E(x)}{t}.$$

The set-convergence of (2.19) reduces to:

$$\{w \;:\; w = \lim_{t\downarrow 0} Q_t\} = \{w \;:\; \exists (t_k)_k \text{ such that } w = \lim_k Q_{t_k}\}.$$

So Q_t converges in the classical way. Hence we have:

Proposition 2.6. *Under* (2.11) *the following are equivalent:*

(i) The function $\bar{\text{co}}E$ *is twice epi-differentiable at* x.

(ii) The function $\bar{\text{co}}E$ *is twice directionally differentiable at* x.

Proof. Since the function $\bar{\text{co}}E$ is continuously differentiable with a locally lipschitzian gradient, the pointwise and epi-convergence of the second-order difference quotient Δ_t are equivalent (see Proposition 3.1 in [45]). □

Hence studying the existence of second-order epi-derivatives is equivalent to proving the existence of second-order directional derivatives.

2.7 Second-order expansion of the closed convex hull of a function using marginal functions

Introduction

We apply estimates of the lower second-order directional derivative of marginal functions to the convex hull.

Given a real-valued function ψ, we define the marginal function φ by:

$$\varphi(u) = \inf\{\psi(u, X) \ : \ X \in \mathcal{I}(u)\}.$$

At least two types of derivatives for marginal functions lead to interesting results. Approximate directional derivatives are based on the spirit of the ϵ-subdifferential. For example, in the convex unconstrained case Hiriart–Urruty [23] computed the first- and second-order directional derivatives of φ.

We choose to use the other type which is based on a Taylor expansion along a line. Gauvin [20, 17, 18, 19], Rockafellar [50] and Janin [28] gave estimates of the directional derivative using first- or second-order multiplier sets. To ensure the existence of at least one Kuhn–Tucker vector, they assumed a constraint-qualification. Unfortunately that constraint qualification does not hold in our setting.

If we take a compact constraint set which does not depend on u, and ψ is directionally differentiable, Furukawa [16] proved that φ is directionally differentiable at u in any direction d with:

$$D\varphi(u; d) = \min_{X\in\mathcal{I}_1(u)} D\psi(u, X; d),$$

where $\mathcal{I}_1(u) = \{X \in K \ : \ \varphi(u) = \psi(u, X)\}$ is the set of first-order active parameters.

In a broad setting, Hiriart–Urruty [22] gave estimates of Clarke's generalized gradient. Closer to our study, Correa and Seeger [13] computed the first-order directional derivative.

Much less is known about second-order directional derivatives. If the constraint set does not depend on u and is compact, Kawasaki [29, 30, 31, 32] gave estimates of the lower second-order directional derivative. He noted an envelope-like effect: "a group of affine functions, whose derivatives are of course zero, often forms and *envelope* with positive second-derivative". However his assumptions are too restrictive to our setting: he takes a fixed compact constraint set and assumes ψ is twice continuously differentiable.

The convex hull $\operatorname{co} E$ of a real-valued function E can be written:

$$\operatorname{co} E(x) = \inf\{\sum_{i=1}^{p} \bar\lambda_i E(x_i) \ : \ \bar\lambda \in \Delta_p \text{ and } \sum_{i=1}^{p} \bar\lambda_i x_i = x\}, \tag{2.20}$$

where Δ_p is the unit simplex of $\mathbb{R}^p$ and $x_i \neq x_j$ for $i \neq j$.

An easy manipulation of (2.20) allows us to apply recent results of Correa and Barrientos [11].

We assume E is 1-coercive (in that case $\bar{\operatorname{co}} E = \operatorname{co} E$). Then the infimum (2.20) is attained at a convex combination $\bar\lambda_1, \dots, \bar\lambda_p$ associated with the phases $x_1, \dots, x_p$ with $1 \le p \le n+1$. It is also attained at the convex combination $\bar\lambda_1, \dots, \bar\lambda_{p-1}, \tilde\lambda_p, \dots \tilde\lambda_{n+1}$ associated with $x_1, \dots, x_{p-1}, \tilde x_p, \dots \tilde x_{n+1}$ where $\tilde\lambda_i = \bar\lambda_p/(n+1-p)$ for $i = p, \dots n+1$, and $\tilde x_i = x_p$ for $i = p, \dots n+1$. So it is not restrictive to assume all coefficients λ_i are positive. Consequently it is sufficient to take λ in $\operatorname{int} \Delta_{n+1}$ in (2.20).

For now on we name $\lambda = (\lambda_1, \lambda')^T \in \mathbb{R}^{n+1}$ a row vector with $\lambda_1 > 0$ and $\lambda' \in \mathbb{R}^n$. Similarly we name $X = (x_1, X')$ with $X' = (x_2, \dots x_{n+1})$ and $x_i \in \mathbb{R}^n$.

We define the following open subset of $\mathbb{R}^n$:

$$\Omega_n = \{\lambda' \in \mathbb{R}^n \ : \ \sum_{i=2}^{n+1} \lambda_i < 1 \text{ and } \lambda_i > 0 \text{ for } i = 2, \ldots, n+1\}.$$

We choose to take λ' in Ω_n even though we do not need all λ_i to be positive but only the positiveness of λ_1. We could associate to a null λ_i the same $\tilde{x}_i$ as above. However computing the minimum on an open set simplifies our analysis.

To apply Theorem 2.5 page 103, we must have a fixed constraint set. Hence we use the following formula:

$$\bar{\text{co}} E(x) = \min_{\lambda' \in \Omega_n} \varphi(x, (1 - \sum_{i=2}^{n+1} \lambda_i, \lambda')), \tag{2.21}$$

where the function φ is defined by:

$$\varphi(x, \lambda) = \min_{X' \in \mathbb{R}^{n^2}} \psi(x, \lambda, X'), \tag{2.22}$$

and the function ψ by:

$$\psi(x, \lambda, X') = \lambda_1 E((x - \sum_{i=2}^{n+1} \lambda_i x_i)/\lambda_1) + \lambda_2 E(x_2) + \cdots + \lambda_{n+1} E(x_{n+1}).$$

We have to study two different marginal functions. Problem (2.22) is smooth with an unbounded constraint set, while problem (2.21) is nonsmooth with a bounded constraint set.

For notational convenience we still name $x_1 = (x - \sum_{i=2}^{n+1} \lambda_i x_i)/\lambda_1$, keeping in mind that it is *only* a notation and no longer a free variable contrary to $x_2, \ldots x_{n+1}$. Similarly, $\lambda_1 = 1 - \sum_{i=2}^{n+1} \lambda_i$ is only a notation for problem (2.21), but $\lambda_1, \ldots \lambda_{n+1}$ are free variables in (2.22).

Remark 2.11. We could write $\bar{\text{co}} E$ as:

$$\bar{\text{co}} E(x) = \min_{X'} \Phi(x, X'), \qquad \Phi(x, X') = \min_{\lambda \in \Delta_{n+1}} \psi(x, \lambda, X').$$

However the matrix $\nabla^2_{\lambda\lambda} \psi(x, \lambda, X') = \lambda_1^{-1} X^T \nabla^2 E(x_1) X$ is never positive, so contrary to decomposition (2.21)–(2.22) for which $\nabla^2_{X'X'} \psi$ may be positive, we can never apply Proposition 2.7 page 103 to obtain second-order information on ϕ. Eventually, we choose to use the intermediate marginal function φ instead of ϕ for technical reasons.

After summarizing our main tool, we study the smoothness of φ. Next we deduce some results on the smoothness of $\bar{\text{co}}E$.

2.7.1 Main tool

We name u_0 a point in $\mathbb{R}^m$, d a direction in $\mathbb{R}^m$, and $\mathcal{C}$ a constraint set in $\mathbb{R}^p$. To a given function $h : \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$, we associate the marginal function $g : \mathbb{R}^m \to \mathbb{R}$ by $g(u) = \inf\{h(u,\mu) \ : \ \mu \in \mathcal{C}\}$. We always assume the set of minimizers $\mathcal{I}_1(u_0) = \{\mu \in \mathcal{C} \ : \ g(u_o) = h(u_0,\mu)\}$ is nonempty.

To prove $Dg(u_0;d) = \lim_{t\to 0^+}(g(u_0+td) - g(u_0))/t$ exists, we make the following assumptions:

i). Either $\mathcal{C}$ is compact or the function $q_1 : \mathbb{R}^+ \times \mathcal{C} \to \mathbb{R}$ defined by: $q_1(t,\mu) = (h(u_0+td,\mu) - g(u_0))/t$, satisfies:

   (P) For every sequence t_n in $\mathbb{R}^+$ converging to 0, there is a sequence ϵ_n in $\mathbb{R}^+$ (the set of positive real numbers) converging to 0 and a sequence μ_n in $\{\mu \in \mathcal{C} \ : \ \inf_{\mu'\in\mathcal{C}} q_1(t_n,\mu') \geq q_1(t_n,\mu) - \epsilon_n\}$ having at least one cluster point μ_0 in $\mathcal{C}$.

ii). The function $(t,\mu) \in \mathbb{R}^+ \times \mathcal{C} \mapsto h(u_0+td,\mu)$ is upper semi-continuous (usc) in $\{0\} \times \mathcal{C}$.

iii). Either, h is subregular (regular in Clarke's sense [9]), or for every μ' in $\mathcal{I}_1(u_0)$ there exists $\lim_{\substack{t\to 0^+\\ \mu\to\mu'}}(h(u_0+td,\mu) - h(u_0,\mu))/t$.

Now we can state the first-order result we will use.

Theorem 2.4 (R. Correa & O. Barrientos [11])**.**
If Assumptions i)–iii) hold, the function g has a directional derivative given by:

$$Dg(u_0;d) = \min_{\mu\in\mathcal{I}_1(u_0)} D_u h(u_0,\mu;d).$$

Moreover, $\mathcal{I}_2(u_0;d) = \mathcal{I}_1(u_0) \cap \mathcal{M}_1(0)$ is the set of points at which the minimum is attained, where:
$\mathcal{M}_1(0) = \{\mu_0 \in \mathcal{C} \ : \ \liminf_{t\to 0}\inf_{\mu\in\mathcal{C}} q_1(t,\mu) \geq \liminf_{\substack{t\to 0^+\\ \mu\to\mu_0}} q_1(t,\mu)\} \subset \mathcal{I}_1(u_0)\}.$

A similar argument may be applied to obtain an estimate of the lower second-order directional derivative. We need two additional hypotheses:

iv). Either $\mathcal{C}$ is compact or the function $q_2 : \mathbb{R}^+ \times \mathcal{C} \to \mathbb{R}$ defined by: $q_2(t,\mu) = (h(u_0+td,\mu) - g(u_0) - tDg(u_0;d))/t^2$ satisfies property (P) page 102.

v). For every μ' in $\mathcal{I}_2(u_0;d) = \{\mu' \in \mathcal{I}_1(u_0) \ : \ Dg(u_0;d) = D_\mu h(u_0,\mu';d)\}$, there exists $\lim_{\substack{t\to 0^+\\ \mu\to\mu'}}(h(u_0+td,\mu) - h(u_0,\mu) - tD_u h(u_0,\mu;d))/t^2$.

Theorem 2.5 (Correa and Barrientos [11])**.**
Under Assumptions i)–v), we have:

$$\underline{D}^2 g(u_0;d) = \min_{\mu\in\mathcal{I}_2(u_0;d)} [D^2_{uu}h(u_0,\mu;d) - A_2(u_0,\mu;d)], \tag{2.23}$$

and the set of points where the minimum is attained is $\mathcal{I}_2(u_0;d)\cap\mathcal{M}_2(0)$.

We name $D^2_{uu}h(u_0,\mu;d)$ the de la Vallée-Poussin second-order directional derivative of the function $h(.,\mu)$. We define
$\mathcal{M}_2(0) = \{\mu_0 \in \mathcal{C} \ : \ \liminf_{t\to 0^+}\inf_{\mu\in\mathcal{C}} q_2(t,\mu) \geq \liminf_{\substack{t\to 0^+\\ \mu\to\mu_0}} q_2(t,\mu)\}$,

$$A_2(u_0,\mu';d) = -\liminf_{\substack{t\to 0^+\\ \mu\to\mu'}} \frac{h(u_0,\mu) - g(u_0) + t(D_u h(u_0,\mu;d) - Dg(u_0;d))}{t^2/2}.$$

We always have $0 \leq A_2(u_0,\mu;d) < +\infty$.

