Handout

Review of Linear Algebra, Matrix Computations, Derivatives and Convexity

MIE 1624H October 3, 2023

Review of derivatives, gradients and Hessians:

- Given a function f of n variables $x_1, x_2, \ldots, x_n$, we use the following notations to represent the vector of variables and the function: $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^T$, $f(\boldsymbol{x}) = f(x_1, x_2, \ldots, x_n)$
- The gradient extends the notion of derivative, the Hessian matrix – that of second derivative.
- We define the *partial derivative* relative to variable x_i, written as $\frac{\partial f}{\partial x_i}$, to be the derivative of f with respect to x_i treating all variables except x_i as constant.
- The gradient of f at $\boldsymbol{x}$, written as $\nabla f(\boldsymbol{x})$, is

$$\nabla f(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

  The gradient of f is a multivariate function of $\boldsymbol{x}$, $f(\boldsymbol{x}) \in \mathbb{R}, \nabla f(\boldsymbol{x}) \in \mathbb{R}^n$.

- The gradient vector $\nabla f(\boldsymbol{x})$ gives the direction of steepest ascent of the function f at point $\boldsymbol{x}$. The gradient acts like the derivative in that small changes around a given point $\boldsymbol{x}^*$ can be estimated using the gradient (see first-order Taylor series expansion and finite difference method).
- Second partial derivatives $\frac{\partial^2 f}{\partial x_i \partial x_j}$ are obtained from $f(\boldsymbol{x})$ by taking the derivative relative to x_i (this yields the first partial derivative $\frac{\partial f}{\partial x_i}$) and then by taking the derivative of $\frac{\partial f}{\partial x_i}$ relative to x_j. So, we can compute $\frac{\partial^2 f}{\partial x_1 \partial x_1} = \frac{\partial^2 f}{\partial x_1^2}$, $\frac{\partial^2 f}{\partial x_1 \partial x_2}$ and so on. This values are arranged into the *Hessian* matrix:

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

  The Hessian matrix is a symmetric matrix, that is $\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i}$.

Computing gradients and Hessians:

Example

Compute the gradient and the Hessian of the function $f(x_1, x_2) = x_1^2 - 3x_1x_2 + x_2^2$ at the point $\boldsymbol{x} = (x_1, x_2)^T = (1, 1)^T$.

$$\nabla f(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{pmatrix} = \begin{pmatrix} 2x_1 - 3x_2 \\ -3x_1 + 2x_2 \end{pmatrix} = \begin{pmatrix} -1 \\ -1 \end{pmatrix}$$

$$\nabla^2 f(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{pmatrix} = \begin{pmatrix} 2 & -3 \\ -3 & 2 \end{pmatrix}$$

Taylor series expansion:

Second-order Taylor series expansion:

$$f(\boldsymbol{x}) = f(\boldsymbol{x}_0) + \nabla f(\boldsymbol{x}_0)^T (\boldsymbol{x} - \boldsymbol{x}_0) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}_0)^T \nabla^2 f(\boldsymbol{x}_0)(\boldsymbol{x} - \boldsymbol{x}_0)$$

First-order Taylor series expansion:

$$f(\boldsymbol{x}) = f(\boldsymbol{x}_0) + \nabla f(\boldsymbol{x}_0)^T (\boldsymbol{x} - \boldsymbol{x}_0)$$

Example

$f(x_1, x_2) = x_1^2 - 3x_1x_2 + x_2^2$, compute $f(1.01, 1.01)$ using first- and second-order Taylor series expansion at the point $\boldsymbol{x}_0 = (1, 1)^T$.

