Iterative Algorithms in Optimization, Variational Analysis and Fixed Point Theory

Unit 02: Smooth optimization and gradient descent.

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Descent directions

Let $A \subset \mathbb{R}^N$ be nonempty and open, and let $f : A \to \mathbb{R}$. A vector $d \neq 0$ is a descent direction for f at x if there is $\Gamma > 0$ such that

$$f(x + \gamma d) < f(x) \qquad \text{for all } \gamma \in (0, \Gamma).$$

The numbers $\gamma \in (0, \Gamma)$ are descent step sizes.

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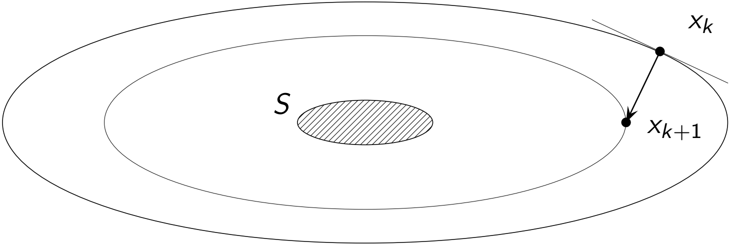
Remark

If f is differentiable at x and $\nabla f(x) \neq 0$, then $-\nabla f(x)$ is the steepest descent direction, and the set of all descent directions is the halfspace

$$\left\{ d \in \mathbb{R}^N : \nabla f(x) \cdot d < 0 \right\}.$$

Gradient descent

From $x_0 \in \mathbb{R}^N$, iterate $x_{k+1} = x_k - \gamma \nabla f(x_k)$



L-smoothness

A differentiable function $f : A \subset \mathbb{R}^N \to \mathbb{R}$ is L-smooth, with $L > 0$, if

$$\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|$$

for all $x, y \in A$.

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for all $x, y \in A$.

Proposition (Descent Lemma)

If f is L-smooth and A is convex, then

$$|f(y) - f(x) - \nabla f(x) \cdot (y - x)| \leq \frac{L}{2}\|x - y\|^2$$

for all $x, y \in A$.

Estimating descent step sizes

Proposition

Let $A \neq \emptyset$ be open and convex, and let $f : A \to \mathbb{R}$ be $L-$smooth. Then,

$$f\left(x - \gamma \nabla f(x)\right) \leq f(x) + \gamma \left(\frac{\gamma L}{2} - 1 \right) \|\nabla f(x)\|^2$$

for all sufficiently small $\gamma > 0$.[a]

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[a] Sufficiently small to remain in A.

There are reasons to take $\gamma = \frac{1}{L}$.

Convergence and complexity

Proposition

Let $f : \mathbb{R}^N \to \mathbb{R}$ be L-smooth and bounded from below. Iterate $x_{k+1} = x_k - \gamma_k \nabla f(x_k)$, where $\inf_{k\geq 0} \gamma_k(2 - \gamma_k L) > 0$.

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1. $\exists \lim\limits_{k\to\infty} f(x_k) \in \mathbb{R}$, *and* $\lim\limits_{k\to\infty} \|\nabla f(x_k)\| = 0$.
2. *Cluster points are critical: if $x_{j_k} \to \hat{x}$, then $\nabla f(\hat{x}) = 0$.*

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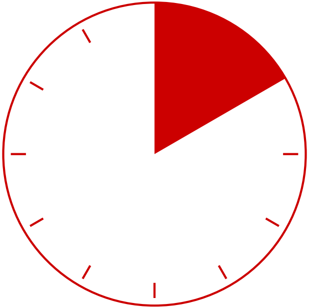
3. *If* f *has no critical points, then* $\lim\limits_{k \to \infty} \|x_k\| = +\infty$.
4. *There is* $C > 0$ *such that* $\min \left\{ \|\nabla f(x_j)\| : 1 \leq j \leq k \right\} \leq \dfrac{C}{\sqrt{k}}$.

Break



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  - Armijo: $f(x_k + \gamma_k d_k) \leq f(x_k) + \sigma \gamma_k \nabla f(x_k) \cdot d_k \quad (A)$.

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  - Wolfe: (A), plus $\nabla f(x_k + \gamma_k d_k) \cdot d_k \geq \tau \nabla f(x_k) \cdot d_k$.
  - Strong Wolfe: (A), plus $|\nabla f(x_k + \gamma_k d_k) \cdot d_k| \leq \tau |\nabla f(x_k) \cdot d_k|$.