After applying Theorem 2.5, two problems remain: Does $D^2 g(u_0;d)$ exists? And how can we compute $A_2(u_0,\mu';d)$?

We note that if $A_2(u_0,\mu';d) = 0$ at μ' in $\mathcal{I}_2(u_0;d)\cap\mathcal{M}_2(0)$ then $D^2 g(u_0;d)$ exists (see [11]). Except from that particular case, where there is no envelope-like effect, we will use the next Proposition.

Proposition 2.7 (Correa and Barrientos [11])**.** *We assume $\mathcal{C}$ is an open subset of $\mathbb{R}^p$ and for all μ in $\mathcal{I}_2(u_0;d)$ the function h is twice differentiable at (u_0,μ). If $\nabla^2_{\mu\mu}h(u_0,\mu)$ is positive, we can write:*

$$A_2(u_0,\mu;d) = \langle(\nabla^2_{\mu\mu}h(u_0,\mu))^{-1}\nabla^2_{\mu u}h(u_0,\mu)d, \nabla^2_{\mu u}h(u_0,\mu)d\rangle.$$

Although the Proposition is a consequence of more general results from [11], we provide a proof (simplified to our setting) to emphasize the main arguments.

Proof. The proof is twofold. First we prove an inequality, then we show that equality holds.

Step 1. We apply Taylor's Theorem to $h(u_0,.)$ and to $\langle\nabla_u h(u_0,.)$ at μ and we use the necessary optimality condition $\nabla_\mu h(u_0,\mu)=0$ to obtain:

$$-A_2(u_0,\mu;d)=\liminf_{\substack{t\to 0^+\\ \mu'\to\mu}} \frac{\langle\nabla^2_{\mu\mu}h(u_0,\mu)(\mu'-\mu),\mu'-\mu\rangle}{t^2} + 2\frac{\langle\nabla^2_{\mu u}h(u_0,\mu)d,\mu'-\mu\rangle}{t} + 2\frac{\theta_1(\|\mu'-\mu\|^2)}{t^2} + 2\frac{\theta_2(\|\mu'-\mu\|)}{t}.$$

Where $\theta_i(\eta)/\eta=\epsilon_i(\eta)$ converges to 0 when η goes to 0^+ $(i=1,2)$. (We note that for the sequence $\mu'=\mu+t^2\tilde{d}$, we find again $-A_2(u_0,\mu;d)\le 0$).

Now we take $\mu'=\mu+t\tilde{d}$. Since $\mathcal{C}$ is open, μ' is in $\mathcal{C}$ for t small enough. We obtain $-A_2(u_0,\mu;d)\le Q(\tilde{d})=\langle A\tilde{d},\tilde{d}\rangle+2\langle b,\tilde{d}\rangle$, for all $\tilde{d}$ in $\mathbb{R}^p$, where $A=\nabla^2_{\mu\mu}h(u_0,\mu)$ and $b=\nabla^2_{\mu u}h(u_0,\mu)d$.

For $\tilde{d}=-A^{-1}b$, the minimum of Q, we obtain $A_2(u_0,\mu;d)\ge\langle A^{-1}b,b\rangle$.

Step 2: We prove that, in fact, equality holds in the above inequality. To begin with, there are sequences $t_n\to 0^+$ and $\mu\to\mu_n$ s.t.

$$-A_2(u_0,\mu;d)=\lim_n \frac{\langle A(\mu_n-\mu),\mu_n-\mu\rangle}{t_n^2}+2\frac{\langle b,\mu_n-\mu\rangle}{t_n} + 2\frac{\theta_1(\|\mu_n-\mu\|^2)}{t_n^2}+2\frac{\theta_2(\|\mu_n-\mu\|)}{t_n}. \tag{2.24}$$

Using an argument by contradiction we are going to prove that the sequence $(\mu_n-\mu)/t_n$ is bounded. Suppose it is not, extracting a subsequence and renaming it, we assume $\lim\|\mu_n-\mu\|/t_n=+\infty$. Since there are $\epsilon'_1>0$ and $\epsilon'_2>0$ such that $2\epsilon_1(\|\mu_n-\mu\|^2)\ge-\epsilon'_1$ and $2\epsilon_2(\|\mu_n-\mu\|)\ge-\epsilon'_2$, we find:

$$\begin{aligned}\frac{\langle A(\mu_n-\mu),\mu_n-\mu\rangle}{t^2}&+2\frac{\langle b,\mu_n-\mu\rangle}{t}+2\frac{\theta_1(\|\mu_n-\mu\|^2)}{t^2}+2\frac{\theta_2(\|\mu_n-\mu\|)}{t}\\ &\ge c\left\|\frac{\mu_n-\mu}{t_n}\right\|^2-2\|b\|\left\|\frac{\mu_n-\mu}{t_n}\right\|-\epsilon'_1\left\|\frac{\mu_n-\mu}{t_n}\right\|^2-\epsilon'_2\left\|\frac{\mu_n-\mu}{t_n}\right\|,\\ &\ge\left\|\frac{\mu_n-\mu}{t_n}\right\|\left[(c-\epsilon'_1)\left\|\frac{\mu_n-\mu}{t_n}\right\|-2\|b\|-\epsilon'_2\right].\end{aligned}$$

Hence $-A_2(u_0,\mu;d) \geq +\infty$. This contradiction proves that the sequence $(\mu_n - \mu)/t_n$ is bounded.

We immediately deduce $\lim_n 2(\theta_1(\|\mu_n-\mu\|^2))/t_n^2 + 2(\theta_2(\|\mu_n-\mu\|))/t_n = 0$. Extracting a subsequence if necessary, we may suppose that $(\mu_n-\mu)/t_n$ converges towards a direction $\bar{d}$. From (2.24) we deduce $-A_2(u_0,\mu;d) = Q(\bar{d})$, which ends the proof. □

Remark 2.12. If $A = \nabla^2_{\mu\mu}h(u_0,\mu)$ is only nonnegative (the necessary second-order optimality conditions tells us that A is always nonnegative), we may use the Moore–Penrose pseudo-inverse [25] to find:

$$A_2(u_0,\mu;d) \geq \langle \nabla^2_{\mu\mu}h(u_0,\mu)^+\nabla^2_{\mu u}h(u_0,\mu)d, \nabla^2_{\mu u}h(u_0,\mu)d\rangle. \tag{2.25}$$

Indeed, we write $\mathbb{R}^p = \mathrm{Im}A \oplus \mathrm{Ker}A$. For any direction δ in $\mathbb{R}^p$, we name $\delta^I \in \mathrm{Im}A$, and $\delta^K \in \mathrm{Ker}A$ such that $\delta = \delta^I + \delta^K$ and $\langle \delta^I, \delta^K\rangle = 0$. We have:

$$\begin{aligned} Q(\delta) &= \langle A\delta^I, \delta^I\rangle + 2\langle b, \delta^I\rangle + 2\langle b, \delta^K\rangle, \\ &\geq -A_2(u_0,\mu;d), \end{aligned}$$

for all $\delta \in \mathbb{R}^p$ (with $b = \nabla^2_{\mu u}h(u_0,\mu)d$). In particular, we have:

$$Q(\delta^K) = 2\langle b, \delta^K\rangle \geq -A_2(u_0,\mu;d).$$

If we suppose b does not belong to $\mathrm{Im}A$, we can build a sequence $\delta^K_n = -nb^K$ to obtain $-A_2(u_0,\mu;d) \leq \lim_n Q(\delta^K_n) = -\infty$, which cannot hold. Consequently b belongs to $\mathrm{Im}A$. We take $\delta = -A^+b$ to obtain (2.25). However, we do not obtain equality: an extra-term may appear from higher order information. In other words, the sequence $(\mu^K_n - \mu^K)/t_n$ may go to infinity when A is not positive.

2.7.2 What we know about φ

We assume E is twice continuously differentiable and 1-coercive (we note that λ_1 is always positive). We consider:

$$\varphi(x,\lambda) = \min_{X'\in\mathbb{R}^{n^2}} \psi(x,\lambda,X'). \tag{2.22}$$

We are going to check each hypothesis of Theorem 2.4 page 102. We denote $u_0 = (x_0,\lambda)$.

- We consider $q_1(t, X') = (\psi(u_0 + td, X') - \varphi(u_0))/t$, and we take a positive sequence t_n converging to 0. We need to find a sequence of positive numbers ϵ_n converging to 0 such that X'_n has a cluster point and:

$$\frac{\varphi(u_0 + t_n d) - \varphi(u_0)}{t_n} \geq \frac{\psi(u_0 + t_n d, X'_n) - \varphi(u_0)}{t_n} - \epsilon_n.$$

  For X'_n in $\mathcal{J}_1(x, \lambda) = \{X' \in \mathbb{R}^{n^2} \ : \ \varphi(x, \lambda) = \psi(x, \lambda, X')\}$, the Inequality clearly holds. An argument similar to the proof of Proposition 2.4 page 94 shows that $\mathcal{J}_1$ is locally bounded. Hence X'_n has a cluster point.

- Since ψ is continuous, Assumption (ii) holds.

- Similarly, (iii) holds because ψ is continuously differentiable.

We deduce that

$$(2.26) \quad D\varphi(x_0, \lambda_0; d) = \min_{X' \in \mathcal{J}_1(x_0, \lambda_0)} [\langle \nabla E(x_1), d^x \rangle + \sum_{i=1}^{n+1} [E(x_i) - \langle \nabla E(x_1), x_i \rangle] d_i^\lambda],$$

with $d = (d^x, d^\lambda)$ (d is a column vector). Indeed, the function ψ is twice differentiable at (x, λ, X') with $\nabla \psi = (\nabla_x \psi, \nabla_\lambda \psi, \nabla'_X \psi)$, where:

$$\nabla_x \psi(x, \lambda, X') = \nabla E(x_1) \in \mathbb{R}^n,$$

$$\nabla_\lambda \psi(x, \lambda, X') = \begin{pmatrix} E(x_1) - \langle \nabla E(x_1), x_1 \rangle \\ \vdots \\ E(x_{n+1}) - \langle \nabla E(x_1), x_{n+1} \rangle \end{pmatrix} \in \mathbb{R}^{n+1},$$

$$\text{and } \nabla'_X \psi(x, \lambda, X') = \begin{pmatrix} \lambda_2 (\nabla E(x_2) - \nabla E(x_1)) \\ \vdots \\ \lambda_{n+1} (\nabla E(x_{n+1}) - \nabla E(x_1)) \end{pmatrix} \in \mathbb{R}^{n^2}.$$

Remark 2.13. If λ is associated to a phase decomposition of x, the expression

$$[\langle \nabla E(x_1), d^x \rangle + \sum_{i=1}^{n+1} [E(x_i) - \langle \nabla E(x_1), x_i \rangle] d_i^\lambda]$$

is constant on $\mathcal{J}_1(x_0, \lambda_0)$. So φ is differentiable at any such λ.

We now check the hypotheses of Theorem 2.5 page 103.

- As for (i), (iv) holds because $\mathcal{J}_1$ is locally bounded.

- Since ψ is twice continuously differentiable, (v) holds.

We deduce:

$$\underline{D}^2\varphi(x_0,\lambda_0;d) = \min_{X'\in\mathcal{J}_2(x_0,\lambda_0;d)}[\langle\nabla^2_{uu}\psi(x_0,\lambda_0,X')d,d\rangle - B_2(x_0,\lambda_0,X';d)]. \tag{2.27}$$

We denote

$$\nabla^2_{uu}\psi = \begin{pmatrix}\nabla^2_{xx}\psi & \nabla^2_{x\lambda}\psi, \\ \nabla^2_{\lambda x}\psi & \nabla^2_{\lambda\lambda}\psi\end{pmatrix}$$
$$\nabla^2_{X'u}\psi d = \nabla^2_{X'x}\psi d^x + \nabla^2_{X'\lambda}\psi d^\lambda,$$
$$J_2(x_0,\lambda_0;d) = \{X' \in \mathcal{J}_1(x_0,\lambda_0) \;:\; D\varphi(x_0,\lambda_0;d) = \langle\nabla'_X\psi(x_0,\lambda_0,X'),d\rangle\}.$$

We recall that:

$$\lambda^T = (\lambda_1,\lambda'^T) \in \mathbb{R}^{n+1}, \qquad \lambda'^T = (\lambda_2,\dots,\lambda_{n+1}) \in \mathbb{R}^n,$$
$$X = (x_1,X') \in \mathbb{R}^{n\times(n+1)}, \qquad X' = (x_2,\dots,x_{n+1}) \in \mathbb{R}^{n\times n},$$

and $M_1 = \nabla^2 E(x_1)$. We write $\mathrm{Diag}(\lambda_2\nabla^2E(x_2),\dots,\lambda_{n+1}\nabla^2E(x_{n+1}))$ the block diagonal matrix.

