# CS 2601 Linear and Convex Optimization

## 2. Math review

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# Outline

- First-order conditions for unconstrained local min

- Second-order conditions for unconstrained local min

# Review: Derivative

$\boldsymbol{x}$ is an interior point of $X \subset \mathbb{R}^n$ if there exists $\epsilon > 0$ s.t. $B(\boldsymbol{x}, \epsilon) \subset X$.

The interior of $X$, denoted by $\operatorname{int} X$, is the set of interior points of $X$.

A function $\boldsymbol{f} : X \subset \mathbb{R}^n \to \mathbb{R}^m$ is differentiable at $\boldsymbol{x}_0 \in \operatorname{int} X$, if there exists a matrix[1] $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ s.t.

$$\lim_{\Delta \boldsymbol{x} \to \boldsymbol{0}} \frac{\boldsymbol{f}(\boldsymbol{x}_0 + \Delta \boldsymbol{x}) - \boldsymbol{f}(\boldsymbol{x}_0) - \boldsymbol{A} \Delta \boldsymbol{x}}{\|\Delta \boldsymbol{x}\|} = \boldsymbol{0}$$

i.e.

$$\Delta \boldsymbol{f} := \boldsymbol{f}(\boldsymbol{x}_0 + \Delta \boldsymbol{x}) - \boldsymbol{f}(\boldsymbol{x}_0) = \boldsymbol{A} \Delta \boldsymbol{x} + o(\|\Delta \boldsymbol{x}\|)$$

The affine function $\boldsymbol{f}(\boldsymbol{x}_0) + \boldsymbol{A}(\boldsymbol{x} - \boldsymbol{x}_0)$ is the first-order approximation of $\boldsymbol{f}$ at $\boldsymbol{x}_0$,

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{x}_0) + \boldsymbol{A}(\boldsymbol{x} - \boldsymbol{x}_0) + o(\|\boldsymbol{x} - \boldsymbol{x}_0\|)$$

[1] More precisely, a linear transformation represented by matrix $\boldsymbol{A}$

# Review: Derivative

The matrix $\boldsymbol{A}$ is called the derivative of $\boldsymbol{f}$ at $\boldsymbol{x}_0$, and we write

$$\boldsymbol{f}'(\boldsymbol{x}_0) = D\boldsymbol{f}(\boldsymbol{x}_0) = \boldsymbol{A}$$

The derivative is given by the Jacobian matrix of $\boldsymbol{f} = (f_1, \ldots, f_m)^T$

$$\boldsymbol{f}'(\boldsymbol{x}_0) = \begin{bmatrix} \frac{\partial f_1(\boldsymbol{x}_0)}{\partial x_1} & \frac{\partial f_1(\boldsymbol{x}_0)}{\partial x_2} & \cdots & \frac{\partial f_1(\boldsymbol{x}_0)}{\partial x_n} \\ \frac{\partial f_2(\boldsymbol{x}_0)}{\partial x_1} & \frac{\partial f_2(\boldsymbol{x}_0)}{\partial x_2} & \cdots & \frac{\partial f_2(\boldsymbol{x}_0)}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m(\boldsymbol{x}_0)}{\partial x_1} & \frac{\partial f_m(\boldsymbol{x}_0)}{\partial x_2} & \cdots & \frac{\partial f_m(\boldsymbol{x}_0)}{\partial x_n} \end{bmatrix}$$

i.e.

$$[\boldsymbol{f}'(\boldsymbol{x}_0)]_{ij} = \frac{\partial f_i(\boldsymbol{x}_0)}{\partial x_j}, \quad i = 1, \ldots, m; j = 1, \ldots, n$$

Note

$$f_i(\boldsymbol{x}_0 + \Delta \boldsymbol{x}) = f_i(\boldsymbol{x}_0) + \sum_{j=1}^{n} \frac{\partial f_i(\boldsymbol{x}_0)}{\partial x_j} \Delta x_j + o(\|\Delta \boldsymbol{x}\|), \quad i = 1, 2, \ldots, m$$

# Review: Derivative

Example. An affine function $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}$ from $\mathbb{R}^n$ to $\mathbb{R}^m$ has derivative $\boldsymbol{f}'(\boldsymbol{x}) = \boldsymbol{A}$ at all $\boldsymbol{x}$. In particular, when $m = 1$, $f(\boldsymbol{x}) = \boldsymbol{a}^T\boldsymbol{x} + b$ has derivative $f'(\boldsymbol{x}) = \boldsymbol{a}^T$, which is a $1 \times n$ matrix, i.e. a row vector.

Proof. In component form,

$$f_i(\boldsymbol{x}) = \sum_{k=1}^{n} A_{ik}x_k + b_i = A_{i1}x_1 + A_{i2}x_2 + \cdots + A_{in}x_n + b_i$$

so

$$\frac{\partial f_i(\boldsymbol{x}_0)}{\partial x_j} = A_{ij} \implies \boldsymbol{f}'(\boldsymbol{x}_0) = \boldsymbol{A}$$

Alternative proof.

$$\boldsymbol{f}(\boldsymbol{x}_0 + \Delta\boldsymbol{x}) - \boldsymbol{f}(\boldsymbol{x}_0) = \boldsymbol{A}\Delta\boldsymbol{x} \implies \boldsymbol{f}'(\boldsymbol{x}_0) = \boldsymbol{A}$$

# Review: Derivative

Example. For symmetric $A$, $f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j$ has derivative

$$f'(\boldsymbol{x}) = 2\boldsymbol{x}^T \boldsymbol{A}$$

Proof.

$$\frac{\partial f}{\partial x_k} = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} \left( x_j \frac{\partial x_i}{\partial x_k} + x_i \frac{\partial x_j}{\partial x_k} \right) = \sum_{j=1}^{n} A_{kj} x_j + \sum_{i=1}^{n} A_{ik} x_i = 2 \sum_{i=1}^{n} x_i A_{ik}$$

Alternatively,

$$f(\boldsymbol{x}_0 + \Delta \boldsymbol{x}) - f(\boldsymbol{x}_0) = \boldsymbol{x}_0^T (\boldsymbol{A} + \boldsymbol{A}^T) \Delta \boldsymbol{x} + \underbrace{\Delta \boldsymbol{x}^T \boldsymbol{A} \Delta \boldsymbol{x}}_{= o(\|\Delta \boldsymbol{x}\|)}$$

Note. For general $\boldsymbol{A}$, $f'(\boldsymbol{x}) = \boldsymbol{x}^T (\boldsymbol{A} + \boldsymbol{A}^T)$. This can also be obtained by noting $\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} = \boldsymbol{x}^T \tilde{\boldsymbol{A}} \boldsymbol{x}$ and $f'(\boldsymbol{x}) = 2\boldsymbol{x}^T \tilde{\boldsymbol{A}}$, where $\tilde{\boldsymbol{A}} = \frac{1}{2}(\boldsymbol{A} + \boldsymbol{A}^T)$.

