Optimization methods
Lecture 5: Introduction to numerical optimization methods. Gradient descent

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Brief reminder of the previous lectures

- How convexity of the problem helps to solve it
- Disciplined convex programming
- CVXPy
- Optimality conditions

Problem statement

$$
\begin{aligned}
&\min_{\mathbf{x} \in S} f_0(\mathbf{x}) \\
\text{s.t. } & f_j(\mathbf{x}) = 0,\ j = 1, \dots, m \\
& g_k(\mathbf{x}) \leq 0,\ k = 1, \dots, p
\end{aligned}
$$

where $S \subseteq \mathbb{R}^n,\ f_j : S \to \mathbb{R},\ j = 0, \dots, m,$
$g_k : S \to \mathbb{R},\ k = 1, \dots, p$

- All functions here are at least continuous
- **Nonlinear** optimization problems are numerically intractable in general case

Reminder of analytical results

First order necessary condition

If $\mathbf{x}^*$ is a local minimizer of differentiable function $f(\mathbf{x})$, then

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If $\mathbf{x}^*$ is a local minimizer of twice differentiable function $f(\mathbf{x})$, then

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Sufficient condition

Let $f(\mathbf{x})$ be twice differentiable functio, and $\mathbf{x}^*$ satisfies the following conditions

$$f'(\mathbf{x}^*) = 0 \quad f''(\mathbf{x}^*) \succ 0,$$

then $\mathbf{x}^*$ is a local minimizer of $f(\mathbf{x})$

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- Information about the problem

General scheme

- Initial guess $\mathbf{x}_0$
- Desired tolerance ε
- Update solution approximation

Questions

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2. How the next point is computed?

Stopping criteria

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3. Necessary condition

$$\|f'(\mathbf{x}_k)\|_2 < \varepsilon$$

How to update point

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Line search

1. Find a direction $\mathbf{h}_k$
2. After that compute «optimal» value α_k

How to compare optimization methods?

For fixed class of problems the following ways of comparison are possible

1. Complexity
2. Convergence speed
3. Experiments

Convergence speed

1. Sublinear
$$\|\mathbf{x}_{k+1} - \mathbf{x}^*\|_2 \leq Ck^{\alpha},$$
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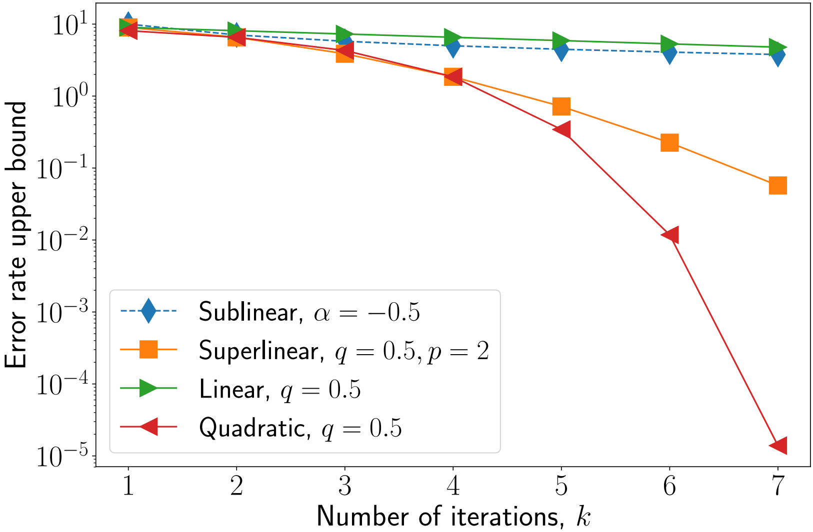
4. Quadratic
$$\|\mathbf{x}_{k+1} - \mathbf{x}^*\|_2 \leq C\|\mathbf{x}_k - \mathbf{x}^*\|_2^2, \qquad \text{or} \qquad \|\mathbf{x}_{k+1} - \mathbf{x}^*\|_2 \leq Cq^{2^k}$$
where $q \in (0, 1)$ and $0 < C < \infty$

Comparison of convergence speed



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  - theoretical estimate without any experiments

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  - what type of convergence can we expect
- convergence speed estimate
  - theoretical estimate without any experiments
  - identification of factors that affect convergence
  - sometimes it is possible to set number of iterations in advance to achieve pre-defined tolerance

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- convergence estimate depends on the unknown constants
- rounding errors are out of scope

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Q: do higher-order methods exist?

