Lecture 3: Convex non-smooth optimisation: the proximal operator, forward-backward splitting

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Inverse problems in biological imaging

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Subdifferentiability

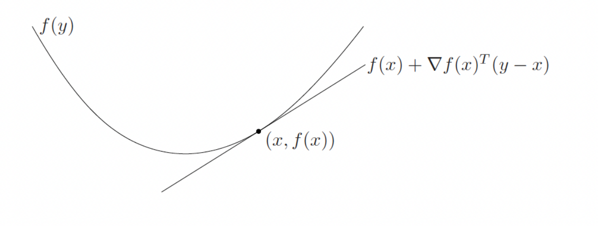
A preliminary observation

We saw that for f differentiable:

$$f \text{ is convex} \quad \Leftrightarrow \quad (\forall x, y \in \mathbb{R}^n) \quad f(y) \geq \underbrace{f(x) + \nabla f(x)^T (y - x)}_{=:\phi(y;x)}$$

Or, in other words:

- the function $\phi(y; x)$ is an affine lower bound/estimator of f
- the tangent to f is below f at all points.



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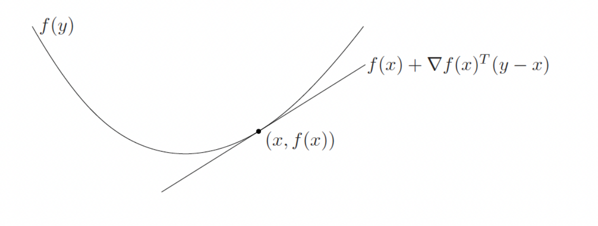

...what if f is not differentiable (but convex)?

Subdifferential and subgradients

Look at the *non-nice* component (typically, the regularisation) g of the original problem we want to solve:

$$\min_{x \in \mathbb{R}^n} \left\{ F(x) := \cancel{f(x)} + g(x) \right\},$$

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Subdifferentials and subgradients

Let g be a proper and **convex** function. Then, a vector $p \in \mathbb{R}^n$ is a *subgradient* of g at point $x \in \mathrm{dom}(g)$ iff:

$$g(y) \geq g(x) + \langle p, y - x\rangle = g(x) + p^T(y - x), \qquad \forall y \in \mathrm{dom}(g)$$

The set of all subgradients at a point $x \in \mathbb{R}^n$ is called the *subdifferential* of g in x, and it is the denoted by:

$$\partial g(x) = \{p \in \mathbb{R}^n : p \text{ is a subgradient of } g \text{ at point } x\}$$

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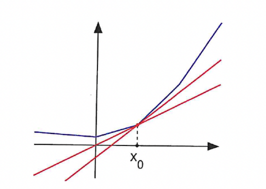
Interpretation:

- $p \in \partial g(x)$ if and only if $\phi(y; x) = g(x) + p^T(y - x)$ is a lower affine bound for g.
- $\partial g(x)$ collects all the **slopes** of the straight lines passing through x.

Remarks

In general, $\partial g(x)$ contains many elements ("many derivatives at each point").



Multiple subgradients at a non-differentiable point x_0.

However, one can show that if g is differentiable in x, then:

$$\partial g(x) = \{\nabla g(x)\},$$

i.e. the only element in $\partial g(x)$ is the (classical) gradient of g in x.

Exercise: compute $\partial g(x)$ at all $x \in \mathbb{R}$ for the 1D function $g(x) = |x|$ and provide a graphical representation of the result.

Separable functions

Very often, the n-dimensional function you deal with, can be nicely expressed as the sum of 1D components. For instance, think of:

- **norms** $\|x\|_p^p,\ p \geq 1$: $\|x\|_p^p = \sum_{i=1}^n |x_i|^p$, hence least-square terms $\|Ax - y\|_2^2 = \sum_{i=1}^m ((Ax)_i - y_i)^2 \dots$
- **sum of norms**, e.g. $g(x) = \|x\|_1 + \frac{\lambda}{2}\|x\|_2^2 = \sum_{i=1}^n \left(|x_i| + \lambda |x_i|^2\right)$.
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- ...