# Review: Gradient

For a real-valued function $f : \mathbb{R}^n \to \mathbb{R}$, the gradient of $f$ at $\boldsymbol{x}$, denoted by $\nabla f(\boldsymbol{x})$, is the transpose of $f'(\boldsymbol{x})$,

$$\nabla f(\boldsymbol{x}) = [f'(\boldsymbol{x})]^T, \quad [\nabla f(\boldsymbol{x})]_i = \frac{\partial f(\boldsymbol{x})}{\partial x_i}, \quad i = 1, \ldots, n$$

$\nabla f(\boldsymbol{x})$ is a column vector and satisfies

$$f'(\boldsymbol{x})\Delta\boldsymbol{x} = \langle \nabla f(\boldsymbol{x}), \Delta\boldsymbol{x} \rangle = \nabla f(\boldsymbol{x})^T \Delta\boldsymbol{x}$$

The first-order approximation of $f$ at $\boldsymbol{x}_0$ is

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

Example. For symmetric $\boldsymbol{A}$, the gradient of $f(\boldsymbol{x}) = \boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}^T\boldsymbol{x} + c$ is

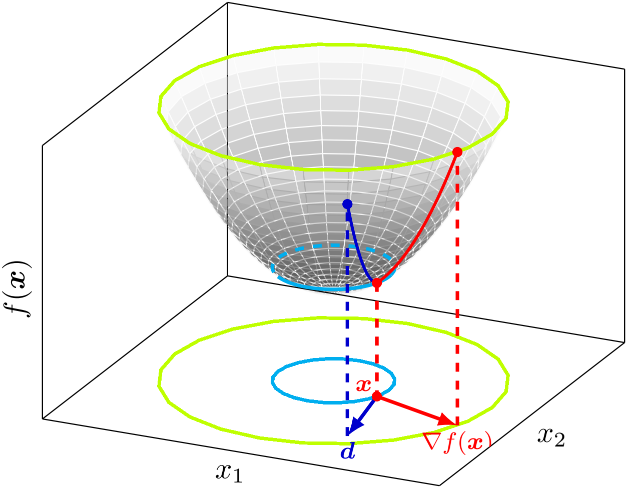
$$\nabla f(\boldsymbol{x}) = 2\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}$$

# Review: Gradient

$\nabla f(\boldsymbol{x})$ is the direction of fastest rate of increase of $f$ at $\boldsymbol{x}$,

$$f(\boldsymbol{x}+\boldsymbol{d}) - f(\boldsymbol{x}) \approx \nabla f(\boldsymbol{x})^T \boldsymbol{d} \leq \|\nabla f(\boldsymbol{x})\| \cdot \|\boldsymbol{d}\|$$

where equality holds in the last step iff $\boldsymbol{d} = \alpha \nabla f(\boldsymbol{x})$ for some $\alpha \geq 0$.



# Review: Chain rule

If $\boldsymbol{f} : X \subset \mathbb{R}^n \to \mathbb{R}^m$ is differentiable at $\boldsymbol{x}_0 \in X$, $\boldsymbol{g} : Y \subset \mathbb{R}^m \to \mathbb{R}^p$ is differentiable at $\boldsymbol{y}_0 = \boldsymbol{f}(\boldsymbol{x}_0)$, then the composition of $\boldsymbol{f}$ and $\boldsymbol{g}$ defined by $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{g}(\boldsymbol{f}(\boldsymbol{x}))$ is differentiable at $\boldsymbol{x}_0$, and

$$\boldsymbol{h}'(\boldsymbol{x}_0) = \boldsymbol{g}'(\boldsymbol{y}_0)\boldsymbol{f}'(\boldsymbol{x}_0) = \boldsymbol{g}'(\boldsymbol{f}(\boldsymbol{x}_0))\boldsymbol{f}'(\boldsymbol{x}_0)$$

Note. The order is important since $\boldsymbol{g}'(\boldsymbol{y}_0) \in \mathbb{R}^{p\times m}$ and $\boldsymbol{f}'(\boldsymbol{x}_0) \in \mathbb{R}^{m\times n}$ are matrices. In general $\boldsymbol{f}'(\boldsymbol{x}_0)\boldsymbol{g}'(\boldsymbol{y}_0)$ is undefined.

$$\begin{array}{ccccc}
\mathbb{R}^n & \xrightarrow{\boldsymbol{f}} & \mathbb{R}^m & \xrightarrow{\boldsymbol{g}} & \mathbb{R}^p \\
\boldsymbol{x}_0 & \mapsto & \boldsymbol{y}_0 = \boldsymbol{f}(\boldsymbol{x}_0) & \mapsto & \boldsymbol{z}_0 = \boldsymbol{h}(\boldsymbol{x}_0) = \boldsymbol{g}(\boldsymbol{y}_0) \\
\Delta\boldsymbol{x} & \overset{\boldsymbol{f}'}{\mapsto} & \Delta\boldsymbol{y} \approx \boldsymbol{f}'(\boldsymbol{x}_0)\Delta\boldsymbol{x} & \overset{\boldsymbol{g}'}{\mapsto} & \Delta\boldsymbol{z} \approx \boldsymbol{g}'(\boldsymbol{y}_0)\Delta\boldsymbol{y} \approx \boldsymbol{g}'(\boldsymbol{y}_0)\boldsymbol{f}'(\boldsymbol{x}_0)\Delta\boldsymbol{x}
\end{array}$$

In component form,

$$[\boldsymbol{h}'(\boldsymbol{x}_0)]_{ij} = \frac{\partial h_i(\boldsymbol{x}_0)}{\partial x_j} = \sum_{k=1}^{m} \frac{\partial g_i(\boldsymbol{y}_0)}{\partial y_k} \cdot \frac{\partial f_k(\boldsymbol{x}_0)}{\partial x_j} = \sum_{k=1}^{m} [\boldsymbol{g}'(\boldsymbol{y}_0)]_{ik} [\boldsymbol{f}'(\boldsymbol{x}_0)]_{kj}$$

