# Lecture 5-6

## CM50264: Machine Learning 1

## Optimization Basics 1

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# Previously in decision trees ...

We are given a dataset

$$D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\} \subset \mathcal{X} \times \mathcal{Y} \subset \mathbb{R}^n \times \mathbb{R}.$$

Training a decision tree:

- Grow a tree from a rootnote.
- At each node, *split* the data into *children* nodes.
- Splits are chosen using a splitting criterion, e.g. the information gain ($IG$).

At each splitting stage, a single feature $x_*$ is selected from $n$-possible features $\{x^1, \ldots, x^n\}$ ($\mathbf{x} = [x^1, \ldots, x^n]^\top$) by

- evaluating $IG(x^i)$ for each feature $x^i$.
- selecting the index $i$ that achieves the highest information gain $IG$.

# Previously in decision trees ...

A single feature $x^*$ is selected from $n$-possible features $\{x^i\}_{i=1}^n$ ($\mathbf{x} = [x^1, \ldots, x^n]^\top$) by

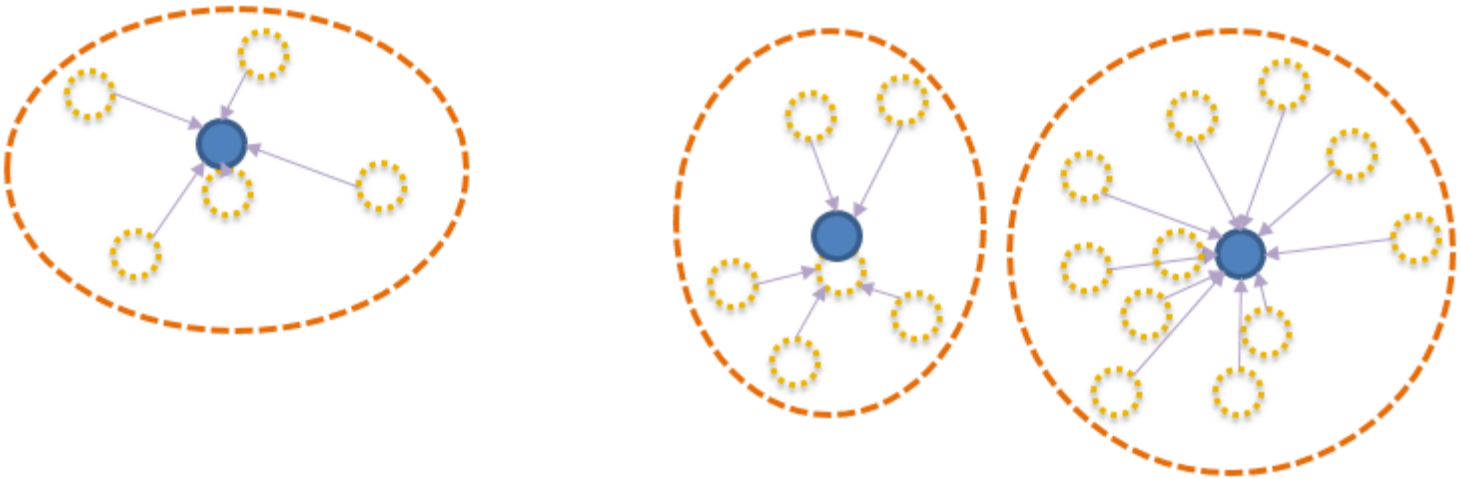
- evaluating the information gain $IG(x^i)$ for each feature $x^i$.
- selecting the index $i$ that achieves the highest information gain $IG$.

Let's formalize this ...

- We are given a candidate set $\mathcal{C} = \{x^1, \ldots, x^n\}$ and a function $IG : \mathcal{X} \to \mathbb{R}$.
- The optimal feature $x^*$ is found by maximizing $IG$:

$$x^* = \arg\max_{x \in \mathcal{C}} IG(x).$$

# In W4 clustering ...



Given a dataset $D = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{R}^n$, our goal is to find cluster centers $\{\mathbf{c}_1, \mathbf{c}_2, \mathbf{c}_3\} \subset \mathbb{R}^n$ that minimizes the average quantization (or reconstruction) error:

$$\mathcal{O}(\{\mathbf{c}_1, \mathbf{c}_2, \mathbf{c}_3\}) = \sum_{i=1}^{N} \|\mathbf{x}_i - \mathbf{c}(\mathbf{x}_i)\|^2.$$

# Regression problem ...

We are given a training dataset

$$D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\} \subset \mathcal{X} \times \mathcal{Y} \subset \mathbb{R}^n \times \mathbb{R}.$$

Our goal is to find a function

$$f : \mathbb{R}^n \to \mathbb{R}$$

such that its output $f(\mathbf{x}')$ for an unseen input $\mathbf{x}' \notin D$ is close to the underlying ground-truth output $y'$:

We want to find a function $f^*$ that minimizes

$$\int l(f(\mathbf{x}), y) dP(\mathbf{x}, y),$$

for a loss function $l(\cdot, \cdot) : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$, e.g.

$$l(f(\mathbf{x}), y) = (f(\mathbf{x}) - y)^2.$$

# Regression problem ...

$$D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\} \subset \mathcal{X} \times \mathcal{Y} \subset \mathbb{R}^n \times \mathbb{R}.$$

We wish to minimize

$$\mathcal{O}(f) = \int (f(\mathbf{x}) - y)^2 dP(\mathbf{x}, y).$$

However, in practice, we do not have access to the underlying data generation process $P(\mathbf{x}, y)$.

Instead, we minimize the empirical mean squared error:

$$\mathcal{O}'(f) = \frac{1}{N} \sum_{i=1}^{N} (f(\mathbf{x}_i) - y_i)^2.$$

# Regression problem ...

Our objective function

$$\mathcal{O}'(f) = \frac{1}{N}\sum_{i=1}^{N}(f(\mathbf{x}_i) - y_i)^2.$$

Our goal is to find a function $f^* : \mathbb{R}^n \to \mathbb{R}$ that minimizes $\mathcal{O}'$:

$$f^* = \underset{f \in \text{All possible functions from } \mathbb{R}^n \text{ to } \mathbb{R}}{\arg\min} \mathcal{O}'(f).$$

A related problem:

$$f^* = \underset{f \in \text{All continuous functions from } \mathbb{R}^n \text{ to } \mathbb{R}}{\arg\min} \mathcal{O}'(f).$$

Another related problem:

$$f^* = \underset{f \in \text{All linear functions from } \mathbb{R}^n \text{ to } \mathbb{R}}{\arg\min} \mathcal{O}'(f).$$

# Regression problem ...

$$f^* = \underset{f \in \text{All linear functions from } \mathbb{R}^n \text{ to } \mathbb{R}}{\arg\min} \mathcal{O}'(f). \tag{1}$$

A linear function $f : \mathbb{R}^n \to \mathbb{R}$ is represented as

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}.$$

A linear function $f$ is uniquely determined by a vector $\mathbf{w}$:
$f$ is *parametrized* by $\mathbf{w} \in \mathbb{R}^n$.

Problem (1) is equivalent to

$$\begin{aligned}\mathbf{w}^* &= \underset{\mathbf{w} \in \mathbb{R}^n}{\arg\min} \frac{1}{N} \sum_{i=1}^{N} (f(\mathbf{x}_i) - y_i)^2 \\ &= \underset{\mathbf{w} \in \mathbb{R}^n}{\arg\min} \frac{1}{N} \sum_{i=1}^{N} (\mathbf{w}^\top \mathbf{x}_i - y_i)^2.\end{aligned}$$

# Why optimization?

- Many (most) machine learning problems are eventually formulated as optimization, e.g.
  - Training decision trees.
  - Training linear (or nonlinear) regression.
  - Discovering cluster structure.
  - Training neural networks.
  - Gunnar Rätsch, "*Machine learning is statistics combined with optimization.*"
- A typical procedure for solving a machine learning problem is
  - (I) Reformulate the problem into an optimization: a (objective) function $f$ and its parameters $\mathbf{x}$.
  - (II) Simplify the optimization problem, if necessary.
  - (III) Choose a proper optimization algorithm.

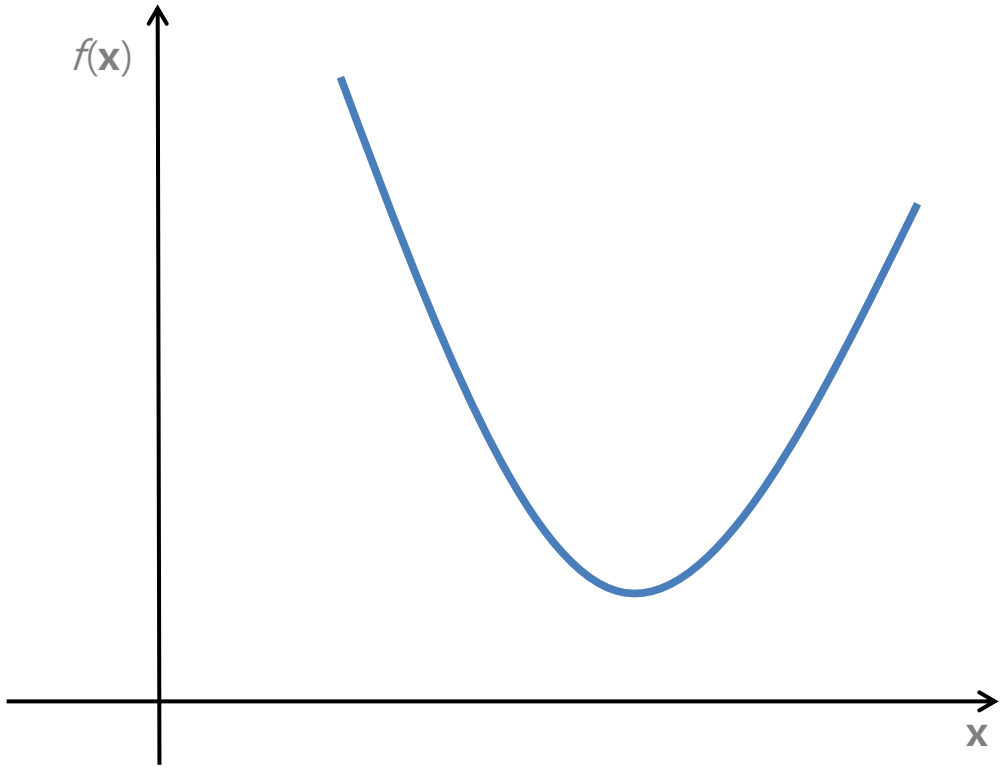
# Previously in decision trees ...