Definition (separable function)

Let g be a proper and convex function. We say that g is *separable* if there exist proper, univariate convex functions $g_i : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ such that

$$g(x) = \sum_{i=1}^n g_i(x_i), \qquad \forall x = (x_1, \ldots, x_n) \in \mathbb{R}^n.$$

Subdifferential of separable functions

Let g b proper, convex and separable. Then, for all $x \in \mathrm{dom}(g)$:

$$\partial g(x) = (\partial g_1(x_1)) \times \ldots \times (\partial g_n(x_n)).$$

Exercise: compute $\partial g(x)$ at all $x \in \mathbb{R}^n$ of $g : \mathbb{R}^n \to \mathbb{R}$, $g(x) = \|x\|_1$ using the results above. Then, compute $\partial F(x)$ of $F(x) := \frac{1}{2}\|Ax - y\|_2^2 + \lambda \|x\|_1$.

Optimality conditions

We have now the tools to introduce optimality conditions in the convex, proper, l.s.c. but **non-differentiable** case.

Optimality conditions for minimisers (non-smooth case)

Let g be proper, convex and l.s.c. ($g \in \Gamma_0(\mathbb{R}^n)$). Then:

$$x^* \in \arg\min_{x \in \mathbb{R}^n} g(x) \qquad \Longleftrightarrow \qquad 0 \in \partial g(x^*)$$

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Interpretation:

- The set $\partial g(x^*)$ is, in general, multivalued but as soon as the vector $0 \in \mathbb{R}^n$ belongs to it, then x^* is a minimiser.
- If g is differentiable, the result reads $0 = \nabla g(x^*)$, which is the Fermat's theorem. The result above is a generalisation to the non-smooth case.

Going towards the solution of the composite problem

Go back to the original, composite, **non-smooth** (since g is) problem:

$$\boxed{\underset{x\in\mathbb{R}^n}{\arg\min} \quad \{F(x) := f(x) + g(x)\}}$$

Using the rules above we have:

$$x^* \in \underset{x\in\mathbb{R}^n}{\arg\min}\, F(x) \Leftrightarrow 0 \in \partial F(x^*) = \underbrace{\partial f(x^*)}_{f \text{ is smooth}} + \partial g(x^*) = \{\nabla f(x^*)\} + \partial g(x^*)$$

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Definition (stationary point)

A point $x^* \in \mathbb{R}^n$ verifying:

$$0 \in \{\nabla f(x^*)\} + \partial g(x^*) \quad \Leftrightarrow \quad -\nabla f(x^*) \in \partial g(x^*)$$

is said to be a **stationary point** of the composite functional $F := f + g$.

Example: stationary points in constrained programming problems

Let $C \subset \mathbb{R}^n$ be a closed and convex set. Let us define the indicator function of C as:

$$\iota_C(x) := \begin{cases} 0 & \text{if } x \in C \\ +\infty & \text{if } x \notin C \end{cases}$$

The function $\iota_C(x)$ is proper, convex and l.s.c.

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Consider:

$$\underset{x \in C}{\arg\min}\ f(x) \quad \Leftrightarrow \quad \underset{x \in \mathbb{R}^n}{\arg\min}\ f(x) + \iota_C(x)$$

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Consider:

$$\arg\min_{x \in C} \; f(x) \quad \Leftrightarrow \quad \arg\min_{x \in \mathbb{R}^n} \; f(x) + \iota_C(x)$$

Stationary points $x^* \in C$ need to satisfy:

$$-\nabla f(x^*) \in \partial \iota_C(x^*)$$

By definition of subdifferential we have that $y \in \iota_C(x^*)$ if and only if:

$$\underbrace{\iota_C(z)}_{=0} \geq \underbrace{\iota_C(x^*)}_{=0} + y^T(z - x^*) \qquad \text{for all } z \in C$$

Equivalently:

$$y^T(z - x^*) \leq 0 \qquad \text{for all } z \in C$$

The set: $N_C(x^*) := \{ y \in \mathbb{R}^n : y^T(z - x^*) \leq 0 \}$ is **the normal cone** of C at x^*.

The proximal operator

Proximal operator: definition

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Relations with activation functions in the context of deep networks.

