

Exemple Kepler's problem

Find the parallelepiped of maximum volume inscribed in the ellipsoid

$$\mathcal{E} = \{x \in \mathbb{R}^3, \underbrace{x_1^2/a_1^2 + x_2^2/a_2^2 + x_3^2/a_3^2 = 1}_{\text{ellipsoid constraint}}\}$$

Write the problem as a canonical optimisation problem

$$\begin{aligned} & \inf_{x_1^2/a_1^2 + x_2^2/a_2^2 + x_3^2/a_3^2 = 1} f(x), \quad f(x) = -\prod_{i=1}^3 x_i \\ & \left. \begin{array}{l} x_1 \geq 0 \\ x_2 \geq 0 \\ x_3 \geq 0 \end{array} \right\} \text{these constraints are} \\ & \qquad \qquad \qquad \qquad \qquad \qquad \text{necessarily inactive at } x^* \\ & \qquad \qquad \qquad \qquad \qquad \qquad \text{because otherwise} \\ & \qquad \qquad \qquad \qquad \qquad \qquad V(x^*) = 0 \end{aligned}$$

- ▶ Can we apply KKT theorem?
- ▶ Which constraints are active ?
- ▶ Lagrangian ?

Exemple Kepler's problem

$x_1 = 0$ or $x_2 = 0$ or $x_3 = 0 \Rightarrow f(x) = 0$! inequality constraints are inactive

$$\ell(x, y) = - \prod_{i=1}^3 x_i + y(x_1^2/a_1^2 + x_2^2/a_2^2 + x_3^2/a_3^2 - 1)$$

Gradient

Exemple Kepler's problem

$$\begin{cases} (-x_2x_3 + 2yx_1/a_1^2 = 0) \times x_1 \\ (-x_1x_3 + 2yx_2/a_2^2 = 0) \times x_2 \\ (-x_2x_1 + 2yx_3/a_3^2 = 0) \times x_3 \end{cases}$$

then sum the 3 equations:

then find x^*

Exemple Kepler's problem

$$-3x_1x_2x_3 + 2y \underbrace{\left(x_1^2/a_1^2 + x_2^2/a_2^2 + x_3^2/a_3^2 \right)}_{=1} = 0$$

$$-x_2x_3 + 2yx_1/a_1^2 = 0$$

$$-x_1x_3 + 2yx_2/a_2^2 = 0$$

$$-x_2x_1 + 2yx_3/a_3^2 = 0$$

We multiply each equation by the corresponding x_i component

$$-x_2x_3x_1 + 2yx_1^2/a_1^2 = 0$$

$$-x_1x_3x_2 + 2yx_2^2/a_2^2 = 0$$

$$-x_2x_1x_3 + 2yx_3^2/a_3^2 = 0$$

Then sum $-3 \prod x_i + 2y = 0$ from which $x_2x_3 = 2y/(3x_1)$ Then inserting in the first equation leads to

$$-2y/(3x_1) + 2yx_1/a_1^2 = 2y(x_1/a_1^2 - 1/(3x_1)) = 0$$

Exemple Kepler's problem

$x_1 = 0$ is impossible (or $\prod x_i = 0$ therefore $3x_1^2 = a_1^2$). We obtain similarly

$$x_i = \frac{a_i}{\sqrt{3}}, \quad i = 1, \dots, 3$$

Finally we get

$$Vol = 8 \prod x_i = 8 \frac{\prod a_i}{3\sqrt{3}}, \quad y = \frac{3 \prod x_i}{2} = \frac{\prod a_i}{2\sqrt{3}}$$

$$y = \frac{3}{2} \frac{\prod a_i}{(\sqrt{3})^3} = \frac{\prod a_i}{2\sqrt{3}}$$

Exemple

Let the function

$$f(x) = f(0) + \langle \nabla f(0), x \rangle + \frac{1}{2} \langle Hf(0)x, x \rangle$$

degree 2 $\Rightarrow f(x) = \frac{1}{2} \langle Ax, x \rangle + \langle b, x \rangle + c$

$$f(x) = 2x_1^2 + 3x_2^2 + 2x_1x_2.$$

and domain $K = \{x_1^2 + 4x_2^2 \leq 1 \text{ and } x_1 + x_2 \geq 1\} = \mathcal{D}_a$

Seek $\inf_{x \in K} f(x)$

1. Show that f has a global minimum over \mathbb{R}^2 and calculate it
2. Show that K is nonempty convex.
3. Draw K in solid lines and isovalues of $f(x)$ in dotted lines
4. Write the Lagrangian for the problem (P).
5. Write the 1st order optimality conditions (or KKT conditions).
6. Use the drawing and the result of question 1 to decide which of the two constraints will be active at least.
7. Calculate x^* and the associated Lagrange multipliers.