- A single feature $x^*$ is selected from $n$-possible features $\{x^i\}_{i=1}^n$ by
  - evaluating the information gain $IG(x^i)$ for each feature $x^i$.
  - selecting the index $i$ that achieves the highest information gain $IG$.
- Equivalently,
  - We are given a candidate set $\mathcal{C} = \{x^1, \ldots, x^n\}$ and a function $IG : \mathcal{X} \to \mathbb{R}$.
  - The best solution $x^*$ is obtained as the maximizer of $IG$:

$$x^* = \arg\max_{x \in \mathcal{C}} IG(x).$$

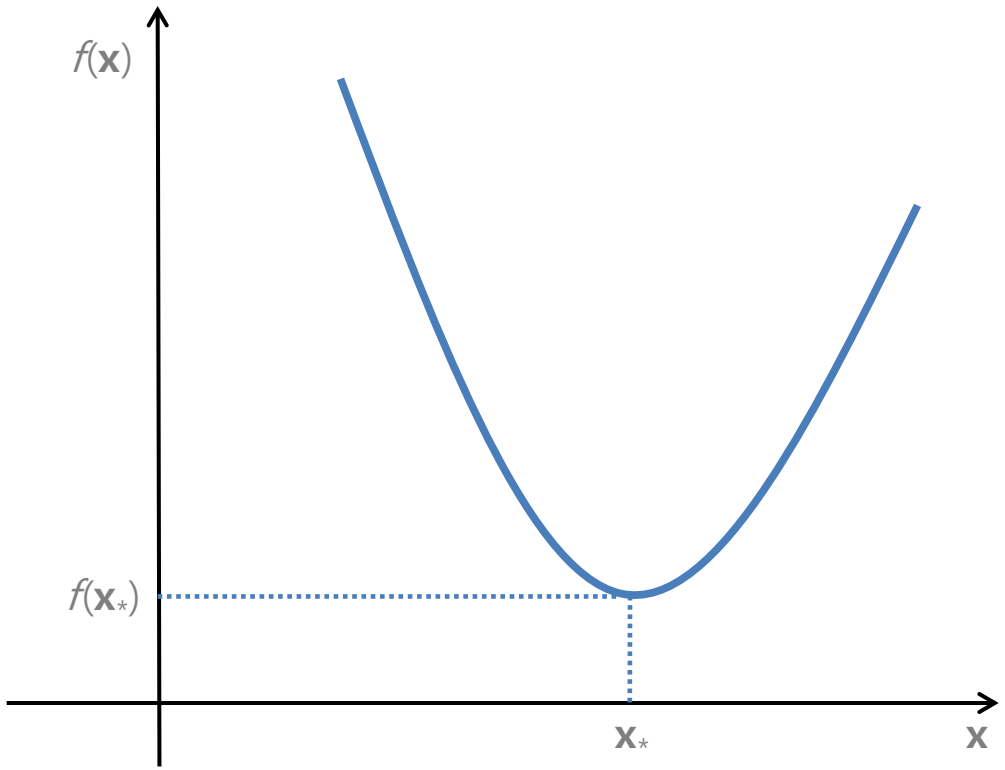
- We solved this optimization problem by evaluating $IG$ of all candidates in $\mathcal{C}$;
  Impossible when $|\mathcal{C}| = \infty$.

# A simple 1D optimization (minimization) problem



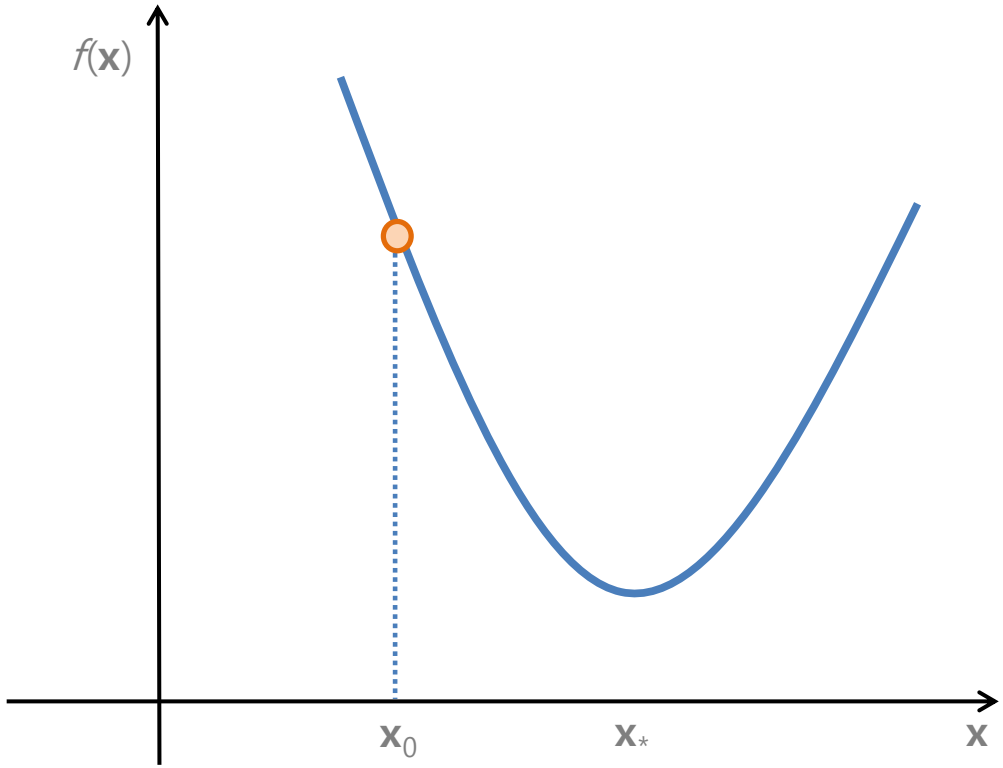

Our objective function $f$ is one-dimensional: $f : \mathbb{R} \to \mathbb{R}$.

# A simple 1D optimization (minimization) problem



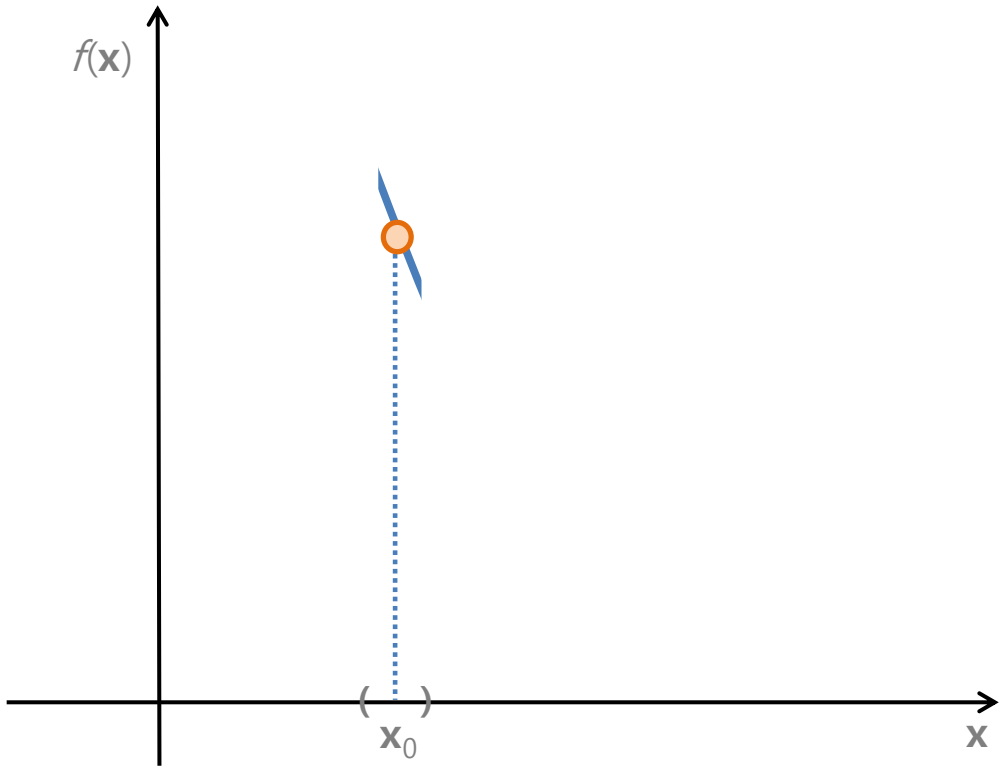

Visually inspecting the graph of $f$ shows that $\mathbf{x}_*$ is the optimum point.
For general high-dimensional problems ($f : \mathbb{R}^n \to \mathbb{R}$), this approach is not applicable.

