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FUNDAMENTALS OF OPTIMIZATION

Unconstrained convex optimization

CONTENT

- Unconstrained optimization problems
- Descent method
- Gradient descent method
- Newton method
- Subgradient method

Unconstrained convex optimization

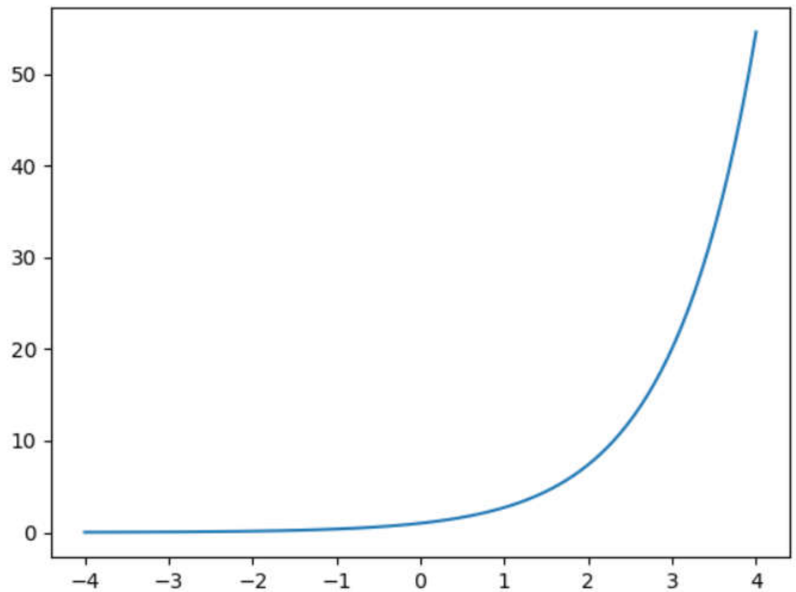
- Unconstrained, smooth convex optimization problem:

$$\min f(x)$$

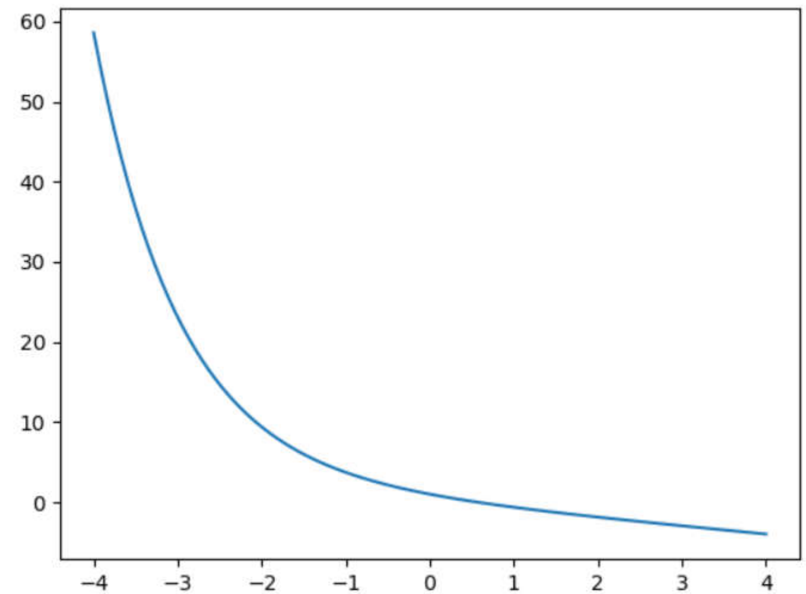
  - $f: R^n \rightarrow R$ is convex and twice differentiable
  - ***dom*** $f = R$: no constraint
  - Assumption: the problem is solvable with $f^* = \min_x f(x)$ and $x^* = \text{argMin}_x f(x)$
- To find x, solve equation $\nabla f(x^*) = 0$: not easy to solve analytically
- Iterative scheme is preferred: compute minimizing sequence $x^{(0)}, x^{(1)}, \ldots$ s.t. $f(x^{(k)}) \rightarrow f(x^*)$ as $k \rightarrow \infty$
- The algorithm stops at some point $x^{(k)}$ when the error is within acceptable tolerance: $f(x^{(k)}) - f^* \leq \varepsilon$