Example

1. Compute $\nabla f(x) = (4x_1 + 2x_2, 2x_1 + 6x_2)^T$ and $Hf(x) = \begin{pmatrix} 4 & 2 \\ 2 & 6 \end{pmatrix}$. The Hessian eigenvalues are $(5 \pm \sqrt{5})/2$. Donc

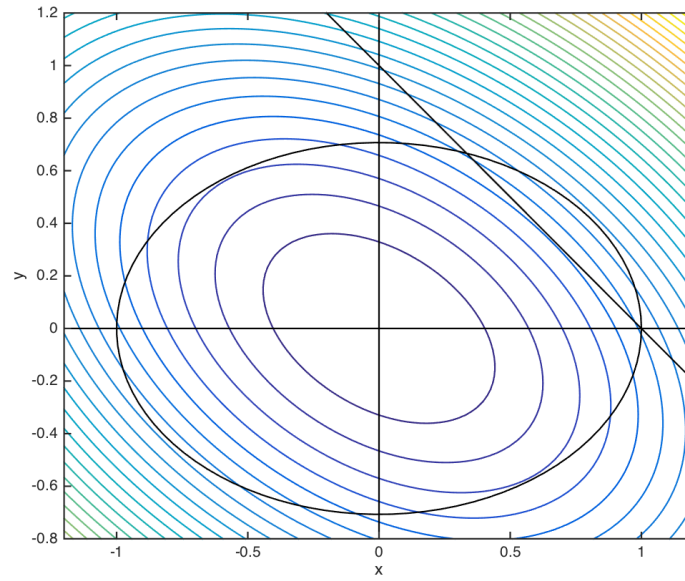
$$f(x) = f(0) + \langle \nabla f(0), x \rangle + \frac{1}{2} \langle Hf(0)x, x \rangle$$

is a quadratic form with a symmetric positive definite matrix, so the minimum 0 is reached in $x = (0, 0)$ and unique.

Example

1. On considère $K = \{x_1^2 + 4x_2^2 \leq 1 \text{ et } x_1 + x_2 \geq 1\}$. Le point $(1, 0) \in K \neq \emptyset$. L'ensemble $\{x_1^2 + 4x_2^2 \leq 1\}$ est l'ellipse de demi grand axe $x_1 \in [-1, 1]$, $x_2 = 0$ et de demi petit axe $x_1 = 0$, $x_2 \in [-1/2, 1/2]$. Il est donc convexe. Le demi plan $\{x_1 + x_2 \geq 1\}$ est lui aussi convexe. L'intersection non vide de 2 convexes est convexe.

Exemple



Exemple

1. On applique la méthode des multiplicateurs de Lagrange:

$$\ell(x, y) = f(x) + y_1(x_1^2 + 4x_2^2 - 1) + y_2(1 - x_1 - x_2)$$

Exemple

1. si (x_1^*, x_2^*) minimise f on K il existe $y_1 \geq 0$ et $y_2 \geq 0$ tels que

$$\nabla_x \ell(x^*, y^*) = \begin{pmatrix} 4x_1^* + 2x_2^* + 2y_1^*x_1^* - y_2^* \\ 2x_1^* + 6x_2^* + 8y_1^*x_2^* - y_2^* \end{pmatrix} = 0_{\mathbb{R}^2},$$

$$y_1^* ((x_1^*)^2 + 4(x_2^*)^2 - 1) = 0,$$

$$y_2^* (1 - x_1^* - x_2^*) = 0$$

Exemple

Comme le minimum global de $f(x)$ n'appartient pas à K , l'une des deux contraintes au moins est forcément active. Vu la convexité de f on prévoit que le minimum sera atteint sur le segment $\{x_1 + x_2 = 1\} \cap K$ et le maximum sur l'arc $\{x_1^2 + 4x_2^2 = 1\} \cap K$.

