Optimization methods
Lecture 6: Introduction to numerical optimization methods. Gradient descent

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Brief reminder of the previous lecture

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

Problem statement

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

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

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

Reminder of analytical results

First order necessary condition

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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

```
def GeneralScheme(x, epsilon):
    while StopCriterion(x) > epsilon:
        OracleResponse = RequestOracle(x)
        UpdateInformation(I, x, OracleResponse)
        x = NextPoint(I, x)
    return x
```

Questions

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3. What is information model?
4. How the next point is computed?

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4. Duality gap

$$f_k - g(\boldsymbol{\lambda}_k, \boldsymbol{\mu}_k) \leq \varepsilon$$

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Main idea

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OOP analogue

- oracle is a virtual method of base class
- every particular problem is a derived class
- oracle is defined for every problem according to the general definition in the base class

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Black-box concept

1. Only oracle responses are available for numerical method
2. Oracle responses are local

Information about the problem

1. Every oracle response gives local information about function behavior at current point
2. We can aggregate all oracle responses and update information about global properties of the objective function:
   - curvature
   - descent direction
   - etc

How to update point

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Trust-region method

1. Find α-neighborhood of $\mathbf{x}_k$
2. Construct in this neighborhood the simple model of the objective function
3. Find a direction $\mathbf{h}_k$, that is minimized the model and does not violate constraints

How to compare optimization methods?

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

1. Complexity
   - analytical: number of query to oracle to solve the problem with tolerance ε
   - arithmetic: total number of operations to solve the problem with tolerance ε
2. Convergence speed
3. Experiments

Convergence speed

1. Sublinear

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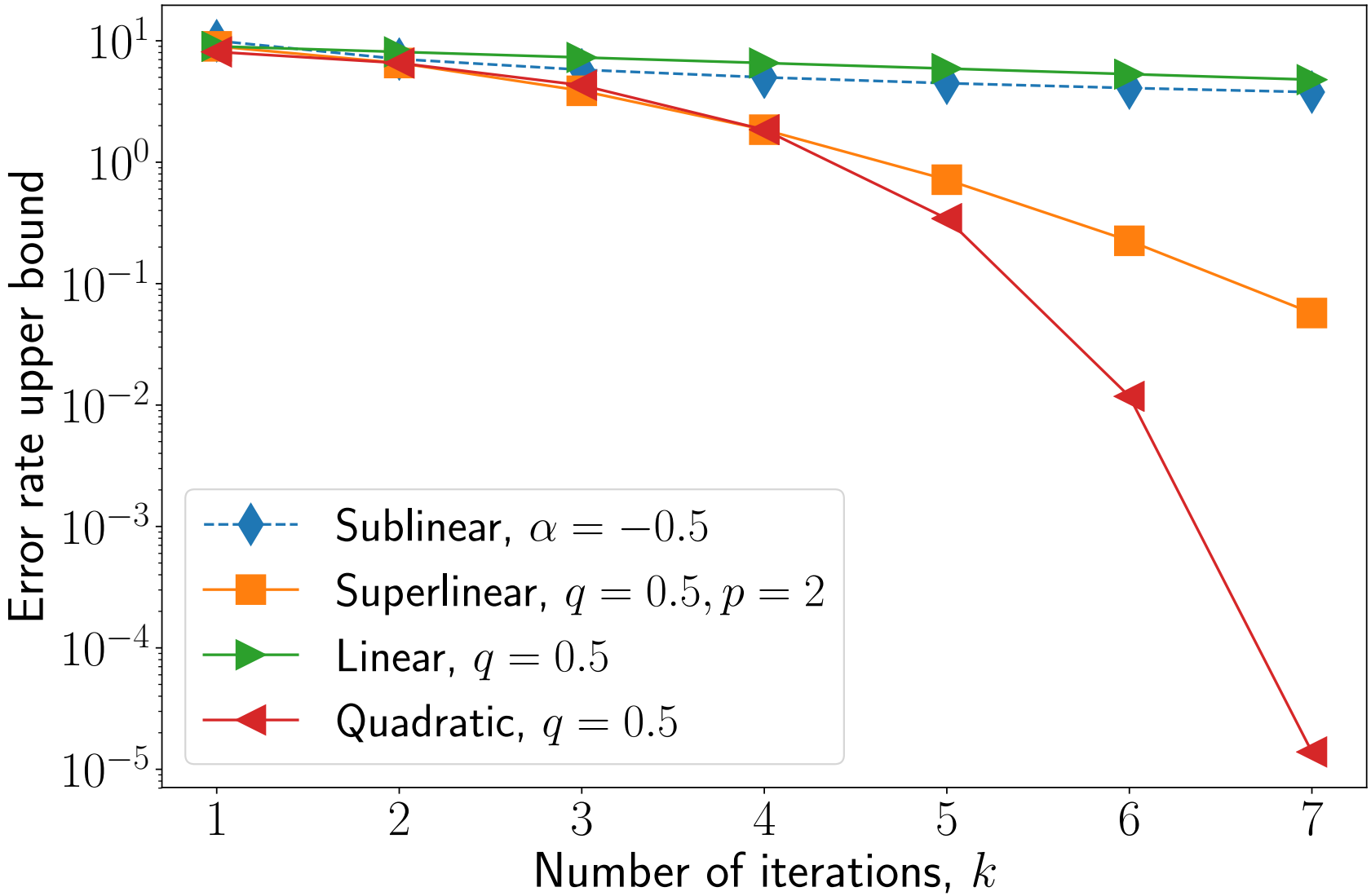
4. Quadratic

$$\|\mathbf{x}_{k+1} - \mathbf{x}^*\|_2 \leq C\|\mathbf{x}_k - \mathbf{x}^*\|_2^2, \qquad \text{or} \qquad \|\mathbf{x}_{k+1} - \mathbf{x}^*\|_2 \leq Cq^{2^k}$$

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

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

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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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 $\sum_{k=1}^{\infty} \alpha_k = \infty$, 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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- $\alpha_k^* = \arg\max_{\alpha_k} \left(\alpha_k - \frac{L\alpha_k^2}{2}\right) = \frac{1}{L}$
- $f(\mathbf{x}_k) - f(\mathbf{x}_{k+1}) \geq \frac{1}{2L}\|f'(\mathbf{x}_k)\|_2^2$

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

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

What affect the linear convergence?

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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