MATH529 – Fundamentals of Optimization
Unconstrained Optimization II

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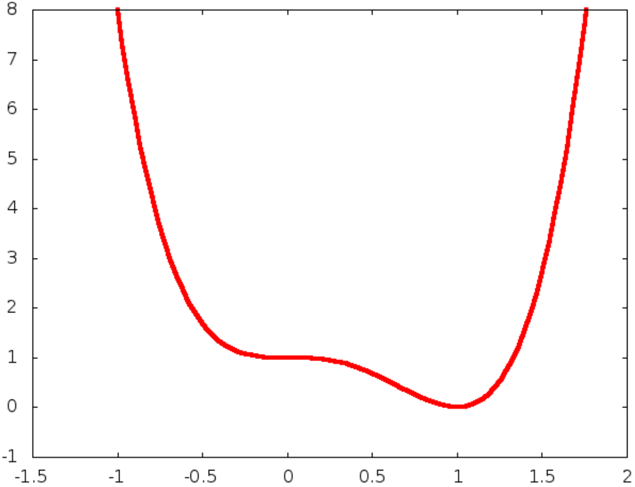
Recap

Example

Find the local and global minimizers and maximizers on $\mathbb{R}$ of $f(x) = 3x^4 - 4x^3 + 1$.

Graph of $f(x) = 3x^4 - 4x^3 + 1$.



Optimization via Calculus

Two theorems summarize the basic facts about **global** optimization of one variable functions.

Theorem (1st order condition (Necessary, but not sufficient))

Suppose that $f(x)$ is a differentiable function on $\mathbb{R}$ (or the function's domain I). If $x^\star$ is a global minimizer of $f(x)$, then $f'(x^\star) = 0$.

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Suppose that $f(x)$ is a differentiable function on $\mathbb{R}$ (or the function's domain I). If $x^\star$ is a global minimizer of $f(x)$, then $f'(x^\star) = 0$.

Theorem (2nd order condition (Sufficient, but not necessary))

Suppose that $f(x)$, $f'(x)$, and $f''(x)$ are all continuous on $\mathbb{R}$ (or I) and that $x^\star$ is a critical point of $f(x)$.

a) If $f''(x) \geq 0$ for all $x \in \mathbb{R}$ (or I), then $x^\star$ is a global minimizer of $f(x)$ on $\mathbb{R}$ (or I).
b) If $f''(x) > 0$ for all $x \in I$ such that $x \neq x^\star$, then $x^\star$ is a strict global minimizer of $f(x)$ on $\mathbb{R}$ (or I).

Local optimization is easier to verify.

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Optimization via Calculus

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Theorem (1st order condition (Necessary, but not sufficient))

Suppose that $f(x)$ *is a differentiable function on* $\mathbb{R}$ *(or* I*). If* $x^\star$ *is a local minimizer of* $f(x)$*, then* $f'(x^\star) = 0$.

Theorem (2nd order condition (Sufficient, but not necessary))

Suppose that $f(x)$, $f'(x)$, *and* $f''(x)$ *are all continuous on* $\mathbb{R}$ *(or* I*) and that* $x^\star$ *is a critical point of* $f(x)$.

If $f''(x^\star) > 0$, *then* $x^\star$ *is a strict local minimizer of* $f(x)$.

Exercise

Find the local and global minimizers and maximizers on $I = (-1, 1)$ of $f(x) = \ln(1 - x^2)$.

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Extend theorems that allow us to identify and classifly local minimizers of one variable functions to multivariable cases.

Notation:

A vector in $\mathbb{R}^n$ is an ordered n-tuple $\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix}$ of real numbers called *components* of $\mathbf{x}$.

If $\mathbf{x}$ and $\mathbf{y}$ are vectors in $\mathbb{R}^n$, then their *dot product* or *inner product* is defined by

$$\mathbf{x} \cdot \mathbf{y} = \mathbf{x}^T \mathbf{y} = (x_1, x_2, x_3, \ldots, x_n) \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{pmatrix} = \sum_{i=1}^{n} x_i y_i$$

where $\mathbf{x}^T$ is the *transpose* of $\mathbf{x}$.

Optimization via Calculus

Notation:
If $f(\mathbf{x})$ is a function of n variables with continuous first and second partial derivatives on $\mathbb{R}^n$, then the *gradient* of $f(\mathbf{x})$ is the vector

$$\nabla f = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \frac{\partial f}{\partial x_3} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

Optimization via Calculus

Notation: The *Hessian* of $f(\mathbf{x})$, denoted by $\nabla^2 f$ or Hf, is the symmetric $n \times n$ matrix

$$\nabla^2 f = Hf = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \frac{\partial^2 f}{\partial x_1 \partial x_3} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \frac{\partial^2 f}{\partial x_2 \partial x_3} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \frac{\partial^2 f}{\partial x_3 \partial x_1} & \frac{\partial^2 f}{\partial x_3 \partial x_2} & \frac{\partial^2 f}{\partial x_3^2} & \cdots & \frac{\partial^2 f}{\partial x_3 \partial x_n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \frac{\partial^2 f}{\partial x_n \partial x_3} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{pmatrix}$$