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Q: do higher-order methods exist?
A: yes, but they are still mostly under development to make them a technology not art. Original paper[1]

[1] Nesterov Y. Implementable tensor methods in unconstrained convex optimization //Mathematical Programming. – 2019. – P. 1-27.

How can we use previous points?

1. One-step methods

$$\mathbf{x}_{k+1} = \Phi(\mathbf{x}_k)$$

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1. One-step methods

$$\mathbf{x}_{k+1} = \Phi(\mathbf{x}_k)$$

2. Multi-step methods

$$\mathbf{x}_{k+1} = \Phi(\mathbf{x}_k, \mathbf{x}_{k-1}, \ldots)$$

Main facts from intro

- Why do we need numerical methods
- General scheme
- How can we compare optimization methods
- Zoo of problems and methods

Descent methods

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Definition

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Remark

There exist methods that do not require monotonic decreasing of the objective function but converge faster

L-smooth function: reminder

Definition

Let $L > 0$. A function f is called L-smooth if it is differentiable and satisfies

$$\|f'(\mathbf{x}) - f'(\mathbf{y})\|_2 \leq L\|\mathbf{x} - \mathbf{y}\|_2.$$

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Descent lemma

Let f be an L-smooth function. Then for any $\mathbf{x}, \mathbf{y}$

$$f(\mathbf{y}) \leq f(\mathbf{x}) + \langle f'(\mathbf{x}), \mathbf{y} - \mathbf{x}\rangle + \frac{L}{2}\|\mathbf{y} - \mathbf{x}\|_2^2$$

Gradient descent

Global upper bound for function f at point $\mathbf{x}_k$:

$$f(\mathbf{y}) \leq f(\mathbf{x}_k) + \langle f'(\mathbf{x}_k), \mathbf{y} - \mathbf{x}_k \rangle + \frac{L}{2} \|\mathbf{y} - \mathbf{x}_k\|_2^2 \equiv g(\mathbf{y}),$$

where $\lambda_{\max}(f''(\mathbf{x})) \leq L$ for all feasible $\mathbf{x}$.

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where $\lambda_{\max}(f''(\mathbf{x})) \leq L$ for all feasible $\mathbf{x}$.
The right-hand side is a quadratic form such that its minimizer has analytical expression:

$$\begin{aligned}
& g'(\mathbf{y}^*) = 0 \\
& f'(\mathbf{x}_k) + L(\mathbf{y}^* - \mathbf{x}_k) = 0 \\
& \mathbf{y}^* = \mathbf{x}_k - \frac{1}{L} f'(\mathbf{x}_k) \equiv \mathbf{x}_{k+1}
\end{aligned}$$

This approach estimates step size as $\frac{1}{L}$.

Step size selection

- Constant step size $\alpha_k \equiv \text{const} < \frac{2}{L}$
- Decreasing sequence such that $\sum\limits_{k=1}^{\infty} \alpha_k = \infty$, e.g. $\frac{1}{k}, \frac{1}{\sqrt{k}}$
- Adaptive step size
- The steepest descent rule: the search of the best α_k

Important note

The best step size does not provide better theoretical convergence rate

Convergence to a stationary point

$$f(\mathbf{x}_{k+1}) \leq f(\mathbf{x}_k) + \langle f'(\mathbf{x}_k), \mathbf{x}_{k+1} - \mathbf{x}_k \rangle + \frac{L}{2}\|\mathbf{x}_{k+1} - \mathbf{x}_k\|_2^2 =$$

$$f(\mathbf{x}_k) - \alpha_k \|f'(\mathbf{x}_k)\|_2^2 + \frac{L\alpha_k^2}{2}\|f'(\mathbf{x}_k)\|_2^2 =$$

$$f(\mathbf{x}_k) - \left(\alpha_k - \frac{L\alpha_k^2}{2}\right)\|f'(\mathbf{x}_k)\|_2^2$$