We easily compute all partial Hessians at (x,λ,X').

$$\nabla^2_{xx}\psi = \lambda_1^{-1}M_1, \qquad \nabla^2_{x\lambda}\psi = -\lambda_1^{-1}M_1X,$$
$$\nabla^2_{xX'}\psi = -\lambda_1^{-1}\lambda'^TM_1, \quad \nabla^2_{\lambda\lambda}\psi = \lambda_1^{-1}X^TM_1X,$$
$$\nabla^2_{X'X'}\psi = \lambda_1^{-1}\lambda'\lambda'^TM_1 + \mathrm{Diag}(\lambda_2\nabla^2E(x_2),\dots,\lambda_{n+1}\nabla^2E(x_{n+1})),$$
$$\nabla^2_{X'\lambda}\psi = \lambda_1^{-1}\lambda'X^TM_1 + \begin{pmatrix}0 & \nabla E(x_2)-\nabla E(x_1) & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & \nabla E(x_{n+1})-\nabla E(x_1)\end{pmatrix}.$$

We sum up our results.

Proposition 2.8. *If E is 1-coercive and twice continuously differentiable, the function φ is directionally differentiable and Formulas* (2.26) *and* (2.27) *hold.*

This last Proposition calls for several remarks.

Remark 2.14. If all Hessians $M_i = \nabla^2 E(x_i)$ are positive for $i = 1, \dots, n+1$, we may apply Proposition 2.7 page 103 to compute:

$$B_2(x_0, \lambda_0, X'; d) = \lambda_1^{-1} \langle M_1 (\sum d_i^\lambda x_i - d^x), \sum d_i^\lambda x_i - d^x \rangle \\ - \langle (\sum_{i=1}^{n+1} \lambda_i M_i^{-1})^{-1} (\sum d_i^\lambda x_i - d^x), \sum d_i^\lambda x_i - d^x \rangle.$$

Hence we have:

$$\underline{D}^2 \varphi(x_0, \lambda_0; d) = \min_{X' \in \mathcal{J}_2(x_0, \lambda_0; d)} [\langle \begin{pmatrix} M & -MX \\ -X^T M & X^T M X \end{pmatrix} d, d \rangle],$$

with $M = (\sum_{i=1}^{n+1} \lambda_i M_i^{-1})^{-1}$.

Remark 2.15. Since the $n+1$ vectors $x_1, \dots, x_{n+1}$ are not linearly independent in $\mathbb{R}^n$, the matrix $X^T M X$ has rank less than n. Hence the matrix $\nabla^2_{\lambda\lambda} \varphi$ is never positive.

Remark 2.16. When φ is twice differentiable, its Hessian is:

$$\begin{pmatrix} M & -MX \\ -X^T M & X^T M X \end{pmatrix}.$$

Before turning to the smoothness of $\bar{\text{co}} E$, we note that to apply Theorem 2.4 page 102 to $\bar{\text{co}} E$, it is sufficient to prove that φ is subregular in Clarke's sense.

Lemma 2.15 (Correa and Jofre [12]). *Let $\varphi(u) = \min_{X'} \psi(u, X')$. If the mapping $(u, X') \mapsto \nabla_u \psi(u, X')$ is continuous at any point in $\{u\} \times \mathcal{J}_1(u)$ and the set-valued function is* sequentially semi-continuous*, then the marginal function φ is subregular at u.*

If the function E is twice continuously differentiable and 1-coercive, both assumptions hold, hence φ is subregular.

We first give the definition of a sequentially semi-continuous set-valued function.

Definition 2.4 (Correa and Seeger [13]). A set-valued function $\mathcal{J}_1$ is *sequentially semi-continuous* (ssc) at u if for any sequence u_n converging to u, there are $X' \in \mathcal{J}_1(u)$ and a sequence $X'_n \in \mathcal{J}_1(u_n)$ such that X' is a cluster point of X'_n.

Proof. To apply Theorem 6.1 in [12], we only need to prove that $\mathcal{J}_1$ is ssc. We may apply Remark 2.1 in [13] because $\mathcal{J}_1$ is usc and closed but it is easier to give a straight proof.

We take u_n converging to u. Since $\mathcal{J}_1$ is locally bounded, taking any sequence $X' \in \mathcal{J}_1(u_n)$ there is a subsequence X'_{n_k} which converges. We name X' its limit. Now using: $\varphi(u_{n_k}) = \psi(u_{n_k}, X'_{n_k})$ and the continuity of both φ and ψ, we deduce: $\varphi(u) = \psi(u, X')$. Consequently X' belongs to $\mathcal{J}_1(u)$. □

2.7.3 What we may deduce on $\bar{\text{co}}E$

First we state a general lemma. The only nontrivial part is the upper semi-continuity of $\mathcal{I}_1$.

Lemma 2.16 (Clarke [10]). *Let V be an open subset of $\mathbb{R}^n$ and suppose the function φ is continuous on $V \times \Delta_{n+1}$. Then $\mathcal{I}_1(x) = \{\lambda \ : \ \varphi(x,\lambda) = \bar{\text{co}}E(x)\}$ is a nonempty compact set for any x in V. In addition $\bar{\text{co}}E$ is continuous on V and the set-valued function $x \mapsto \mathcal{I}_1(x)$ is upper semi-continuous on V.*

We are now ready to apply Theorem 2.4 page 102 to the marginal function.

$$\bar{\text{co}}E(x) = \min_{\lambda' \in \Omega_n} \varphi(x, (1 - \sum_{i=2}^{n+1} \lambda_i, \lambda')). \tag{2.21}$$

Theorem 2.6. *We assume E is twice continuously differentiable and 1-coercive. Then its convex hull $\bar{\text{co}}E$ is differentiable in any direction d at any point x with:*

$$\nabla \bar{\text{co}}E(x) = \nabla E(x_1),$$

where $x_1 = (x - \sum_2^{n+1} \lambda_i x_i)/\lambda_1$ and $X' = (x_2, \ldots, x_{n+1})$ is any point in $\mathcal{J}_1(x_0, \lambda)$.

In addition if the limit $\lim_{\substack{t \to 0^+ \\ \lambda \to \tilde{\lambda}}} (\varphi(x_0 + td, \lambda) - \varphi(x_0, \lambda) - tD_x\varphi(x_0, \lambda; d))/t^2$ exists for $\tilde{\lambda}$ in $\mathcal{I}_2(x_0; d) = \{\lambda \in \mathcal{I}_1(x_0) \ : \ D\bar{\text{co}}E(x_0; d) = D_x\varphi(x_0, \lambda; d)\}$, we have:

$$\underline{D}^2 \bar{\text{co}}E(x; d) = \min_{\lambda \in \mathcal{I}_2(x;d)} [D^2_{xx}\varphi(x, \lambda; d) - A_2(x, \lambda; d)].$$

Remark 2.17. We cannot apply Proposition 2.7 page 103, because the matrix $\nabla^2_{\lambda\lambda}\varphi$ is never positive.

We know that (see Remark 2.25 page 105):

$$\underline{D}^2\varphi(x_0,\lambda_0;d) \leq \min_{X'\in\mathcal{J}_2(x_0,\lambda_0;d)}[\langle\begin{pmatrix} M & -MX \\ -X^TM & X^TMX\end{pmatrix} d, d\rangle],$$

with $M = (M_1\sum_{i=2}^{n+1}\lambda_i M_i^+ + \lambda_1 I)^{-1}M_1$. If all matrices M_i are positive definite, equality holds and $M = (\sum_{i=1}^{n+1}\lambda_i M_i^{-1})^{-1}$. Consequently, if φ is smooth enough, we have:

$$\underline{D}^2\bar{\text{co}}E(x_0;d) \leq \min_{\lambda\in\mathcal{I}_2(x;d)}\langle Md, d\rangle.$$

If all matrices M_i are positive, we find Inequality (11) page 8 in [1]. We note that the Inequality does not take into account the envelope-like effect due to λ. Its proof in [1] uses an inf-convolution argument which does not require any smoothness assumption on φ.

We end this section with two examples. In the first one φ is not twice differentiable yet $\bar{\text{co}}E$ is twice directionally differentiable. In the second, both functions are twice continuously differentiable.

Example 2.5. We consider $E(t,s) = (t^2-1)^2 + s^2$ and $x_0 = (0,1)$. The phases are unique: $x_1 = (1,1)$, $x_2 = x_3 = (-1,1)$. We choose $\lambda = (1/2, 1/4, 1/4)$. When $|t| < 1$, we easily compute $\bar{\text{co}}E(t,s) = s^2$. Hence $\bar{\text{co}}E$ is twice differentiable with:

$$\nabla^2\bar{\text{co}}E(t,s) = \begin{pmatrix} 0 & 0 \\ 0 & 2\end{pmatrix}$$

for all (t,s) with $|t| < 1$. We apply Theorem 2.4 page 102 to φ to deduce:

$$\underline{D}^2\varphi(x_0,\lambda;d) = \langle\begin{pmatrix} 8 & 0 & -8 & 8 & 8 \\ 0 & 2 & -2 & -2 & -2 \\ -8 & -2 & 10 & -6 & -6 \\ 8 & -2 & -6 & 10 & 10 \\ 8 & -2 & -6 & 10 & 10\end{pmatrix} d, d\rangle.$$

In fact, φ can be written as $\varphi(x,\lambda) = \min(F_1(x,\lambda), F_2(x,\lambda), F_3(x,\lambda))$, with $F_i(x,\lambda) = \psi(x,\lambda,X_i'(x,\lambda))$ and $X_i'(x,\lambda)$ is a root of $\nabla_{X'}\psi(x,\lambda,X_i'(x,\lambda)) = 0$.

If φ was twice continuously differentiable, we could apply Proposition 2.7 page 103 and Theorem 2.5 page 103. We would obtain

$$A_2(x_0; d) \geq \nabla^2_{x\lambda}\varphi(\nabla^2_{\lambda\lambda}\varphi)^+\nabla^2_{\lambda x}\varphi = \begin{pmatrix} 8 & 0 \\ 0 & 2 \end{pmatrix}.$$

We would deduce the following contradiction when $d_2 \neq 0$:

$$0 < \langle \begin{pmatrix} 8 & 0 \\ 0 & 2 \end{pmatrix} d, d\rangle = \langle \nabla^2 \bar{\text{co}}E(x_0)d, d\rangle = \langle \nabla^2\varphi(x_0, \lambda)d, d\rangle - A_2(x_0; d) \leq 0.$$

Consequently φ is not twice continuously differentiable at (x_0, λ). Indeed we cannot hope $d \mapsto D^2\varphi(x_0, \lambda; d)$ to be quadratic when it exists.

Example 2.6. We take $E(s, t) = (s^2 + t^2 - 1)^4$, at $x_0 = (0, 0)$ with $\lambda = (1/2, 1/4, 1/4)$. We easily compute $\bar{\text{co}}E(x) = 0$ when $\|x\| \leq 1$. Hence $\bar{\text{co}}E$ is twice continuously differentiable on the open unit ball. We have:

$$0 \leq \underline{D}^2\varphi(x_0, \lambda) \leq \overline{D}^2\varphi(x_0, \lambda) \leq \langle M_i d, d\rangle \leq 0.$$

So φ is twice continuously differentiable on a neighborhood of (x_0, λ) and we find that $\bar{\text{co}}E$ is twice continuously differentiable with a null Hessian.

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Chapitre 3

Formule explicite du Hessien de la rgularise de Moreau-Yosida d'une fonction convexe f en fonction de l'pi-diffrentielle seconde de f

Introduction

Ce chapitre fait suite a des discussions et questions souleves par C. Lemarchal l'occasion du colloque franco-allemand de Dijon (27 juin–2 juillet 1994).

La rgularise Moreau–Yosida F d'une fonction convexe f est dfinie par :

$$F(x) = \min_{y \in \mathbb{R}^n} [f(y) + \frac{1}{2}\|x - y\|^2] = (f \Box \frac{1}{2}\|.\|^2)(x),$$

o $\Box$ dsigne l'oprateur d'inf-convolution.