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Proximal operator

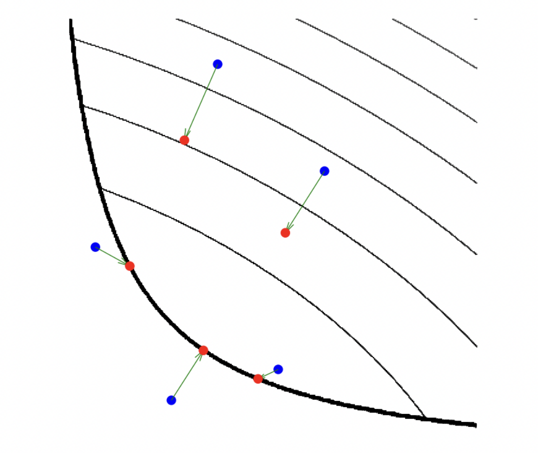
Let $g : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ be a proper, convex, l.s.c. function. Then, the *proximal operator* of g with parameter $\gamma > 0$ is defined as the function $\text{prox}_{\gamma g} : \mathbb{R}^n \to \mathbb{R}^n$ defined for all $x \in \mathbb{R}^n$ by:

$$\text{prox}_{\gamma g}(x) := \underset{y \in \mathbb{R}^n}{\arg\min}\ \gamma g(y) + \frac{1}{2}\|y - x\|^2 = \underset{y \in \mathbb{R}^n}{\arg\min}\ \underbrace{g(y) + \frac{1}{2\gamma}\|y - x\|^2}_{=:h(x;y)}$$

Remarks:

- For a fixed $x \in \mathbb{R}^n$, the function $h(y;x)$ is the sum of a convex + strictly convex function, hence it is strictly convex. Hence, it has a **unique** minimiser, the proximal point $\text{prox}_{\gamma g}(x)$.
- If g is not assumed to be convex, then there may be multiple minimisers... Exercise (if time allows).

Graphical interpretation



Thin black lines: level lines of g. **Thick** black lines: graph of the function. Blue points: evaluation points are moved to the red points in the minimisation with an amount depending on γ. Note: points are moved to the minimum of the function.

Relation with subdifferentials

For $\gamma > 0$ and $x \in \mathbb{R}^n$, let $z := \operatorname{prox}_{\gamma g}(x)$. We have:

$$\begin{aligned}
z := \operatorname{prox}_{\gamma g}(x) \qquad &\Leftrightarrow \qquad z = \operatorname*{arg\,min}_{y \in \mathbb{R}^n} g(y) + \frac{1}{2\gamma}\|y - x\|^2 \\
\text{(optimality)} \qquad &\Leftrightarrow \qquad 0 \in \partial g(z) + \frac{1}{\gamma}(z - x) \\
\text{(rearranging)} \qquad &\Leftrightarrow \qquad x \in z + \gamma \partial g(z) \\
\text{(using operators)} \qquad &\Leftrightarrow \qquad x \in (Id + \gamma \partial g)(z) \\
\text{(uniqueness)} \qquad &\Leftrightarrow \qquad z = (Id + \gamma \partial g)^{-1}(x)
\end{aligned}$$

Characterisations of the proximal operator

Characterisations of prox operator

Let $g : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ be a proper and convex function and $x, z \in \mathbb{R}^n$. The following claims are equivalent ($\gamma = 1$):

- $z = \mathrm{prox}_g(x)$
- $x - z \in \partial g(z)$
- $(x - z)^T (y - z) \leq g(y) - g(z)$ for all $y \in \mathbb{R}^n$

Proof:

By definition:

$$z = \arg\min_{y \in \mathbb{R}^n} g(y) + \frac{1}{2\gamma} \|y - x\|^2.$$

By optimality theorem and the sum rule of subddiferential calculus, we get:

$$0 \in \partial g(z) + z - x \Leftrightarrow x - z \in \partial g(z).$$

By applying the definition of subdifferential to the vector $w = x - z$, we get:

$$g(y) \geq g(z) + w^T (y - z) = g(z) + (x - z)^T (y - z), \qquad \text{for all } y \in \mathbb{R}^n.$$

Proximal operator and implicit gradient descent

Subgradient descent? For $x_0 \in \mathbb{R}^n$, τ_k suitably chosen

$$x_{k+1} = x_k - \tau_k p_k, \quad \text{where } p_k \in \partial g(x_k), \quad \|p_k\| = 1$$

It turns out that this iteration scheme is **very slow** so not practically used...

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It turns out that this iteration scheme is **very slow** so not practically used...