First-order Taylor series expansion:

$$f(1.01, 1.01) = f(1, 1) + \nabla f(1, 1)^T \begin{pmatrix} 1.01 - 1 \\ 1.01 - 1 \end{pmatrix} = -1 + (-1, -1) \begin{pmatrix} 0.01 \\ 0.01 \end{pmatrix} = -1.02$$

Second-order Taylor series expansion:

$$f(1.01, 1.01) = f(1, 1) + \nabla f(1, 1)^T \begin{pmatrix} 0.01 \\ 0.01 \end{pmatrix} + \frac{1}{2}(0.01, 0.01)\nabla^2 f(1, 1) \begin{pmatrix} 0.01 \\ 0.01 \end{pmatrix} =$$

$$= -1 + (-1, -1) \begin{pmatrix} 0.01 \\ 0.01 \end{pmatrix} + \frac{1}{2}(0.01, 0.01) \begin{pmatrix} 2 & -3 \\ -3 & 2 \end{pmatrix} \begin{pmatrix} 0.01 \\ 0.01 \end{pmatrix} = -1.0201$$

Convex functions:

Definition A function f is convex if for any $\boldsymbol{x}^1,\ \boldsymbol{x}^2 \in C$ and $0 \le \lambda \le 1$

$$f(\lambda \boldsymbol{x}^1 + (1-\lambda)\boldsymbol{x}^2) \le \lambda f(\boldsymbol{x}^1) + (1-\lambda) f(\boldsymbol{x}^2).$$

A square matrix $\boldsymbol{A}$ said to be positive definite (PD) if $\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} > 0$ for all $\boldsymbol{x} \neq 0$.

A square matrix $\boldsymbol{A}$ said to be positive semidefinite (PSD) if $\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} \ge 0$ for all $\boldsymbol{x}$.

Hessian $\nabla f^2(\boldsymbol{x})$ is PD $\Longrightarrow$ strictly convex function.

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Gradient $\nabla f(\bar{\boldsymbol{x}}) = 0$ and Hessian $\nabla f^2(\bar{\boldsymbol{x}})$ is PSD $\Longrightarrow$ $\bar{\boldsymbol{x}}$ is a minimum of the function f.

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Checking a matrix for PD and PSD by computing principal minors:

Leading principal minors D_k, $k = 1, 2, \ldots, n$ of a matrix $\boldsymbol{A} = (a_{ij})_{[n \times n]}$ are defined as

$$D_k = \det \begin{pmatrix} a_{11} & \ldots & a_{1k} \\ \vdots & & \vdots \\ a_{k1} & \ldots & a_{kk} \end{pmatrix}$$

A square matrix $\boldsymbol{A}$ is PD $\Leftrightarrow$ $D_k > 0$ for all $k = 1, 2, \ldots, n$.

Example

Consider the function $f(\boldsymbol{x}) = 3x_1^2 + 3x_2^2 + 5x_3^2 - 2x_1x_2$. The corresponding Hessian matrix is

$$\nabla^2 f(\boldsymbol{x}) = 2 \cdot \begin{pmatrix} 3 & -1 & 0 \\ -1 & 3 & 0 \\ 0 & 0 & 5 \end{pmatrix}$$

Leading principal minors of $\nabla^2 f(\boldsymbol{x})$ are

$$D_1 = 2 \cdot 3 = 6 > 0, \qquad D_2 = 2^2 \cdot \det \begin{pmatrix} 3 & -1 \\ -1 & 3 \end{pmatrix} = 2^2 \cdot [3 \cdot 3 - (-1)(-1)] = 4 \cdot 8 = 32 > 0,$$

$$\begin{aligned} D_3 &= 2^3 \cdot \det \begin{pmatrix} 3 & -1 & 0 \\ -1 & 3 & 0 \\ 0 & 0 & 5 \end{pmatrix} \\ &= 2^3 \cdot ([3 \cdot 3 \cdot 5 + 0 \cdot 0 \cdot (-1) + 0 \cdot 0 \cdot (-1)] - [0 \cdot 0 \cdot 3 + 0 \cdot 0 \cdot 3 + (-1) \cdot (-1) \cdot 5]) \\ &= 8 \cdot 40 = 320 > 0 \end{aligned}$$

So, the Hessian is positive definite (PD) and the function is strictly convex.

A square matrix $\boldsymbol{A}$ is PSD $\Leftrightarrow$ all the principal minors of $\boldsymbol{A}$ are ≥ 0.

