Numerical Optimization

Unit 2: Multivariable optimization problems

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Partial derivative of a two variable function

- Given a two variable function $f(x_1, x_2)$.
- The partial derivative of f with respect to x_i is

$$\begin{cases} \dfrac{\partial f}{\partial x_1} = \lim_{h \to 0} \dfrac{f(x_1 + h, x_2) - f(x_1, x_2)}{h} \\ \\ \dfrac{\partial f}{\partial x_2} = \lim_{h \to 0} \dfrac{f(x_1, x_2 + h) - f(x_1, x_2)}{h} \end{cases}$$

- The meaning of partial derivative: let $F(x_1) = f(x_1, v)$ and $G(x_2) = f(u, x_2)$,

$$\frac{\partial f}{\partial x_1}(x_1, v) = F'(x_1).$$

$$\frac{\partial f}{\partial x_2}(u, x_2) = G'(x_2).$$

Gradient

Definition

The gradient of a function $f : \mathbb{R}^n \to \mathbb{R}$ is a **vector** in $\mathbb{R}^n$ defined as

$$\vec{g} = \nabla f(\vec{x}) = \begin{pmatrix} \partial f / \partial x_1 \\ \vdots \\ \partial f / \partial x_n \end{pmatrix}, \text{where } \vec{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

Directional derivative

Definition

The directional derivative of a function $f : \mathbb{R}^n \to \mathbb{R}$ in the direction $\vec{p}$ is defined as

$$D(f(\vec{x}), \vec{p}) = lim_{h \to 0} \frac{f(\vec{x} + h\vec{p}) - f(x)}{h}$$

.

Remark

If $f : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable in a neighborhood of $\vec{x}$,

$$D(f(\vec{x}), \vec{p}) = \nabla f(x)^T \vec{p},$$

for any vector $\vec{p}$.

The descent directions

- A direction $\vec{p}$ is called a **descent direction** of $f(\vec{x})$ at $\vec{x}$ if $D(f(\vec{x_0}), \vec{p}) < 0$.
- If f is smooth enough, $\vec{p}$ is a descent direction if $f(\vec{x}_0)^T \vec{p} < 0$.
- Which direction $\vec{p}$ makes $f(\vec{x_0} + \vec{p})$ decreasing most?
    - Mean Value theorem

$$f(\vec{x_0} + \vec{p}) = f(\vec{x_0}) + \nabla f(\vec{x_0} + \alpha \vec{p})^\top \vec{p}$$

    - $\vec{p} = -\nabla f(\vec{x_0})$ is called the steepest descent direction of $f(x)$ at x_0.

$$\begin{aligned} f(\vec{x_0} + \vec{p}) &= f(\vec{x_0}) + \nabla f(\vec{x_0} + \alpha \vec{p})^\top \vec{p} \\ &\approx f(\vec{x_0}) - \nabla f(\vec{x_0})^T \nabla f(\vec{x_0}) \end{aligned}$$

The steepest descent algorithm

The steepest descent algorithm

For $k = 1, 2, \ldots$ until convergence
  Compute $\vec{p_k} = -\nabla f(x_k)$
  Find $\alpha_k \in (0, 1)$ s,t, $F(\alpha_k) = f(\vec{x_k} + \alpha_k \vec{p_k})$ is minimized.
  $\vec{x_{k+1}} = \vec{x_k} + \alpha_k \vec{p_k}$

- You can use any single variable optimization techniques to compute α_k.
- If $F(\alpha_k) = f(\vec{x_k} + \alpha_k \vec{p_k})$ is a quadratic function, α_k has a theoretical formula. (will be derived in next slides.)
- If $F(\alpha_k) = f(\vec{x_k} + \alpha_k \vec{p_k})$ is more than a quadratic function, we may approximate it by a quadratic model and use the formula to solve α_k.
- Higher order polynomial approximation will be mentioned in the line search algorithm.