# Review: Chain rule

Example. $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b})$ has derivative $\boldsymbol{h}'(\boldsymbol{x}_0) = \boldsymbol{f}'(\boldsymbol{A}\boldsymbol{x}_0 + \boldsymbol{b})\boldsymbol{A}$. If $f$ is real-valued,

$$\nabla h(\boldsymbol{x}_0) = \boldsymbol{A}^T [f'(\boldsymbol{A}\boldsymbol{x}_0 + \boldsymbol{b})]^T = \boldsymbol{A}^T \nabla f(\boldsymbol{A}\boldsymbol{x}_0 + \boldsymbol{b})$$

Example. Given $f : \mathbb{R}^n \to \mathbb{R}$ and $\boldsymbol{x}, \boldsymbol{d} \in \mathbb{R}^n$, define

$$g(t) = f(\boldsymbol{x} + t\boldsymbol{d})$$

Then

$$g'(t) = f'(\boldsymbol{x} + t\boldsymbol{d})\boldsymbol{d} = \nabla f(\boldsymbol{x} + t\boldsymbol{d})^T \boldsymbol{d} = \boldsymbol{d}^T \nabla f(\boldsymbol{x} + t\boldsymbol{d})$$

Note. $g$ is the restriction of $f$ to the straight line through $\boldsymbol{x}$ with direction $\boldsymbol{d}$. We can often get useful information about $f$ by looking at $g$, which is usually easier to deal with.

# First-order necessary condition

Consider unconstrained optimization problem, i.e. $X = \mathbb{R}^n$.

Theorem. If $\boldsymbol{x}^*$ is a local minimum of $f$ and $f$ is differentiable at $\boldsymbol{x}^*$, then its gradient at $\boldsymbol{x}^*$ vanishes, i.e.

$$\nabla f(\boldsymbol{x}^*) = \left( \frac{\partial f(\boldsymbol{x}^*)}{\partial x_1}, \ldots, \frac{\partial f(\boldsymbol{x}^*)}{\partial x_n} \right)^T = \mathbf{0}.$$

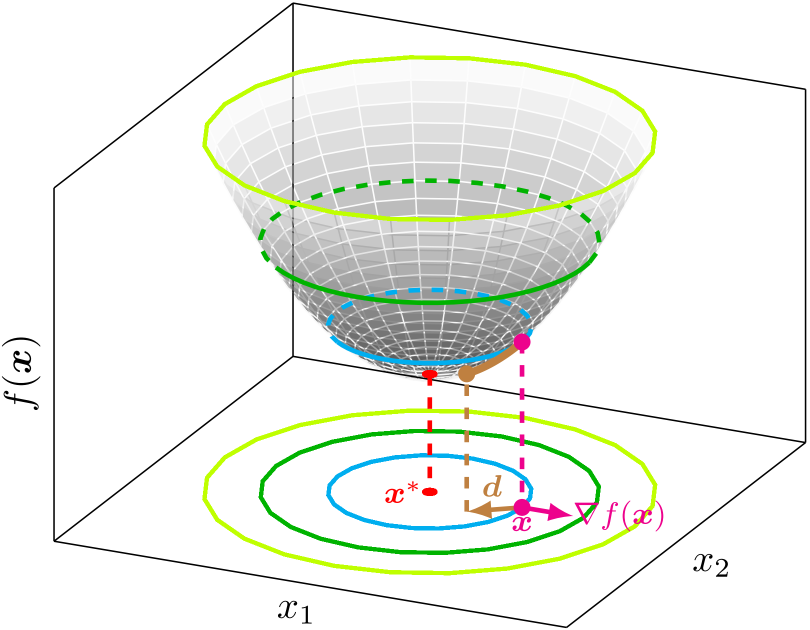
Proof. Let $\boldsymbol{d} \in \mathbb{R}^n$. Define $g(t) = f(\boldsymbol{x}^* + t\boldsymbol{d})$.

- Since $\boldsymbol{x}^*$ is a local minimum, $g(t) \geq g(0)$
- For $t > 0$,

$$\frac{g(t) - g(0)}{t} \geq 0 \implies g'(0) = \lim_{t \downarrow 0} \frac{g(t) - g(0)}{t} \geq 0$$

- By chain rule, $g'(0) = \sum_{i=1}^n d_i \frac{\partial f(\boldsymbol{x}^*)}{\partial x_i} = \boldsymbol{d}^T \nabla f(\boldsymbol{x}^*) \geq 0$
- Setting $\boldsymbol{d} = -\nabla f(\boldsymbol{x}^*) \implies \|\nabla f(\boldsymbol{x}^*)\|^2 \leq 0 \implies \nabla f(\boldsymbol{x}^*) = \mathbf{0}$

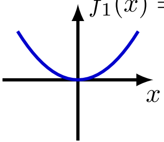
# First-order Necessary Condition (cont'd)



# First-order Necessary Condition (cont'd)

A point $\boldsymbol{x}^*$ with $\nabla f(\boldsymbol{x}^*) = \mathbf{0}$ is called a stationary point of $f$.

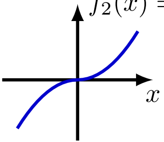
$f_1(x) = x^2$




$x^* = 0$

minimum

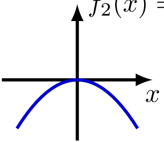
$f_2(x) = x|x|$




$x^* = 0$

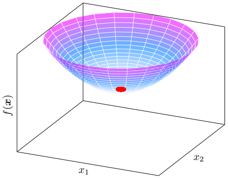
inflection point

$f_2(x) = -x^2$



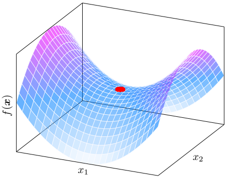

$x^* = 0$

maximum



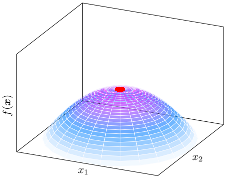

$f(\boldsymbol{x}) = x_1^2 + x_2^2$

minimum



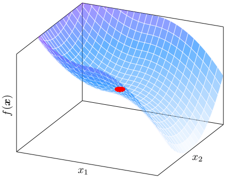

$f(\boldsymbol{x}) = x_1^2 - x_2^2$

saddle point




$f(\boldsymbol{x}) = -x_1^2 - x_2^2$

maximum




$f(\boldsymbol{x}) = -x_1|x_1| + x_2^2$

Note. Will see stationarity is sufficient for convex optimization.

