

CentraleSupélec

ST7 – Optimization

Part VIII: Some iterative algorithms

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迭代算法.

Problem

Let \mathcal{H} be a Hilbert space.

Let $f: \mathcal{H} \rightarrow \mathbb{R}$ be Gâteaux differentiable.

C - 非空闭凸子集、

Let C be a nonempty closed convex subset of \mathcal{H} .

We want to

$$\text{Find } \hat{x} \in \underset{x \in C}{\text{Argmin}} f(x).$$

Objective: Build a sequence $(x_n)_{n \in \mathbb{N}}$ converging to a minimizer.

收敛性.

Principle of first-order methods

- ▶ If f is Fréchet differentiable, then, at iteration n , we have

$$(\forall x \in \mathcal{H}) \quad \underline{f(x) = f(x_n) + \langle \nabla f(x_n) \mid x - x_n \rangle + o(\|x - x_n\|)}.$$

So if $\|x_{n+1} - x_n\|$ is small enough and x_{n+1} is chosen such that

$$\langle \nabla f(x_n) \mid x_{n+1} - x_n \rangle < 0$$

then $f(x_{n+1}) < f(x_n)$.

- ▶ In particular, the **steepest descent direction** is given by

$$x_{n+1} - x_n = -\gamma_n \nabla f(x_n), \quad \gamma_n \in]0, +\infty[.$$

learning rate.

Principle of first-order methods

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- ▶ In particular, the steepest descent direction is given by

$$x_{n+1} - x_n = -\gamma_n \nabla f(x_n), \quad \gamma_n \in]0, +\infty[.$$

- ▶ To secure that the solution belongs to C we can add a projection step.
- ▶ A relaxation parameter λ_n can also be added.

(松弛变量)

Projected gradient algorithm

The **gradient algorithm** has the following form:

$$(\forall n \in \mathbb{N}) \quad x_{n+1} = x_n - \gamma_n \nabla f(x_n)$$

where $\gamma_n \in]0, +\infty[$ is the **stepsize**. 步长. ?

Projected gradient algorithm

The projected gradient algorithm has the following form:

$$(\forall n \in \mathbb{N}) \quad x_{n+1} = P_C(x_n - \gamma_n \nabla f(x_n))$$

where $\gamma_n \in]0, +\infty[$.

projection.

Projected gradient algorithm

The projected gradient algorithm has the following form:

$$(\forall n \in \mathbb{N}) \quad x_{n+1} = x_n + \lambda_n (P_C(x_n - \gamma_n \nabla f(x_n)) - x_n)$$

where $\gamma_n \in]0, +\infty[$ and $\lambda_n \in]0, 1]$. *relaxation.*

Remark: x is a fixed point of the projected gradient iteration if and only if $x \in C$ and

$$(\forall y \in C) \quad \langle \nabla f(x) \mid y - x \rangle \geq 0.$$

不动点迭代:

下一步迭代只与当前步的迭代点有关，
与其他迭代点无关。

Projected gradient algorithm

The **projected gradient algorithm** has the following form:

$$(\forall n \in \mathbb{N}) \quad x_{n+1} = x_n + \lambda_n (P_C(x_n - \gamma_n \nabla f(x_n)) - x_n)$$

where $\gamma_n \in]0, +\infty[$ and $\lambda_n \in]0, 1]$.

Proof: If x is a fixed point, then 不动点.

$$\begin{aligned} x &= x + \lambda_n (P_C(x - \gamma_n \nabla f(x)) - x) \\ \Leftrightarrow x &= P_C(x - \gamma_n \nabla f(x)). \end{aligned}$$

According to the characterization of the projection, for every $y \in C$,

$$\begin{aligned} \langle x - \gamma_n \nabla f(x) - x \mid y - x \rangle &\leq 0 \\ \Leftrightarrow \langle \nabla f(x) \mid y - x \rangle &\geq 0. \end{aligned}$$

投影的基本性质.

