MATH529 – Fundamentals of Optimization
Unconstrained Optimization III

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Recap

Optimization via Calculus

Definition

Let A be an $n \times n$ symmetric matrix and $Q_A(\mathbf{x}) = \mathbf{x}^T A\mathbf{x}$ its associated quadratic form. Then A and $Q_A(\mathbf{x})$ are called:

- positive definite if $Q_A(\mathbf{x}) > 0$ for all $\mathbf{x} \in \mathbb{R}$, except $\mathbf{x} = \mathbf{0}$.
- positive semidefinite if $Q_A(\mathbf{x}) \geq 0$ for all $\mathbf{x} \in \mathbb{R}$.
- negative definite if $Q_A(\mathbf{x}) < 0$ for all $\mathbf{x} \in \mathbb{R}$, except $\mathbf{x} = \mathbf{0}$.
- negative semidefinite if $Q_A(\mathbf{x}) \leq 0$ for all $\mathbf{x} \in \mathbb{R}$.
- indefinite if $Q_A(\mathbf{x}) > 0$ for some $\mathbf{x} \in \mathbb{R}$ and $Q_A(\mathbf{x}) < 0$ for other $\mathbf{x} \in \mathbb{R}$.

Optimization via Calculus

In view of this definition, we can say that

Theorem

Suppose that $\mathbf{x}^\star$ is a stationary point of a function $f(\mathbf{x})$ with continuous first and second partial derivatives on $\mathbb{R}^n$. Then:

- $\mathbf{x}^\star$ *is a* **global minimizer** *of $f(\mathbf{x})$ if $Hf(\mathbf{x})$ is positive semidefinite on $\mathbb{R}^n$;*
- $\mathbf{x}^\star$ *is a* **strict global minimizer** *of $f(\mathbf{x})$ if $Hf(\mathbf{x})$ is positive definite on $\mathbb{R}^n$;*
- $\mathbf{x}^\star$ *is a* **strict local minimizer** *of $f(\mathbf{x})$ if $Hf(\mathbf{x}^\star)$ is positive definite;*
- $\mathbf{x}^\star$ *is a* **saddle point** *of $f(\mathbf{x})$ if $Hf(\mathbf{x}^\star)$ is indefinite;*

Optimization via Calculus

Example

$f(x, y) = (1 - x)^2 + 100(y - x^2)^2$

Optimization via Calculus

Example

$f(x, y) = \frac{x^2}{2} + \frac{y^2}{2} + xy + 8$

Example

$f(x, y) = x^4 - y^4$

There are two methods to determine whether a matrix is positive (negative) (semi)definite:

- Using determinants
- Using eigenvalues

Optimization via Calculus

Determining positive (negative) definiteness using determinants.

Let

$$
A = \begin{array}{c}
\begin{array}{ccccc} \Delta_1 & \Delta_2 & \Delta_3 & & \end{array} \\
\begin{pmatrix}
a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\
a_{12} & a_{22} & a_{23} & \cdots & a_{2n} \\
a_{13} & a_{23} & a_{33} & \cdots & a_{3n} \\
\vdots & & & & \vdots \\
a_{1n} & a_{2n} & a_{3n} & \cdots & a_{nn}
\end{pmatrix}
\end{array},
\qquad
\begin{aligned}
\Delta_1 &= a_{11}, \\
\Delta_2 &= \det \begin{pmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{pmatrix}, \\
&\vdots \\
\Delta_n &= \det A.
\end{aligned}
$$

Optimization via Calculus

Determining positive (negative) (semi)definiteness using determinants.

Theorem (Determining positive or negative (semi)definiteness)

If A is an $n \times n$ symmetric matrix and if Δ_k is the kth principal minor of A for $1 \leq k \leq n$, then:

- *A is positive definite if and only if $\Delta_k > 0$ for $1 \leq k \leq n$;*
- *A is negative definite if and only if $(-1)^k \Delta_k > 0$ for $1 \leq k \leq n$ (in other words, the sign of Δ_k alternates starting with $\Delta_k < 0$).*
- *A is positive semidefinite if $\Delta_k > 0$ for $1 \leq k \leq n-1$ and $\Delta_n = 0$;* **Note: not an iff!**
- *A is negative semidefinite if $(-1)^k \Delta_k > 0$ for $1 \leq k \leq n-1$ and $\Delta_n = 0$;*

Optimization via Calculus

Example

Find the local and global minimizers and maximizers of $f(\mathbf{x}) = x_1^3 + x_2^3 + x_3^2 - 3x_1x_2 + x_1x_3^2 + 2$.

Optimization via Calculus

Determining positive (negative) (semi)definiteness using eigenvalues.

Since Hessians are symmetric, the following facts follow:

- The eigenvalues of a Hessian are real.
- The eigenvectors of distinct eigenvalues are orthogonal (or if an eigenvalue has multiplicity k, one can find k orthogonal vectors).

Optimization via Calculus

Determining positive (negative) (semi)definiteness using eigenvalues.

By definition, an eigenvalue of an $n \times n$ matrix A, denoted by λ, is a real or complex number such that $A\mathbf{p} = \lambda\mathbf{p}$, where $\mathbf{p} \neq \mathbf{0}$ is called an eigenvector of A.

If we form a square matrix P with the n eigenvectors of A as columns, then we can write

$$AP = PD$$

where D is a diagonal matrix the eigenvalues λ_i, $i = 1, \ldots, n$ down the main diagonal.

Optimization via Calculus

Determining positive (negative) (semi)definiteness using eigenvalues.

Since P is orthogonal, $P^{-1} = P^T$, and therefore we can write

$$P^T AP = D$$

which means that in the quadratic form

$$Q_A(\mathbf{x}) = \mathbf{x}^T A\mathbf{x}$$

we can substitute $\mathbf{x} = P\mathbf{y}$, yielding

$$Q_A(\mathbf{x}) = (P\mathbf{y})^T A(P\mathbf{y}) = \mathbf{y}^T P^T AP\mathbf{y} = \mathbf{y}^T D\mathbf{y} = \lambda_1 y_1^2 + \ldots + \lambda_n y_n^2.$$

So the sign of $Q_A(\mathbf{x})$ depends on the signs of the eigenvalues of A.

Determining positive (negative) (semi)definiteness using eigenvalues.

Theorem (Determining positive or negative (semi)definiteness)

If A is an $n \times n$ symmetric matrix, then:

- *A is positive definite if and only if all its eigenvalues are positive ($\lambda_i > 0$, for all $i = 1 \dots n$);*
- *A is negative definite if and only if all its eigenvalues are negative ($\lambda_i < 0$, for all $i = 1 \dots n$);*
- *A is positive semidefinite if and only if all its eigenvalues are nonnegative ($\lambda_i \geq 0$, for all $i = 1 \dots n$);*
- *A is negative semidefinite if and only if all its eigenvalues are nonpositive ($\lambda_i \leq 0$, for all $i = 1 \dots n$);*
- *A is indefinite if and only if A has at least one positive and one negative eigenvalue.*