Convex functions

A function $f : A \subset \mathbb{R}^N \to \mathbb{R}$ is convex if A is convex and

$$f\big(\lambda x + (1-\lambda)y\big) \leq \lambda f(x) + (1-\lambda)f(y) \quad \forall x, y \in A,\ \lambda \in (0,1).$$

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If $f : \mathbb{R}^N \to \mathbb{R}$ is convex and L-smooth, then

$$\frac{1}{L}\|\nabla f(y) - \nabla f(x)\|^2 \leq \big(\nabla f(y) - \nabla f(x)\big) \cdot (y - x) \qquad \forall x, y \in \mathbb{R}^N.$$

Convex functions and gradient descent

Theorem

Let $f : \mathbb{R}^N \to \mathbb{R}$ *be convex and L-smooth. Iterate* $x_{k+1} = x_k - \gamma \nabla f(x_k)$ *with* $0 < \gamma < \frac{2}{L}$.

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1. $\lim_{k\to\infty} f(x_k) = \inf(f)$.
2. *If f has minimizers, then x_k converges to one of them, and*

$$f(x_k) - \min(f) \leq \frac{\mathrm{dist}(x_0, S)^2}{\gamma(2 - \gamma L)k}.$$

Moreover, $\lim_{k\to\infty} k\left[f(x_k) - \min(f)\right] = 0.$

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Quadratic functions

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$$Q(x) = \frac{1}{2}x^T Px + c^T x + d,$$

where $P = A^T A \in \mathbb{R}^{N\times N}$ is symmetric and positive semidefinite, $c = -A^T b \in \mathbb{R}^N$ and $d = \frac{1}{2}\|b\|^2 \in \mathbb{R}$.

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Such functions are always convex and bounded from below.

A tiny bit of linear algebra and geometry

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4. If μ is the smallest eigenvalue of P, then $\|Ax\|^2 = x^T P x \geq \mu \|x\|^2$ for all $x \in \mathbb{R}^N$. Moreover,

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5. $\|Ax\|^2 = x^T P x \leq L\|x\|^2$, where L is the largest eigenvalue of P.

If $\mu > 0$, the ratio $\kappa = \frac{L}{\mu}$ is the condition number of P.

Consequences for Q and for gradient descent

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If P is invertible, then $\min(Q) = 0$ and Q has exactly one minimizer

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Proposition

Iterate $x_{k+1} = x_k - \gamma_k \nabla Q(x_k)$, *with* $\gamma_k \equiv \frac{2}{L+\mu}$. *For each* $k \geq 1$, *we have*

$$\|x_k - \hat{x}\| \leq \left(\frac{L-\mu}{L+\mu}\right)^k \|x_0 - \hat{x}\| = \left(\frac{\kappa - 1}{\kappa + 1}\right)^k \|x_0 - \hat{x}\|.$$

General case

If P is not invertible, then

$$\min(Q) = \frac{1}{2}\,\mathrm{dist}\left(b, \mathrm{ran}(A)\right)^2,$$

and $u \in S$ if, and only if, $Au = \mathrm{Proj}_{\mathrm{ran}(A)}\, b$.

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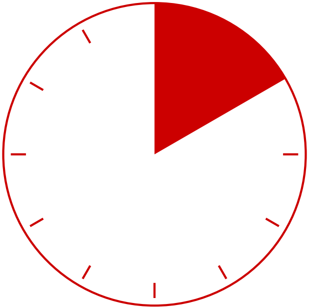

From quadratic to non quadratic functions I

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for all $x, y \in \mathbb{R}^N$ and $\theta \in (0,1)$. If $\ker(A) = \{0\}$, then

$$Q\big(\theta x + (1-\theta)y\big) \leq \theta Q(x) + (1-\theta)Q(y) - \mu\frac{\theta(1-\theta)}{2}\|x-y\|^2.$$

A function $f : \mathbb{R}^N \to \mathbb{R}$ that satisfies such an inequality is called $\mu-$strongly convex. It must be continuous and must have exactly one minimizer.

Polyak-Łojasiewicz inequality

If f is $\mu-$ strongly convex, it satisfies the Polyak-Łojasiewicz inequality with constant μ:

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Example

Show that $Q(x) = \frac{1}{2}\|Ax - b\|^2$ satisfies a Polyak-Łojasiewicz inequality, even if $\ker(A)$ is nontrivial.