# A simple 1D optimization (minimization) problem



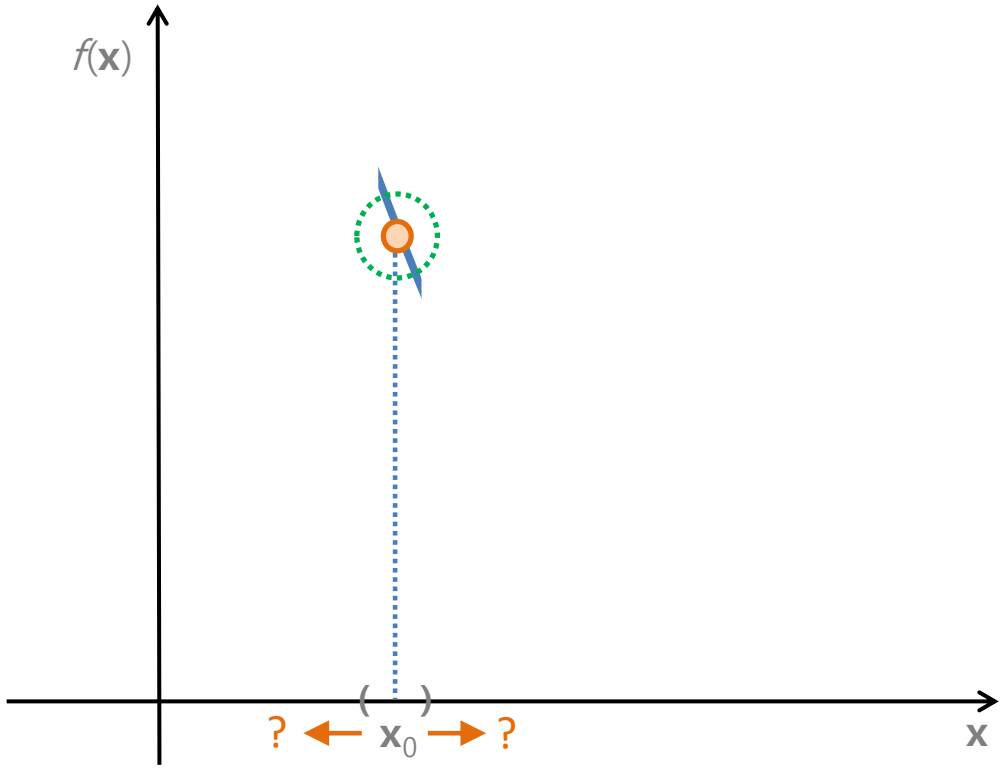

An iterative optimization method starts with an initial guess (or the initial solution) $\mathbf{x}_0$.

# A simple 1D optimization (minimization) problem



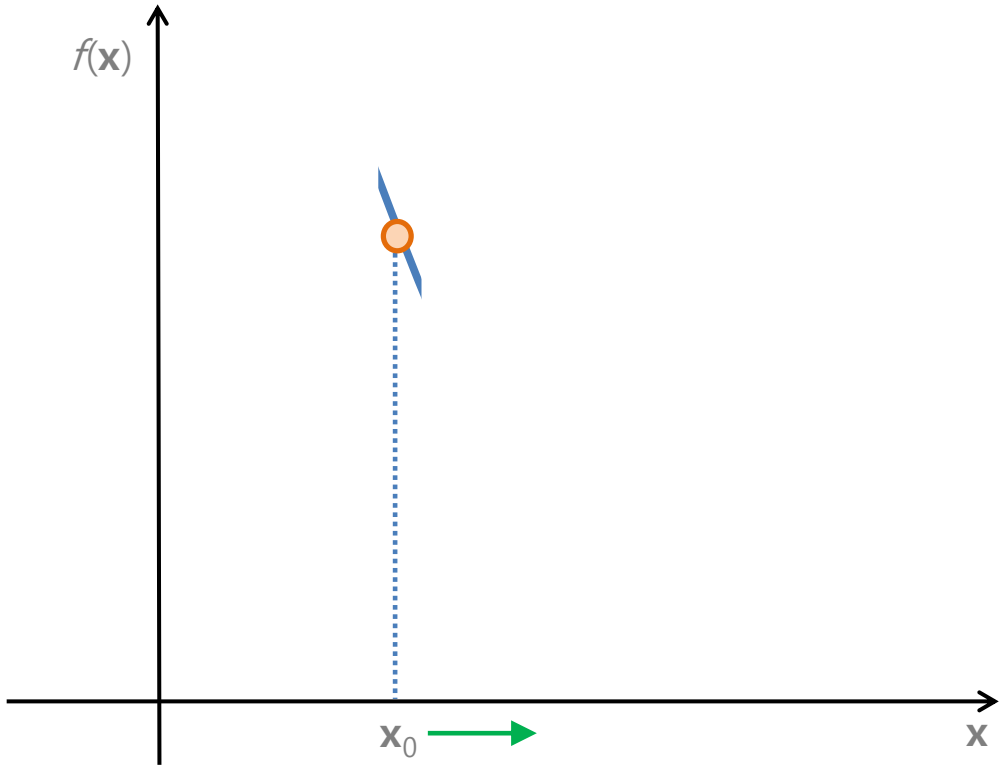

We cannot see the entire graph of $f$.
Instead, we can observe $f$ in a (very small) local neighborhood of the zero-th solution $\mathbf{x}_0$.

# A simple 1D optimization (minimization) problem




By inspecting $f$ values around $\mathbf{x}_0$, we can decide which direction to explore.

# A simple 1D optimization (minimization) problem

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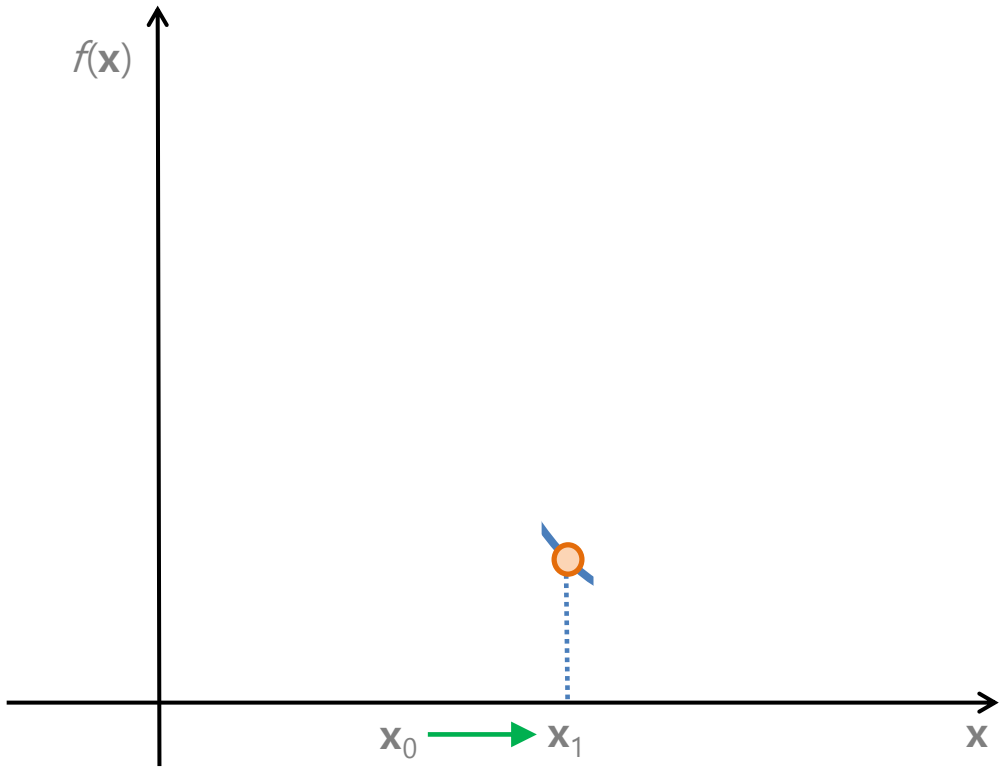
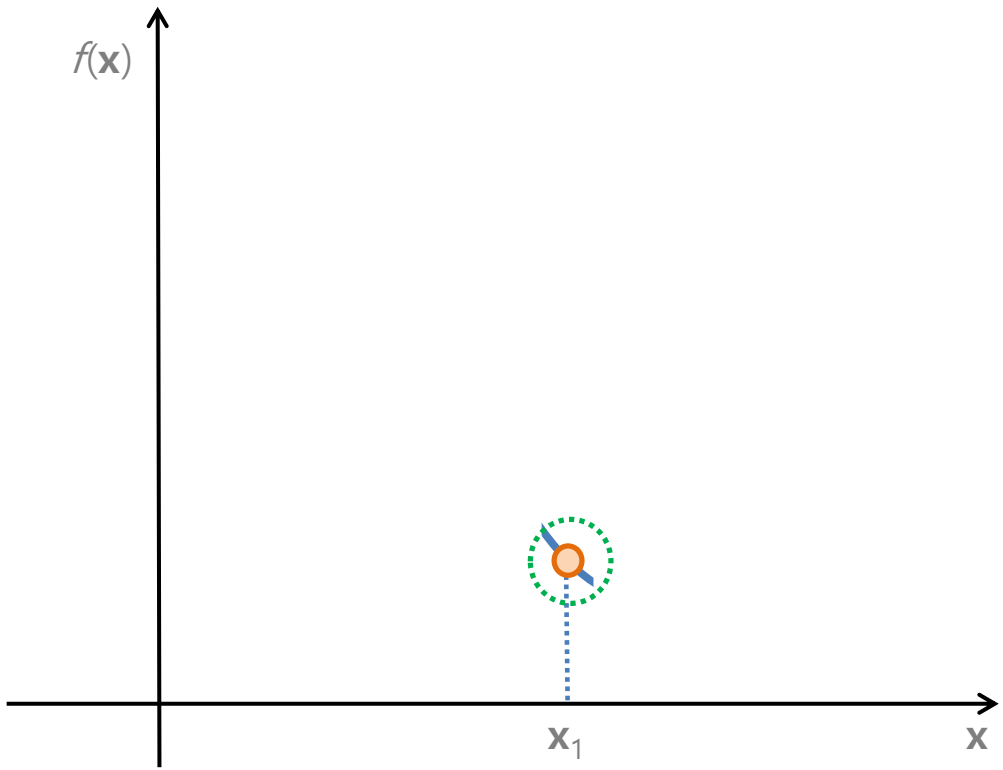
# A simple 1D optimization (minimization) problem