The *principal minor* is

$$\boldsymbol{A}(i_1\ i_2 \dots i_p) = \det \begin{pmatrix} a_{i_1 i_1} & \dots & a_{i_1 i_p} \\ \vdots & & \vdots \\ a_{i_p i_1} & \dots & a_{i_p i_p} \end{pmatrix}, \text{where } 1 \leq i_1 < i_2 < \dots < i_p \leq n,\ p \leq n.$$

Checking if symmetric matrix is PD or PSD by computing its eigenvalues:

Definition Any number λ such that the equation $\boldsymbol{A}\boldsymbol{x} = \lambda \boldsymbol{x}$ has a non-zero vector-solution $\boldsymbol{x}$ is called an eigenvalue (or a characteristic root) of the equation.

A symmetric matrix is PD if its eigenvalues $\lambda_i > 0$ for all $i = 1, 2, \dots, n$ and PSD if $\lambda_i \geq 0$.

How to calculate eigenvalues: $\boldsymbol{A}\boldsymbol{x} - \lambda\boldsymbol{x} = 0 \Rightarrow (\boldsymbol{A} - \lambda\boldsymbol{I})\boldsymbol{x} = 0$. Since $\boldsymbol{x}$ is non-zero, the determinant of $(\boldsymbol{A} - \lambda\boldsymbol{I})$ should vanish. Therefore all eigenvalues can be calculated as roots of the equation (which is often called the characteristic equation of $\boldsymbol{A}$):

$$\det(\boldsymbol{A} - \lambda\boldsymbol{I}) = 0.$$

Example

Consider the Hessian matrix

$$\nabla^2 f(\boldsymbol{x}) = \begin{pmatrix} 3 & -1 & 0 \\ -1 & 3 & 0 \\ 0 & 0 & 5 \end{pmatrix}$$

Computing eigenvalues

$$\det(\nabla^2 f(\boldsymbol{x}) - \lambda\boldsymbol{I}) = \det \begin{pmatrix} 3-\lambda & -1 & 0 \\ -1 & 3-\lambda & 0 \\ 0 & 0 & 5-\lambda \end{pmatrix} = (5-\lambda)(\lambda^2 - 6\lambda + 8) = (5-\lambda)(\lambda-2)(\lambda-4) = 0.$$

Therefore, the eigenvalues are $\lambda = 2$, $\lambda = 4$ and $\lambda = 5$. As all of them are strictly positive, the Hessian is positive definite (PD).

Try computing eigenvalues and determinants in Python:

```
import numpy as np
H = np.matrix( ((3,-1,0), (-1,3,0), (0,0,5)) )
eigenvalues, eigenvectors = np.linalg.eig(H)
determinant = np.linalg.det(H)
```

Properties of convex functions:

- if f is convex function, its sublevel set $f(\boldsymbol{x}) \leq \alpha$ is convex;
- positive multiple of convex function is convex:

  f convex, $\alpha \geq 0 \quad \Longrightarrow \quad \alpha f$ convex
- sum of convex functions is convex:

  f_1, f_2 convex $\quad \Longrightarrow \quad f_1 + f_2$ convex
- pointwise maximum of convex functions is convex:

  f_1, f_2 convex $\quad \Longrightarrow \quad \max\{f_1(\boldsymbol{x}), f_2(\boldsymbol{x})\}$ convex

  (corresponds to intersections of epigraphs)
- affine transformation of domain:

  f convex $\quad \Longrightarrow \quad f(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b})$ convex

Composition rules:

Composite function

$$f(x) = h(g(x))$$

is convex if:

- g convex; h convex nondecreasing
- g concave; h convex nonincreasing

Proof (differentiable functions, $x \in \Re$):

$$f'' = h''(g')^2 + g''h'$$

Examples:

- $f(x) = e^{g(x)}$ is convex if g is convex
- $f(x) = 1/g(x)$ is convex if g is concave, positive
- $f(x) = g(x)^p,\ p \geq 1$ is convex if $g(x)$ is convex, positive