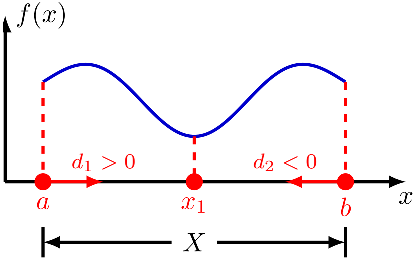
# First-order Necessary Condition (cont'd)

For constrained optimization problem, i.e. $X \neq \mathbb{R}^n$,

- if $\boldsymbol{x}^*$ is in the interior of $X$, i.e. $B(\boldsymbol{x}^*, \epsilon) \subset X$ for some $\epsilon > 0$, then the proof still works, so $\nabla f(\boldsymbol{x}^*) = \boldsymbol{0}$
- otherwise, the proof shows $\boldsymbol{d}^T \nabla f(\boldsymbol{x}^*) \geq 0$ for any feasible direction $\boldsymbol{d}$ at $\boldsymbol{x}^*$
  - $\boldsymbol{d}$ is a feasible direction at $x \in X$ if $\boldsymbol{x} + \alpha \boldsymbol{d} \in X$ for all sufficiently small $\alpha > 0$
- will revisit later

Example. $X = [a, b]$

- $f'(x_1) = 0$
- $d_1 f'(a) \geq 0 \implies f'(a) \geq 0$
- $d_2 f'(b) \geq 0 \implies f'(b) \leq 0$



# Outline

- First-order conditions for unconstrained local min

- Second-order conditions for unconstrained local min

# Review: Second derivative

The second-order partial derivatives of $f : X \subset \mathbb{R}^n \to \mathbb{R}$ at $\boldsymbol{x}_0 \in \operatorname{int} X$ are

$$\frac{\partial^2 f(\boldsymbol{x}_0)}{\partial x_i \partial x_j}, \quad i, j = 1, 2, \ldots, n$$

The Hessian (matrix) of $f$ at $\boldsymbol{x}_0$, denoted by $\nabla^2 f(\boldsymbol{x}_0)$, is given by

$$[\nabla^2 f(\boldsymbol{x}_0)]_{ij} = \frac{\partial^2 f(\boldsymbol{x}_0)}{\partial x_i \partial x_j}, \quad i, j = 1, 2, \ldots, n$$

Note. Do not confuse with Jacobian matrix of vector-valued function.

If $\dfrac{\partial^2 f(\boldsymbol{x})}{\partial x_i \partial x_j}$ and $\dfrac{\partial^2 f(\boldsymbol{x})}{\partial x_j \partial x_i}$ exist in a neighborhood of $\boldsymbol{x}_0$ and are continuous at $\boldsymbol{x}_0$, then

$$\frac{\partial^2 f(\boldsymbol{x}_0)}{\partial x_i \partial x_j} = \frac{\partial^2 f(\boldsymbol{x}_0)}{\partial x_j \partial x_i}$$

so $\nabla^2 f(\boldsymbol{x}_0)$ is symmetric.

Will assume twice continuous differentiability when considering $\nabla^2 f$.

# Review: Second derivative

Example. For an affine function $f(\boldsymbol{x}) = \boldsymbol{b}^T\boldsymbol{x} + \boldsymbol{c}$

$$\nabla f^2(\boldsymbol{x}) = \boldsymbol{O}$$

Example. For a quadratic function $f(\boldsymbol{x}) = \boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x}$ with a symmetric $\boldsymbol{A}$,

$$\nabla^2 f(\boldsymbol{x}) = 2\boldsymbol{A}$$

Proof. Recall $f'(\boldsymbol{x}) = 2\boldsymbol{x}^T\boldsymbol{A}$, i.e.

$$\frac{\partial f(\boldsymbol{x})}{\partial x_j} = 2\sum_{k=1}^{n} x_k A_{kj}$$

so

$$\frac{\partial^2 f(\boldsymbol{x})}{\partial x_i \partial x_j} = 2\sum_{k=1}^{n} \frac{\partial x_k}{\partial x_i} A_{kj} = 2A_{ij}$$

# Review: Chain rule for second derivative

The composition with affine function $g(\boldsymbol{x}) = f(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b})$ has Hessian

$$\nabla^2 g(\boldsymbol{x}) = \boldsymbol{A}^T \nabla^2 f(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b})\boldsymbol{A}$$

Proof. Let $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}$, i.e. $y_k = \sum_i A_{ki} x_i$. Recall $\nabla g(\boldsymbol{x}) = \boldsymbol{A}^T \nabla f(\boldsymbol{y})$, i.e.

$$\frac{\partial g(\boldsymbol{x})}{\partial x_j} = \sum_k \frac{\partial f(\boldsymbol{y})}{\partial y_k} \frac{\partial y_k}{\partial x_j} = \sum_k \frac{\partial f(\boldsymbol{y})}{\partial y_k} A_{kj}$$

$$\frac{\partial^2 g(\boldsymbol{x})}{\partial x_i \partial x_j} = \sum_k \frac{\partial}{\partial x_i} \frac{\partial f(\boldsymbol{y})}{\partial y_k} A_{kj} = \sum_k \sum_\ell \frac{\partial^2 f(\boldsymbol{y})}{\partial y_\ell \partial y_k} A_{\ell i} A_{kj} = [\boldsymbol{A}^T \nabla^2 f(\boldsymbol{y}) \boldsymbol{A}]_{ij}$$

Special case. For $g(t) = f(\boldsymbol{x} + t\boldsymbol{d})$,

$$g''(t) = \boldsymbol{d}^T \nabla^2 f(\boldsymbol{x} + t\boldsymbol{d})\boldsymbol{d}$$

Proof. Set $\boldsymbol{A} \leftarrow \boldsymbol{d}$, $\boldsymbol{x} \leftarrow t$, $\boldsymbol{b} \leftarrow \boldsymbol{x}$ in the general formula above.