Pour le minimum on cherche donc $x, y_2 > 0$ tels que

$$\begin{aligned}4x_1^* + 2x_2^* &= y_1^* \\2x_1^* + 6x_2^* &= y_2^* \\x_1^{*2} + 4x_2^{*2} &< 1 \\x_1^* + x_2^* &= 1\end{aligned}$$

ce qui conduit à $x_1^* = 2/3$, $x_2^* = 1/3$, $y_2^* = 10/3$, $y_1^* = 0$ et $f(x^*) = 5/3$.

Algorithms for constrained optimization

$$\begin{cases} \inf & f(x) \\ \text{s.c.} & c^E(x) = 0 \\ \text{s.c.} & c^I(x) \leq 0 \\ & x \in \mathbb{R}^n \end{cases}$$

with

$$\begin{aligned} f & : \mathbb{R}^n \longrightarrow \mathbb{R}, \\ c^E & : \mathbb{R}^n \longrightarrow \mathbb{R}^m, \\ c^I & : \mathbb{R}^n \longrightarrow \mathbb{R}^p, \\ f \ c & \text{ smooth.} \end{aligned}$$

- Change of unknowns

Algorithms for constrained optimization

best ever method: use the python

scipy.optimize
package

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- ▶ Projection

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- ▶ Penalisation

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- ▶ SQP algorithm $\Leftrightarrow \begin{pmatrix} \nabla_x l(x,y) = 0_{\mathbb{R}^n} \\ \nabla_y l(x,y) = 0_{\mathbb{R}^m} \end{pmatrix}$ $m+n$ system solved by Newton
- ▶ Change of unknowns
- ▶ Projection
- ▶ Penalisation
- ▶ Methods using Lagrange multipliers

Change of unknowns

$$\min_{x_1^2 + x_2^2 = 1} x_1^4 + x_2^4 \Rightarrow \begin{cases} x_1 = \cos \theta \\ x_2 = \sin \theta \end{cases}$$

diffeomorphism $\varphi : \mathbb{R}^n \rightarrow K \subset \mathbb{R}^n$

Examples:

- $K = (\mathbb{R}_+)^n \rightarrow$ set $x = y^2$ and optimize without constraints with respect to y .

$$\varphi : (\mathbb{R}^*)^n \rightarrow (\mathbb{R}^{+*})^n, x_i = \varphi_i(y) = y_i^2$$

$$\min_{\substack{x \geq 0 \\ x \in (\mathbb{R}^+)^n}} f(x)$$

$$\tilde{f}(y) = f\left(\begin{pmatrix} y_1^2 \\ \vdots \\ y_n^2 \end{pmatrix}\right) \quad \min_{\mathbb{R}^D} \tilde{f}(y)$$
$$x_i^* = y_i^{*2}$$

Change of unknowns

$$\tilde{f}(\theta^*) = \underset{\text{RWD}}{\text{inv}} f(\theta)$$

$$x_i^* = \frac{a_i + b_i}{2} + \frac{b_i - a_i}{2} \cos \theta_i$$

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- ▶ $K = \prod_{i=1, \dots, n} [a_i, b_i] \rightarrow$ set $x_i = \frac{a_i + b_i}{2} + \frac{b_i - a_i}{2} \cos \theta_i$ and optimize without constraints with respect to θ_i

$$\varphi : \mathbb{R}^n \rightarrow K, x_i = \varphi_i(\theta_i)$$

$$a_i \leq x_i \leq b_i$$

where $f(x)$

$$\tilde{f}(\theta) = f \begin{pmatrix} \frac{a_1 + b_1}{2} + \frac{b_1 - a_1}{2} \cos \theta_1 \\ \vdots \\ \frac{a_n + b_n}{2} + \frac{b_n - a_n}{2} \cos \theta_n \end{pmatrix}$$

Consequence of the change of unknowns on the calculation of the gradient

if you know $\nabla f(x)$

$$x = \varphi(y) \quad \tilde{f}(y) = f(\varphi(y)) \quad \nabla \tilde{f}(y)$$
$$\nabla \tilde{f}(y) = J\varphi(y) \nabla f(\varphi(y))$$

φ diffeomorphism $\Rightarrow J\varphi$ defined on $\varphi^{-1}(\overset{\circ}{K})$