Optimization via Calculus

Definition

Suppose $f(\mathbf{x})$ is a real-valued function defined on a subset D of $\mathbb{R}^n$. A point $\mathbf{x}^\star$ in D is:

- A **global minimizer** for $f(\mathbf{x})$ on D if $f(\mathbf{x}^\star) \leq f(\mathbf{x})$ for all $\mathbf{x} \in D$;

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- A **critical point** (also called a **stationary point**) of $f(\mathbf{x})$ if the first partial derivatives of $f(\mathbf{x})$ exist at $\mathbf{x}^\star$ and $\frac{\partial f}{\partial x_i} = 0$, for $i = 1, 2, 3 \ldots, n$.

Theorem (Multivariable Taylor's formula)

Suppose that $\mathbf{x}$, $\mathbf{x}^\star$ *are points in* $\mathbb{R}^n$ *and that* $f(\mathbf{x})$ *is a real-valued function of* n *variables with continuous first and second partial derivatives on some open set containing the line segment* $[\mathbf{x}^\star, \mathbf{x}] = \{\mathbf{w} \in \mathbb{R}^n : \mathbf{w} = \mathbf{x}^\star + t(\mathbf{x} - \mathbf{x}^\star)\,,\, 0 \leq t \leq 1\}$ *joining* $\mathbf{x}^\star$ *and* $\mathbf{x}$. *Then, there exists a* $\mathbf{z} \in [\mathbf{x}^\star, \mathbf{x}]$ *such that*

$$f(\mathbf{x}) = f(\mathbf{x}^\star) + \nabla f(\mathbf{x}^\star)^T(\mathbf{x} - \mathbf{x}^\star) + \frac{1}{2}(\mathbf{x} - \mathbf{x}^\star)^T Hf(\mathbf{z})(\mathbf{x} - \mathbf{x}^\star)$$

Optimization via Calculus

Theorem (Local minimizer identification)

Suppose that $f(\mathbf{x})$ is a real-valued function for which all first partial derivatives of $f(\mathbf{x})$ exist on a subset $D \in \mathbb{R}^n$. If $\mathbf{x}^\star$ is an interior point of D that is a local minimizer of $f(\mathbf{x})$, then $\nabla f(\mathbf{x}^\star) = \mathbf{0}$.

Theorem (Classification of minimizers (maximizers))

Suppose that $\mathbf{x}^\star$ *is a critical 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* $(\mathbf{x}-\mathbf{x}^\star)^T Hf(\mathbf{z})(\mathbf{x}-\mathbf{x}^\star) \geq 0$ *for all* $\mathbf{x} \in \mathbb{R}^n$ *and all* $\mathbf{z} \in [\mathbf{x}^\star, \mathbf{x}]$*;*
- $\mathbf{x}^\star$ *is a* **strict global minimizer** *of* $f(\mathbf{x})$ *if* $(\mathbf{x}-\mathbf{x}^\star)^T Hf(\mathbf{z})(\mathbf{x}-\mathbf{x}^\star) > 0$ *for all* $\mathbf{x} \in \mathbb{R}^n$ *such that* $\mathbf{x} \neq \mathbf{x}^\star$ *and for all* $\mathbf{z} \in [\mathbf{x}^\star, \mathbf{x}]$*;*
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Optimization via Calculus

Practical ways to use the previous theorem:

Conditions that involve the form $(\mathbf{x} - \mathbf{x}^\star)^T Hf(\mathbf{z})(\mathbf{x} - \mathbf{x}^\star)$, or in general $\mathbf{v}^T A \mathbf{v}$, where A is a symmetric square matrix, call for methods to **identify whether A (in our case the Hessian of the objective function) is positive or negative (semi)definite**.

Quadratic forms:

Let

$$A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix}.$$

The quadratic form $Q_A(\mathbf{x}) = \mathbf{x}^T A\mathbf{x} = a_{11}x_1^2 + a_{12}x_1x_2 + a_{13}x_1x_3 + \ldots + a_{ij}x_ix_j + \ldots + a_{ii}x_i^2 + \ldots + a_{nn}x_n^2$.

Example

Write the quadratic form associated with the following matrix:

$$A = \begin{pmatrix} -1 & 0 & 2 & -3 \\ 0 & 2 & 1/2 & -1 \\ 2 & 1/2 & 0 & 4 \\ -3 & -1 & 4 & 5 \end{pmatrix}.$$

Determining whether a quadratic form $Q_A(\mathbf{x}) > 0$ for all $\mathbf{x} \in \mathbb{R}^n$.
Example in class . . . .