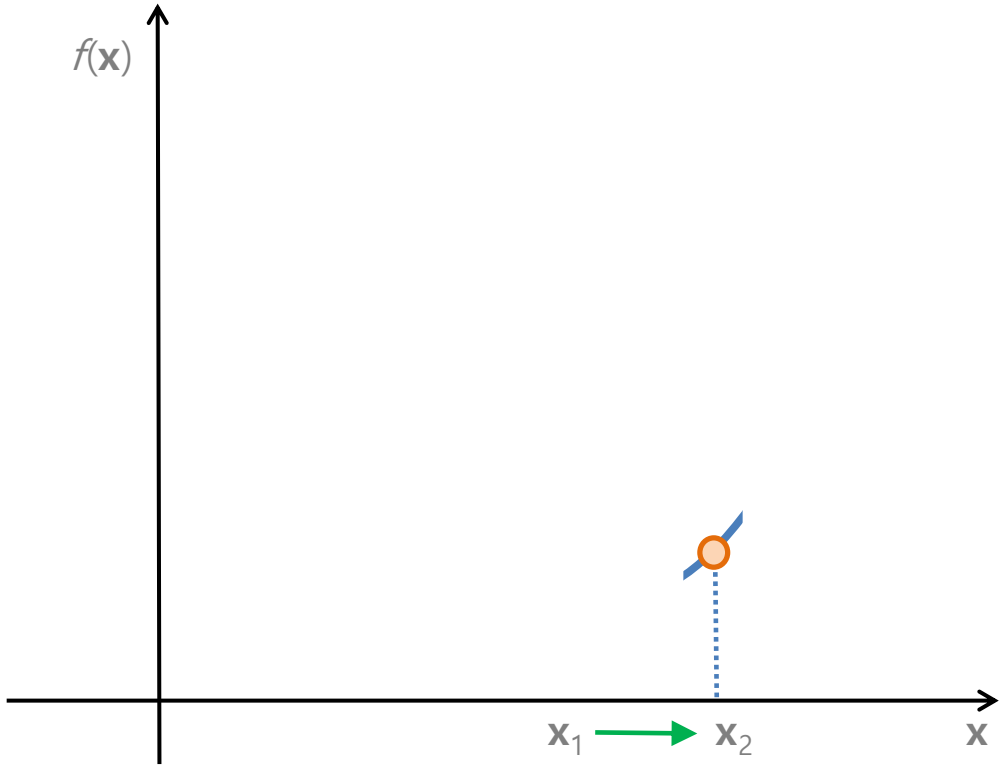

Now we are at the first solution $\mathbf{x}_1$.

# A simple 1D optimization (minimization) problem



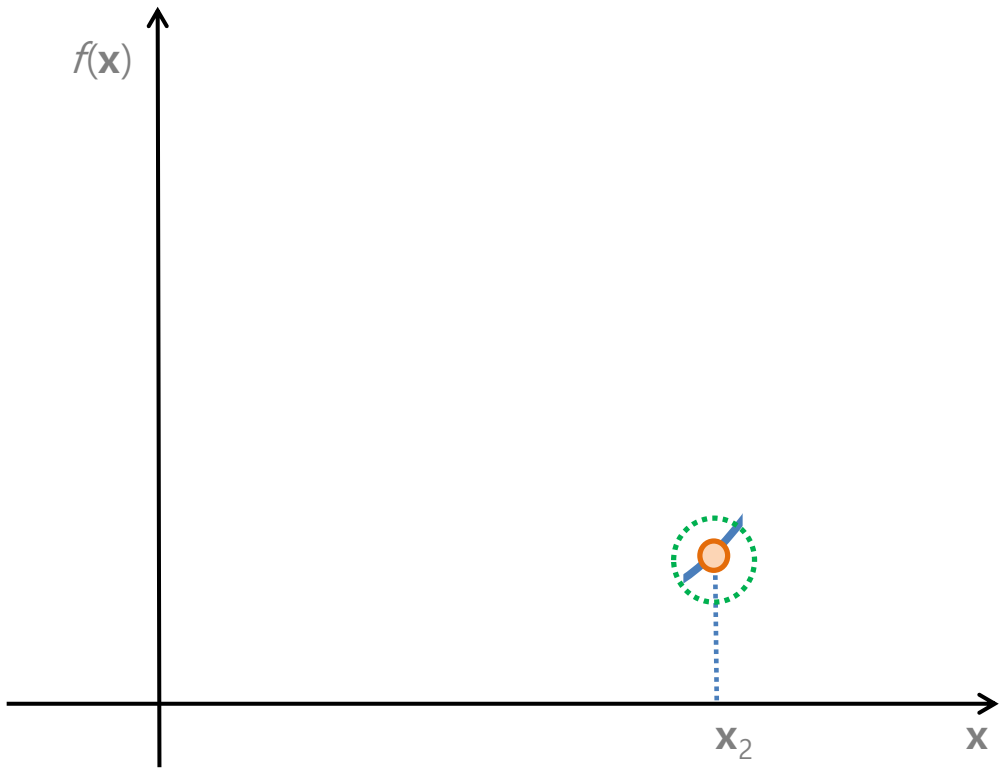

Again, observing $f$ in a neighborhood, we decide the next direction to move.

# A simple 1D optimization (minimization) problem



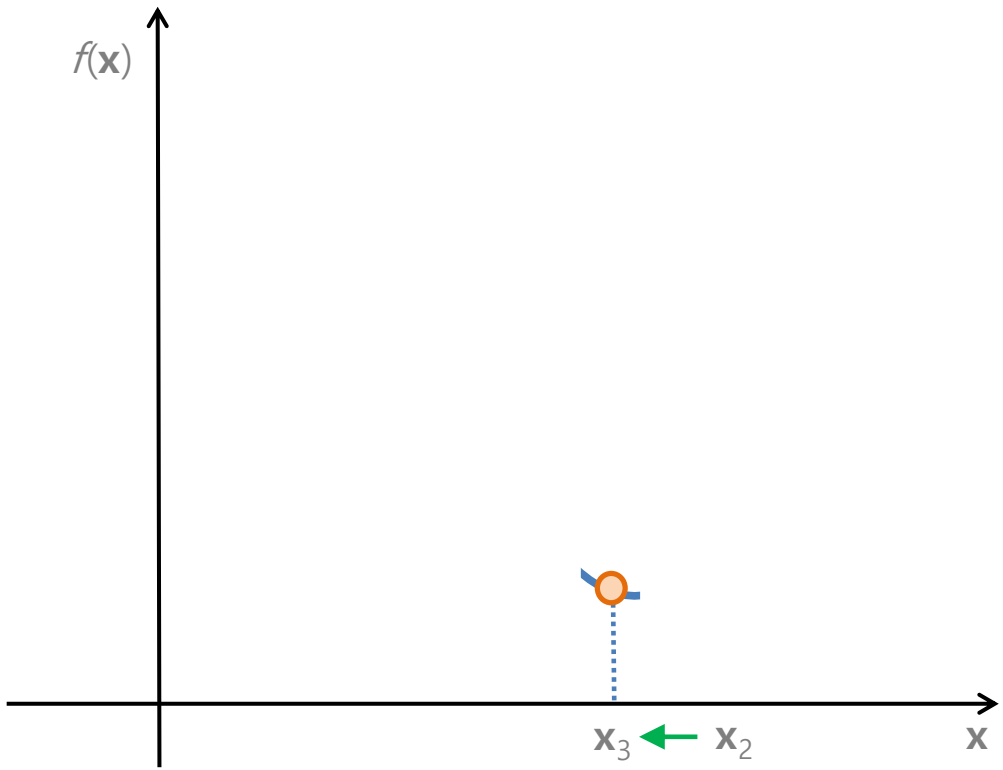

Now we are at the second solution $\mathbf{x}_2$.