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 $\tilde{f}(y) = f \circ \varphi(y) = f(x)$

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φ diffeomorphism $\Rightarrow J_\varphi$ defined on $\varphi^{-1}(\overset{\circ}{K})$
 $\tilde{f}(y) = f \circ \varphi(y) = f(x) \quad \nabla_y \tilde{f}(y) = J(y) \nabla_x f(x)$ avec $J(x)$ jacobian matrix of φ

Example of change of unknowns

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$$J(y) = \begin{pmatrix} 2y_1 & 0 & \cdots & 0 \\ 0 & 2y_2 & \cdots & 0 \\ \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 2y_n \end{pmatrix} = \begin{pmatrix} 2\sqrt{x_1} & 0 & \cdots & 0 \\ 0 & 2\sqrt{x_2} & \cdots & 0 \\ \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 2\sqrt{x_n} \end{pmatrix},$$

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$$\begin{aligned} \tilde{f}(y) &= f(y_1^2, \dots, y_n^2), & \nabla_y \tilde{f}(y) &= J(y) \nabla f(x) \\ \frac{\partial \tilde{f}(y)}{\partial y_i} &= 2y_i \frac{\partial f}{\partial x_i}(y_1^2, \dots, y_n^2) \end{aligned}$$

Projection and projected gradient methods

loop of gradient descent

$$x_{k+1}^* = x_k - \alpha_k \nabla f(x_k)$$
$$x_{k+1} = P_K(x_{k+1}^*) \quad \text{projection of } x_{k+1}^* \text{ on } K$$

Inequality constraints \Leftrightarrow Belong to a non empty closed convex set $K \subset \mathbb{R}^n$.
(not necessarily bounded)

$$\inf_{x \in K} f(x)$$

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Theorem

Necessary local optimality condition Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ a differentiable function and K a convex non empty subset of \mathbb{R}^n . Let x^* a local minimizer of f in K then

$$\langle \nabla f(x^*), x - x^* \rangle \geq 0, \forall x \in K$$

necessary

sufficient

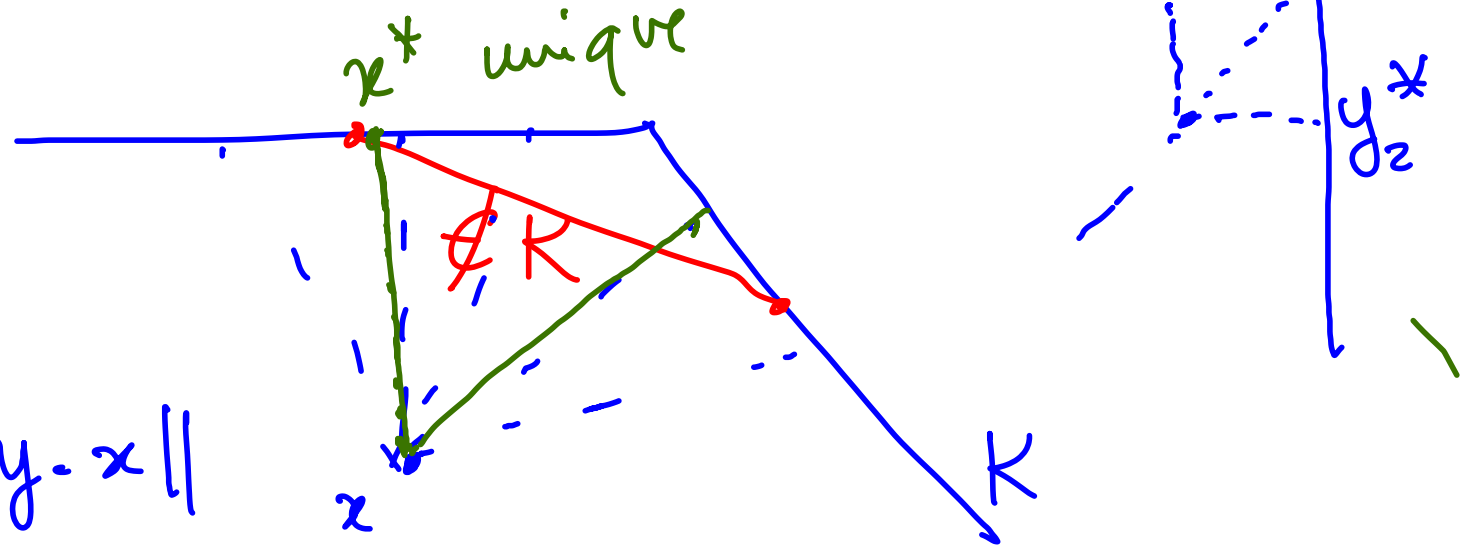
If moreover f is convex the condition becomes ~~necessary~~, ie any point x^* satisfying it is a global minimum of f on K .