A way to improve the speed of convergence is to move from an **explicit** to an **implicit** update, i.e. considering for $k \geq 0$

$$x_{k+1} = x_k - \tau_k \underbrace{\cancel{p_k}}_{p_{k+1}}, \quad \text{where } p_{k+1} \in \partial g(x_{k+1})$$

Equivalently, we get the **proximal algorithm**

$$\begin{aligned} x_{k+1} \in x_k - \tau_k \partial g(x_{k+1}) &\Leftrightarrow x_k \in x_{k+1} + \tau_k \partial g(x_{k+1}) \\ x_k \in (I + \tau_k \partial g)(x_{k+1}) &\Leftrightarrow x_{k+1} \in (I + \tau_k \partial g)^{-1}(x_k) \\ \Leftrightarrow x_{k+1} = \operatorname{prox}_{\tau_k g}(x_k) & \end{aligned}$$

Note: same convergence speed as gradient descent $O(1/k)$.

Computation of proximal operators: examples

Let $C \subset \mathbb{R}^n$ be a closed and convex set. Recall indicator function of C as:

$$\iota_C(x) := \begin{cases} 0 & \text{if } x \in C \\ +\infty & \text{if } x \notin C \end{cases}$$

The function $\iota_C(x)$ is proper, convex and l.s.c. Proximal operator?

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$$\mathrm{prox}_{\gamma \iota_C}(x) = \arg\min_{y \in \mathbb{R}^n} \; \iota_C(y) + \frac{1}{2\gamma}\|y - x\|^2 = \arg\min_{y \in C} \frac{1}{2\gamma}\|y - x\|^2 = P_C(x),$$

the **projection** of x onto C (the closest point $y \in C$ to x).

The notion of prox for functions g more general than ι_C is the reason why the prox operator is often referred to as *generalised projection*.

Computation of proximal points: examples

Fix for now $\gamma = 1$.

- (Constant) If $g(x) = c$, $c \in \mathbb{R}$ for every x (constant function). Then:

$$\text{prox}_g(x) = \underset{y \in \mathbb{R}^n}{\arg\min}\ c + \frac{1}{2}\|x - y\|^2 = x$$

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- (Linear) If $g(x) = a^T x + b$, for $a \in \mathbb{R}^n$ and $b \in \mathbb{R}$. Then:

$$\begin{aligned} \operatorname{prox}_g(x) &= \operatorname*{arg\,min}_{y \in \mathbb{R}^n} \; a^T y + b + \frac{1}{2}\|y - x\|^2 \\ &= \operatorname*{arg\,min}_{y \in \mathbb{R}^n} \; a^T x + b - \frac{1}{2}\|a\|^2 + \frac{1}{2}\|y - (x - a)\|^2 = x - a \quad \text{(translation)} \end{aligned}$$

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- (Quadratic) If $g(x) = \frac{1}{2}x^T A x + b^T x + c$ with $A \in \mathbb{R}^{n \times n}$ and SPD, $b \in \mathbb{R}^n$ and $c \in \mathbb{R}$. Then:

$$\mathrm{prox}_g(x) = \arg\min_{y \in \mathbb{R}^n} \; \frac{1}{2} y^T A y + b^T y + c + \frac{1}{2}\|y - x\|^2$$

  Take the gradient and set it to 0:

$$A\hat{y} + b + \hat{y} - x = 0 \quad \Rightarrow \quad (A + \mathrm{Id})\hat{y} = x - b \quad \Rightarrow \quad \hat{y} = (A + \mathrm{Id})^{-1}(x - b)$$

Computation of proximal points: properties

Exercise: compute, for $\tau > 0$ $\text{prox}_{\tau g}(x)$ where $g(x) = |x|$. Plot the result as a function of x.

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Proximal operator of separable functions

Let $g : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ be proper, convex, l.s.c. and **separable**, i.e. $g(x) = \sum_{i=1}^n g_i(x_i)$ for proper, convex, l.s.c. 1D functions $g_i : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$. Then for $\gamma > 0$

$$\text{prox}_{\gamma g}(x) = \left(\text{prox}_{\gamma g_1}(x_1), \dots, \text{prox}_{\gamma g_n}(x_n)\right),$$

so the prox of a multi-dimensional function can be computed as the vector of prox's of their components g_i.

Exercise: For $\tau > 0$, give the expression of the proximal operator $\text{prox}_{\tau g}(x)$ with $g(x) = \|x\|_1$ for $x \in \mathbb{R}^n$.

Exercise: Behaviour of prox w.r.t. scaling/quadratic perturbations.