Local minimizer

- x^* is a local minimizer for f: $R^n \rightarrow R$ if $f(x^*) \leq f(x)$ for $||x^*-x|| \leq \varepsilon$ ($\varepsilon > 0$ is a constant)
- x^* is a global minimizer for f: $R^n \rightarrow R$ if $f(x^*) \leq f(x)$ for all $x \in R^n$



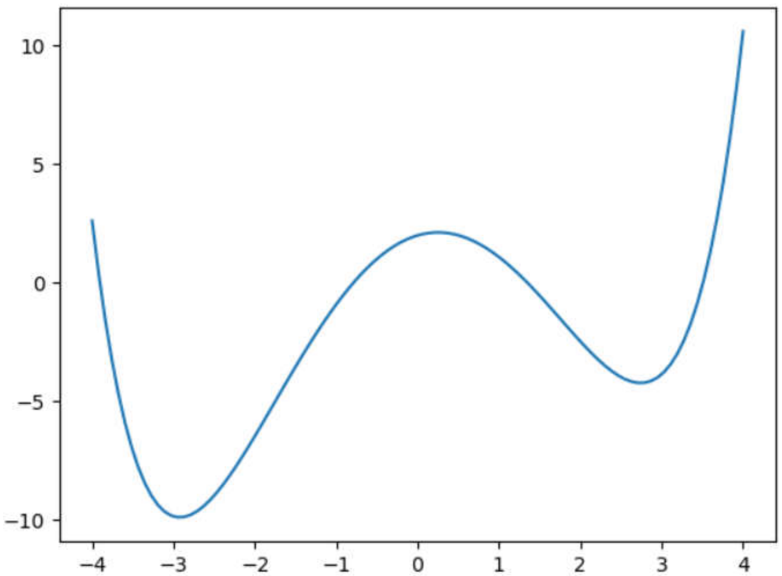
$f(x) = e^x$ has no minimizer



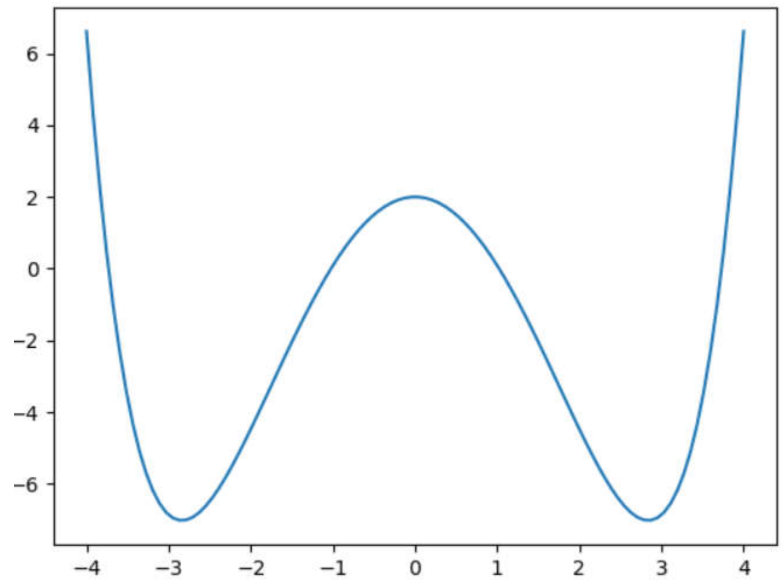
$f(x) = -x + e^{-x}$ has no minimizer

Local minimizer

- x^* is a local minimizer for f: $R^n \rightarrow R$ if $f(x^*) \le f(x)$ for $||x^*-x|| \le \varepsilon$ ($\varepsilon > 0$ is a constant)
- x^* is a global minimizer for f: $R^n \rightarrow R$ if $f(x^*) \le f(x)$ for all $x \in R^n$