Counter example

K not convex set

$$\begin{aligned} \|P_K(x) - x\| &= \inf_{y \in K} \|y - x\| \\ &= \inf_{y \in K} f_x(y) \end{aligned}$$

f_x concave and strictly convex still holds
 $\exists y^*$ solution



Definition/proposition of the projection on a convex set

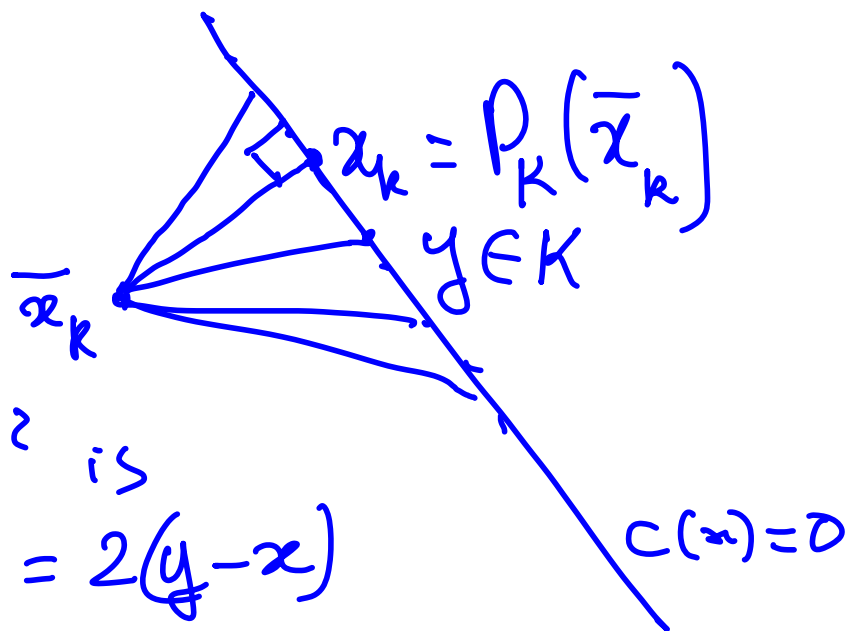
orthogonal projection:

$$f_x(y^*) = \inf_{y \in K} f_x(x) = P^*$$

if K is convex then P^* is global and unique y^* is unique.

Let K a non empty closed convex set in \mathbb{R}^n . The projection of a point $x \in \mathbb{R}^n$ on K , denoted $P_K(x)$, is defined as the unique solution

$$\|P_K(x) - x\|^2 = \inf_{y \in K} \|x - y\|_2^2 = f_x(x)$$



Why does $P_K(x) \exists!$?

for fixed x $f_x(y) = \|y - x\|^2$ is strictly convex $\nabla f_x(y) = 2(y - x)$

$f_x(y)$ concave $\Rightarrow \exists$ minimum.