Projected gradient descent

For proper, differentiable, convex f and convex, closed $C \in \mathbb{R}^n$:

$$\arg\min_{x \in C} \; f(x) = \arg\min_{x \in \mathbb{R}^n} \; f(x) + \iota_C(x)$$

PGD algorithm

Input: $x_0 \in \mathbb{R}^n$ (initial guess), $\tau \in \left(0, \frac{2}{L}\right)$ (step-size)

Iterate for $k \geq 0$:

$$x_{k+\frac{1}{2}} = x_k - \tau \nabla f(x_k)$$

$$x_{k+1} = P_C(x_{k+\frac{1}{2}}) = \arg\min_{y \in C} \; \frac{1}{2}\|y - x_{k+\frac{1}{2}}\|^2$$

$$= \arg\min_{y \in \mathbb{R}^n} \; \iota_C(y) + \frac{1}{2}\|y - x_{k+\frac{1}{2}}\|^2 = \mathrm{prox}_{\iota_C}(x_{k+\frac{1}{2}})$$

till **convergence**.

$\Rightarrow$ the algorithm converges to a minimiser of f

- First: gradient step, next projection step
- Note: the projection on C requires the solution of an inner minimisation problem: not always explicit!

Forward-backward splitting a.k.a. proximal gradient descent

Why all this?

So far, we have discussed:

- **gradient descent** for minimising proper convex, differentiable functions f
- **implicit gradient descent** (proximal operators) for minimising proper convex (non-differentiable) functions g

Idea: combine the two ideas for solving the original, composite problem

$$\boxed{\min_{x \in \mathbb{R}^n} \left\{ F(x) := f(x) + g(x) \right\},}$$

Why all this?

So far, we have discussed:

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Idea: combine the two ideas for solving the original, composite problem

$$\boxed{\min_{x \in \mathbb{R}^n} \; \{F(x) := f(x) + g(x)\},}$$

Forward-backward splitting (FB/FBS) algorithm

Input: $x_0 \in \mathbb{R}^n$, $\tau \in \left(0, \frac{2}{L}\right)$

For $k \geq 0$, iterate:

$$x_{k+1} = \mathrm{prox}_{\tau g}\left(x_k - \tau \nabla f(x_k)\right) \Leftrightarrow \begin{cases} x_{k+1/2} & = x_k - \tau \nabla f(x_k) \\ x_{k+1} & = \mathrm{prox}_{\tau g}(x_{k+1/2}) \end{cases}$$

till convergence.

Such scheme alternates explicit (forward) and implicit (backward) gradient descent for minimising f and g alternatively. It's called **forward-backward** splitting algorithm or **proximal gradient** algorithm.

Main ingredients:

- Nice (smooth) part: proper, convex, differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ with L-Lipschitz continuous gradient

$$(\forall x, y \in \mathbb{R}^n) \quad \|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|$$

- Non-nice (non-smooth) part: proper, l.s.c., convex (non-smooth) function $f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$

Typically, we assume that g is *easily proximable*, i.e. the proximal operator of g can be computed in closed form (examples are $g(x) = \iota_C(x)$, $g(x) = \|x\|_1$, $g(x) = \|x\|_1 + \iota_{\geq 0}(x)$, $g(x) = \|x\|_1 + \frac{\lambda}{2}\|x\|_2^2 \ldots$).

Main features

Forward-backward splitting (FB/FBS) algorithm[1]

Input: $x_0 \in \mathbb{R}^n$, $\tau \in \left(0, \frac{1}{L}\right)$

For $k \geq 0$, iterate:

$$x_{k+1} = \mathrm{prox}_{\tau g}\left(x_k - \tau \nabla f(x_k)\right)$$

till convergence.

- Step-size: same bound depending on L as for GD.
- If g is easily proximable: no inner minimisation. Otherwise: need to solve a nested minimisation problem up to some accuracy (**inexact** algorithms)
- Computational cost/complexity: evaluation of ∇f may be costly (matrix/vector products), number of iterations before convergence depends on τ.
  * Too small τ: unnecessary too many iterations
  * Too big τ: risk of moving to a point z for which $f(x) > f(x_k)$...