# Review: Second-order Taylor expansion

The second-order Taylor expansion for $g : \mathbb{R} \to \mathbb{R}$ takes the form

$$g(a+t) = g(a) + g'(a)t + \frac{1}{2}g''(a)t^2 + o(|t|^2) \tag{T1}$$

The second-order Taylor expansion for $f : \mathbb{R}^n \to \mathbb{R}$ takes the form

$$f(\boldsymbol{x}+\boldsymbol{d}) = f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T\boldsymbol{d} + \frac{1}{2}\boldsymbol{d}^T\nabla^2 f(\boldsymbol{x})\boldsymbol{d} + o(\|\boldsymbol{d}\|^2) \tag{T2}$$

i.e.

$$f(\boldsymbol{x}+\boldsymbol{d}) = f(\boldsymbol{x}) + \sum_{i=1}^{n}\frac{\partial f(\boldsymbol{x})}{\partial x_i}d_i + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\partial^2 f(\boldsymbol{x})}{\partial x_i \partial x_j}d_i d_j + o(\|\boldsymbol{d}\|^2)$$

Note. (T2) can be obtained by applying (T1) to $g(t) = f(\boldsymbol{x} + t\hat{\boldsymbol{d}})$ at $a = 0$ and $t = \|\boldsymbol{d}\|$, where $\hat{\boldsymbol{d}}$ is the unit vector in the direction $\boldsymbol{d}$, i.e. $\boldsymbol{d} = \|\boldsymbol{d}\|\hat{\boldsymbol{d}}$,

$$g(\|\boldsymbol{d}\|) = g(0) + g'(0)\|\boldsymbol{d}\| + \frac{1}{2}g''(0)\|\boldsymbol{d}\|^2 + o(\|\boldsymbol{d}\|^2)$$

By the chain rule, $g'(0) = \nabla f(\boldsymbol{x})^T\hat{\boldsymbol{d}}, \quad g''(0) = \hat{\boldsymbol{d}}^T\nabla^2 f(\boldsymbol{x})\hat{\boldsymbol{d}}$

# Review: Second-order Taylor expansion

For a quadratic function $f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}^T\boldsymbol{x} + c$, the second-order Taylor expansion is exact with no $o(\|\boldsymbol{d}\|^2)$ term, i.e.

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

Note. This can be used to find the expressions for $\nabla f$ and $\nabla^2 f$.

Assume $A$ is symmetric; otherwise, replace $A$ by $\tilde{A} = \frac{1}{2}(A + A^T)$.

$$\begin{aligned} f(\boldsymbol{x}+\boldsymbol{d}) &= (\boldsymbol{x}+\boldsymbol{d})^T\boldsymbol{A}(\boldsymbol{x}+\boldsymbol{d}) + \boldsymbol{b}^T(\boldsymbol{x}+\boldsymbol{d}) + c \\ &= \boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} + \boldsymbol{d}^T\boldsymbol{A}\boldsymbol{x} + \boldsymbol{x}^T\boldsymbol{A}\boldsymbol{d} + \boldsymbol{d}^T\boldsymbol{A}\boldsymbol{d} + \boldsymbol{b}^T\boldsymbol{x} + \boldsymbol{b}^T\boldsymbol{d} + c \\ &= f(\boldsymbol{x}) + (2\boldsymbol{A}\boldsymbol{x}+\boldsymbol{b})^T\boldsymbol{d} + \frac{1}{2}\boldsymbol{d}^T(2\boldsymbol{A})\boldsymbol{d} \end{aligned}$$

Comparison with the Taylor expansion shows that

$$\nabla f(\boldsymbol{x}) = 2\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}, \quad \nabla^2 f(\boldsymbol{x}) = 2\boldsymbol{A}.$$

# Review: Definite matrices

A matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is positive semidefinite, denoted by $\boldsymbol{A} \succeq \boldsymbol{O}$, if

1. it is symmetric, i.e. $\boldsymbol{A} = \boldsymbol{A}^T$
2. $\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} \geq 0, \forall \boldsymbol{x} \in \mathbb{R}^n$

It is positive definite, denoted by $\boldsymbol{A} \succ \boldsymbol{O}$, if condition 2 is replaced by

2′. $\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} > 0, \forall \boldsymbol{x} \in \mathbb{R}^n$ and $\boldsymbol{x} \neq \boldsymbol{0}$.

Note. For a quadratic form $\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}$, can always assume $\boldsymbol{A}$ is symmetric, since

$$\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} = \boldsymbol{x}^T \boldsymbol{A}^T \boldsymbol{x} = \boldsymbol{x}^T \left( \frac{\boldsymbol{A} + \boldsymbol{A}^T}{2} \right) \boldsymbol{x}$$

$\boldsymbol{A}$ is negative (semi)definite if $-\boldsymbol{A}$ is positive (semi)definite.

$\boldsymbol{A}$ is indefinite if it is neither positive semidefinite nor negative semidefinite, i.e. there exists $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathbb{R}^n$ s.t.

$$\boldsymbol{x}_1^T \boldsymbol{A} \boldsymbol{x}_1 > 0 > \boldsymbol{x}_2^T \boldsymbol{A} \boldsymbol{x}_2$$

# Review: Test for positive definiteness

A vector $\boldsymbol{x}$ is an eigenvector of a matrix $\boldsymbol{A}$ with associated eigenvalue $\lambda$ if

$$\boldsymbol{A}\boldsymbol{x} = \lambda \boldsymbol{x}$$

We can find all eigenvalues by solving $\det(\lambda \boldsymbol{I} - \boldsymbol{A}) = 0$.

Theorem. Let $\boldsymbol{A}$ be a symmetric matrix.

- $\boldsymbol{A} \succ \boldsymbol{O}$ iff all its eigenvalues $\lambda > 0$.
- $\boldsymbol{A} \succeq \boldsymbol{O}$ iff all its eigenvalues $\lambda \geq 0$.