Quadratic model

- If $f(\vec{x})$ is a quadratic function, we can write it as

$$f(x,y) = ax^2 + bxy + cy^2 + dx + ey + f(0,0).$$

- If f is smooth, the derivatives of f are

$$\frac{\partial f}{\partial x} = 2ax + by + d, \quad \frac{\partial f}{\partial y} = 2cy + bx + e$$

$$\frac{\partial^2 f}{\partial x^2} = 2a, \quad \frac{\partial^2 f}{\partial y^2} = 2c, \quad \frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x} = b.$$

- Let $\vec{x} = \begin{pmatrix} x \\ y \end{pmatrix}$, $f(\vec{x})$ can be expressed as

$$f(\vec{x}) = \frac{1}{2}\vec{x}^{\,T} \begin{pmatrix} 2a & b \\ b & 2c \end{pmatrix} \vec{x} + \vec{x}^{\,T} \begin{pmatrix} d \\ e \end{pmatrix} + f(\vec{0}).$$

Gradient and Hessian

- The gradient of f, as defined before, is

$$g(\vec{x}) = \nabla f(\vec{x}) = \begin{pmatrix} \dfrac{\partial f}{\partial x} \\ \dfrac{\partial f}{\partial y} \end{pmatrix} = \begin{pmatrix} 2a & b \\ b & 2c \end{pmatrix} \vec{x} + \begin{pmatrix} d \\ e \end{pmatrix}$$

- The second derivative, which is a matrix called **Hessian**, is

$$\nabla^2 f(\vec{x}) = H(\vec{x}) = \begin{pmatrix} \dfrac{\partial f}{\partial x^2} & \dfrac{\partial f}{\partial x \partial y} \\ \dfrac{\partial f}{\partial y \partial x} & \dfrac{\partial f}{\partial y^2} \end{pmatrix} = \begin{pmatrix} 2a & b \\ b & 2c \end{pmatrix}$$

- Therefore, $f(\vec{x}) = 1/2\vec{x}^{\,T} H(\vec{0})\vec{x} + g(\vec{0})^T \vec{x} + f(\vec{0})$,

$$\nabla f(\vec{x}) = H\vec{x} + \vec{g}, \text{ and } \nabla^2 f = H$$

- In the following lectures, we assume H is symmetric. Thus, $H = H^T$.

Optimal α_k for quadratic model

- We denote $H_k = H(\vec{x}_k)$, $\vec{g_k} = \vec{g}(\vec{x}_k)$, and $f_k = f(\vec{x}_k)$.
- Also, $H = H(\vec{0})$, $\vec{g} = \vec{g}(\vec{0})$, and $f = f(\vec{0})$.

$$
\begin{aligned}
F(\alpha) &= f(\vec{x}_k + \alpha\vec{p}_k) \\
&= \frac{1}{2}(\vec{x}_k + \alpha\vec{p}_k)^T H(\vec{x}_k + \alpha\vec{p}_k) + g^T(\vec{x}_k + \alpha\vec{p}_k) + f(\vec{0}) \\
&= \frac{1}{2}\vec{x}_k{}^T H\vec{x}_k + g^T\vec{x_k} + f(\vec{0}) + \alpha(H\vec{x}_k + \vec{g})^T\vec{p}_k + \frac{\alpha^2}{2}\vec{p}_k{}^T H\vec{p}_k \\
&= f_k + \alpha\vec{g}_k^T\vec{p}_k + \frac{\alpha^2}{2}\vec{p}_k{}^T H\vec{p}_k \\
F'(\alpha) &= \vec{g}_k{}^T\vec{p}_k + \alpha\vec{p}_k{}^T H\vec{p}_k
\end{aligned}
$$

The optimal solution of α_k is at $F'(\alpha) = 0$, which is $\alpha_k = \dfrac{-\vec{g}_k{}^T\vec{p}_k}{\vec{p}_k{}^T H\vec{p}_k}$

Optimal condition

Theorem (Necessary and sufficient condition of optimality)

- *Let $f : \mathbb{R}^n \to \mathbb{R}$ be continuously differentiable in D. If $\vec{x}^* \in D$ is a local minimizer, $\nabla f(\vec{x}^*) = 0$ and $\nabla^2 f(\vec{x})$ is* **positive semidefinite**.
- *If $\nabla f(\vec{x}^*) = 0$ and $\nabla^2 f(\vec{x})$ is* **positive definite**, *then $\vec{x}^*$ is a local minimizer.*