# A simple 1D optimization (minimization) problem



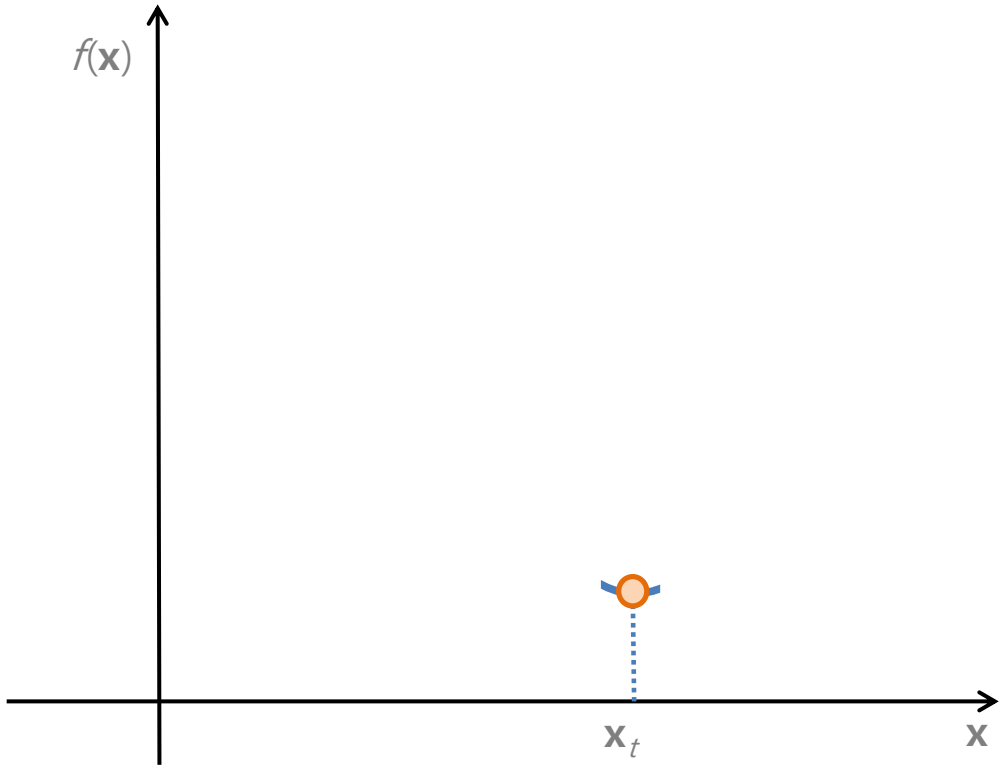

Decide the next direction to move.

# A simple 1D optimization (minimization) problem



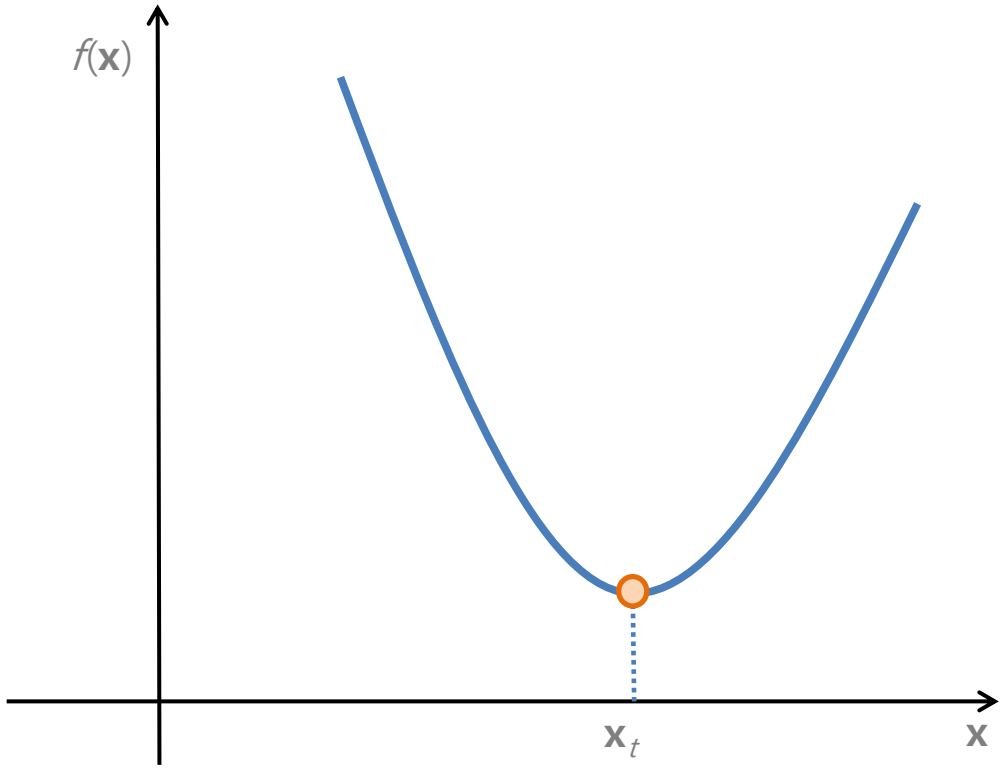

Decide the next direction to move.

# A simple 1D optimization (minimization) problem



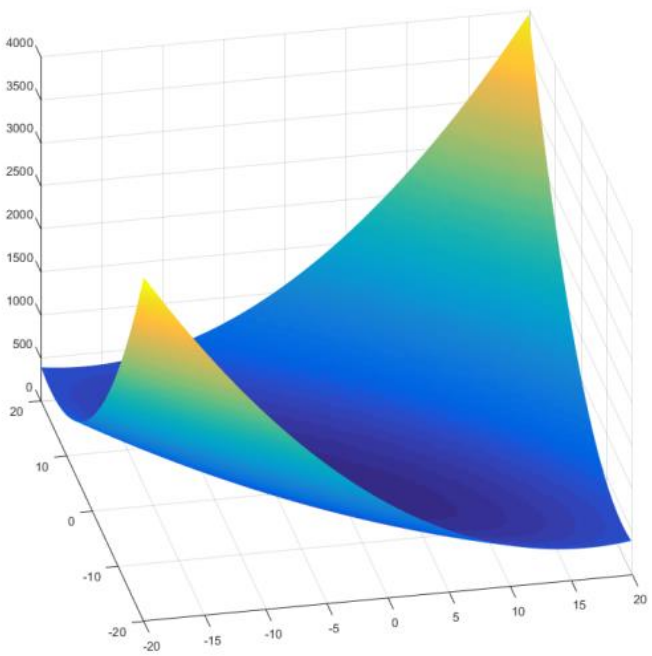

After a few iterations, we arrive at the optimum $\mathbf{x}_t = \mathbf{x}_*$.

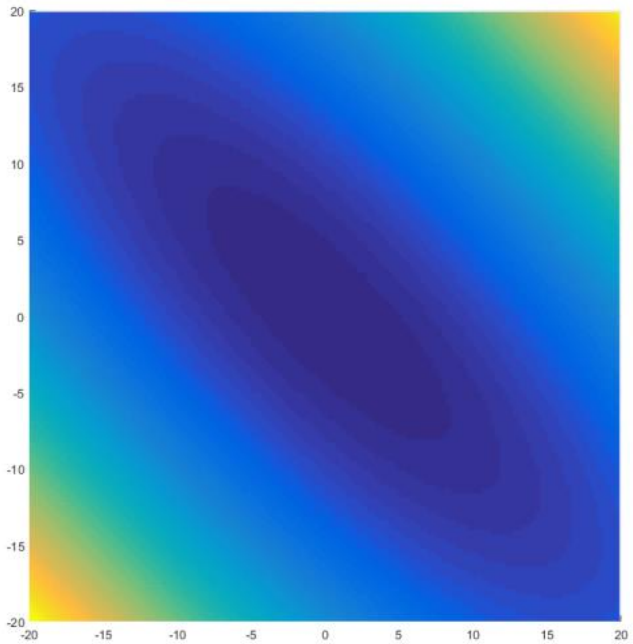
# A simple 1D optimization (minimization) problem




After a few iterations, we arrive at the optimum $\mathbf{x}_t = \mathbf{x}_*$.

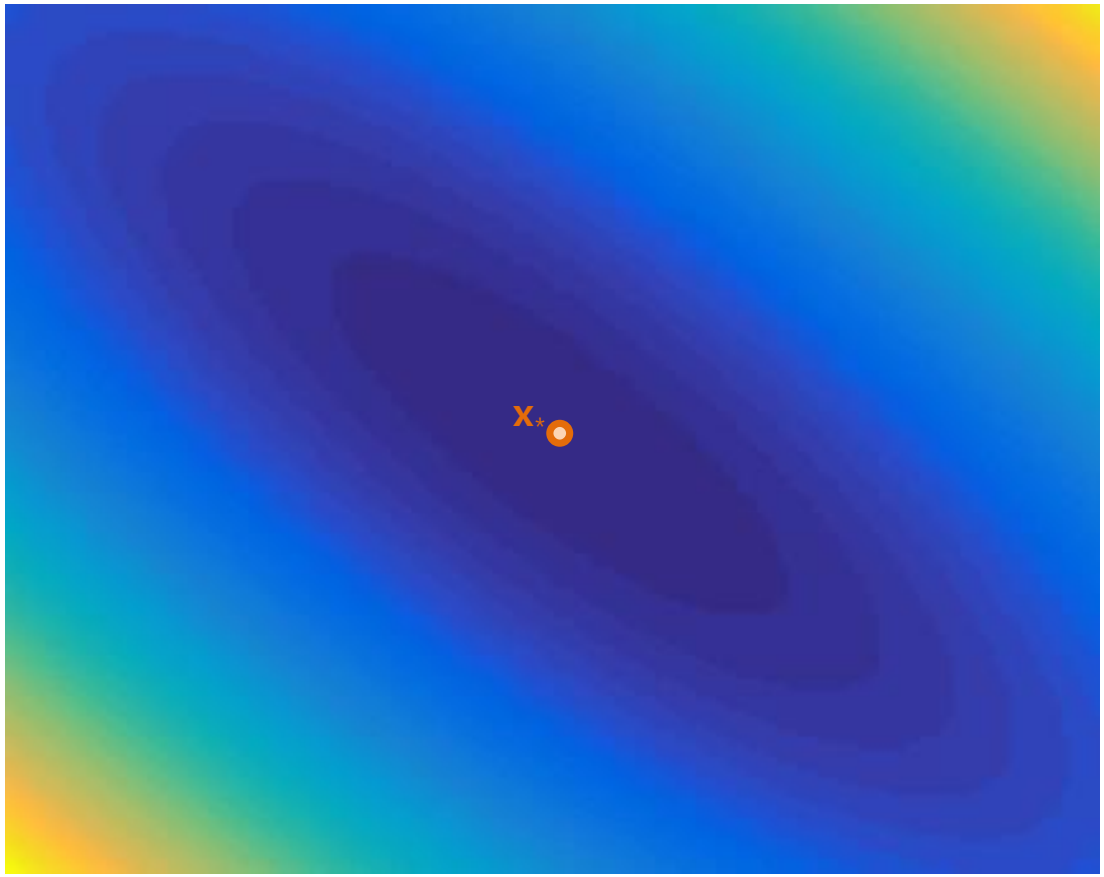
# A simple 2D optimization problem




Our objective function $f$ is two-dimensional: $f : \mathbb{R}^2 \to \mathbb{R}$.