Exmaple. $\boldsymbol{A} = \begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix}$ is positive definite.

$$\det(\lambda \boldsymbol{I} - \boldsymbol{A}) = (\lambda - 1)(\lambda - 5) - 4 = 0 \implies \lambda = 3 \pm 2\sqrt{2} > 0$$

Exmaple. $\boldsymbol{A} = \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}$ is positive semidefinite.

$$\det(\lambda \boldsymbol{I} - \boldsymbol{A}) = (\lambda - 1)(\lambda - 4) - 4 = 0 \implies \lambda_1 = 0, \lambda_2 = 5$$

# Review: Test for positive definiteness

Given matrix $\boldsymbol{A} = (a_{ij}) \in \mathbb{R}^{n\times n}$, a $k \times k$ principal submatrix of $\boldsymbol{A}$ consists of $k$ rows and $k$ columns with the same indices $I = \{i_1 < i_2 < \cdots < i_k\}$,

$$\boldsymbol{A}_I = \begin{pmatrix} a_{i_1 i_1} & \cdots & a_{i_1 i_k} \\ \vdots & \ddots & \vdots \\ a_{i_k i_1} & \cdots & a_{i_k i_k} \end{pmatrix}$$

A principal minor of order $k$ of $\boldsymbol{A}$ is $\det \boldsymbol{A}_I$ for some $I$ with $|I| = k$.

If $I = \{1, 2, \ldots, k\}$, $D_k(\boldsymbol{A}) \triangleq \det \boldsymbol{A}_I$ is called the leading principal minor of order $k$.

Theorem (Sylvester). Let $\boldsymbol{A}$ be a symmetric matrix.

- $\boldsymbol{A} \succ \boldsymbol{O}$ iff $D_k(\boldsymbol{A}) > 0$ for $k = 1, 2, \ldots, n$.
- $\boldsymbol{A} \succeq \boldsymbol{O}$ iff $\det \boldsymbol{A}_I \geq 0$ for all $I \subset \{1, 2, \ldots, n\}$

Note. For positive semidefiniteness, we need to check all principal minors, not just the leading principal minors.

# Review: Test for positive definiteness

Exmaple. $\boldsymbol{A} = \begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix}$ is positive definite.

$$D_1(\boldsymbol{A}) = \det(1) = 1 > 0, \quad D_2(\boldsymbol{A}) = \det \boldsymbol{A} = 1 > 0$$

Example. $\boldsymbol{A} = \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}$ is positive semidefinite.

$$D_1(A) = \det(1) = 1,\ \det \boldsymbol{A}_{\{2\}} = \det(4) = 4,\ D_2(\boldsymbol{A}) = \det \boldsymbol{A} = 0$$

Note. It is not enough to check $D_k(A) \geq 0$ for all $k$!

Example. $\boldsymbol{A} = \begin{pmatrix} 0 & 0 \\ 0 & -2 \end{pmatrix}$ is negative semidefinite,

$$D_1(\boldsymbol{A}) = \det(0) = 0, \quad D_2(\boldsymbol{A}) = \det \boldsymbol{A} = 0,$$

but

$$\det \boldsymbol{A}_{\{2\}} = \det(-2) = -2 < 0$$

# Review: Test for positive definiteness

Exmaple. $\boldsymbol{A} = \begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix}$ is positive definite.

- Use definition,

$$\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} = x_1^2 + 4x_1x_2 + 5x_2^2 = (x_1 + 2x_2)^2 + x_2^2 \geq 0, \quad \forall \boldsymbol{x} \in \mathbb{R}^2$$

with equality $\iff \begin{cases} x_1 + 2x_2 = 0 \\ x_2 = 0 \end{cases} \iff \boldsymbol{x} = 0$

- Find eigenvalues by solving $\det(\lambda \boldsymbol{I} - \boldsymbol{A}) = 0$

$$\det \begin{pmatrix} \lambda - 1 & -2 \\ -2 & \lambda - 5 \end{pmatrix} = (\lambda - 1)(\lambda - 5) - 4 = 0 \implies \lambda = 3 \pm 2\sqrt{2} > 0$$

- Check leading principal minors

$$D_1(\boldsymbol{A}) = \det(1) = 1 > 0, \quad D_2(\boldsymbol{A}) = \det \boldsymbol{A} = 1 > 0$$

# Review: Test for positive definiteness

Exmaple. $\boldsymbol{A} = \begin{pmatrix} 1 & 2 & 1 \\ 2 & 5 & 8 \\ 1 & 8 & 1 \end{pmatrix}$ is not positive definite.

Check leading principal minors

$$D_1(\boldsymbol{A}) = \det(1) = 1 > 0, \quad D_2(\boldsymbol{A}) = \det \begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix} = 1 > 0$$

$$D_3(\boldsymbol{A}) = \det \boldsymbol{A} = 1 \times \begin{vmatrix} 5 & 8 \\ 8 & 1 \end{vmatrix} - 2 \times \begin{vmatrix} 2 & 8 \\ 1 & 1 \end{vmatrix} + 1 \times \begin{vmatrix} 2 & 5 \\ 1 & 8 \end{vmatrix} = -36 < 0$$

Can also check eigenvalues, e.g. using `numpy.linalg.eig`,

$$\lambda_1 = 11.69585173, \quad \lambda_2 = 0.58307572, \quad \lambda_3 = -5.27892745$$

# Review: Eigendecomposition

A symmetric matrix $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ has the following eigendecomposition

$$\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^T = \sum_{i=1}^{n} \lambda_i \boldsymbol{v}_i \boldsymbol{v}_i^T$$

where $\boldsymbol{\Lambda} = \text{diag}\{\lambda_1, \ldots, \lambda_n\}$, $\boldsymbol{Q} = (\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n)$ is an orthogonal matrix, i.e. $\boldsymbol{Q}^T\boldsymbol{Q} = \boldsymbol{Q}\boldsymbol{Q}^T = \boldsymbol{I}$, and $\boldsymbol{A}\boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i$.

Example. $\boldsymbol{A} = \frac{1}{4}\begin{pmatrix} 3 & -1 \\ -1 & 3 \end{pmatrix}$ has eigenvalues $\lambda_1 = \frac{1}{2}$ and $\lambda_2 = 1$, with corresponding eigenvectors $\boldsymbol{v}_1 = \frac{1}{\sqrt{2}}(1,1)^T$ and $\boldsymbol{v}_2 = \frac{1}{\sqrt{2}}(-1,1)^T$. The eigendecomposition is

$$\boldsymbol{A} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}^T + \begin{pmatrix} \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}\begin{pmatrix} \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}^T$$

# Review: Eigendecomposition

Consider the linear transformation $\boldsymbol{x} \mapsto \boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$.