$f(x) = e^x + e^{-x} - 3x^2 + x$ has one local minimizer and one global minimizer



$f(x) = e^x + e^{-x} - 3x^2$ has two global minimizers

Local minimizer

- **Theorem** (Necessary condition for local minimum) If x^* is a local minimizer for f: $R^n \rightarrow R$, then $\nabla f(x^*) = 0$ (x^* is also called *stationary point* for f)

Local minimizer

Example

- $f(x,y) = x^2 + y^2 - 2xy + x$
- $\nabla f(x) = \begin{pmatrix} 2x - 2y + 1 \\ 2y - 2x \end{pmatrix} = 0$ has no solution

→ there is no minimizer of $f(x,y)$

Local minimizer

- **Theorem** (Sufficient condition for a local minimum) Assume x^* is a stationary point and that $\nabla^2 f(x^*)$ is positive definite, then x^* is a local minimizer

$$\nabla^2 f(x) = \begin{pmatrix} \frac{\partial^2 f(x)}{\partial x_1 \partial x_1} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial xn} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial x_2 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial xn} \\ \cdots & & & \\ \frac{\partial^2 f(x)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x)}{\partial xn \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial xn \partial xn} \end{pmatrix}$$

Local minimizer

- Matrix A_{nxn} is called positive definite if

$$A^i = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,i} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,i} \\ & \cdots\cdots & & \\ a_{i,1} \;..\; & a_{i,2} & \cdots & a_{i,i} \end{pmatrix}, \quad \det(A^i) > 0,\ i = 1,\ldots,n$$

Local minimizer

- **Example** $f(x,y) = e^{x^2+y^2}$

$\nabla f(x,y) = \begin{pmatrix} 2xe^{x^2+y^2} \\ 2ye^{x^2+y^2} \end{pmatrix}$ = 0 has unique solution $x^* = (0,0)$

$\nabla^2 f(0,0) = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$ > 0 → (0,0) is a minimizer of f

Local minimizer

- **Example** Find a minimizer of $f(x,y) = x^2 + y^2 - 2xy - x$?

Descent method

Determine starting point $x^{(0)} \in R^n$;

$k \leftarrow 0$;

while(stop condition not reach){

  Determine a search direction $p_k \in R^n$;

  Determine a step size $\alpha_k > 0$ s.t. $f(x^{(k)} + \alpha_k p_k) < f(x^{(k)})$;

  $x^{(k+1)} \leftarrow x^{(k)} + \alpha_k p_k$;

  $k \leftarrow k+1$;

}

Stop condition may be

- $|| \nabla f(x^k)|| \le \varepsilon$
- $||x^{k+1} - x^k|| \le \varepsilon$
- $k > K$ (maximum number of iterations)

Gradient descent method

- Gradient descent schema

$$x^{(k)} = x^{(k-1)} - \alpha_k \nabla f(x^{(k-1)})$$

init $x^{(0)}$;

$k = 1$;

while stop condition not reach{

  specify constant α_k;

  $x^{(k)} = x^{(k-1)} - \alpha_k \nabla f(x^{(k-1)})$;

  $k = k + 1$;

}

- α_k might be specified in such a way that $f(x^{(k-1)} - \alpha_k \nabla f(x^{(k-1)}))$ is minimized: $\frac{\partial f}{\partial \alpha_k} = 0$

Gradient descent method

Example $f(x_1,x_2,x_3) = x_1^2 + x_2^2 + x_3^2 - x_1x_2 - x_2x_3 + x_1 + x_3 \rightarrow \min$?