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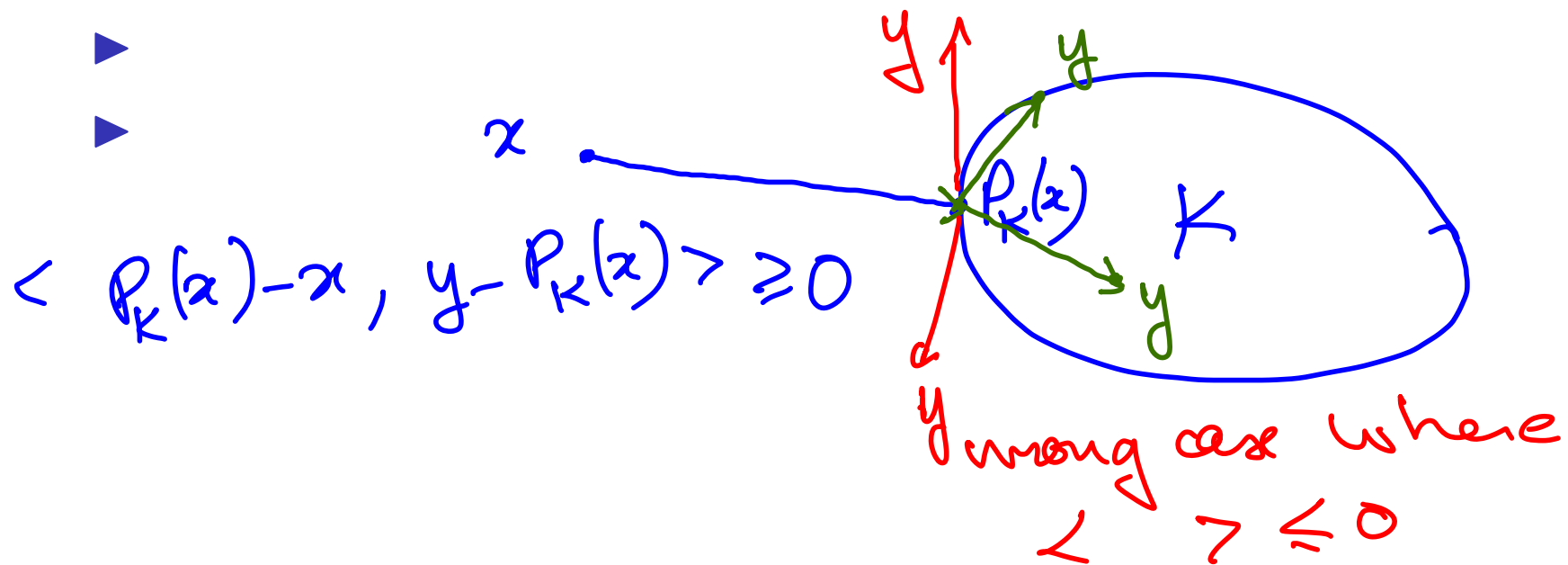
$$f(y) = \|y - x\|^2 \quad \inf_{y \in K} \|x - y\|_2^2 = \underset{y \in K}{\text{arg}} f_x(y)$$

Furthermore $P_K(x)$ is the only point in K satisfying

$$\langle P_K(x) - x, y - P_K(x) \rangle \geq 0, \quad \forall y \in K$$

Proof

- ▶ Existence of $P_K(x)$ as minimum on a closed set of $f(y) = \|x - y\|^2$ coercive (Theorem 1.1)



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- ▶

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- ▶ Equivalence between the two properties:
 \Rightarrow for $y \in K$ and $\theta \in [0, 1]$, $\theta y + (1 - \theta)P_K(x) \in K$
 - ▶ Develop $\|x - P_K(x)\|^2 \leq \|\theta y + (1 - \theta)P_K(x) - x\|^2$
 - ▶ Simplify θ
 - ▶ Do $\theta = 0$

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 - ▶ Simplify θ
 - ▶ Do $\theta = 0$ \Leftarrow for $y \in K$ develop

$$\begin{aligned}\|x - y\|^2 &= \|x - P_K(x) + P_K(x) - y\|^2 \\ &= \|x - P_K(x)\|^2 + \|P_K(x) - y\|^2 + 2\langle x - P_K(x), P_K(x) - y \rangle \\ &\geq \|x - P_K(x)\|^2\end{aligned}$$

Particular cases of projection on a convex.