Definition

- A matrix H is called **positive definite** if for any nonzero vector $\vec{v} \in \mathbb{R}^n$, $\vec{v}^\top H \vec{v} > 0$.
- H is called **positive semidefinite** if $\vec{v}^\top H \vec{v} \geq 0$ for all $\vec{v} \in \mathbb{R}^n$.
- H is **negative definite** or **negative semidefinite** if $-H$ is positive definite or positive semidefinite.
- H is **indefinite** if it is neither positive semidefinite nor negative semidefinite.

Convergence of the steepest descent method

Theorem (Convergence theorem of the steepest descent method)

If the steepest descent method converges to a local minimizer $\vec{x}^*$, where $\nabla^2 f(\vec{x})$ is positive definite, and $e_{\max}$ and $e_{\min}$ are the largest and the smallest eigenvalue of $\nabla^2 f(\vec{x})$, then

$$\lim_{k\to\infty} \frac{\|\vec{x}_{k+1} - \vec{x}^*\|}{\|\vec{x}_k - \vec{x}^*\|} \leq \left(\frac{e_{\max} - e_{\min}}{e_{\max} + e_{\min}}\right)$$

Definition

For a scalar λ and an unit vector v, (λ, v) is an eigenpair of of a matrix H if $Hv = \lambda v$. The scalar λ is called an eigenvalue of H, and v is called an eigenvector.

Newton's method

- We use the quadratic model to find the step length α_k. Can we use the quadratic model to find the search direction $\vec{p}_k$?
- Yes, we can. Recall the quadratic model (now $\vec{p}$ is the variable.)

$$f(\vec{x}_k + \vec{p}) \approx \frac{1}{2}\vec{p}^{\,T} H_k \vec{p} + \vec{p}^{\,T} \vec{g}_k + f_k$$

- Compute the gradient $\nabla_{\vec{p}} f(\vec{x}_k + \vec{p}) = H_k \vec{p} + \vec{g}_k$
- The solution of $\nabla_{\vec{p}} f(\vec{x}_k + \vec{p}) = 0$ is $\vec{p}_k = -H_k^{-1} \vec{g}_k$.
- Newton's method uses p_k as the search direction

Newton's method

1. Given an initial guess $\vec{x}_0$
2. For $k = 0, 1, 2, \ldots$ until converge

$$\vec{x}_{k+1} = \vec{x}_k - H_k^{-1} \vec{g}_k.$$

Descent direction

- The direction $p_k = -H_k^{-1} g_k$ is called Newton's direction
- Is p_k a descent direction? (what's the definition of descent directions?)
- We only need to check if $\vec{g}_k{}^T \vec{p}_k < 0$.

$$\vec{g}_k^T \vec{p}_k = -\vec{g}_k^T H_k^{-1} \vec{g}_k.$$

  Thus, $\vec{p}_k$ is a descent direction if H^{-1} is positive definite.
- For a symmetric matrix H, the following conditions are equivalent

- H is positive definite.
- H^{-1} is positive definite.
- All the eigenvalues of H are positive.

Some properties of eigenvalues/eigenvectors

- A symmetric matrix H, of order n has n real eigenvalues and n real and linearly independent (orthogonal) eigenvectors

$$Hv_1 = \lambda_1 v_1, \quad Hv_2 = \lambda_2 v_2, \quad ..., Hv_n = \lambda_n v_n$$

- Let $V = [v_1 \;\; v_2 \; ... \; v_n]$, $\Lambda = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix}$, $HV = V\Lambda$.

- If $\lambda_1, \; \lambda_2, ..., \lambda_n$ are nonzero, since $H = V\Lambda V^{-1}$,

$$H^{-1} = V\Lambda^{-1}V^{-1}, \;\; \Lambda^{-1} = \begin{bmatrix} 1/\lambda_1 & & & \\ & 1/\lambda_2 & & \\ & & \ddots & \\ & & & 1/\lambda_n \end{bmatrix}$$

The eigenvalues of H^{-1} are $\dfrac{1}{\lambda_1}, \; \dfrac{1}{\lambda_2}, ..., \dfrac{1}{\lambda_n}$.