简单约束的凸优化问题

这一讲讨论简单约束可微凸优化问题

$$\min \{f(x) \mid x \in \Omega\}$$

的梯度算法, 其中 Ω 是 \mathbb{R}^n 中的凸闭集, 并假设到 Ω 上的投影是容易实现的. 在第一讲中就已经提到, 简单约束可微凸优化问题等价于求变分不等式

$$\text{VI}(\Omega, \nabla f) \quad x \in \Omega, \quad (x' - x)^T \nabla f(x) \geq 0, \quad \forall x' \in \Omega$$

的解. 这一讲的投影梯度方法, 分别是收缩算法和下降算法, 都不要用到函数值 $f(x)$, 只要对给定的 x , 能提供 $\nabla f(x)$. 收缩算法保证迭代点向解集靠近. 下降算法则隐含了目标函数值下降, 尽管目标函数值在计算过程中从不出现.

设 x^* 是变分不等式 $\text{VI}(\Omega, \nabla f)$ 的解. 由于 $\tilde{x} = P_\Omega[x - \beta \nabla f(x)] \in \Omega$, 因此根据变分不等式的定义有第一个基本不等式

$$(F1) \quad (\tilde{x} - x^*)^T \beta \nabla f(x^*) \geq 0.$$

由于 \tilde{x} 是 $x - \beta \nabla f(x)$ 在 Ω 上的投影, $x^* \in \Omega$, 根据投影的基本性质, 有

$$(F12) \quad (\tilde{x} - x^*)^T ([x - \beta \nabla f(x)] - \tilde{x}) \geq 0.$$

Projected gradient algorithm

The **projected gradient algorithm** has the following form:

$$(\forall n \in \mathbb{N}) \quad x_{n+1} = x_n + \lambda_n (P_C(x_n - \gamma_n \nabla f(x_n)) - x_n)$$

where $\gamma_n \in]0, +\infty[$ and $\lambda_n \in]0, 1]$.

Remark:

- ▶ x is a fixed point of the projected gradient iteration if and only if $x \in C$ and

$$\text{凸的} (\forall y \in C) \quad \langle \nabla f(x) | y - x \rangle \geq 0.$$

- ▶ When f is convex, x is a fixed point of the projected gradient iteration if and only if x is a global minimizer of f over C .

全局最小值.

Convergence in the convex case 收敛性.

Cocoercity property 强制性.

Assume that f is convex and has a Lipschitzian gradient with constant $\beta \in]0, +\infty[$, i.e.

$$(\forall (x, y) \in \mathcal{H}^2) \quad \|\nabla f(x) - \nabla f(y)\| \leq \beta \|x - y\|.$$

Then

$$(\forall (x, y) \in \mathcal{H}^2) \quad \beta \langle \nabla f(x) - \nabla f(y) | x - y \rangle \geq \|\nabla f(x) - \nabla f(y)\|^2.$$

Convergence in the convex case

Cocoercity property

Assume that f is convex and has a Lipschitzian gradient with constant $\beta \in]0, +\infty[$. Then

$$(\forall (x, y) \in \mathcal{H}^2) \quad \beta \langle \nabla f(x) - \nabla f(y) \mid x - y \rangle \geq \|\nabla f(x) - \nabla f(y)\|^2.$$

Convergence theorem

Assume that f is convex and has a Lipschitzian gradient with constant $\beta \in]0, +\infty[$.

Assume that $D = \text{Argmin}_{x \in C} f(x) \neq \emptyset$.

Assume that $\inf_{n \in \mathbb{N}} \gamma_n > 0$, $\sup_{n \in \mathbb{N}} \gamma_n < 2/\beta$, $\inf_{n \in \mathbb{N}} \lambda_n > 0$, and $\sup_{n \in \mathbb{N}} \lambda_n \leq 1$.

Then the sequence $(x_n)_{n \in \mathbb{N}}$ generated by the projected gradient algorithm is Fejér monotone with respect to D , i.e.

$$(\forall x \in D)(\forall n \in \mathbb{N}) \quad \|x_{n+1} - x\| \leq \|x_n - x\|.$$

Convergence in the convex case

Convergence theorem

Assume that f is convex and has a Lipschitzian gradient with constant $\beta \in]0, +\infty[$.