Orthogonal projection of x on a subset K

$$P_K(x) := \operatorname{argmin}_{y \in K} \|x - y\|.$$

Specific cases that can be solved explicitly

Projection on an intersection of half spaces

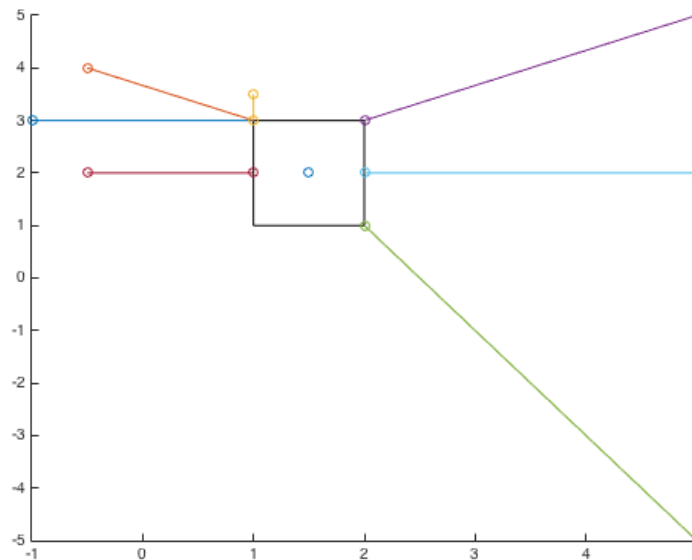
Supposons que $K = \{x \in \mathbb{R}^n, x_i \geq a_i, i \in I, x_j \leq b_j, j \in J\}$ avec $I, J \subset \{1, \dots, n\}$. On a alors

$$P_K(x)_i = \begin{cases} \max(a_i, x_i), & \text{pour } i \in I \setminus J \\ \min(b_i, x_i), & \text{pour } i \in J \setminus I \\ \min(b_i, \max(a_i, x_i)), & \text{pour } i \in I \cap J \end{cases}$$

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Projection on a line (A, \vec{v})

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Euler inequation

Let $f : K \subset E \rightarrow \mathbb{R}$, where K is a convex included in E , a Hilbert space. We suppose that f is differentiable in $x^* \in K$. If x^* is a local minimum of f over K , then x^* satisfies the Euler inequality:

$$Df(x^*)(y - x^*) \geq 0, \forall y \in K.$$

Algorithm of the projected gradient

Data: Function f , convex K , step $(\alpha_k)_{k \geq 0}$, tolerance τ , max number of iterations k_{\max}

Result: $\min_{x \in K} f(x)$

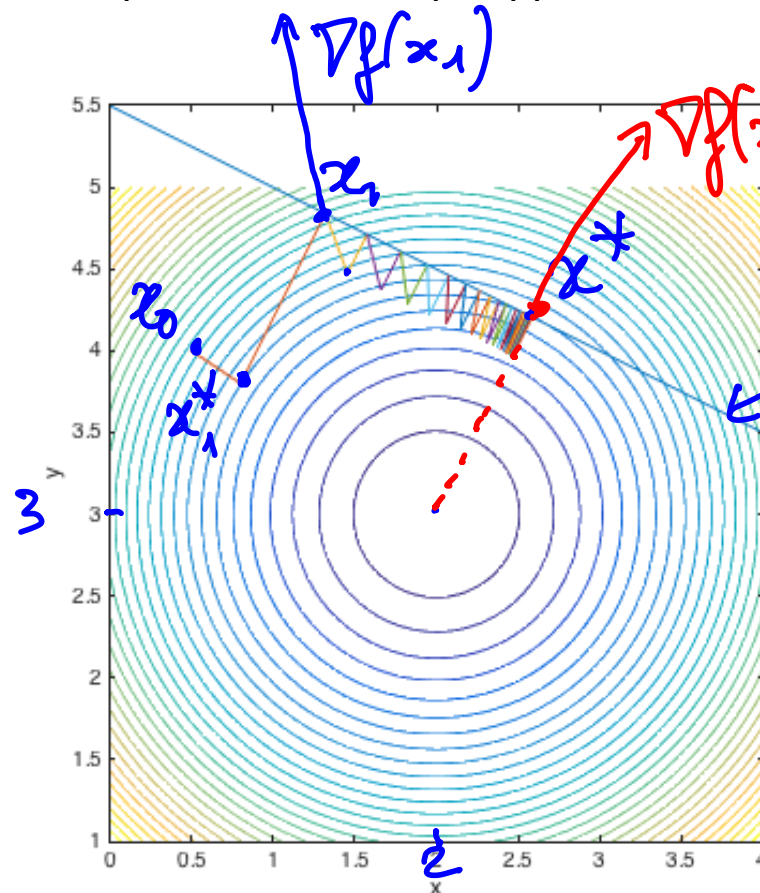
Initialisation : choice of $x_0 \in \mathbb{R}^n$

while $\|x^{k+1} - x^k\| \geq \tau$ or $k < k_{\max}$ **do**

 | Solve $x^{k+1} = P_K(x^k - \alpha_k \nabla f(x^k))$, $k \leftarrow k + 1$

end

$x^* = x_k$



$f(x) = \|x - x_c\|^2$
 $x_c = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$
 line $c(x) = 0$
 linear constraint