How to solve $H\vec{p} = -\vec{g}$?

- For a symmetric positive definite matrix H, $H\vec{p} = -\vec{g}$ can be solved by Cholesky decomposition, which is similar to LU decomposition, but is only half computational cost of LU decomposition.
- Let $H = \begin{bmatrix} h_{11} & h_{12} & h_{13} \\ h_{21} & h_{22} & h_{23} \\ h_{31} & h_{32} & h_{33} \end{bmatrix}$, where $h_{12} = h_{21},\ h_{13} = h_{31},\ h_{23} = h_{32}$.

  Cholesky decomposition makes $H = LL^T$, where L is a lower triangular matrix, $L = \begin{bmatrix} \ell_{11} & & \\ \ell_{21} & \ell_{22} & \\ \ell_{31} & \ell_{32} & \ell_{33} \end{bmatrix}$
- Using Cholesky decomposition, $H\vec{p} = -\vec{g}$ can be solved by
  1. Compute $H = LL^T$
  2. $\vec{p} = -(L^T)^{-1}L^{-1}\vec{g}$
- In Matlab, use $p = -H \setminus g$. Don't use $inv(H)$.

The Cholesky decomposition

For $i = 1, 2, ..., n$
$$\ell_{ii} = \sqrt{h_{ii}}$$
For $j = i+1, i+2, ..., n$
$$\ell_{ji} = \frac{h_{ji}}{\ell_{ii}}$$
For $k = i+1, i+2, ..., j$
$$h_{jk} = h_{jk} - \ell_{ji}\ell_{ki}$$

$$\begin{bmatrix} h_{11} & h_{12} & h_{13} \\ h_{21} & h_{22} & h_{23} \\ h_{31} & h_{32} & h_{33} \end{bmatrix} = LL^T = \begin{bmatrix} \ell_{11}^2 & \ell_{11}\ell_{21} & \ell_{11}\ell_{31} \\ \ell_{11}\ell_{21} & \ell_{21}^2 + \ell_{22}^2 & \ell_{21}\ell_{31} + \ell_{22}\ell_{32} \\ \ell_{11}\ell_{33} & \ell_{21}\ell_{31} + \ell_{22}\ell_{32} & \ell_{31}^2 + \ell_{32}^2 + \ell_{33}^2 \end{bmatrix}$$

$$\begin{aligned} \ell_{11} &= \sqrt{h_{11}} \\ \ell_{21} &= h_{21}/\ell_{11} \\ \ell_{31} &= h_{31}/\ell_{11} \end{aligned} \qquad \begin{aligned} h_{22}^{(2)} &= h_{22} - \ell_{21}\ell_{21} \\ h_{32}^{(2)} &= h_{32} - \ell_{21}\ell_{31} \\ h_{33}^{(2)} &= h_{33} - \ell_{31}\ell_{31} \end{aligned} \qquad \begin{aligned} \ell_{22} &= \sqrt{h_{22}^{(2)}} \\ \ell_{32} &= h_{32}^{(2)}/\ell_{22} \\ \ell_{33} &= \sqrt{h_{33}^{(2)} - \ell_{32}\ell_{32}} \end{aligned}$$

Convergence of Newton's method

Theorem

Suppose f is twice differentiable. $\nabla^2 f$ is continuous in a neighborhood of $\vec{x}^*$ and $\nabla^2 f(\vec{x}^*)$ is positive definite, and if $\vec{x}_0$ is sufficiently close to $\vec{x}^*$, the sequence converges to $\vec{x}^*$ quadratically.

Three problems of Newton's method

1. H may not be positive definite $\Rightarrow$ Modified Newton's method + Line search.
2. H is expensive to compute $\Rightarrow$ Quasi-Newton.
3. H^{-1} is expensive to compute $\Rightarrow$ Conjugate gradient.