Recall $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n$ form an orthonormal basis of $\mathbb{R}^n$, so

$$\boldsymbol{x} = \boldsymbol{Q}\tilde{\boldsymbol{x}} = \sum_{i=1}^{n} \tilde{x}_i \boldsymbol{v}_i, \quad \boldsymbol{y} = \boldsymbol{Q}\tilde{\boldsymbol{y}} = \sum_{i=1}^{n} \tilde{y}_i \boldsymbol{v}_i$$

where

$$\tilde{\boldsymbol{x}} = \boldsymbol{Q}^T \boldsymbol{x}, \quad \tilde{\boldsymbol{y}} = \boldsymbol{Q}^T \boldsymbol{y},$$

Thus

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x} \iff \boldsymbol{Q}^T \boldsymbol{y} = \boldsymbol{Q}^T \boldsymbol{A}\boldsymbol{Q}\tilde{\boldsymbol{x}} \iff \tilde{\boldsymbol{y}} = \boldsymbol{\Lambda}\tilde{\boldsymbol{x}}$$

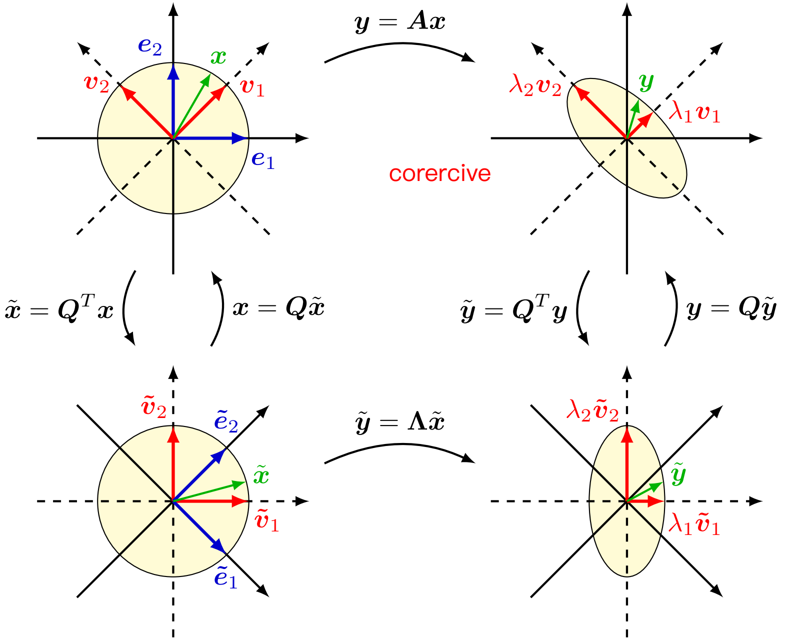
In components,

$$\tilde{x}_i = \boldsymbol{v}_i^T \boldsymbol{x}, \quad \tilde{y}_i = \boldsymbol{v}_i^T \boldsymbol{y}$$

so

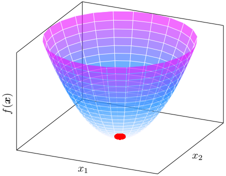
$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x} = \sum_{i=1}^{n} \lambda_i \boldsymbol{v}_i \boldsymbol{v}_i^T \boldsymbol{x} = \sum_{i=1}^{n} (\lambda_i \tilde{x}_i) \boldsymbol{v}_i \iff \tilde{y}_i = \lambda_i \tilde{x}_i$$

# Review: Eigendecomposition



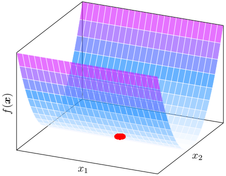
# Review: Geometry of quadratic forms

Quadratic form $f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}$ in $\mathbb{R}^2$



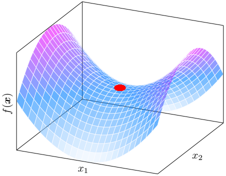

$\boldsymbol{A} = \text{diag}\{1, 1\}$

positive definite



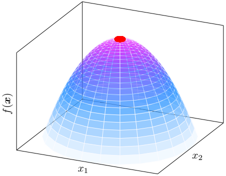

$\boldsymbol{A} = \text{diag}\{0, 1\}$

positive semidefinite



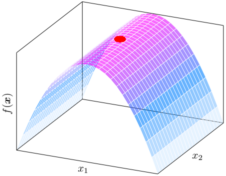

$\boldsymbol{A} = \text{diag}\{1, -1\}$

indefinite




$\boldsymbol{A} = \text{diag}\{-1, -1\}$

negative definite

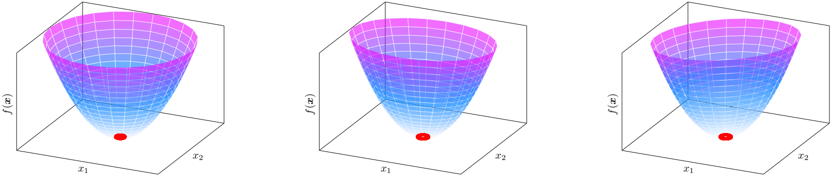



$\boldsymbol{A} = \text{diag}\{-1, 0\}$

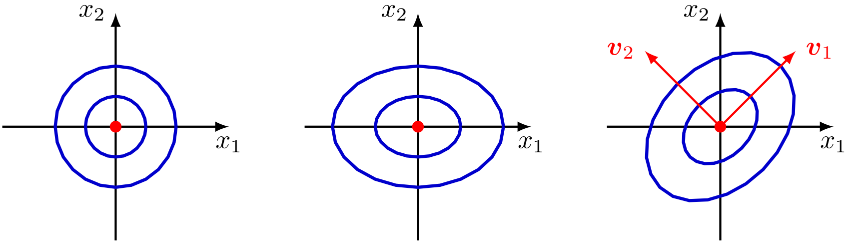
negative semidefinite

# Review: Geometry of quadratic forms

Quadratic form $f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}$ in $\mathbb{R}^2$




$\boldsymbol{A} = \text{diag}\{1, 1\}$ $\quad$ $\boldsymbol{A} = \text{diag}\{\frac{1}{2}, 1\}$ $\quad$ $\boldsymbol{A} = \frac{1}{4}\begin{pmatrix} 3 & -1 \\ -1 & 3 \end{pmatrix}$



# Review: Bounds on quadratic forms

**Proposition.** For a symmetric matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$,

$$\lambda_{\min} \|\boldsymbol{x}\|_2^2 \leq \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} \leq \lambda_{\max} \|\boldsymbol{x}\|_2^2, \quad \forall \boldsymbol{x} \in \mathbb{R}^n$$

where $\lambda_{\max}$ and $\lambda_{\min}$ are the largest and the smallest eigenvalues of $\boldsymbol{A}$, respectively.