Lemarchal et Sagastizábal [12, 13] ont tudis le Hessien de la rgularise Moreau–Yosida F en utilisant le calcul diffrentiel usuel et la transforme de Legendre–Fenchel (voir aussi les travaux de Az [3]).

Contrairement [12], nous abordons le problme avec des outils trs diffrents.

Les publications de Rockafellar [17, 18, 19, 20] sur l'pi-diffrentielle, en particulier [20], laissent penser que cette notion de diffrentiation est plus adapte notre contexte. Cette intuition a t confirme par les articles de Noll [14] et de Borwein et Noll [4]. Ce dernier donne une caractrisation du Hessien mais ne calcule pas de formule explicite. Par ailleurs, une rcente communication de Qi [15] recensant un certain nombre de conditions suffisantes d'existence du Hessien montre l'activit de ce domaine.

Unes des ides de base nos rsultats est d'utiliser la transformation de Legendre–Fenchel en liaison avec l'pi-diffrentiation. Cette ide semble naturelle car la rgularit de f mais aussi celle de sa transforme de Legendre–Fenchel f^* est directement lie l'existence du Hessien de la rgularise F. De plus, l'ensemble des fonctions partiellement quadratiques (dfinies page 121 et correspondant aux « generalized purely quadratic functions » de [17]) est stable par transforme de Legendre–Fenchel. Enfin la formule de Moreau (Proposition 1.14 dans [16]) :

$$f\Box\frac{1}{2}\|.\|^2 + f^*\Box\frac{1}{2}\|.\|^2 = \frac{1}{2}\|.\|^2$$

explicite le lien naturel entre f, f^* et le noyau quadratique $1/2||.||^2$.

Nous consacrons la majorit de notre tude au cas du noyau quadratique. Comme l'ont remarqu Lemarchal et Sagastizábal [12], il est trs intressant, d'un point de vue algorithmique, de considrer des mtriques diffrentes, c'est--dire d'effectuer l'opration : $f\Box\frac{1}{2}\langle M.,.\rangle$; o M est une matrice dfinie positive. D'un point de vue thorique, effectuer l'inf-convolution avec une matrice dfinie positive ou avec la matrice identit ne prsente gure de diffrence. Nous prsentons donc nos rsultats pour la matrice identit ; ils se traduisent directement au cas d'une matrice dfinie positive.

Plusieurs auteurs ont propos des gnralisations de la rgularisation de Moreau-Yosida. L'ide gnrale est de remplacer le noyau quadratique $1/2\|.\|^2$ par une fonction jouant le rle de distance. On obtient ainsi la rgularise par une distance de Bregman ou par une fonction entropie [21]. Nous proposons ici une troisime gnralisation sous la forme d'un noyau N jouant le rle d'une norme. Cette approche permet une extension immdiate de la dmarche applique au noyau quadratique.

Dans une premire partie, nous rappelons les principaux rsultats ncessaires notre tude. La seconde partie dveloppe les relations entre pi-diffrentielle de F et de f, ainsi que diverses notions de rgularit seconde. Nous disposerons alors des outils ncessaires pour donner des formules explicites que nous utiliserons pour retrouver certains rsultats de [12]. Nous tendrons ensuite notre tude des noyaux plus gnraux en dveloppant plus particulirement la rgularisation par la « ball-pen function » [10, 14].

3.1 pi-diffrentiation, proto-diffrentiation et rgularise de Moreau-Yosida

Nous utilisons beaucoup de rsultats sur l'pi-diffrentiation, la proto-diffrentiation, l'pi-convergence ainsi que sur la classe des fonctions partiellement quadratiques. Ils sont rsums dans la premire partie de cette section. Nous rappelons ensuite brivement la rgularit de F et posons nos notations.

3.1.1 pi-diffrentiabilit et proto-diffrentiabilit

Dans toute la suite $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ dsigne une fonction convexe, semi-continue infrieurement (sci) et propre ($f \not\equiv +\infty$).

La notion d'pi-convergence est au cœur de ce chapitre. Nous en donnons une dfinition plus facilement manipulable que celle donne dans [1] (c'est une lgre extension de la notion usuelle due Noll [14]).

Une suite de fonctions $\varphi_k : \mathbb{R}^n \to (-\infty, +\infty]$ propres, semi-continues infrieurement, valeurs tendues, *pi-converge* vers un rel θ en $\xi \in \mathbb{R}^n$, si les deux conditions suivantes sont satisfaites :

$$\text{il existe une suite } (\bar{\xi}_k)_k \text{ tel que } \bar{\xi}_k \to \xi \text{ et } \varphi_k(\bar{\xi}_k) \to \theta; \tag{3.1}$$

$$\text{pour toute suite } (\xi_k)_k \text{ convergeant vers } \xi \text{ , } \liminf_{k\to\infty} \varphi_k(\xi_k) \geq \theta. \tag{3.2}$$

On dira que la suite $(\varphi_k(\xi))_{k\in\mathbb{R}^n}$ pi-converge vers une fonction $\varphi : \mathbb{R}^n \to \overline{\mathbb{R}}$ si elle pi-converge pour tout $\xi \in \mathbb{R}^n$ vers $\varphi(\xi)$. On notera : $\varphi_k(\xi_k) \xrightarrow[\xi_k]{e} \xi$.

Ce type de convergence a t appliqu par Rockafellar [16, 18, 19] au quotient diffrentiel :

$$\Delta_t(\xi) = \frac{f(x+t\xi) - f(x) - t\langle v, \xi\rangle}{t^2/2}, \text{ avec } t > 0 \text{ et } v \in \partial f(x).$$

On dira que f est *deux fois pi-diffrentiable* en x relativement $v \in \partial f(x)$ si $\Delta_t(\xi)$ pi-converge pour tout ξ vers une fonction $f''_{x,v}$ qui vrifie $f''_{x,v}(0) > -\infty$.

La fonction limite $f''_{x,v}$ est alors convexe, sci, propre, positivement homogne de degr deux, $f''_{x,v}(0) = 0$ et pour tout ξ, $f''_{x,v}(\xi) \geq 0$ (ces rsultats sont dtaills dans [20]).

L'pi-convergence du quotient Δ_t correspond un dveloppement au second ordre —au sens de l'pi-convergence— de la fonction f. Comme pour les notions de diffrentiabilit classiques, le dveloppement au second ordre de f est li au dveloppement au premier ordre d'une « drive ». Dans le cadre de l'pi-convergence, cette ide est formalise par la proto-diffrentiabilit [19] qui nous permet de relier l'pi-drive seconde avec la drive seconde classique.

Une multifonction $G : \mathbb{R}^n \rightrightarrows \mathbb{R}^n$ est *proto-diffrentiable* en x relativement $v \in G(x)$ si le graphe de l'application :

$$\phi_t : \xi \longmapsto \frac{G(x+t\xi) - v}{t} \ , \ t > 0,$$

converge dans $\mathbb{R}^n \times \mathbb{R}^n$ (au sens de Painlev–Kuratowski). L'ensemble limite est alors interprt comme le graphe d'une multifonction note $G^{'}_{x,v}$.

Remarque 3.1. Nous utilisons ici les notions de convergence d'ensembles exposes dans [2]. L'pi-convergence correspond la convergence des pigraphes de la suite de fonctions tandis que la proto-diffrentiabilit est dfinie par rapport la convergence des graphes.

Le lien entre la proto-diffrentiabilit du sous-diffrentiel de l'analyse convexe ∂f et l'pi-diffrentiation seconde de f est effectu dans [20] ; nous utiliserons le rsultat suivant :

Théorème 3.1 (Thorme 2.2, Rockafellar [20]).
Les propositions suivantes sont quivalentes :
(i) f est deux fois pi-diffrentiable en x relativement v.
(ii) ∂f est proto-diffrentiable en x relativement v.
Quand elles sont vrifies, on a pour tout ξ :

$$\partial \left(\frac{1}{2} f^{''}_{x,v} \right)(\xi) = (\partial f)^{'}_{x,v}(\xi).$$

La notion de proto-diffrentiabilit permet aussi de faire le lien avec la notion de diffrentiabilit classique.

Théorème 3.2 (Thorme 3.2, Rockafellar [19]). *Soit $G : \mathbb{R}^n \to \mathbb{R}^n$ une application. Les propositions suivantes sont quivalentes :*

(i) G est diffrentiable en x.
(ii) G est continue en x, proto-diffrentiable en x relativement $v = G(x)$ et $G'_{x,v}$ est linaire.

La transforme de Legendre–Fenchel constitue —avec l'pi-diffrentiation— l'un des principaux outils de notre analyse. La proposition suivante montre que l'opration de double pi-diffrentiation « commute » avec la transformation de Legendre–Fenchel.

Proposition 3.1 (Thorme 2.4, [20])**.** *Les propositions suivantes sont quivalentes :*
(i) f est deux fois pi-diffrentiable en x relativement $v \in \partial f(x)$.
(ii) f^* est deux fois pi-diffrentiable en v relativement $x \in \partial f^*(v)$.
Quand elles sont vrifies, on a :

$$\left(\frac{1}{2} f''_{x,v}\right)^* = \frac{1}{2} (f^*)''_{v,x} .$$

Nous aurons aussi besoin de calculer l'pi-drive seconde d'une somme. Toutefois l'addition rclame plus de rgularit de la part d'une des deux fonctions.

Proposition 3.2 (Proposition 2.10, [18])**.** *Si g est deux fois pi-diffrentiable en x relativement v et k est deux fois diffrentiable en x alors $h = g + k$ est deux fois pi-diffrentiable en x relativement $u = v + \nabla k(x)$ et pour tout ξ :*

$$h''_{x,u}(\xi) = f''_{x,v}(\xi) + \langle \nabla^2 k(x)\xi, \xi \rangle.$$

Une des difficults techniques de ce chapitre est que la transforme de Legendre–Fenchel d'une fonction quadratique pure (sans terme linaire) n'est pas toujours une fonction quadratique pure. Toutefois cette transforme est une fonction partiellement quadratique. Ces fonctions ont t tudies par Hiriart–Urruty et Lemarchal (chap. X de [10]) et par Rockafellar [16]. Nous rappelons brivement leurs rsultats.

Une fonction $\varphi : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ convexe, sci, propre, positivement homogne de degr deux est dite *partiellement quadratique* (ou « Generalized purely quadratic ») s'il existe une matrice R symtrique, semi-dfinie positive et H un sous-espace vectoriel de $\mathbb{R}^n$ tels que pour tout ξ :

$$\varphi(\xi) = \frac{1}{2}\langle R\xi, \xi\rangle + I_H(\xi).$$

La notation I_H dsigne l'indicatrice de H ($I_H(\xi)$ est nulle pour ξ dans H et est gale a $+\infty$ en dehors de H).

Contrairement l'ensemble des fonctions quadratiques pures, l'ensemble des fonctions partiellement quadratiques est stable par transforme de Legendre–Fenchel.

Proposition 3.3 (Hiriart–Urruty et Lemarchal [10])**.**
La fonction φ dfinie ci-dessus a pour conjugue :

$$\varphi^*(s) = \frac{1}{2}\langle (P_H \circ R \circ P_H)^- s, s\rangle + I_{\mathrm{Im}(R)+H^\perp}(s).$$

La notation P_H dsigne l'oprateur de projection orthogonale sur H et $(.)^-$ reprsente le pseudo-inverse de Moore–Penrose [10]. L'image de R, note $\mathrm{Im}(R)$, est dfinie par : $\mathrm{Im}(R) = \{y \in \mathbb{R}^n \,; \exists x \in \mathbb{R}^n, y = Rx\}$.

Nous disposons maintenant des outils ncessaires notre tude. Avant d'tudier la rgularit au second ordre, nous rappelons quelques proprits de la rgularise de Moreau-Yosida tout en fixant les notations utilises par la suite.

3.1.2 Rgularise de Moreau-Yosida

La rgularise de Moreau-Yosida est l'application F dfinie par :

$$x \mapsto F(x) = \min_{y\in\mathbb{R}^n}[f(y) + \frac{1}{2}\|x-y\|^2] = (f\Box\frac{1}{2}\|.\|^2)(x) \;; \tag{3.3}$$

o $\Box$ dsigne l'oprateur d'inf-convolution.