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Convergence to a stationary point

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- $f(\mathbf{x}_k) - f(\mathbf{x}_{k+1}) \geq \frac{1}{2L}\|f'(\mathbf{x}_k)\|_2^2$
- $\frac{1}{2L}\sum_{k=0}^{T} \|f'(\mathbf{x}_k)\|_2^2 \leq f(\mathbf{x}_0) - f(\mathbf{x}_{T+1}) \leq f(\mathbf{x}_0) - f^*$

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- f is bounded below, $\|f'(\mathbf{x}_k)\|_2 \to 0, \; k \to \infty$

Convergence: convex function

Theorem

Let f be convex function with Lipschitz gradient and $\alpha = \frac{1}{L}$, then gradient descent converges like

$$f(\mathbf{x}_{k+1}) - f^* \leq \frac{2L\|\mathbf{x} - \mathbf{x}_0\|_2^2}{k+4} = \mathcal{O}(1/k)$$

Convergence: strongly convex case

- As a consequence of strongly convexity

$$f(\mathbf{z}) \geq f(\mathbf{x}_k) + \langle f'(\mathbf{x}_k), \mathbf{z} - \mathbf{x}_k \rangle + \frac{\mu}{2}\|\mathbf{z} - \mathbf{x}_k\|_2^2$$

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- Minimize both sides by $\mathbf{z}$

$$f(\mathbf{x}^*) \geq f(\mathbf{x}_k) - \frac{1}{2\mu} \|f'(\mathbf{x}_k)\|_2^2, \quad \|f'(\mathbf{x}_k)\|_2^2 \geq 2\mu(f(\mathbf{x}_k) - f^*)$$

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- Remember that $\alpha_k \equiv \frac{1}{L}$

$$f^* \leq f(\mathbf{x}_{k+1}) \leq f(\mathbf{x}_k) - \frac{1}{2L} \|f'(\mathbf{x}_k)\|_2^2$$

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$$f^* \leq f(\mathbf{x}_{k+1}) \leq f(\mathbf{x}_k) - \frac{1}{2L} \|f'(\mathbf{x}_k)\|_2^2$$

- And finally get linear convergence

$$f(\mathbf{x}_{k+1}) - f^* \leq \left(1 - \frac{1}{\kappa}\right) (f(\mathbf{x}_k) - f^*)$$

Theorem about strongly convex functions

Theorem

Let f be L-smooth and μ-strongly convex, $\alpha_k = \frac{2}{\mu+L}$, then gradient descent converges like

$$f(\mathbf{x}_k) - f^* \leq \frac{L}{2}\left(\frac{L-\mu}{L+\mu}\right)^{2k} \|\mathbf{x}_0 - \mathbf{x}^*\|_2^2$$

What affect the linear convergence?

$$q^* = \frac{L-\mu}{L+\mu} = \frac{L/\mu - 1}{L/\mu + 1} = \frac{\kappa - 1}{\kappa + 1},$$

where κ is an estimate of condition number of $f''(\mathbf{x})$.

What affect the linear convergence?

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where κ is an estimate of condition number of $f''(\mathbf{x})$.

- If $\kappa \gg 1$, $q^* \to 1 \Rightarrow$, we have very slow convergence. For example, if $\kappa = 100$, then $q^* \approx 0.98$

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- If $\kappa \gg 1$, $q^* \to 1 \Rightarrow$, we have very slow convergence. For example, if $\kappa = 100$, then $q^* \approx 0.98$
- If $\kappa \simeq 1$, $q^* \to 0 \Rightarrow$ implies acceleration of convergence. For example, if $\kappa = 4$, then $q^* = 0.6$

Can we do better?

What do we know by now?

- Gradient descent converges like $\mathcal{O}(1/k)$ for convex L-smooth functions
- Gradient descent converges linearly with factor $q = \frac{\kappa-1}{\kappa+1}$ for strongly convex L-smooth functions

Q: do methods with faster convergence exist and how can we derive them?

Take home message

- General scheme of numerical optimization methods
- Convergence speed
- Gradient descent
- Properties and convergence theorems