Newton method

- Second-order Taylor approximation g of f at x is

$$f(x+h) \approx g(x+h) = f(x) + h\nabla f(x) + \frac{1}{2}h^2\ \nabla^2 f(x)$$

- Which is a convex quadratic function of h
- g(x+h) is minimized when $\frac{\partial g}{\partial h} = 0 \rightarrow h = -\nabla^2 f(x)^{-1}\nabla f(x)$

Newton method

Generate $x^{(0)}$; // starting point

$k = 0$;

while stop condition not reach{

  $x^{(k+1)} \leftarrow x^{(k)} - \nabla^2 f(x^{(k)})^{-1} \nabla f(x^{(k)})$;

  $k = k + 1$;

}

Newton method

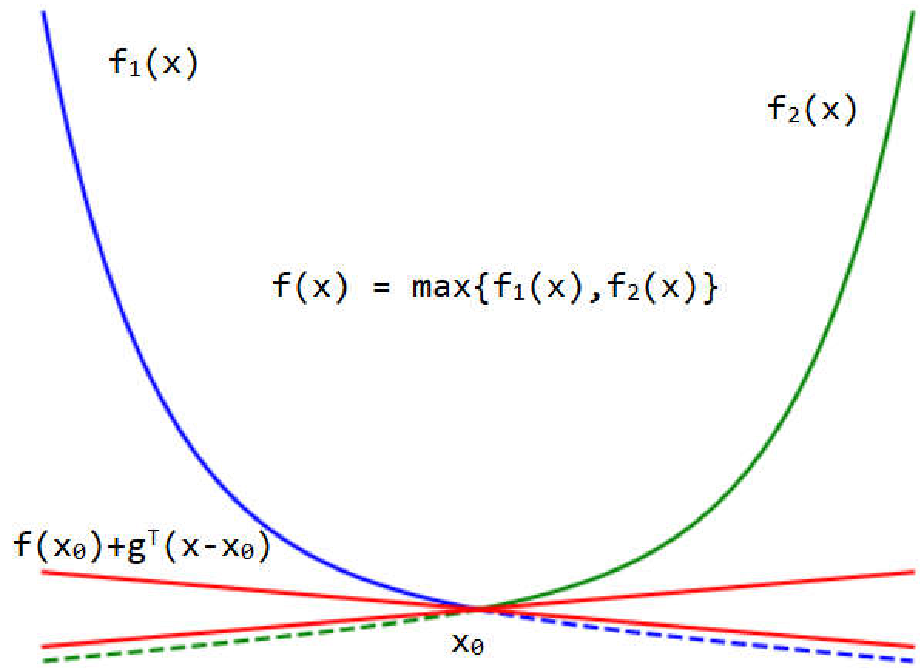
Step	x	y	f
Initialization	[0,0,0]	[1, 1, 1]	0
Step 1	[-1., -1., -1.]	[-2.46519033e-32 1.11022302e-16 2.22044605e-16]	-1.0000000000000004
Step 2	[-1., -1., -1.]	[0., 0., 0.]	-1

Subgradient method

- For minimize nondifferentiable convex function
- Subgradient method is not a descent method: the function value can increase

Subgradient method

- Subgradient of *f* at *x*
  - Any vector *g* such that $f(x') \geq f(x) + g^T(x'-x)$
  - If f is differentiable, only possible choice is $g^{(k)} = \nabla f(x^{(k)})$, → the subgradient method reduces to the gradient method



Basic subgradient method

$$x^{(k+1)} = x^{(k)} - \alpha_k g^{(k)}$$

- $x^{(k)}$: is at the k^{th} iteration
- $g^{(k)}$: any subgradient of f at $x^{(k)}$
- $\alpha_k > 0$ is the k^{th} step size
- Note: subgradient is not a descent method, thus $f_{best}^{(k)} = \min\{f(x^{(1)}), f(x^{(2)}), \ldots, f(x^{(k)})\}$