La fonction F a les proprits suivantes :

- F est convexe, valeurs finies, diffrentiable, de gradient 1-Lipschitz *i.e.* pour tout $x_1, x_2 \in \mathbb{R}^n$:

$$\|\nabla F(x_1) - \nabla F(x_2)\| \leq \|x_1 - x_2\|.$$

– le minimum (3.3) est atteint en un point unique $p(x)$ appel *point proximal* de x (on notera $p = p(x)$ lorsqu'il n'y a pas d'ambigut sur x). On note G le gradient de F en x ; il vrifie $G = x - p(x)$. Le point proximal $p(x)$ est l'unique solution de l'quation multivoque :

$$x - p(x) \in \partial f(p(x)).$$

– l'application $x \mapsto p(x)$ est 1-Lipschitz, *i.e.*, pour tout $x_1, x_2 \in \mathbb{R}^n$:

$$\|p(x_1) - p(x_2)\| \leq \|x_1 - x_2\|.$$

Dans la suite, x dsigne un point de $\mathbb{R}^n$, p son point proximal et G le gradient de F en x.

3.2 Analyse au second ordre : gnralits

Nous donnons une caractrisation de l'pi-diffrentiabilit de f l'aide f^*, F, ∂f, ∂f^* ou de ∇F. Dans une deuxime sous-partie, nous traduisons l'existence d'un dveloppement au second ordre de f en terme de dveloppement au premier ordre de ∂f et d'pi-diffrentiabilit.

Cette courte section rassemble des rsultats parpills dans la littrature.

3.2.1 pi-diffrentiation et rgularisation de Moreau-Yosida

Ce premier thorme montre toute la puissance de la notion d'pi-diffrentiabilit seconde. En effet, il *caractrise* les cas o F est deux fois pi-diffrentiable. On obtient ainsi des conditions ncessaires d'existence d'un Hessien pour F.

Théorème 3.3. *Les propositions suivantes sont quivalentes :*
(i) f est deux fois pi-diffrentiable en p relativement $G \in \partial f(p)$.
(ii) f^* est deux fois pi-diffrentiable en G relativement $p \in \partial f^*(G)$.
(iii) F est deux fois pi-diffrentiable en $x = p + G$ relativement $G = \nabla F(x)$.
(iv) F^* est deux fois pi-diffrentiable en G relativement $x \in \partial F^*(G)$.
(v) ∂f est proto-diffrentiable en p relativement $G \in \partial f(p)$.
(vi) ∂f^* est proto-diffrentiable en G relativement $p \in \partial f^*(G)$.
(vii) ∇F est proto-diffrentiable en $x = p + G$ relativement $G = \nabla F(x)$.
(viii) ∇F^* est proto-diffrentiable en G relativement $x \in \partial F^*(G)$.

Si l'une de ces conditions est vrifie, on a la formule suivante :

$$F''_{x,G} = f''_{p,G} \Box \|.\|^2.$$

Preuve. Le thorme 3.1 assure les quivalences entre (i) et (v), (ii) et (vi), (iii) et (vii) ainsi qu'entre (iv) et (viii). La proposition 3.1 implique les quivalences entre (i) et (ii) et entre (iii) et (iv). On conclut en appliquant la proposition 3.2 avec $F^* = f^* + \frac{1}{2}\|.\|^2$ pour obtenir l'quivalence entre (ii) et (iv). □

La rgularit au second ordre de F apparat ainsi fondamentalement diffrente du comportement de F au premier ordre. En effet, f peut tre extrmement irrgulire, F sera toujours continment diffrentiable. Par contre, on ne peut esprer de rgularit au second ordre sur F si f n'admet pas des proprits de rgularit au second ordre.

3.2.2 Analyse au second ordre d'une fonction convexe

Pour clarifier la situation, nous sommes amens tudier les diffrents cas possibles de rgularit au second ordre d'une fonction convexe, sci, propre, valeurs tendues.

Théorème 3.4. *Les propositions suivantes sont quivalentes :*

(1). f est deux fois pi-diffrentiable en p relativement G et $f''_{p,G}$ est quadratique pure, i.e., sans terme linaire et valeurs finies.

(2). ∂f admet une approximation au premier ordre en p, i.e., il existe une matrice carre R de dimension n, symtrique, semi-dfinie positive telle que :

$$\forall h \in \mathbb{R}^n, \forall s \in \partial f(p+h)\ ,\ s = \nabla f(p) + Rh + o(h).$$

(3). f admet une approximation quadratique en p, i.e., il existe une matrice carre R de dimension n, symtrique, semi-dfinie positive telle que :

$$\forall h \in \mathbb{R}^n\ ,\ f(p+h) = f(p) + \nabla f(p)h + \frac{1}{2}\langle Rh, h\rangle + o(\|h\|^2).$$

Ces trois propositions sont vraies ds que :

(4). f est deux fois diffrentiable en p.

Preuve. La dmonstration se scinde en trois parties.

– L'quivalence entre (1) et (2) est dmontr par le thorme 3.1 de [4] ou le thorme 2.12 de [9]. Comme Borwein et Noll [4] l'ont remarqu, la convexit de f intervient fortement dans ce rsultat.

– Pour prouver que (1) est quivalent (3), il suffit de remarquer que la proprit (1) quivaut Δ_t pi-converge vers la fonction quadratique pure $f''_{p,G}$. De mme, la proprit (3) quivaut Δ_t converge ponctuellement vers la forme linaire $\langle R.,.\rangle$. L'quivalence se dduit alors du corollaire 3.3 de [14] ou de la proposition 6.1 de [4].

– L'implication (4) $\Rightarrow$ (3) est triviale ; la rciproque est fausse car (3) n'implique pas la diffrentiabilit de f dans un voisinage de p. $\square$

Remarque 3.2. Le thorme prcdent mrite plusieurs commentaires.

– La proprit (1) entrane la diffrentiabilit de f en p. Une preuve directe de ce rsultat est donne par le thorme 4.1 de [19].

– La proprit (2) implique directement l'existence d'un Hessien F (il suffit d'appliquer le thorme 2 de [15]).

– Comme ∇F est 1-Lipschitz, la convergence ponctuelle et l'pi-convergence de :

$$\Delta^F_{t,x,\nabla F(x)}(h) = \frac{F(x+th) - F(x) - t\langle \nabla F(x), h\rangle}{t^2/2}$$

sont quivalentes (proposition 3.1 de [14]) ; ainsi les proprits (1)–(4) du prcdent thorme appliqu la fonction F sont quivalentes.

3.3 Formules explicites du Hessien de F

Nous pouvons maintenant donner des formules explicites du Hessien de F et les illustrer par divers exemples.

3.3.1 Caractrisation, Formules

Théorème 3.5. *Les propositions suivantes sont quivalentes :*

(1). F est deux fois diffrentiable en $x = p + G$ avec $G = \nabla F(x)$.

(2). f est deux fois pi-diffrentiable en p relativement G et $f''_{p,G}$ est partiellement quadratique.

(3). f^* est deux fois pi-diffrentiable en G relativement p et $(f^*)''_{G,p}$ est partiellement quadratique.

• *En posant* $Q = \nabla^2 F(x)$, *on obtient les formules suivantes :*

$$(3.4)\quad \begin{cases} \frac{1}{2} f''_{p,G} & = \frac{1}{2} \left\langle \left(P_{Im(Q)} \circ (Q^- - I) \circ P_{Im(Q)} \right)^- .,. \right\rangle + I_{Im(Q^- - I)+Ker(Q)} \\ \frac{1}{2} (f^*)''_{G,p} & = \frac{1}{2} \left\langle (Q^- - I) .,. \right\rangle + I_{Im(Q)} \end{cases}$$

• *Rciproquement, si* $\frac{1}{2} f''_{p,G}(\xi) = \frac{1}{2} \langle R\xi, \xi \rangle + I_H(\xi)$, *o* H *est un sous-espace vectoriel de* $\mathbb{R}^n$ *et* R *est une matrice* $n \times n$, *symtrique, semi-dfinie positive sur* H, *un calcul similaire donne :*

$$(3.5)\qquad \frac{1}{2} (f^*)''_{G,p}(\xi) = \frac{1}{2} \left\langle (P_H \circ R \circ P_H)^- \xi, \xi \right\rangle + I_{Im(R)+H^\perp}(\xi),$$

$$(3.6)\qquad \nabla^2 F(x) = \left[P_{Im(R)+H^\perp} \circ \left[I + (P_H \circ R \circ P_H)^- \right] \circ P_{Im(R)+H^\perp} \right]^- .$$

• *Si on a* $\frac{1}{2} (f^*)''_{G,p}(\xi) = \frac{1}{2} \langle S\xi, \xi \rangle + I_K(\xi)$, *o* K *est un sous-espace vectoriel de* $\mathbb{R}^n$ *et* S *est une matrice* $n \times n$, *symtrique, semi-dfinie positive sur* K, *on en dduit le Hessien de* F *:*

$$(3.7)\qquad \nabla^2 F(x) = \left[P_K \circ [I + S] \circ P_K \right]^- .$$

Remarque 3.3. Il s'agit d'une *caractrisation* de la diffrentiabilit au second ordre de F. Les formules (3.4), (3.5)–(3.6) et (3.7) permettent de traduire l'pi-diffrentiabilit de f en fonction du Hessien de F.

Preuve. L'quivalence entre (2) et (3) se dduit des propositions 3.3 et 3.1.

Dmontrons que la proprit (1) quivaut (2).

En appliquant le thorme 3.2 puis le thorme 3.1 (en remarquant que $F''_{x,G}(0) = 0$), la proprit (1) est quivalente aux proprits suivantes :

– « ∇F est diffrentiable en x » ;

– « ∇F est continue en x, proto-diffrentiable en x relativement G et $(\nabla F)'_{x,G}$ est linaire » ;

– « F est deux fois pi-diffrentiable en x relativement G et $F''_{x,G}$ est quadratique pure » ;

– « f est deux fois pi-diffrentiable en p relativement G et $F''_{x,G}$ est quadratique pure ».

On calcule alors $\partial(\frac{1}{2}F''_{x,G})(\xi) = (\nabla F)'_{x,G}(\xi) = \nabla^2 F(x)\xi$, et on dduit :

$$\frac{1}{2}F''_{x,G}(\xi) = \frac{1}{2}\left\langle \nabla^2 F(x)\xi, \xi \right\rangle.$$

Pour $Q = \nabla^2 F(x)$, la proposition 3.3 donne $\left(\frac{1}{2}F''_{x,G}\right)^* = \frac{1}{2}\left\langle Q^- ., . \right\rangle + I_{Im(Q)}$. Par ailleurs, la proposition 3.2 entrane $\left(\frac{1}{2}F''_{x,G}\right)^* = \frac{1}{2}(f^*)''_{G,p} + \frac{1}{2}\|.\|^2$. On obtient ainsi $\left(\frac{1}{2}f''_{p,G}\right)^*(\xi) = \frac{1}{2}\left\langle (Q^- - I)\xi, \xi \right\rangle + I_{Im(Q)}(\xi)$. En utilisant nouveau la proposition 3.3, on obtient l'implication (1) $\Rightarrow$ (2) et les formules (3.4).

Pour la rciproque et la formule (3.6), on applique la proposition 3.3 $f''_{p,G}$ pour obtenir : $\frac{1}{2}(f^*)''_{G,p} = \frac{1}{2}\langle S., .\rangle + I_K$, avec $S = (P_H \circ R \circ P_H)^-$ et $K = \mathrm{Im}(R) + H^\perp$. On en dduit :

$$\frac{1}{2}F''_{x,G}(\xi) = \frac{1}{2}\left\langle (P_K \circ (I+S) \circ P_K)^- \xi, \xi \right\rangle + I_{Im(I+S)+K^\perp}(\xi).$$

Pour conclure il suffit de remarquer que la matrice $I + S$ est dfinie positive. En effet, $f''_{p,G}$ est convexe donc la matrice R est positive sur H. En utilisant la symtrie de P_H, on obtient, pour tout $\xi \in \mathbb{R}^n$:

$$\langle P_H R P_H \xi, \xi \rangle = \langle R P_H \xi, P_H \xi \rangle \geq 0.$$

Ainsi la matrice S est semi-dfinie positive. Par consquent, la matrice $I + S$ est dfinie positive. On en dduit que $F''_{x,G}$ est quadratique pure ; ce qui dmontre la rciproque et (3.6).

La formule (3.7) se dduit immdiatement de la proposition 3.3. □

Nous donnons trois exemples illustrant le thorme 3.5. Dans le premier, la proposition 6.3 de [4] permet de conclure que le Hessien de F existe. Cette proposition ne s'applique pas aux deux autres exemples.