# A simple 2D optimization problem

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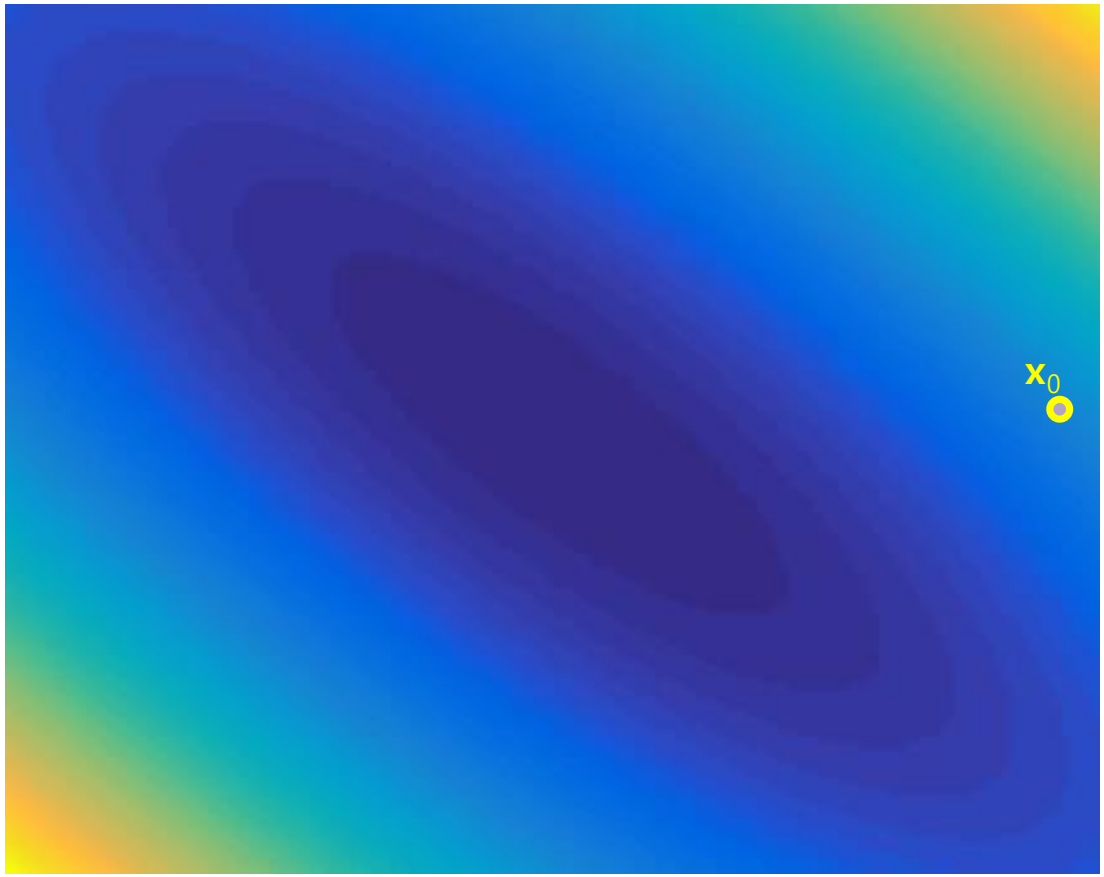
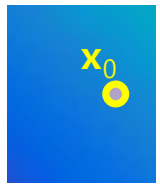
# A simple 2D optimization problem



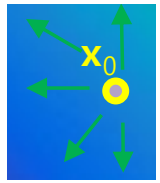

We start the optimization with an initial (zero-th) solution $\mathbf{x}_0$.

# A simple 2D optimization problem



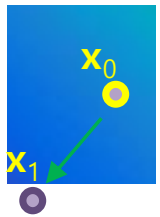

Again, we can observe $f$ only in a small neighborhood of $\mathbf{x}_0$.

# A simple 2D optimization problem




By inspecting $f$ around $\mathbf{x}_0$ ...

# A simple 2D optimization problem

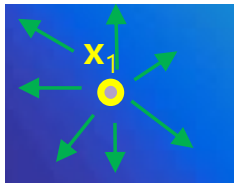



We decide a direction to move (to decrease the $f$ value).

# A simple 2D optimization problem

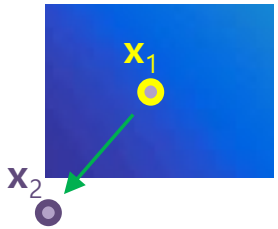







Now we are at the first solution $\mathbf{x}_1$, and observing $f$ around ...

# A simple 2D optimization problem

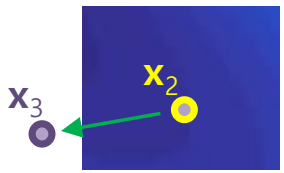



and decide a new direction ...

# A simple 2D optimization problem





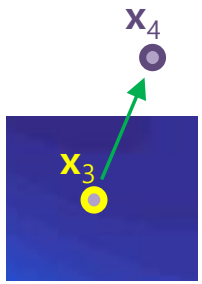



From the second solution to the third ...