Convergence of projected gradient algorithm

Theorem

Let f differentiable sur \mathbb{R}^n and $K \in \mathbb{R}^n$ closed non empty convex subset. Denote by x_k the current solution of the projected gradient algorithm and

$$d(\alpha) = P_K(x_k - \alpha \nabla f(x_k)) - x_k$$

If $d(\alpha) \neq 0$ then $d(\alpha)$ is a descent direction $\forall \alpha > 0$

Proof

Let $\alpha > 0$ fixed. Suppose : $d(\alpha) = p_K(x_k - \alpha \nabla f(x_k)) - x_k \neq 0$.
 $d(\alpha)$ descent direction f in $x_k \Leftrightarrow \langle \nabla f(x_k), d(\alpha) \rangle < 0$

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Indeed $\forall y \in K$,

$$\Leftrightarrow \langle P_K(x_k - \alpha \nabla f(x_k)) - (x_k - \alpha \nabla f(x_k)), y - P_K(x_k - \alpha \nabla f(x_k)) \rangle \geq 0$$

Therefore for all $y \in K$ $\langle d(\alpha) + \alpha \nabla f(x_k), y - x_k - d(\alpha) \rangle \geq 0$

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Therefore for all $y \in K$ $\langle d(\alpha) + \alpha \nabla f(x_k), y - x_k - d(\alpha) \rangle \geq 0$

Since $x_k \in K$ choose $y = x_k$ on a

$$\langle d(\alpha) + \alpha \nabla f(x_k), d(\alpha) \rangle \leq 0 \text{ or } \alpha \langle \nabla f(x_k), d(\alpha) \rangle \leq -\|d(\alpha)\|^2 < 0$$

Convergence of projected gradient algorithm

Theorem

If f is differentiable, α -elliptic and its gradient is C -Lipschitzien, the projected gradient algorithm converges towards x^ quand $k \rightarrow \infty$ for $(\alpha_k)_{k \geq 0}$ sufficiently small: $\alpha_k \leq \frac{2\alpha}{C^2}$ où α and C are two constants such that*

$$\begin{aligned}(\nabla f(x) - \nabla f(y), x - y) &\geq \alpha \|x - y\|^2, \quad \forall x, y \in \mathbb{R}^n, \\ \|\nabla f(x) - \nabla f(y)\| &\leq C \|x - y\|, \quad \forall x, y \in \mathbb{R}^n.\end{aligned}$$

Proof

Compose two contracting applications

- ▶ $x \rightarrow x - \alpha \nabla f(x)$ with conditions on α_k (See unconstrained gradient convergence theorem)

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- ▶ $x \rightarrow x - \alpha \nabla f(x)$ with conditions on α_k (See unconstrained gradient convergence theorem)
- ▶ $x \rightarrow P_K(x)$. indeed

$$\begin{aligned}\|x - y\|^2 &= \|x - y - (P_K(x) - P_K(y)) + (P_K(x) - P_K(y))\|^2 \\ &= \|x - y - (P_K(x) - P_K(y))\|^2 + \\ &\quad \langle x - y - (P_K(x) - P_K(y)), P_K(x) - P_K(y) \rangle + \|P_K(x) - P_K(y)\|^2 \\ &= \|x - y - (P_K(x) - P_K(y))\|^2 \\ &\quad + \langle x - P_K(x), P_K(x) - P_K(y) \rangle \\ &\quad + \langle -y + P_K(y), P_K(x) - P_K(y) \rangle + \|P_K(x) - P_K(y)\|^2\end{aligned}$$

but $\langle x - P_K(x), P_K(x) - P_K(y) \rangle \geq 0$ car $P_K(y) \in K$

Therefore

$$\begin{aligned}\|x - y\|^2 &\geq \|x - y - (P_K(x) - P_K(y))\|^2 + \|P_K(x) - P_K(y)\|^2 \\ &\geq \|P_K(x) - P_K(y)\|^2\end{aligned}$$