Convergence proof

- Notations: x^* is a minimizer of f
- Assumptions
  - Norm of the subgradients is bounded (with a constant G): $||g^{(k)}||_2 \leq G$ (this is the case if, for example, f satisfies the Lipschitz condition $|f(u) - f(v)| \leq G||u\text{-}v||_2$)
  - $||x^{(1)} - x^*||_2^2 \leq R$ (with a known constant R)
- We have $||x^{(k+1)} - x^*||_2^2 = ||x^{(k)} - \alpha_k g^{(k)} - x^*||_2^2$

$= ||x^{(k)} - x^*||_2^2 - 2\alpha_k g^{(k)T}(x^{(k)} - x^*) + \alpha_k^2||g^{(k)}||_2^2$

$\leq ||x^{(k)} - x^*||_2^2 - 2\alpha_k(f(x^{(k)}) - f(x^*)) + \alpha_k^2||g^{(k)}||_2^2$ (due to the fact that $f(x^*) \geq f(x^{(k)}) + g^{(k)T}(x^* - x^{(k)})$) (1)

Convergence proof

- Apply the inequality (1) recursively, we have

$||x^{(k+1)} - x^*||_2^2 \leq ||x^{(1)} - x^*||_2^2 - 2\sum_{i=1}^{k} \alpha_i(f(x^{(i)}) - f^*) + \sum_{i=1}^{k} \alpha_i^2 ||g^{(i)}||_2^2$ (where $f^* = f(x^*)$)

$\rightarrow 2\sum_{i=1}^{k} \alpha_i(f(x^{(i)}) - f^*) \leq R^2 + \sum_{i=1}^{k} \alpha_i^2 ||g^{(i)}||_2^2$

$\rightarrow R^2 + \sum_{i=1}^{k} \alpha_i^2 ||g^{(i)}||_2^2 \geq 2\sum_{i=1}^{k} \alpha_i(f(x^{(i)}) - f^*) \geq 2(\sum_{i=1}^{k} \alpha_i) \min_{i=1,\dots,k}(f(x^{(i)}) - f^*) = 2\sum_{i=1}^{k} \alpha_i(f_{best}^{(k)} - f^*)$

$$\rightarrow f_{best}^{(k)} - f^* \leq \frac{R^2 + \sum_{i=1}^{k} \alpha_i^2 ||g^{(i)}||_2^2}{2\sum_{i=1}^{k} \alpha_i} \qquad (2)$$

Convergence proof

- Different cases
  - Constant step size $\alpha_k = \alpha$

→ $f_{best}^{(k)} - f^* \leq \dfrac{R^2 + G^2\alpha^2 k}{2\alpha k}$

→ $f_{best}^{(k)} - f^*$ converges to $G^2\alpha/2$ when $k \to \infty$

  - Constant step length $\alpha_k = \gamma / ||g^{(k)}||_2$

→ $f_{best}^{(k)} - f^* \leq \dfrac{R^2 + \gamma^2 k}{2\gamma k/G}$

→ $f_{best}^{(k)} - f^*$ converges to $G\gamma/2$ when $k \to \infty$

Convergence proof

- Different cases
  - Square summable but not summable

$||\alpha||_2^2 = \sum_{i=1}^{\infty} \alpha_i^2 < \infty$ and $\sum_{i=1}^{\infty} \alpha_i = \infty$

$$\rightarrow f_{best}^{(k)} - f^* \leq \frac{R^2 + G^2||\alpha||_2^2}{2\sum_{i=1}^{k} \alpha_i}$$

$\rightarrow f_{best}^{(k)} - f^*$ converges to 0 as $k \rightarrow \infty$

Example

$$\text{minimize } f(x) = \max_{i=1,\ldots,m}(a_i^T x + b_i)$$

- Finding subgradient: given x, the index j for which

$$a_j^T x + b_j = \max_{i=1,\ldots,m}(a_i^T x + b_i)$$

→ subgradient at x is $g = a_j$

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Thank you for your attentions!