**Proof.** Recall that $\boldsymbol{A}$ can be orthogonally diagonalized, i.e. $\boldsymbol{A} = \boldsymbol{Q} \boldsymbol{\Lambda} \boldsymbol{Q}^T$, where $\boldsymbol{\Lambda} = \text{diag}\{\lambda_1, \ldots, \lambda_n\}$ and $\boldsymbol{Q}^T \boldsymbol{Q} = \boldsymbol{I}$. Let $\boldsymbol{x} = \boldsymbol{Q} \tilde{\boldsymbol{x}}$.

$$\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} = \tilde{\boldsymbol{x}}^T (\boldsymbol{Q}^T \boldsymbol{A} \boldsymbol{Q}) \tilde{\boldsymbol{x}} = \tilde{\boldsymbol{x}}^T \boldsymbol{\Lambda} \tilde{\boldsymbol{x}} = \sum_{i=1}^n \lambda_i \tilde{x}_i^2 \leq \sum_{i=1}^n \lambda_{\max} \tilde{x}_i^2 = \lambda_{\max} \|\tilde{\boldsymbol{x}}\|_2^2$$

Then use the fact that orthogonal transformations preserve 2-norm, i.e.

$$\|\boldsymbol{x}\|_2^2 = \boldsymbol{x}^T \boldsymbol{x} = (\boldsymbol{Q}\tilde{\boldsymbol{x}})^T (\boldsymbol{Q}\tilde{\boldsymbol{x}}) = \tilde{\boldsymbol{x}}^T (\boldsymbol{Q}^T \boldsymbol{Q}) \tilde{\boldsymbol{x}} = \tilde{\boldsymbol{x}}^T \tilde{\boldsymbol{x}} = \|\tilde{\boldsymbol{x}}\|_2^2.$$

Similarly for $\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} \geq \lambda_{\min} \|\boldsymbol{x}\|_2^2$.

# Second-order necessary condition

Theorem. If $f : \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable and $\boldsymbol{x}^*$ is a local minimum of $f$, then its Hessian matrix $\nabla^2 f(\boldsymbol{x}^*)$ is positive semidefinite, i.e.

$$\boldsymbol{d}^T \nabla^2 f(\boldsymbol{x}^*) \boldsymbol{d} \geq 0, \quad \forall \boldsymbol{d} \in \mathbb{R}^n$$

Proof. Fix $\boldsymbol{d} \in \mathbb{R}^n$. By the first-order necessary condition, $\nabla f(\boldsymbol{x}^*) = \boldsymbol{0}$. By the second-order Taylor expansion, for any $t > 0$,

$$f(\boldsymbol{x}^* + t\boldsymbol{d}) = f(\boldsymbol{x}^*) + \frac{t^2}{2} \boldsymbol{d}^T \nabla^2 f(\boldsymbol{x}) \boldsymbol{d} + o(t^2 \|\boldsymbol{d}\|^2) \geq f(\boldsymbol{x}^*)$$

So

$$\frac{1}{2} \boldsymbol{d}^T \nabla^2 f(\boldsymbol{x}) \boldsymbol{d} + o(\|\boldsymbol{d}\|^2) \geq 0$$

Taking the limit $t \to 0$ yields $\boldsymbol{d}^T \nabla f(\boldsymbol{x}^*) \boldsymbol{d}^T \geq 0$.

Note. Can apply the same argument to $g(t) = f(\boldsymbol{x}^* + t\boldsymbol{d})$ with local minimum $t^* = 0$ and use chain rule to obtain $g''(0) = \boldsymbol{d}^T \nabla^2 f(\boldsymbol{x}^*) \boldsymbol{d} \geq 0$.

# Second-order sufficient condition

Theorem. Suppose $f$ is twice continuously differentiable. If

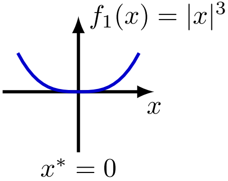
1. $\nabla f(\boldsymbol{x}^*) = 0$
2. $\nabla^2 f(\boldsymbol{x}^*)$ is positive definite, i.e.

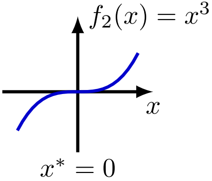
$$\boldsymbol{d}^T \nabla^2 f(\boldsymbol{x}^*) \boldsymbol{d} > 0, \quad \forall \boldsymbol{d} \neq \boldsymbol{0}$$

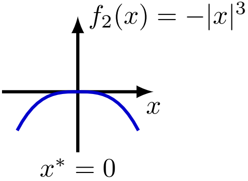
then $\boldsymbol{x}^*$ is a local minimum.

Proof. Use second-order Tayler expansion.

Note. In condition 2, positive definiteness cannot be replaced by positive semidefiniteness.

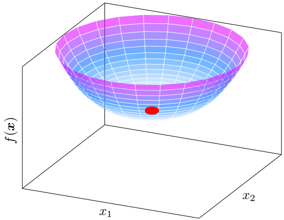


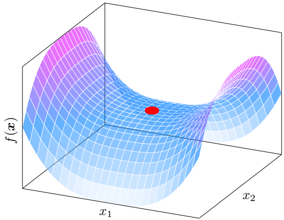



# Second-order sufficient condition (cont'd)

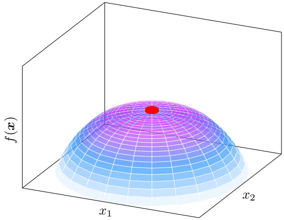
$\nabla f(\mathbf{0}) = \mathbf{0}$ and $\nabla^2 f(\mathbf{0}) = \boldsymbol{O}$ for all examples below.



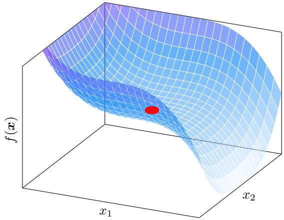

$$f(\boldsymbol{x}) = |x_1|^3 + |x_2|^3$$




$$f(\boldsymbol{x}) = |x_1|^3 - |x_2|^3$$




$$f(\boldsymbol{x}) = -|x_1|^3 - |x_2|^3$$




$$f(\boldsymbol{x}) = -x_1^3 + |x_2|^3$$