Exemple 3.1. Dfinissons la fonction f par :

$$(p_1, p_2) \in \mathbb{R}^2 \mapsto f(p_1, p_2) = |p_1| + \frac{2}{3}|p_2|^{\frac{3}{2}},$$

et considrons $p = (p_1, p_2)$ avec $p_1 > 0$ et $p_2 > 0$. La fonction f est deux fois diffrentiable en p et un calcul direct nous donne :

$$\nabla f(p) = \begin{pmatrix} 1 \\ \sqrt{p_2} \end{pmatrix}, \text{ et } \nabla^2 f(p) = \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{2\sqrt{p_2}} \end{pmatrix} = R.$$

Donc f est deux fois pi-diffrentiable en p relativement $G = \nabla f(p)$ avec $\frac{1}{2} f''_{p,G}(\xi) = \frac{1}{2}\langle R\xi, \xi\rangle$. La proposition 6.3 de [4] s'applique : F admet un Hessien en $x = p + G$.

Exemple 3.2. Appliquons le thorme 3.5 la transforme de Legendre–Fenchel

$$(s_1, s_2) \mapsto f^*(s_1, s_2) = I_{[-1,1]}(s_1) + \frac{1}{3}|s_2|^3$$

de la fonction f de l'exemple 3.1. Le domaine de f^* ne constituant pas tout $\mathbb{R}^n$, on ne peut pas appliquer la proposition 6.3 de [4]. Par contre, la proposition 3.3 donne :

$$\frac{1}{2}(f^*)''_{G,p}(\xi) = \frac{1}{2}\langle R^- \xi, \xi\rangle + I_{\{0\}\times\mathbb{R}}(\xi) \text{ avec } R^- = \begin{pmatrix} 0 & 0 \\ 0 & 2\sqrt{p_2} \end{pmatrix}.$$

Finalement le thorme 3.5 permet de conclure que F est deux fois diffrentiable en $x = (p_1 + 1, p_2 + \sqrt{p_2})$ avec

$$\nabla^2 F(x) = \begin{pmatrix} 0 & 0 \\ 0 & 1 + 2\sqrt{p_2} \end{pmatrix}^- = \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{1+2\sqrt{p_2}} \end{pmatrix}.$$

Exemple 3.3. Considrons la fonction f de l'exemple 3.1 avec $p = (0, 0)$. Calculons $\partial f(p) = [-1, 1] \times \{0\}$. Sachant que $G = x - p = (0, 0)$ appartient $\partial f(p)$, p est le point proximal de $x = (0, 0)$. D'autre part, la fonction f^* est deux fois diffrentiable en G avec

$$\nabla f^*(G) = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ et } \nabla^2 f^*(G) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

D'o f est deux fois pi-diffrentiable en p relativement G, avec pour tout ξ :

$$\frac{1}{2} f''_{p,G}(\xi) = I_{\{(0,0)\}}(\xi).$$

Donc F admet un Hessien en x qui s'crit :

$$\nabla^2 F(x) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Remarque 3.4. Bien que dans ces exemples le thorme 3.4 permette d'affirmer l'existence du Hessien de F en x, le calcul de la conjugue n'est pas toujours facile. Le thorme 3.5 est d'autant plus utile qu'il permet d'viter ce calcul.

Notons aussi que l'exemple 3.1 souligne le lien entre la rgularit de f ou de f^* avec la rgularit de F.

On sait que si f admet une approximation quadratique en p, ou que f^* admet une approximation quadratique en G, alors la rgularis F admet un Hessien en x. L'exemple 3.4 montre que la rciproque est fausse.

Exemple 3.4. On considre la fonction $f(p_1, p_2) = |p_1| + p_2$. Sa conjugue s'crit : $f^*(s_1, s_2) = I_{[-1,1]}(s_1) + I_1(s_2)$. Soit $x = (x_1, x_2) \in \mathbb{R}^2$, un calcul direct du point proximal donne :

$$p(x_1, x_2) = \begin{cases} (x_1 + 1, x_2 - 1) & \text{si } x < -1, \\ \\ (0, x_2 - 1) & \text{si } -1 \leq x \leq 1, \\ \\ (x_1 - 1, x_2 - 1) & \text{si } 1 < x. \end{cases}$$

On en dduit que la matrice jacobienne de p, $p^{'}(x_1, x_2)$ est gale la matrice identit pour $|x_1| > 1$ et la matrice $\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$ pour $|x_1| < 1$. Pour tout $x_2 \in \mathbb{R}$, f n'est pas diffrentiable en $(0, x_2)$ et f^* n'est jamais diffrentiable (car l'intrieur de $\mathrm{Dom}(f^*)$ est vide) ; par contre p est diffrentiable en $(0, x_2)$. Donc F est deux fois diffrentiable en $(0, x_2)$ bien que, ni f, ni f^* n'admettent d'approximation quadratique en p.

Reprenons l'exemple —dvelopp dans la conclusion de [12]— o f est deux fois pi-diffrentiable mais $f^{''}_{p,G}$ n'est pas partiellement quadratique. Un calcul explicite permet de vrifier que $F''_{x,G}$ n'est pas quadratique.

Exemple 3.5. Posons

$$\begin{aligned} e &= (0, 1), \\ B &= \{x \in \mathbb{R}^2, \|x - e\| \leq 1\} = \{x \in \mathbb{R}^2, \frac{1}{2}\|x\|^2 \leq x_2\}, \\ f(p_1, p_2) &= \max(\frac{1}{2}\|p\|^2, \langle e, p \rangle) = \max(\frac{1}{2}(p_1^2 + p_2^2), p_2) = \begin{cases} p_2 & \text{si } p \in B, \\ \frac{1}{2}\|p\|^2 & \text{sinon.} \end{cases} \end{aligned}$$

La fonction f est deux fois pi-diffrentiable [18]. De plus, le point proximal d'un point $x \in \mathbb{R}^2$ s'crit :

$$p(x) = \begin{cases} x - e & \text{si } \|x - 2e\| < 1, \\ \frac{x}{2} & \text{si } \|x - 2e\| > 2, \\ \frac{x - 2e}{\|x - 2e\|} + e & \text{si } 1 \leq \|x - 2e\| \leq 2. \end{cases}$$

Pour $x = (0,0), p(x) = (0,0)$ et $G = \nabla F(x) = (0,0)$. Les drives directionnelles de p sont donnes par :

$$p^{'}(x;d) = \lim_{t \downarrow 0} \frac{p(x+td) - p(x)}{t} = \begin{cases} \begin{pmatrix} d_1/2 \\ d_2/2 \end{pmatrix} & \text{si } d_2 \leq 0, \\ \\ \begin{pmatrix} d_1/2 \\ 0 \end{pmatrix} & \text{si } d_2 > 0. \end{cases}$$

Comme $p^{'}(x;.)$ n'est pas linaire, $F^{''}_{x,G}$ n'est pas quadratique, un calcul immdiat donne :

$$F^{''}_{x,G}(d) = \begin{cases} \frac{1}{2}\|d\|^2 & \text{si } d_2 \leq 0, \\ \frac{1}{2}d_1^2 + d_2^2 & \text{sinon.} \end{cases}$$

3.3.2 Lien avec les rsultats de Lemarchal et Sagastizábal

Lemarchal et Sagastizábal [12] ont obtenu des rsultats de rgularit sans utiliser la notion d'pi-diffrentiabilit. Outre le fait de considrer des fonctions convexes valeurs partout finies, ils introduisent l'hypothse suivante pour contrler la croissance de f en p :

(3.8) Il existe $\epsilon > 0$, $C > 0$ tels que pour tout $h \in \mathbb{R}^n$ vrifiant $\|h\| < \epsilon$,

$$f(p+h) \leq f(p) + f^{'}(p,h) + \frac{1}{2}C\|h\|^2.$$

Cette hypothse devient plus naturelle en considrant le comportement de f au voisinage de $p(x_0)$. Supposons que (3.8) ne soit pas vrifie, f augmente alors plus vite qu'une fonction quadratique. Donc la fonction p est constante et gale $p(x_0)$ sur un voisinage de x ; ce qui implique l'existence d'un Hessien F en x_0.

Cette hypothse admet une interprtation en terme d'pi-diffrentielle seconde :

Proposition 3.4. *Si la fonction f est deux fois pi-diffrentiable en p relativement G, on a :*

- $\text{Dom}(f^{''}_{p,G}) \subseteq U = N_{\partial f(p)}(G) = \{\xi \in \mathbb{R}^n; f^{'}(p,\xi) = \langle G, \xi \rangle\}$.
- *Si l'hypothse* (3.8) *est vrifie alors* $\text{Dom}(f^{''}_{p,G}) = U$.

Preuve. On utilise la proposition 2.8 de [18] pour obtenir :

$$\text{Dom}(f^{''}_{p,G}) \subseteq \{\xi \in \mathbb{R}^n; f^{'}_p(\xi) = \langle G, \xi \rangle\},$$

o f'_p dsigne l'enveloppe sci de $f^{'}(p, .)$.

Soit $\xi \in \mathrm{Dom}(f''_{p,G})$, on a $f'_p(\xi) = \sup_{s\in\partial f(p)}\langle s, \xi\rangle = \langle G, \xi\rangle$.

On rappelle que la *face expose* $\partial f(p)$ en ξ est dfinie par :

$$F_{\partial f(p)}(\xi) = \{s \in \partial f(p)\,;\, \langle s, \xi\rangle = \sup_{s^{'}\in\partial f(p)} \langle s^{'}, \xi\rangle\}.$$

Le corollaire 2.1.3 de chap. VI [10] affirme que les proprits $G \in F_{\partial f(p)}(\xi)$, $\xi \in N_{\partial f(p)}(G)$ et $f'_p(\xi) = \langle G, \xi\rangle$ sont quivalentes. La premire partie de la proposition est ainsi dmontre.

Supposons que l'hypothse (3.8) soit vrifie. Soit ξ tel que $f^{'}(p, \xi) = \langle G, \xi\rangle$. Soit $t > 0$, posons $\xi_t = (1+t)\xi$. Comme $f^{'}(p; .)$ est positivement homogne de degr un, on obtient $f^{'}(p; \xi_t) = (1 + t)\langle G, \xi\rangle = \langle G, \xi_t\rangle$, d'o on en dduit :

$$f(p + t\xi_t) \leq f(p) + f^{'}(p, t\xi_t) + \frac{1}{2}C\|t\xi_t\|^2 \leq f(p) + t\langle G, \xi_t\rangle + \frac{1}{2}C\|t\xi_t\|^2,$$

donc

$$0 \leq \frac{f(p + t\xi_t) - f(p) - t\langle G, \xi_t\rangle}{\frac{1}{2}t^2} \leq C\|\xi_t\|^2.$$

En prenant la limite infrieure dans cette dernire ingalit on obtient :

$$f''_{p,G}(\xi) \leq \liminf_{t\downarrow 0} \Delta_t(\xi_t) \leq C\|\xi\|^2 < \infty.$$

Pour conclure que ξ appartient Dom$(f''_{p,G})$ il suffit alors d'appliquer le lemme ci-dessous. □

Lemme 3.1. *La proprit* $\xi \in \mathrm{Dom}(f''_{p,G})$ *quivaut :*

(3.9) $$\exists\beta > 0\,,\, \exists\xi_t \to \xi \text{ tels que } \Delta_t(\xi_t) = \frac{f(p + t\xi_t) - f(p) - t\langle G, \xi_t\rangle}{\frac{1}{2}t^2} < \beta.$$

Preuve. La dfinition de $f''_{p,G}$ se traduit par les deux proprits suivantes :

(3.1) il existe $\xi_t \to \xi$ tel que $\Delta_t(\xi_t) \to f''_{p,G}(\xi)$,

(3.2) pour tout $\xi_t \to \xi$, $\liminf \Delta_t(\xi_t) \geq f''_{p,G}(\xi)$.

Supposons que ξ appartienne Dom($f''_{p,G}$). La proprit (3.9) se dduit immdiatement de (3.1).

Rciproquement, supposons que (3.9) soit vraie. La proprit (3.2) applique une suite quelconque $\bar{\xi}_t \to \xi$ donne :

$$f''_{p,G}(\xi) \leq \liminf \Delta_t(\bar{\xi}_t) \leq \liminf \Delta_t(\xi_t) < \beta;$$

ce qui signifie que ξ appartient Dom($f''_{p,G}$). □

Comme le montre l'exemple qui suit, l'inclusion de la proposition 3.4 peut tre stricte si l'hypothse (3.8) n'est pas vrifie.