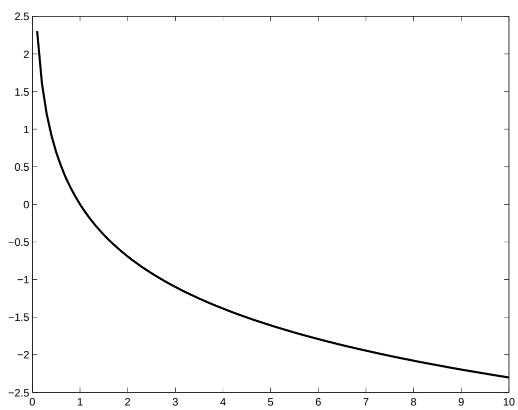
Examples

Show that the function $e^x + \frac{1}{2}x^2$ is convex and solve $\min \; e^x + \frac{1}{2}x^2$**.**

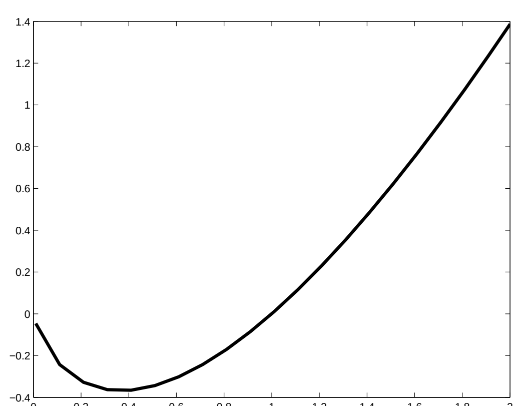
First derivative: A function is increasing if $f' > 0$, decreasing if $f' < 0$ and neither if $f' = 0$.
Second derivative: A function is convex if $f'' > 0$ and concave if $f'' < 0$.
Answer: $f'(x) = e^x + x$ and $f''(x) = e^x + 1 \; > \; 0$. So, f is convex.
Thus, we can find a solution to an optimization problem by solving $f'(x) = 0$, given f is convex.

Find the local/global minimum of the functions if exists:

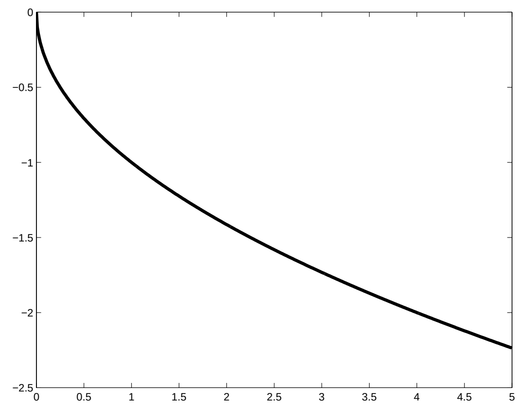
- $-\ln x$
  $f'(x) = -1/x$, $f''(x) = 1/x^2 > 0$ - strictly convex function. $f'(x) = -1/x = 0 \implies x \to \infty$



- $x \ln x$
  $f'(x) = 1 + \ln x$, $f''(x) = 1/x > 0$ on the domain of $\ln x \Rightarrow$ strictly convex function. $f'(x) = 1 + \ln x = 0 \implies x = 0.37$ (global minimum).



- $-\sqrt{x}$ when $x \geq 0$
  $f'(x) = -0.5x^{-1/2}$, $f''(x) = 0.25x^{-3/2} \geq 0$ when $x \geq 0 \Rightarrow$ convex function. $f'(x) = -0.5x^{-1/2} = 0 \implies x \to \infty$.