# A simple 2D optimization problem

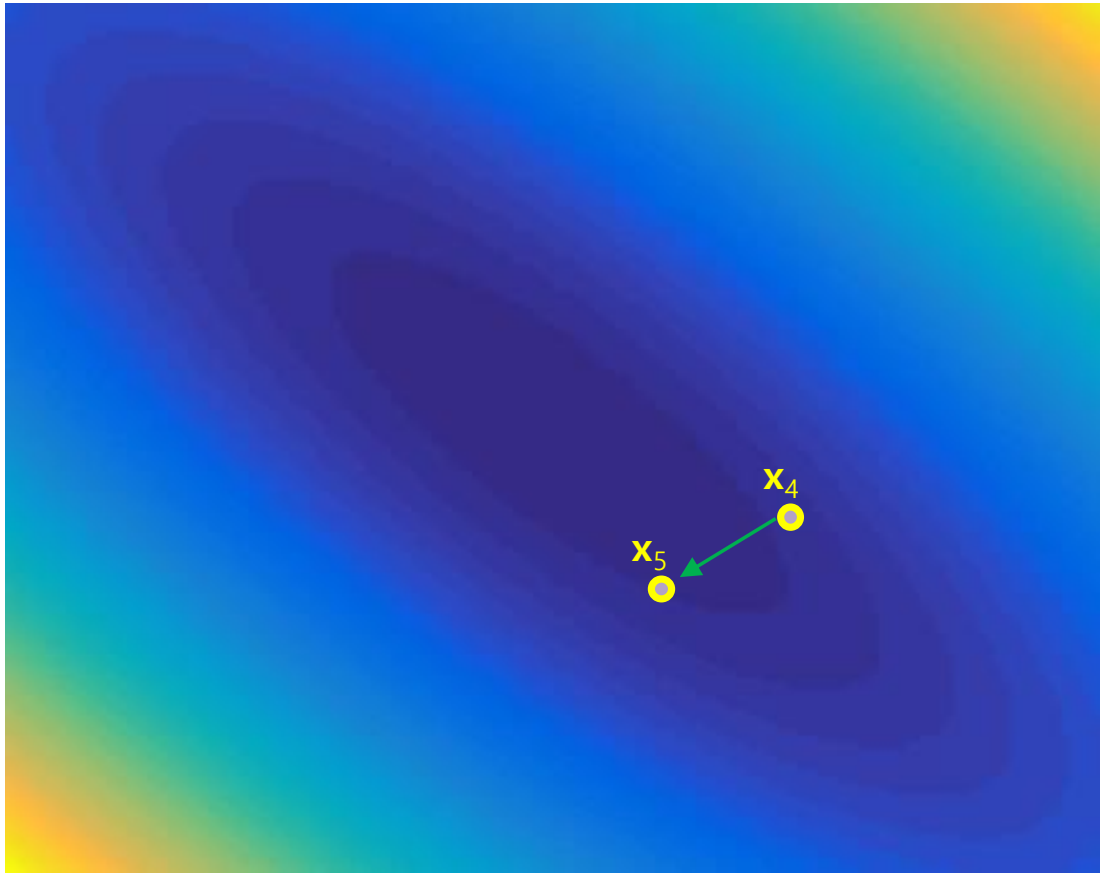






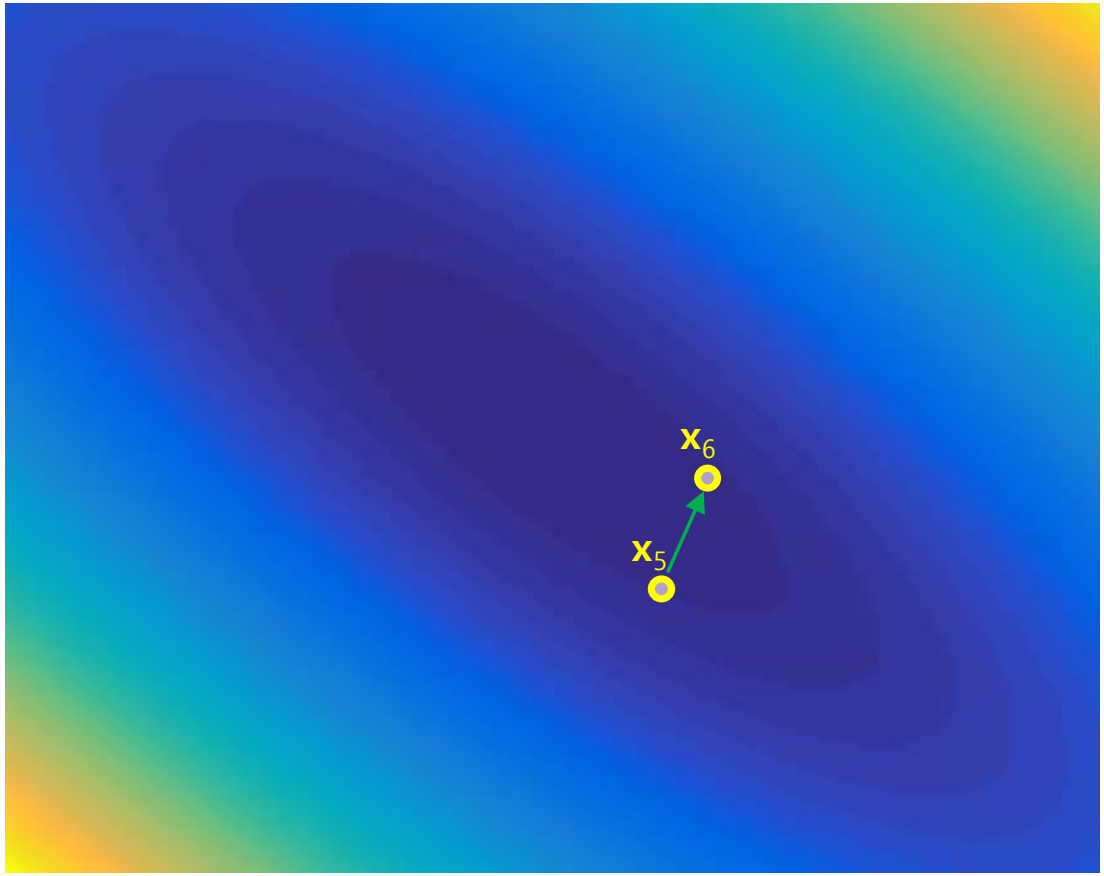

from the third solution to the fourth ...

# A simple 2D optimization problem



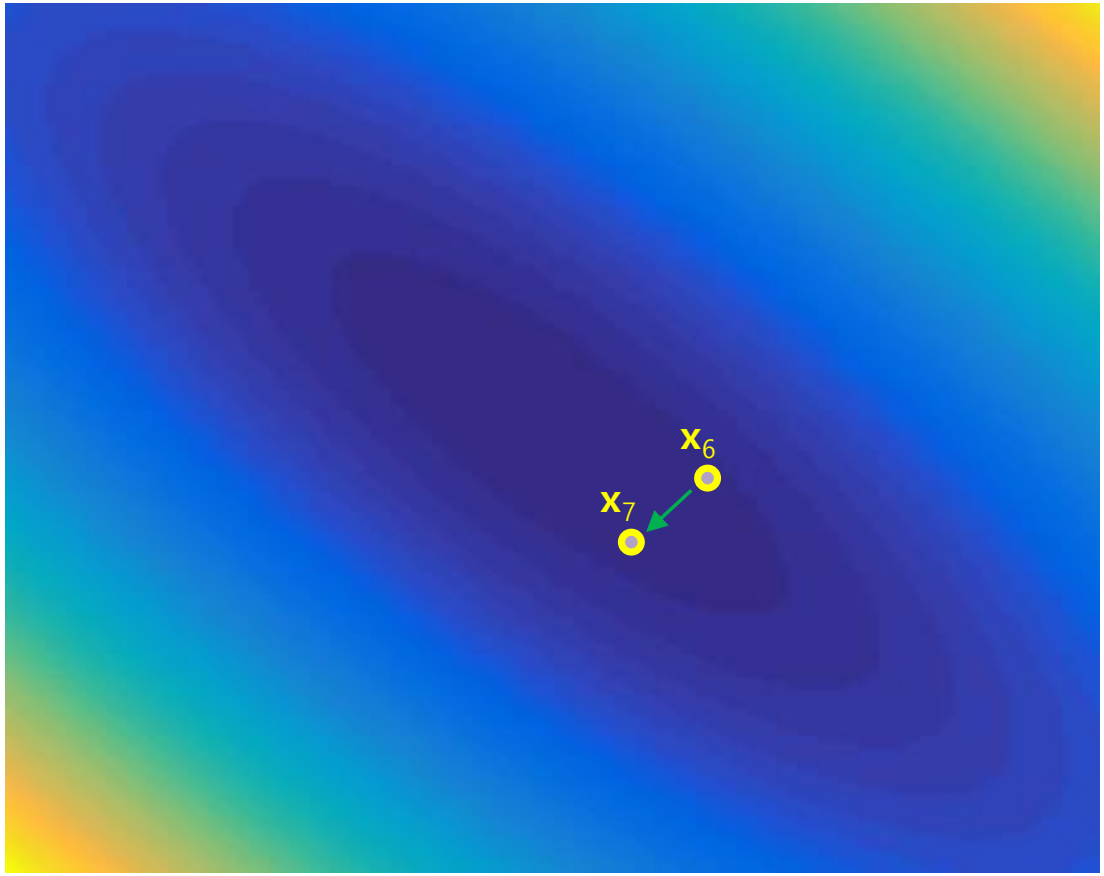

from $\mathbf{x}_4$ to $\mathbf{x}_5$ ...

# A simple 2D optimization problem



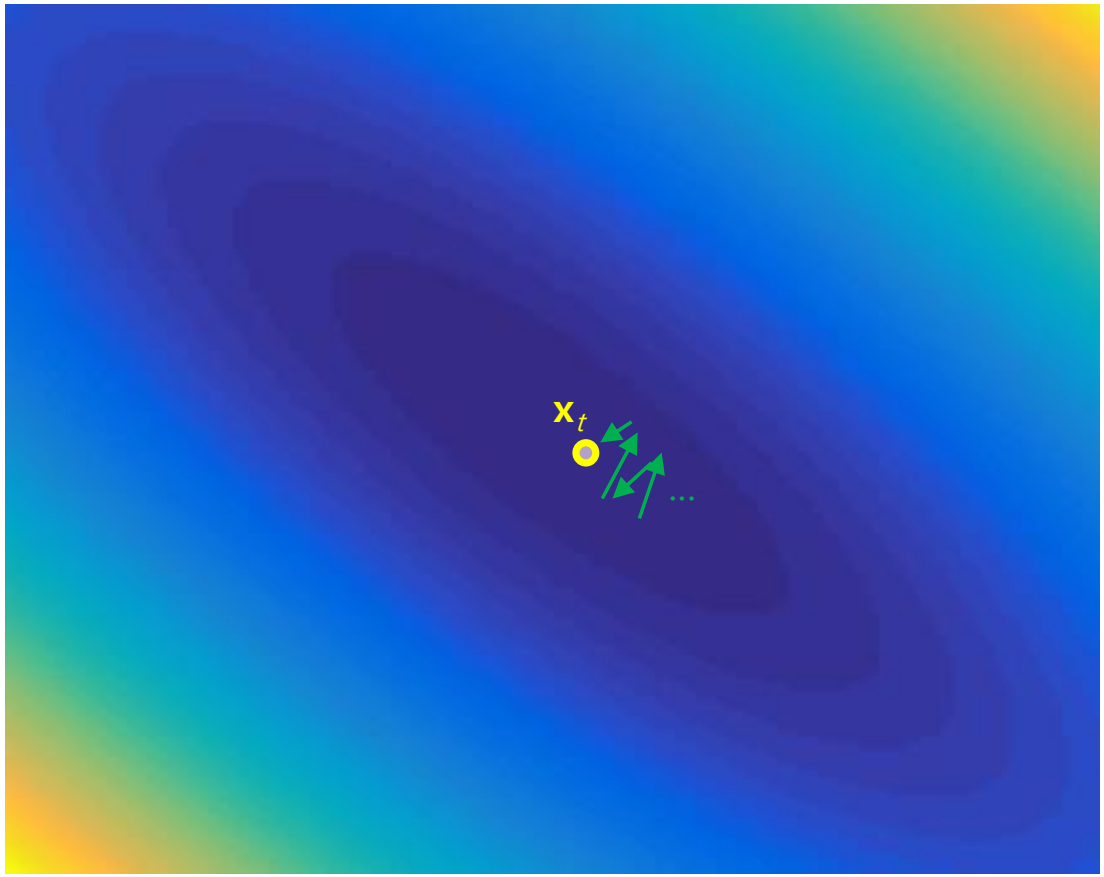

from $\mathbf{x}_5$ to $\mathbf{x}_6$ ...

# A simple 2D optimization problem




from $\mathbf{x}_6$ to $\mathbf{x}_7$ ...

# A simple 2D optimization problem




After a few iterations, we arrive at the optimum $\mathbf{x}_t = \mathbf{x}_*$.