Exemple 3.6. Prenons

$$f(p_1, p_2) = |p_1| + \frac{2}{3}|p_2|^{\frac{3}{2}}.$$

Pour $x = (0,0)$, on calcule $p = (0,0)$, $G = (0,0)$; d'o Dom$(f''_{p,G}) = \{(0,0)\}$. Or $\partial f(p) = [-1,1] \times \{0\}$, le cne normal est donc $U = N_{\partial f(p)}(G) = \{0\} \times \mathbb{R}$. En conclusion, l'inclusion Dom$(f''_{p,G}) \subset U$ est stricte.

Remarque 3.5. Le thorme 3.1 de [12] affirme que si f admet un Hessien gnralis en p alors F admet un Hessien en x. Le thorme 3.4 donne le mme type de rsultat. On peut l'interprter comme une simple application du corollaire 3.3 de [14] qui donne des hypothses sous lesquelles les notions de convergence et d'pi-convergence sont quivalentes. En effet, si on suppose que f admet une approximation quadratique en p (ce qui signifie que pour toute direction d, $\Delta_t(d) \underset{t\downarrow 0}{\longrightarrow} \Delta(d)$), alors pour toute direction d, $\Delta_t(d) \xrightarrow[t\downarrow 0]{e} \Delta(d)$. Dans ce cas, $f''_{p,G}$ existe et est quadratique pure ; par consquent F admet un Hessien.

Quand le Hessien de F existe, quelle est la rgularit de f ? Pour tudier cette question, Lemarchal et Sagastizábal [12] ont suppos que (3.8) tait vrifi et que f admettait un gradient $\nabla f(p)$ en p.

En effet, l'hypothse (3.8) implique que Dom$(f''_{p,G}) = N_{\partial f(p)}(G)$ et l'existence de $\nabla f(p)$ entrane $N_{\partial f(p)}(G) = \mathbb{R}^n$. D'autre part, l'existence de $\nabla^2 F(x)$ assure que $f''_{p,G}$ existe et est partiellement quadratique. Par consquent, f admet une approximation quadratique en p. Par ailleurs, f est suppose diffrentiable en p, donc elle admet un Hessien en p.

Toutefois demander l'existence de $\nabla f(p)$ est trs restrictif comme le montre l'exemple suivant :

Exemple 3.7. Dfinissons

$$(p_1,p_2) \mapsto f(p_1,p_2) = |p_1| + \frac{1}{2}(p_2)^2.$$

Pour $x=(0,0)$, un calcul direct donne $p=(0,0)$ et $G=(0,0)$. Le sous-diffrentiel de f en p s'crit : $\partial f(p) = [-1,1]\times\{0\}$. On en dduit $U = N_{\partial f(p)}(G) = \{0\}\times\mathbb{R}$ et

$$\nabla^2 F(x) = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{2} \end{pmatrix}.$$

En appliquant le thorme 3.5, on obtient :

$$\frac{1}{2} f''_{p,G}(\xi) = \frac{1}{2}\langle \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \xi, \xi\rangle + I_{\{0\}\times\mathbb{R}}(\xi).$$

Comme

$$f'(x;d) = \lim_{t\downarrow 0} \frac{f(x+td)-f(x)}{t} = \lim_{t\downarrow 0} \frac{t|d_1| - \frac{t^2}{2}|d_2|^2}{t} = |d_1|,$$

on obtient, pour tout h,

$$f(0+h) = |h_1| + \frac{|h_2|^2}{2} \leq |h_1| + \frac{1}{2}\left(|h_1|^2 + |h_2|^2\right) = f(0) + f'(0,h) + \frac{1}{2}\|h\|^2.$$

L'hypothse (3.8) est ainsi vrifie.

tant donn que $f''_{p,G}$ n'est pas quadratique pure, f n'admet pas d'approximation quadratique en p pour tout h dans $\mathbb{R}^n$. On peut pourtant remarquer que f admet une approximation quadratique pour toutes les directions d dans U :

$$\forall d \in U, \quad f(p+td) = t|d_1| + \frac{t^2}{2}|d_2|^2 = f(0,0) + t\langle G, d\rangle + \frac{t^2}{2}\langle Dd, d\rangle + o(t^2)$$

avec $D = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$.

Remarque 3.6. Il est intressant de comparer les formules obtenues pour $\nabla^2 F(x)$ dans le cas o f est deux fois diffrentiable en p.

Dans le thorme 3.1 de [13] on obtient, en posant $R = \nabla^2 f(p)$,

$$\nabla^2 F(x) = I - [I+R]^{-1} = (I+R)^{-1}R.$$

En utilisant la formule (3.6) avec $H = \mathbb{R}^n$ et $P_{Im(R)} = RR^-$, on obtient :

$$\begin{aligned} \nabla^2 F(x) &= \left[P_{\mathrm{Im}(R)} \circ (I + R^-) \circ P_{\mathrm{Im}(R)}\right]^- \\ &= \left[RR^-(I+R^-)RR^-\right] \\ &= \left[(I+R)R^-\right]^-. \end{aligned}$$

Le Hessien de F s'crit donc :

$$\nabla^2 F(x) = I - (I+R)^{-1} = (I+R)^{-1}R = R(I+R)^{-1} = \left[(I+R)R^-\right]^-.$$

Quelques manipulations algbriques permettent de vrifier directement l'galit :

$$(I+R)^{-1}R = \left[(I+R)R^-\right]^- \tag{3.10}$$

En effet, pour en dduire l'galit, il suffit d'utiliser les proprits $R^-RR = R$, $RR^-R^- = R^-$ et $RR^- = R^-R$ pour montrer que $((I+R)R^-)^- = (I+R)^{-1}R$.

Une preuve consiste poser $x = ((I+R)R^-)^- y$ et utiliser la dfinition du pseudo-inverse pour obtenir :

$$\begin{cases} (I+R)R^- x = P_{\mathrm{Im}((I+R)R^-)} y, \\ x \in \mathrm{Im}((I+R)R^-). \end{cases}$$

Sachant que $\mathrm{Im}((I+R)R^-) = \mathrm{Im}(R^-) = \mathrm{Im}(R)$, les galits successives suivantes prouvent (3.10) :

$$\begin{aligned} (I+R)R^- x =& P_{\mathrm{Im}(R)} y = RR^- y \\ R(I+R)R^- x =& RRR^- y \\ (I+R)RR^- x =& Ry \text{ or } x = P_{\mathrm{Im}(R)}(x) = RR^- x \\ (I+R)x =& Ry \\ x =& (I+R)^{-1}Ry. \end{aligned}$$

3.4 Extensions d'autres noyaux

Dans [10] et [12], on appelle rgularisation de Moreau-Yosida l'inf-convolution avec le noyau $\frac{1}{2}\langle M.,.\rangle$ o M est une matrice $n \times n$ symtrique dfinie positive. Tous les rsultats que nous avons obtenus s'appliquent, avec de lgres modifications, ce cas.

Il est vident que le noyau $\frac{1}{2}\|.\|^2$ reprsente un cas trs particulier : il vrifie la formule de Moreau et est l'unique solution dans l'ensemble des fonctions convexes, sci, propres de l'quation $g^* = g$ (ce rsultat est dmontr dans [16]).

Dans cette section, nous montrons que si un noyau N vrifie certaines proprits, la rgularise $f \square N$ satisfait le mme type de rsultat que dans le cas du noyau quadratique.

3.4.1 Les rsultats gnraux

Nous allons considrer des noyaux plus gnraux en partant de la proposition suivante qui tend le thorme 3.3.

Proposition 3.5. *Soit $N : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ une fonction convexe, sci, propre telle que N^* soit deux fois diffrentiable en un point $G \in \mathbb{R}^n$ avec $\nabla^2 N^*(G)$ dfinie positive. Dfinissons $F = f \square N$ et notons p un point de $\mathbb{R}^n$. Les deux propositions suivantes sont alors quivalentes :*

1. *f est deux fois pi-diffrentiable en p relativement G.*

2. *F est deux fois pi-diffrentiable en $x = p + \nabla N^*(G)$ relativement G.*

Quand elles sont vrifies, on a :

$$F''_{x,G} = f''_{p,G} \square \langle \left[\nabla^2 N^*(G)\right]^{-1} . \, , . \rangle.$$

Preuve. Les propositions suivantes sont quivalentes :
– f est deux fois pi-diffrentiable en p relativement G,
– f^* est deux fois pi-diffrentiable en G relativement p,
– $F^* = f^* + N^*$ est deux fois pi-diffrentiable en G relativement x,
– $F = f \square N$ est deux fois pi-diffrentiable en x relativement G.

Quand l'une d'elles est vrifie, on a les formules suivantes :

$$\left(\frac{1}{2} f''_{p,G}\right)^* = \frac{1}{2} \left(f^*\right)''_{G,p},$$

$$\left(F^*\right)''_{G,x}(\xi) = \left(f^*\right)''_{G,x}(\xi) + \langle \nabla^2 N^*(G)\xi, \xi \rangle,$$

$$\frac{1}{2} F''_{x,G} = \frac{1}{2} f''_{p,G} \square \left(\frac{1}{2} \langle \nabla^2 N^*(G). , . \rangle\right)^*.$$

Comme $\nabla^2 N^*(G)$ est dfinie positive, on conclut la preuve en crivant :

$$\left(\frac{1}{2}\langle\nabla^2 N^*(G).,.\rangle\right)^* = \frac{1}{2}\left\langle\left[\nabla^2 N^*(G)\right]^{-1}.,.\right\rangle. \quad \square$$

Remarque 3.7. Le rsultats prcdent appelle quelques remarques.

– Il faut s'assurer que f et N ont une minorante affine commune pour que F soit convexe, sci, propre.

– On peut enlever l'hypothse $\nabla^2 N^*(G)$ dfinie positive pour obtenir l'inf-convolution de $f''_{p,G}$ avec une fonction partiellement quadratique.

– La fonction $F''_{x,G}$ est une rgularise de Moreau-Yosida (voir page 123) ; ceci justifie l'attention particulire accorde ce noyau.

La gnralisation du thorme 3.5 —qui caractrise le Hessien de la rgularise de Moreau–Yosida— n'est pas aussi immdiate. Le rsultat est le suivant :

Théorème 3.6. *Sous les hypothses de la proposition 3.5, on a les implications (1) ⇒ (2) ⇒ (3) entre les propositions :*

(1). F est deux fois diffrentiable en x.

(2). f est deux fois pi-diffrentiable en $p = x - \nabla N^*(G)$ relativement $G = \nabla F(x)$ et $f''_{p,G}$ est partiellement quadratique.

(3). F deux fois pi-diffrentiable en $x = p + \nabla N^*(G)$ relativement G et $F''_{x,G}$ est quadratique pure.

Si ∇F est continue en x, les propositions (1), (2) et (3) sont quivalentes et il existe un Hessien F en x dont l'expression est :

$$\nabla^2 F(x) = \left[P_K \circ \left[(P_H \circ R \circ P_H)^- + \nabla^2 N^*(G)\right] \circ P_K\right]^- . \tag{3.11}$$

De plus on obtient les formules suivantes :

• *si (1) est vraie alors, en posant $Q = \nabla^2 F(x)$, on a :*

$$\left(\frac{1}{2} f''_{p,G}\right)^* = \frac{1}{2}\left\langle\left(Q^- - \nabla^2 N(G)\right).,.\right\rangle + I_{\mathrm{Im}(Q)},$$

$$\frac{1}{2} f''_{p,G} = \frac{1}{2}\left\langle\left[P_{\mathrm{Im}(Q)} \circ \left(Q^- - \nabla^2 N(G)\right) \circ P_{\mathrm{Im}(Q)}\right]^- .,.\right\rangle + I_{\mathrm{Im}(Q^- - \nabla^2 N(G)) + \mathrm{Ker}(Q)}.$$

• *si (2) est vraie, on peut crire* $\frac{1}{2}f''_{p,G} = \frac{1}{2}\langle R.,.\rangle + I_H$*, o on dfinit la matrice* B *par* $B = (P_H \circ R \circ P_H)^{-} + \nabla^2 N^*(G)$ *et le sous-espace* K *par* $K = \mathrm{Im}(R) + H^{\perp}$*. L'pi-diffrentielle seconde de* F *s'crit alors :*

$$\frac{1}{2}F''_{x,G}(\xi) = \frac{1}{2}\left\langle (P_K \circ B \circ P_K)^{-}\xi, \xi\right\rangle.$$

Preuve. Il suffit de remarquer que la matrice B est dfinie positive et d'appliquer les mmes arguments que lors de la preuve du thorme 3.5. □

3.4.2 Un cas particulier

On tudie l'exemple de la « ball-pen function » qui apparat dans [16] (page 106) et dans [10]. Son importance est souligne dans un rcent article de Noll [14]. Elle est dfinie par :

$$x \mapsto N(x) = \begin{cases} -\sqrt{1-\|x\|^2} & \text{si } \|x\| \leq 1, \\ +\infty & \text{sinon.} \end{cases} \tag{3.12}$$

Sa conjugue se calcule explicitement et a pour expression :

$$s \mapsto N^*(s) = \sqrt{1+\|s\|^2}. \tag{3.13}$$

La fonction N vrifie les proprits suivantes :

- N est strictement convexe, sci, propre, de domaine $\mathcal{D} = \mathrm{Dom}(N) = B(0,1)$ (la boule unit ferme). De plus, N est deux fois diffrentiable sur $\mathrm{int}(\mathcal{D})$.