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Then the sequence $(x_n)_{n \in \mathbb{N}}$ generated by the projected gradient algorithm is Fejér monotone with respect to D .

Proof: Let $x \in D$. Then, for every $n \in \mathbb{N}$,

$$\begin{aligned}
 & \|P_C(x_n - \gamma_n \nabla f(x_n)) - x\|^2 && x \text{ is a fix point.} \\
 & = \|P_C(x_n - \gamma_n \nabla f(x_n)) - P_C(x - \gamma_n \nabla f(x))\|^2 && x = P_C(x - \gamma_n \nabla f(x)). \\
 & \leq \|x_n - \gamma_n \nabla f(x_n) - x + \gamma_n \nabla f(x)\|^2 && \text{coercivity.} \\
 & = \|x_n - x\|^2 - 2\gamma_n \langle \nabla f(x_n) - \nabla f(x) | x_n - x \rangle + \gamma_n^2 \|\nabla f(x_n) - \nabla f(x)\|^2 \\
 & \leq \|x_n - x\|^2 - \underline{2\gamma_n \beta^{-1} \|\nabla f(x_n) - \nabla f(x)\|^2} + \gamma_n^2 \|\nabla f(x_n) - \nabla f(x)\|^2 \\
 & = \|x_n - x\|^2 - \gamma_n (2\beta^{-1} - \gamma_n) \|\nabla f(x_n) - \nabla f(x)\|^2 \leq \|x_n - x\|^2.
 \end{aligned}$$

Convergence in the convex case

Convergence theorem

Assume that f is convex and has a Lipschitzian gradient with constant $\beta \in]0, +\infty[$.

Assume that $D = \text{Argmin}_{x \in C} f(x) \neq \emptyset$.

Assume that $\inf_{n \in \mathbb{N}} \gamma_n > 0$, $\sup_{n \in \mathbb{N}} \gamma_n < 2/\beta$, $\inf_{n \in \mathbb{N}} \lambda_n > 0$, and $\sup_{n \in \mathbb{N}} \lambda_n \leq 1$.

Then the sequence $(x_n)_{n \in \mathbb{N}}$ generated by the projected gradient algorithm is Fejér monotone with respect to D .

Proof: We deduce that

$$\begin{aligned} \|x_{n+1} - x\| &\leq (1 - \lambda_n) \|x_n - x\| + \lambda_n \|P_C(x_n - \gamma_n \nabla f(x_n)) - x\| \\ &\leq \|x_n - x\|. \end{aligned}$$

This shows that $(x_n)_{n \in \mathbb{N}}$ is Fejér monotone with respect to D .

Convergence in the convex case

Convergence theorem

Assume that f is convex and has a Lipschitzian gradient with constant $\beta \in]0, +\infty[$.

Assume that $\text{Argmin}_{x \in C} f(x) \neq \emptyset$.

Assume that $\inf_{n \in \mathbb{N}} \gamma_n > 0$, $\sup_{n \in \mathbb{N}} \gamma_n < 2/\beta$, $\inf_{n \in \mathbb{N}} \lambda_n > 0$, and $\sup_{n \in \mathbb{N}} \lambda_n \leq 1$.

Then the sequence $(x_n)_{n \in \mathbb{N}}$ generated by the projected gradient algorithm converges weakly to a minimizer of f over C .