Polyak-Łojasiewicz inequality and gradient descent

Proposition

Let $f : \mathbb{R}^N \to \mathbb{R}$ be $L-$smooth and satisfy the Polyak-Łojasiewicz inequality with constant $\mu > 0$. Iterate $x_{k+1} = x_k - \frac{1}{L}\nabla f(x_k)$. Then,

$$f(x_k) - \min(f) \leq \left(1 - \frac{\mu}{L}\right)^k \left(f(x_0) - \min(f)\right),$$

for all $k \geq 1$.

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Remark

If we define the condition number of f as $\kappa = \frac{L}{\mu}$, then $1 - \frac{\mu}{L} = \frac{\kappa - 1}{\kappa}$. How does this compare with the quadratic case? How is the condition number related to the Hessian of f?

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The conjugate gradient method

Consider, as before, the problem of minimizing

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where $A \in \mathbb{R}^{M\times N}$ and $b \in \mathbb{R}^M$. Assume $\ker(A) = \{0\}$.

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The conjugate gradient method iterates

$$x_{k+1} = x_k + \gamma_k d_k$$

for convenient choices of γ_k and d_k, in such a way that $\{d_0, \dots, d_{N-1}\}$ is a basis of $\mathbb{R}^N$ and x_k minimizes Q on the affine subspace

$$x_0 + \mathrm{span}\{d_0, \dots, d_{n-1}\}.$$

The (unique) solution is found in at most N steps.

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If $g_k = 0$, we stop because we have found the solution. Otherwise, we compute γ_k and then x_{k+1} by the exact minimization rule:

$$\gamma_k = \frac{\|g_k\|^2}{\|d_k\|_P^2} \qquad \text{and} \qquad x_{k+1} = x_k + \gamma_k d_k.$$

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$$\gamma_k = \frac{\|g_k\|^2}{\|d_k\|_P^2} \qquad \text{and} \qquad x_{k+1} = x_k + \gamma_k d_k.$$

Finally, update

$$g_{k+1} = Px_{k+1} + c = g_k + P(x_{k+1} - x_k) = g_k + \gamma_k P d_k$$

The conjugate gradient method

Start with $x_0 \in \mathbb{R}^N$ and compute $d_0 = -\nabla Q(x_0) = -Px_0 - c$.

At step k, we know x_k and d_k, and we compute $g_k = \nabla Q(x_k)$.

If $g_k = 0$, we stop because we have found the solution. Otherwise, we compute γ_k and then x_{k+1} by the exact minimization rule:

$$\gamma_k = \frac{\|g_k\|^2}{\|d_k\|_P^2} \qquad \text{and} \qquad x_{k+1} = x_k + \gamma_k d_k.$$

Finally, update

$$g_{k+1} = Px_{k+1} + c = g_k + P(x_{k+1} - x_k) = g_k + \gamma_k P d_k,$$

and

$$d_{k+1} = -g_{k+1} + \beta_k d_k, \qquad \text{with} \qquad \beta_k = \frac{\|g_{k+1}\|^2}{\|g_k\|^2}.$$

Nonlinear extensions

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If $g_k = 0$, we stop; otherwise, we compute (backtracking) γ_k satisfying

$$\begin{aligned} f(x_k + \gamma_k d_k) &\leq f(x_k) + \sigma \gamma_k \, g_k \cdot d_k \\ |\nabla f(x_k + \gamma_k d_k) \cdot d_k| &\leq \tau \, |g_k \cdot d_k|, \end{aligned}$$

with $0 < \sigma < \tau < 1$ (strong Wolfe conditions).

Nonlinear extensions, continued

Then, we update

$$\begin{aligned} x_{k+1} &= x_k + \gamma_k d_k \\ d_{k+1} &= -g_{k+1} + \beta_k d_k, \end{aligned}$$

where several choices for β_k are possible, such as:

- Fletcher-Reeves: $\frac{\|g_{k+1}\|^2}{\|g_k\|^2}$
- Polak-Ribière: $\frac{g_{k+1} \cdot (g_{k+1} - g_k)}{\|g_k\|^2}$
- Hestenes-Stiefel: $\frac{g_{k+1} \cdot (g_{k+1} - g_k)}{d_k \cdot (g_{k+1} - g_k)}$
- Dai-Yuan: $\frac{\|g_{k+1}\|^2}{d_k \cdot (g_{k+1} - g_k)}$