- N^* est strictement convexe, valeurs finies, 1-Lipschitzienne et deux fois diffrentiable sur $\mathbb{R}^n$. Pour tout $s \in \mathbb{R}^n$, on a :

$$\nabla N^*(s) = \frac{s}{\sqrt{1+\|s\|^2}},$$
$$\nabla^2 N^*(s) = \frac{1}{(1+\|s\|^2)^{\frac{3}{2}}}\left[\left(1+\|s\|^2\right)I - ss^{\top}\right].$$

Par ailleurs,

$$\det\left(\nabla^2 N^*(s)\right) = \frac{1}{(1+\|s\|^2)^{\frac{n+2}{2}}} > 0,$$
$$\left[\nabla^2 N^*(s)\right]^{-1} = \sqrt{1+\|s\|^2}\left(I + ss^{\top}\right).$$

Les deux dernires galits se dduisent du lemme ci-dessous.

Lemme 3.2. *Pour u, v appartenant $\mathbb{R}^n$,*

$$\det\left(I + uv^\top\right) = 1 + \langle u, v\rangle,$$
$$\left(I + uv^\top\right)^{-1} = I - \frac{1}{1 + \langle u, v\rangle} uv^\top.$$

Preuve. La formule de l'inverse se dmontre par vrification posteriori.

Pour le calcul du dterminant, on remarque que $uv^\top x = \langle v, x\rangle u$, pour tout $x \in \mathbb{R}^n$. La matrice $uv^\top$ tant de rang 1, elle admet 0 pour valeur propre d'ordre $n-1$; la dernire valeur propre tant $\langle u, v\rangle$. □

La fonction $y \mapsto f(y) + N(x - y)$ tant strictement convexe, sci, propre sur la boule unit compacte, il existe un unique minimum (3.16) not p. Par ailleurs, F est partout finie ($F \leq f - 1$). Comme $F^* = f^* + N^*$ est strictement convexe, F est C^1 sur $\mathbb{R}^n$.

Le point proximal p est caractris par la proposition suivante :

Proposition 3.6. *Les propositions suivantes sont quivalentes :*

(1). p est l'unique minimum du problme (3.16).

(2). p est l'unique solution de l'quation (3.14).

(3). p est l'unique solution de l'quation : $x - p = \nabla N^*(G)$.

Preuve. Montrons que (1) quivaut (2). Sachant que $x = p + (x - p)$ constitue une dcomposition exacte de (3.16), en posant $G = \nabla F(x)$, la proposition 3.4.2 du chap. XI de [10] assure que $\{G\} = \partial f(p) \cap \partial N(x - p)$. Par consquent, $\partial N(x - p)$ est non vide, $G = \nabla N(x - p)$ et p vrifie :

$$\|x - p\| < 1 \text{ et } \frac{x - p}{\sqrt{1 - \|x - p\|^2}} \in \partial f(p). \tag{3.14}$$

Rciproquement, soit $x \in \mathbb{R}^n$ et p solution de (3.14), on a :

$$0 \in \partial f(p) - \nabla N(x - p).$$

Donc p est l'unique minimum de la fonction $y \mapsto f(y) + N(x - y)$.

L'implication (1) $\Rightarrow$ (3) tant vidente, montrons la rciproque. Sachant que $G = \nabla F(x) \in \partial f(p)$, on a $G \in \partial f(p) \cap \partial N(x-p)$. L'inf-convolution est ainsi exacte en p. Le point p est bien l'unique solution de (3.16). $\square$

L'application p admet mme une expression explicite :

Proposition 3.7 (Noll [14])**.** *Soit $p : x \mapsto p(x)$ l'application qui associe x l'unique solution de* (3.16)*, alors :*

$$p = P_{n+1} \circ P_{\mathrm{Epi}(f)} \circ (id \otimes F),$$

avec les notations suivantes :

- $P_{n+1} : \begin{array}{ccc} \mathbb{R}^n \times \mathbb{R} & \to & \mathbb{R}^n \\ (x,t) & \mapsto & x \end{array}$ *est la projection orthogonale le long du vecteur* $e_{n+1} = (0, \ldots, 0, 1)$ *;*
- $P_{\mathrm{Epi}(f)}$ *est la projection orthogonale sur le convexe ferm* $\mathrm{Epi}(f)$ *;*
- $(id \otimes F) : \begin{array}{ccc} \mathbb{R}^n & \to & \mathbb{R}^n \times \mathbb{R} \\ x & \mapsto & (x, F(x)) \end{array}$ *.*

Preuve. Il suffit de montrer que : $(p, f(p)) = P_{\mathrm{Epi}(f)}(x, F(x))$.
Comme $F(x) = f(p) + N(x-p)$, cela revient montrer que pour tout (y,r) dans $\mathrm{Epi}(f)$, on a :

$$\langle x-p, y-p \rangle + N(x-p)(r - f(p)) \leq 0. \tag{3.15}$$

En utilisant les proprits de G ($G \in \partial f(p)$ et $G = \nabla N(x-p)$), on obtient :

$$r - f(p) \geq f(y) - f(p) \geq \langle G, y-p \rangle = \frac{\langle x-p, y-p \rangle}{\sqrt{1 - \|x-p\|^2}} = \frac{\langle x-p, y-p \rangle}{-N(x-p)},$$

ce qui implique (3.15). $\square$

La diffrentiabilit seconde de F est, en fait, directement lie la diffrentiabilit de p. En effet, l'oprateur de projection est localement Lipschitz.

Corollaire 3.1. *L'application p est localement Lipschitz sur $\mathbb{R}^n$, F est C^1 et ∇F est localement Lipschitz. De plus on a l'quivalence :*
(F est deux fois diffrentiable en x) $\Leftrightarrow$ (p est diffrentiable en x).

3.4.3 Exemples de Noyaux rgularisant

La rgularise de Moreau–Yosida a t gnralise en remplaant le noyau quadratique (qui correspond une norme) par une notion de distance. Les nouvelles rgularises ainsi gnres sont de la forme

$$\inf_y [f(y) + \mathcal{D}(x, y)]$$

o $\mathcal{D}(x, y)$ est soit la φ-divergence dfini par $d_\varphi(x, y) = \sum_{i=1}^n y_i \varphi(x_i/y_i)$, soit la distance de Bregman $\mathcal{D}_h(x, y) = h(x) - h(y) - \langle \nabla h(y), x - y \rangle$. Les fonctions h et φ sont des fonctions d'une variable ayant certaines rgularits. Cette approche a t tudie par M. Teboulle [21] et J. Eckstein [8].

La gnralisation de la rgularise de Moreau–Yosida par inf-convolution avec un noyau N n'entre pas dans ce cadre. Elle consiste remplacer le noyau quadratique par une autre fonction jouant le rle d'une norme et non d'une distance. Elle conserve ainsi la proprit de translation de l'inf-convolution qui facilite la manipulation des proprits duales : la conjugue F^* est tout simplement la somme des conjugues.

Comme pour la rgularise de Moreau–Yosida, des proprits globales peuvent tre dduites. Considrons un noyau N tel que N^* soit partout finie et deux fois diffrentiable avec un Hessien dfini positif. Le noyau N est alors strictement convexe, deux fois diffrentiable sur int(Dom(N)) et si le problme

$$F(x) = \inf_{y \in \mathbb{R}} [f(y) + N(x - y)] \tag{3.16}$$

admet une solution, elle est unique. De plus, si N^* est globalement Lipschitz, alors le corollaire 13.3.3 de [16] implique que Dom(N) est born et qu'il existe une solution (3.16).

La fonction $N^*(s) = \exp(\|s\|^2)$ est deux fois diffrentiable avec un Hessien dfini positif. Elle dfini donc un noyau N satisfaisant nos hypothses.

D'autres constructions de noyaux sont possibles, par exemple sous la forme $N^*(s) = h_i(\|s\|^2)$ ou sous la forme $N^*(s) = \sum_{i=1}^n h_i(s_i)$. Les fonctions $h_i : \mathbb{R} \to \mathbb{R}$ sont deux fois diffrentiables avec une drive seconde strictement positive. De telles fonctions sont utilises pour dfinir des φ-divergence, des distances de Bregman ou des entropies. Nous citons les plus classiques ci-dessous. Pour certaines fonctions h_i qui ne sont pas deux fois diffrentiables en tout point, nous ne pouvons qu'appliquer nos rsultats locaux.

Exemple 3.8. On note t un nombre rel.

$$h_1(t) = \begin{cases} t\log t - t + 1 & \text{pour } t \geq 0, \\ \infty & \text{sinon}\,; \end{cases} \qquad h_1^*(s) = e^s - 1\ ;$$

$$h_2(t) = \begin{cases} -\log t + t - 1 & \text{pour } t > 0, \\ \infty & \text{sinon}\,; \end{cases} \qquad h_2^*(s) = \begin{cases} -\log(1-s) & \text{pour } s < 1, \\ \infty & \text{sinon}\,; \end{cases}$$

$$h_3(t) = \begin{cases} t\log t & \text{si } t > 0, \\ 0 & \text{si } t = 0, \\ \infty & \text{sinon}\,; \end{cases} \qquad h_3^*(s) = e^{s-1}\ ;$$

$$h_4(t) = \begin{cases} -\log t & \text{si } t > 0, \\ \infty & \text{sinon}\,; \end{cases} \qquad h_4^*(s) = \begin{cases} -1 - \log(-s) & \text{si } s < 0, \\ \infty & \text{sinon.} \end{cases}$$

$$h_5(t) = \begin{cases} t^p/p & \text{si } t \geq 0, \\ \infty & \text{sinon}\,; \end{cases} \qquad h_5^*(s) = \max\{0, \frac{s^q}{q}\},\ \text{avec } \frac{1}{p} + \frac{1}{q} = 1.$$

La φ-divergence associe la fonction h_1 est connue sous le nom de divergence de Kullback–Liebler. La fonction h_3 est l'entropie de Boltzmann–Shannon, la fonction h_4 l'entropie de Burg et la fonction h_5 correspond une entropie L_p $(1 < p < \infty)$. D'autres fonctions de ce type ont t proposes dans [5, 6, 7, 11].

3.5 Conclusion

Nous avons tabli des liens entre la rgularit d'ordre deux de la rgularise de Moreau-Yosida et l'pi-diffrentielle seconde de la fonction initiale. La thorie de l'pi-diffrentiation est trs bien adapte ce problme, car elle englobe certaines difficults techniques dans la notion d'pi-convergence.

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Perspectives

Ce travail peut être poursuivi dans différentes directions :

- Le développement d'algorithmes de calcul de la transformée de Legendre discrète en ligne (on ajoute les pentes s_j une a une et non toutes en même temps) est une poursuite logique de notre étude. Des applications de l'algorithme LLT sont en cours.

- Nous conjecturons l'existence de la dérivée seconde directionnelle de l'enveloppe convexe d'une fonction régulière 1-coercive. Une démonstration de ce résultat ainsi qu'une formule explicite pourrait avoir des retombées algorithmiques intéressantes et permettrait d'approfondir notre compréhension de la structure de l'enveloppe convexe.

- D'autres conséquences algorithmiques sont à espérer de la clarification du lien entre le U-Hessien et l'épi-dérivée seconde de la régularisée de Moreau-Yosida