梯度投影法，
弱收敛。

Convergence of the function values

Descent lemma

Assume that f is Gâteaux differentiable and has a β -Lipschitzian gradient with $\beta \in]0, +\infty[$. Then,

$$(\forall (x, y) \in \mathcal{H}^2) \quad f(y) \leq f(x) + \langle y - x \mid \nabla f(x) \rangle + \frac{\beta}{2} \|y - x\|^2.$$

Proof: For every $(x, y) \in \mathcal{H}^2$ and $t \in \mathbb{R}$, let $\varphi(t) = f(x + t(y - x))$. φ is differentiable and $\varphi'(t) = \langle y - x \mid \nabla f(x + t(y - x)) \rangle$. We have then

$$\begin{aligned} \varphi(1) - \varphi(0) &= \int_0^1 \varphi'(t) dt \\ \Leftrightarrow f(y) - f(x) - \langle y - x \mid \nabla f(x) \rangle &= \int_0^1 \langle y - x \mid \nabla f(x + t(y - x)) - \nabla f(x) \rangle dt. \end{aligned}$$

In addition, according to the Cauchy-Schwarz inequality,

$$\begin{aligned} &\langle y - x \mid \nabla f(x + t(y - x)) - \nabla f(x) \rangle \\ &\leq \|y - x\| \|\nabla f(x + t(y - x)) - \nabla f(x)\| \leq t\beta \|y - x\|^2. \end{aligned}$$

This leads to $f(y) \leq f(x) + \langle y - x \mid \nabla f(x) \rangle + \frac{\beta}{2} \|y - x\|^2$.

Convergence of the function values 函数值的收敛性.

Descent lemma

Assume that f is Gâteaux differentiable and has a β -Lipschitzian gradient with $\beta \in]0, +\infty[$. Then,

$$(\forall (x, y) \in \mathcal{H}^2) \quad f(y) \leq f(x) + \langle y - x \mid \nabla f(x) \rangle + \frac{\beta}{2} \|y - x\|^2.$$

Convergence theorem

Assume that f is Gâteaux differentiable and has a β -Lipschitzian gradient with $\beta \in]0, +\infty[$. Assume that $\mu = \inf_{x \in C} f(x) > -\infty$.

Assume that $(\forall n \in \mathbb{N}) \lambda_n = 1$ and $\gamma_n \in]0, 1/\beta[$.

Then $(f(x_n))_{n \in \mathbb{N}}$ is a convergent sequence.

Convergence of the function values

Convergence theorem

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Assume that $(\forall n \in \mathbb{N}) \lambda_n = 1$ and $\gamma_n \in]0, 1/\beta[$.

Then $(f(x_n))_{n \in \mathbb{N}}$ is a convergent sequence.

Proof: Let $n \geq 1$. According to the descent lemma,

$$f(x_{n+1}) \leq f(x_n) + \langle \nabla f(x_n) \mid x_{n+1} - x_n \rangle + \frac{\beta}{2} \|x_{n+1} - x_n\|^2$$

Since $x_{n+1} = P_C(x_n - \gamma_n \nabla f(x_n))$ and $x_n \in C$,

$$\begin{aligned} \|x_{n+1} - x_n + \gamma_n \nabla f(x_n)\|^2 &\leq \|x_n - x_n + \gamma_n \nabla f(x_n)\|^2 \\ \Leftrightarrow \|x_{n+1} - x_n\|^2 + 2\gamma_n \langle \nabla f(x_n) \mid x_{n+1} - x_n \rangle &\leq 0 \\ \Leftrightarrow \langle \nabla f(x_n) \mid x_{n+1} - x_n \rangle &\leq -\frac{1}{2\gamma_n} \|x_{n+1} - x_n\|^2. \end{aligned}$$

Therefore,

$$f(x_{n+1}) \leq f(x_n) + \frac{1}{2}(\beta - \gamma_n^{-1})\|x_{n+1} - x_n\|^2 \leq f(x_n).$$

Since $(f(x_n))_{n \in \mathbb{N}}$ is a decaying sequence, lower bounded by μ , it converges.

Convergence of the function values

Convergence theorem

Assume that f is Gâteaux differentiable and has a β -Lipschitzian gradient with $\beta \in]0, +\infty[$. Assume that $\mu = \inf_{x \in C} f(x) > -\infty$. Assume that $(\forall n \in \mathbb{N}) \lambda_n = 1$ and $\gamma_n \in]0, 1/\beta[$. Then $(f(x_n))_{n \in \mathbb{N}}$ is a convergent sequence.