- $(x_1 - 2)^2 + (x_2 + 1)^2 - 2$

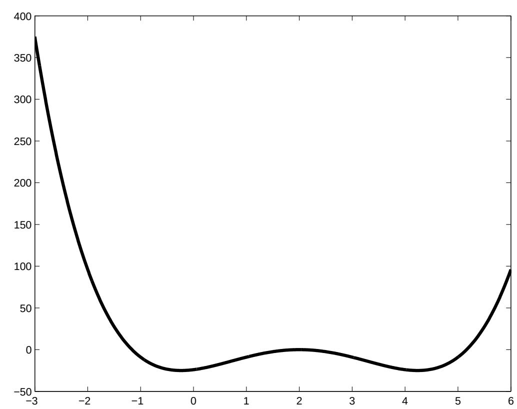
$$\nabla f(x) = \begin{pmatrix} 2(x_1 - 2) \\ 2(x_2 + 1) \end{pmatrix}$$

$$\nabla^2 f(x) = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} \succ 0$$

  As $\nabla^2 f(x)$ is PD, $f(x)$ is strictly convex function.

$$\nabla f(x) = 0 \quad \implies \quad x = \begin{pmatrix} 2 \\ -1 \end{pmatrix} \quad \text{(global minimum).}$$

- $(x - 2)^4 - 10(x - 2)^2$
  $f'(x) = 4(x - 2)^3 - 20(x - 2)$, $f''(x) = 12(x - 2)^2 - 20$ - non-convex, non-concave function.



Example of Newton Method

Consider minimizing the function $f(x_1, x_2) = e^{x_1+x_2-2} + (x_1 - x_2)^2$. Given $\boldsymbol{x}^0 = (1, 1)^T$, apply a full Newton step and compute $\boldsymbol{x}^1$.

$$\begin{aligned}
\nabla f(\boldsymbol{x}) &= \begin{pmatrix} e^{x_1+x_2-2} + 2(x_1 - x_2) \\ e^{x_1+x_2-2} - 2(x_1 - x_2) \end{pmatrix} \\
\nabla^2 f(\boldsymbol{x}) &= \begin{pmatrix} e^{x_1+x_2-2} + 2 & e^{x_1+x_2-2} - 2 \\ e^{x_1+x_2-2} - 2 & e^{x_1+x_2-2} + 2 \end{pmatrix} \\
\boldsymbol{x}^1 &= \boldsymbol{x}^0 - \left(\nabla^2 f(\boldsymbol{x}^0)\right)^{-1} \nabla f(\boldsymbol{x}^0)
\end{aligned}$$

So

$$\begin{aligned}
\nabla f(\boldsymbol{x}^0) &= \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\
\nabla^2 f(\boldsymbol{x}^0) &= \begin{pmatrix} 3 & -1 \\ -1 & 3 \end{pmatrix}
\end{aligned}$$

Instead of inverting matrix $\nabla^2 f(\boldsymbol{x}^0)$, which is costly, we can solve the system of equations. Please note that if we want to compute $\boldsymbol{y} = \boldsymbol{A}^{-1}\boldsymbol{b}$, we can solve the system of equations $\boldsymbol{A}\boldsymbol{y} = \boldsymbol{b}$ to find $\boldsymbol{y}$. So we can solve $\nabla^2 f(\boldsymbol{x}^0) \cdot \boldsymbol{y} = \nabla f(\boldsymbol{x}^0)$ to get $\boldsymbol{y} = (\nabla^2 f(\boldsymbol{x}^0))^{-1} \nabla f(\boldsymbol{x}^0)$.

$$\begin{pmatrix} 3 & -1 \\ -1 & 3 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \Rightarrow \begin{cases} y_1 = 0.5 \\ y_2 = 0.5 \end{cases}$$

Thus,

$$\begin{aligned}
\boldsymbol{x}^1 &= \boldsymbol{x}^0 - \left(\nabla^2 f(\boldsymbol{x}^0)\right)^{-1} \nabla f(\boldsymbol{x}^0) \\
&= \begin{pmatrix} 1 \\ 1 \end{pmatrix} - \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix} = \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix}
\end{aligned}$$

$$f(\boldsymbol{x}^1) = 0.3679 \quad < \quad f(\boldsymbol{x}^0) = 1$$