[1] Combettes, Wajs, 2005

Particular cases, ISTA

- If $g \equiv 0$: smooth-optimisation problem. The FB scheme is nothing but GD.
- If $g(x) = \iota_C(x)$ for closed and convex $C \to$ projected gradient descent.
- If $g(x) = \lambda \|x\|_1$ for $\lambda > 0$, the problem reads

$$\min_{x \in \mathbb{R}^n} \; f(x) + \lambda \|x\|_1, \qquad (*)$$

then the algorithm to solve it is typically known as ISTA.

[2] Daubechies, Defrise, De Mol, 2004

Particular cases, ISTA

- If $g \equiv 0$: smooth-optimisation problem. The FB scheme is nothing but GD.
- If $g(x) = \iota_C(x)$ for closed and convex $C \to$ projected gradient descent.
- If $g(x) = \lambda\|x\|_1$ for $\lambda > 0$, the problem reads

$$\min_{x\in\mathbb{R}^n} \; f(x) + \lambda\|x\|_1, \tag{*}$$

then the algorithm to solve it is typically known as ISTA.

Iterative Soft Thresholding Algorithm (ISTA)[2]

The iteration (*) takes the form:

$$x_{k+1} = \mathcal{T}_{\tau\lambda}(x_k - \tau\nabla f(x_k))$$

where for $z = x_k - \tau\nabla f(x_k)$, $\mathcal{T}_{\tau\lambda}(z)$ is the *soft-thresholding* (or *shrinkage*) operator (prox of the function $g(x) = \lambda\|x\|_1$ with parameter τ) defined by:

$$\mathcal{T}_{\tau\lambda}(z) = (\mathcal{T}_{\tau\lambda}(z_j))_{j=1,\dots,n} = \Big(\left[|z_j| - \lambda\tau\right]_+ \operatorname{sign}(z_j)\Big)_{j=1,\dots,n}$$

[2] Daubechies, Defrise, De Mol, 2004

Convergence properties of proximal gradient descent

Convergence speed

Convergence rate of FBS/PGD

Let $x^0 \in \mathbb{R}^n$, and $(x_k)_k$ the sequence of iterates generated by the FB algorithm. If $\tau \in (0, 2/L)$, there holds:

$$\underbrace{F(x_k)}_{(f+g)(x_k)} - F(x^*) \leq \underbrace{\frac{\|x_0 - x^*\|^2}{2\tau}}_{C(x^0, x^*, \tau):=} \frac{1}{k} = O\left(\frac{1}{k}\right),$$

where x^* is a minimiser of F.

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where x^* is a minimiser of F.

- The point x^* is unknown, so the constant C is.
- The difference between x_k and x^* is measured in function values: the values $F(x_k)$ asymptotically approaches the (unknown) value $F(x^*)$ with speed proportional to $1/k$
- The result can also be written $O(1/k)$ where the constant is unknown, as $\|x_0 - x^*\|^2$ is.

Accelerated forward-backward splitting (FISTA)

Accelerated forward-backward algorithm (FISTA)

Analogous idea as for GD: combine proximal updates with inertia.

Accelerated forward-backward splitting (FISTA)

Input: $x_0 = x^{-1} = y_0 \in \mathbb{R}^n$ (initialisations), $\tau \in \left(0, \frac{1}{L}\right]$ (step-size), $t_0 = 1$

Iterate for $k \geq 0$:

$$y_k = x_k + \frac{t_k - 1}{t_{k+1}}(x_k - x_{k-1})$$
$$x_{k+1} = \mathrm{prox}_{\tau g}(y_k - \tau \nabla f(y_k))$$
$$t_{k+1} = \frac{1 + \sqrt{1 + 4t_k^2}}{2}$$

till **convergence**.

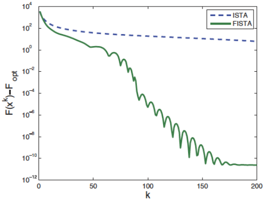
- Proximal operator is evaluated in GD-type applied on the extraploated sequence (y_k)
- Same computational costs as FB: one gradient computation and one prox computation at each iteration + explicit update. Modifications are cheap!

Convergence rates for FISTA

Convergence rate of FISTA

For a convex, smooth function f with L-Lipschitz gradient and convex, proper and l.s.c. function g, the convergence rate for the function values of FISTA for the composite function $F = f + g$ with $\tau \in (0, 1/L]$ is:

$$F(x_k) - F(x^*) \leq \frac{1}{(k+1)^2} \frac{2\|x_0 - x^*\|^2}{\tau}$$



Questions?

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