Remarks:

- ▶ If f is convex, the same result holds when $(\forall n \in \mathbb{N}) \lambda_n \in]0, 1]$ and $\gamma_n \in]0, 2/\beta[$. In addition, $f(x_n) \rightarrow \mu$.
- ▶ In the nonconvex case, there is no guarantee that the limit is μ since the iterates may get stuck in a spurious local minimum.

Metric change 度量变化.

Let $A \in \mathcal{B}(\mathcal{H}, \mathcal{H})$ be a self-adjoint operator which is strongly positive, i.e. there exists $\alpha \in]0, +\infty[$ such that

$$(\forall x \in \mathcal{H}) \quad \langle x | Ax \rangle \geq \alpha \|x\|^2.$$

The inner product induced by A is

$$(\forall (x, y) \in \mathcal{H}^2) \quad \langle x | y \rangle_A = \langle x | Ay \rangle.$$

Remark: When $\mathcal{H} = \mathbb{R}^N$, $A \in \mathbb{R}^{N \times N}$ is strongly positive if and only if A is symmetric positive definite.

Metric change

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The inner product induced by A is

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Let $A \in \mathcal{B}(\mathcal{H}, \mathcal{H})$ be a strongly positive self-adjoint operator.

Let $f: \mathcal{H} \rightarrow \mathbb{R}$ be a Gâteaux differentiable function.

In the Hilbert space $(\mathcal{H}, \langle \cdot | \cdot \rangle_A)$, the gradient of f is $\nabla_A f = A^{-1} \nabla f$.

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Let $A \in \mathcal{B}(\mathcal{H}, \mathcal{H})$ be a strongly positive self-adjoint operator.

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In the Hilbert space $(\mathcal{H}, \langle \cdot | \cdot \rangle_A)$, the gradient of f is $\nabla_A f = A^{-1} \nabla f$.

Proof: The Gâteaux differential is such that

$$\begin{aligned} (\forall (x, y) \in \mathcal{H}^2) \quad f'(x)y &= \langle \nabla f(x) | y \rangle \\ &= \langle AA^{-1} \nabla f(x) | y \rangle \\ &= \langle A^{-1} \nabla f(x) | Ay \rangle \\ &= \langle \underbrace{A^{-1} \nabla f(x)} | y \rangle_A. \end{aligned}$$

Preconditioning

- ▶ Unconstrained optimization: $C = \mathcal{H}$ 无约束优化.
- ▶ Let $A \in \mathcal{B}(\mathcal{H}, \mathcal{H})$ be a strongly positive self-adjoint operator.
- ▶ The gradient algorithm in $(\mathcal{H}, \langle \cdot | \cdot \rangle_A)$ reads

$$\begin{aligned}
 (\forall n \in \mathbb{N}) \quad x_{n+1} &= x_n - \gamma_n \nabla_A f(x_n) \\
 &= x_n - \gamma_n A^{-1} \nabla f(x_n)
 \end{aligned}$$

with $\gamma_n \in]0, +\infty[$.

Preconditioning

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with $\gamma_n \in]0, +\infty[$.

- ▶ Let $(A_n)_{n \in \mathbb{N}}$ be a sequence of strongly positive self-adjoint operators in $\mathcal{B}(\mathcal{H}, \mathcal{H})$. A more general form is

$$\begin{aligned} (\forall n \in \mathbb{N}) \quad x_{n+1} &= x_n - \gamma_n A_n^{-1} \nabla f(x_n) \\ &= x_n - \tilde{A}_n^{-1} \nabla f(x_n), \end{aligned}$$

where $\tilde{A}_n = \gamma_n^{-1} A_n$.

\rightsquigarrow

quasi-Newton algorithm.

拟牛顿法.

Preconditioning

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where $\tilde{A}_n = \gamma_n^{-1} A_n$.

\rightsquigarrow quasi-Newton algorithm.

Remarks:

- ▶ By being more flexible, this algorithm may lead to a faster convergence by a suitable choice of $(\tilde{A}_n)_{n \in \mathbb{N}}$.
- ▶ If f is twice Fréchet differentiable and its Hessian is strongly positive on \mathcal{H} , one can choose

$$(\forall n \in \mathbb{N}) \quad \tilde{A}_n = \nabla^2 f(x_n)$$

\rightsquigarrow Newton's method. 牛顿法.

Preconditioning

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- ▶ By being more flexible, this algorithm may lead to a faster convergence by a suitable choice of $(\tilde{A}_n)_{n \in \mathbb{N}}$.
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\rightsquigarrow **Newton's method**.

- ▶ Newton's method can also be derived from a second-order Taylor expansion of f around x_n at iteration $n \in \mathbb{N}$: = 二阶 Taylor 展开

$$x_{n+1} = \operatorname{argmin}_{x \in \mathcal{H}} f(x_n) + \underbrace{\langle \nabla f(x_n) | x - x_n \rangle}_{f'(x_n)(x-x_n)} + \frac{1}{2} \langle x - x_n | \nabla^2 f(x_n)(x - x_n) \rangle.$$

$f''(x_n)(x-x_n) \sim /2$

Example 1: Uzawa algorithm

Problem

Let $\mathcal{L}: \mathcal{H} \times \mathbb{R}^q \rightarrow \mathbb{R}$ be differentiable with respect to its second argument. We want to find a saddle point of \mathcal{L} over $\mathcal{H} \times [0, +\infty[^q$.

Solution

Set $\lambda_0 \in [0, +\infty[^q$

For $n = 0, 1, \dots$

	Set $\gamma_n \in]0, +\infty[, \rho_n \in]0, 1]$
	$x_n \in \text{Argmin} \mathcal{L}(\cdot, \lambda_n)$
	$\lambda_{n+1} = \lambda_n + \rho_n (P_{[0, +\infty[^q}(\lambda_n + \gamma_n \nabla_{\lambda} \mathcal{L}(x_n, \lambda_n)) - \lambda_n).$

Example 2: DC programming

Problem

Let $f \in \Gamma_0(\mathcal{H})$ and let $g \in \Gamma_0(\mathcal{H})$.

We want to minimize the difference of convex functions $f - g$.

Remark: The problem is equivalent to

$$\begin{aligned} & \underset{x \in \mathcal{H}}{\text{minimize}} \quad f(x) - \sup_{v \in \mathcal{H}} (\langle x \mid v \rangle - g^*(v)) \\ \Leftrightarrow & \underset{(x,v) \in \mathcal{H}^2}{\text{minimize}} \quad f(x) - \langle x \mid v \rangle + g^*(v) \end{aligned}$$

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Solution

If f and g^* are Gâteaux differentiable, we can use the following algorithm:

Set $(x_0, v_0) \in \mathcal{H}^2$

For $n = 0, 1, \dots$

$$\left[\begin{array}{l} \text{Set } \gamma_n \in]0, +\infty[, \mu_n \in]0, +\infty[\\ x_{n+1} = x_n - \gamma_n(\nabla f(x_n) - v_n) \\ v_{n+1} = v_n - \mu_n(\nabla g^*(v_n) - x_{n+1}). \end{array} \right.$$

Exercise

Let \mathcal{H} and \mathcal{G} be real Hilbert spaces and let $L \in \mathcal{B}(\mathcal{H}, \mathcal{G})$. Let $y \in \mathcal{G}$ and let $\alpha \in]0, +\infty[$.

We want to minimize the function defined as

$$(\forall x \in \mathcal{H}) \quad f(x) = \frac{1}{2} \|Lx - y\|^2 + \frac{\alpha}{2} \|x\|^2.$$

1. Give the form of the gradient descent algorithm allowing us to solve this problem.
2. How does Newton's method read for this function ?
3. Consider the case when $\mathcal{H} = \mathbb{R}^N$. Study the convergence of the gradient descent algorithm by performing the eigendecomposition of L^*L .