# Iterative descent algorithm



Summarizing our optimization approach...

(I) $t = 0$; Make an initial guess $\mathbf{x}_t$;

(II) Iterate until the termination condition is met.

(i) Find a direction $\mathbf{p}_t$ to move;

(ii) Decide how much ($\alpha_t$) to move along $\mathbf{p}_t$ direction;

(iii) $\mathbf{x}_{t+1} = \mathbf{x}_t + \alpha_t \mathbf{p}_t$;

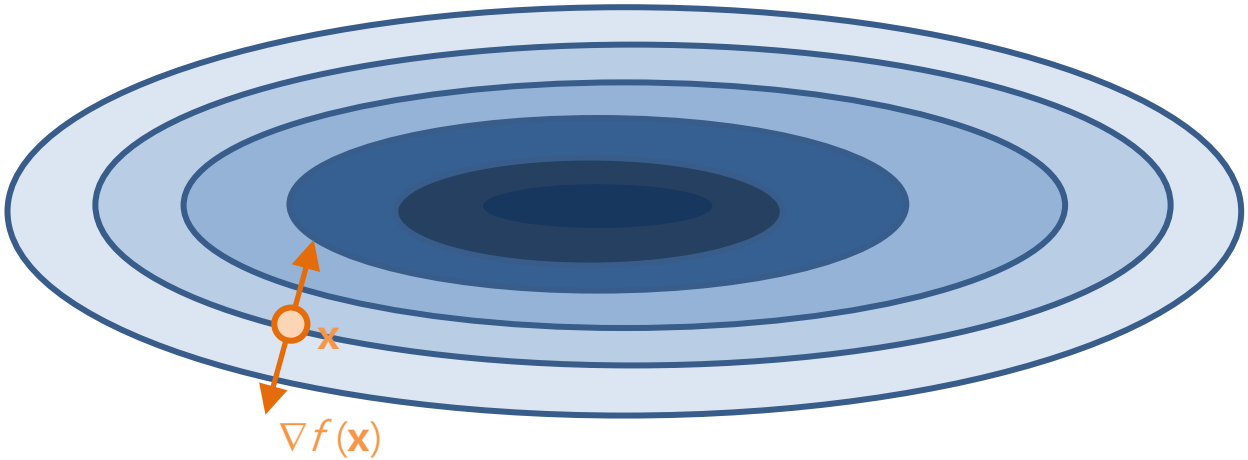
(iv) $t = t + 1$;

How do we decide

- direction to move $\mathbf{p}_t$,
- step size $\alpha_t$,
- when to stop (termination condition)?

# Steepest descent

- How do we decide the direction $\mathbf{p}_t$ to move?
- Steepest descent algorithm chooses the direction along which $f$ decreases most rapidly.
- $f$ increases most rapidly along the gradient $\nabla f$ direction: $\mathbf{p}_t = -\nabla f(\mathbf{x}_t)$.



# Steepest descent



How do we know that $f$ increases most rapidly along $\nabla f$?

Applying Taylor's theorem,

$$f(\mathbf{x}+\alpha\mathbf{p}) = f(\mathbf{x}) + \alpha\mathbf{p}^\top\nabla f(\mathbf{x}) + \frac{1}{2}\alpha^2\mathbf{p}^\top\nabla^2 f(\mathbf{x}+t\mathbf{p})\mathbf{p},$$

for some $t \in (0,\alpha)$.

The rate of change in $f$ along the direction $\mathbf{p}$ is $\alpha$.

The optimum unit vector $\mathbf{p}^*$ ($\|\mathbf{p}^*\| = 1$) that minimizes $\mathbf{p}^\top\nabla f(\mathbf{x})$ is $-\frac{\nabla f(\mathbf{x})}{\|\nabla f(\mathbf{x})\|}$.

# Steepest descent





$$\mathbf{x}_{t+1} = \mathbf{x}_t + \alpha_t \mathbf{p}_t;$$

- $\mathbf{p}_t = -\nabla f(\mathbf{x}_t)$.
- How do we decide the step size $\alpha_t > 0$?
  $\rightarrow$ A simple solution (among others): fix it to a constant value.
- When to terminate the optimization process?
  $\rightarrow$ A simple solution (among others):
  terminate when $\frac{\|f(\mathbf{x}_t)\|}{\|f(\mathbf{x}_0)\|} < T$ for a constant $T > 0$.

# Steepest descent algorithm



Input: the stopping condition parameter $T > 0$ and step size $\alpha > 0$;

(I) $t = 0$; Make an initial guess $\mathbf{x}_t$;

(II) Iterate until $\frac{\|f(\mathbf{x}_t)\|}{\|f(\mathbf{x}_0)\|} < T$.

(i) $\mathbf{x}_{t+1} = \mathbf{x}_t - \alpha \nabla f(\mathbf{x}_t)$;

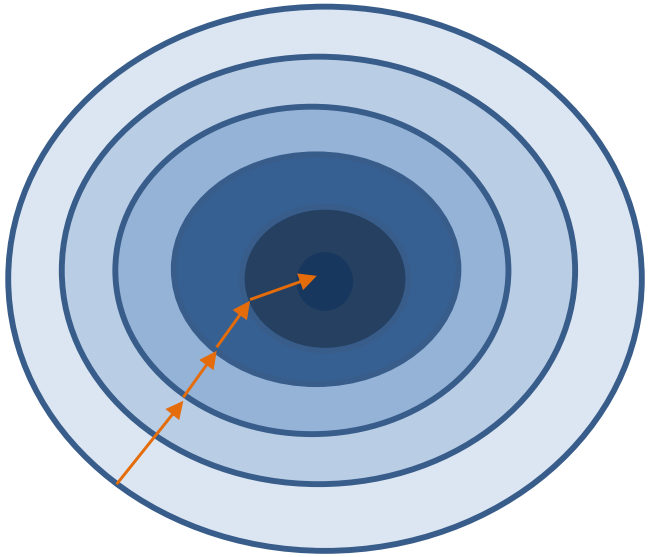
(ii) $t = t + 1$;

# Steepest descent algorithm





Good for isotropic functions.

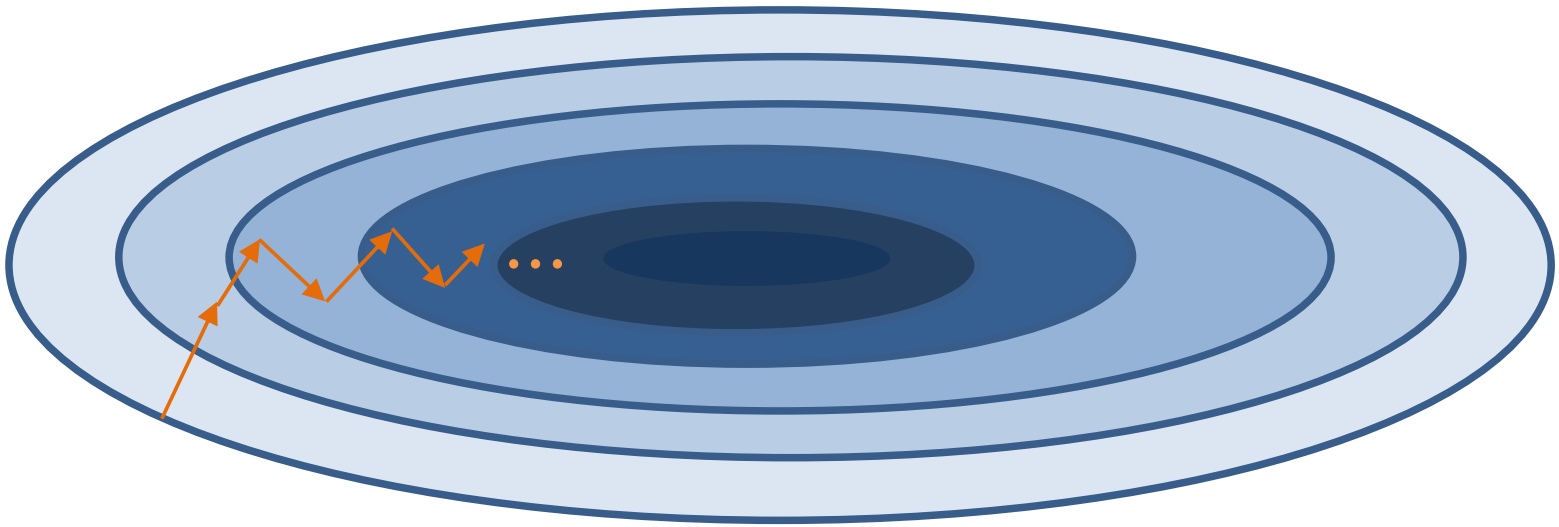


# Steepest descent algorithm





Not good for anisotropic functions.

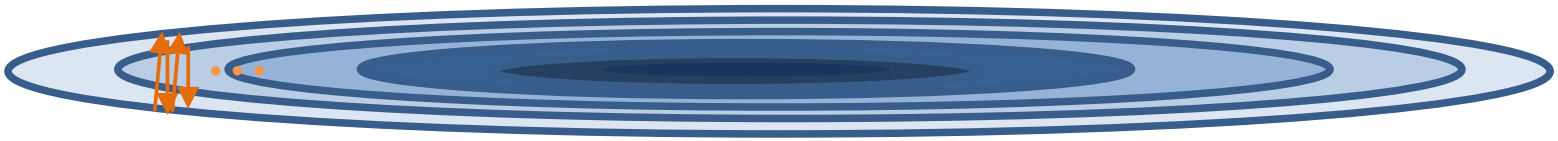


# Steepest descent algorithm



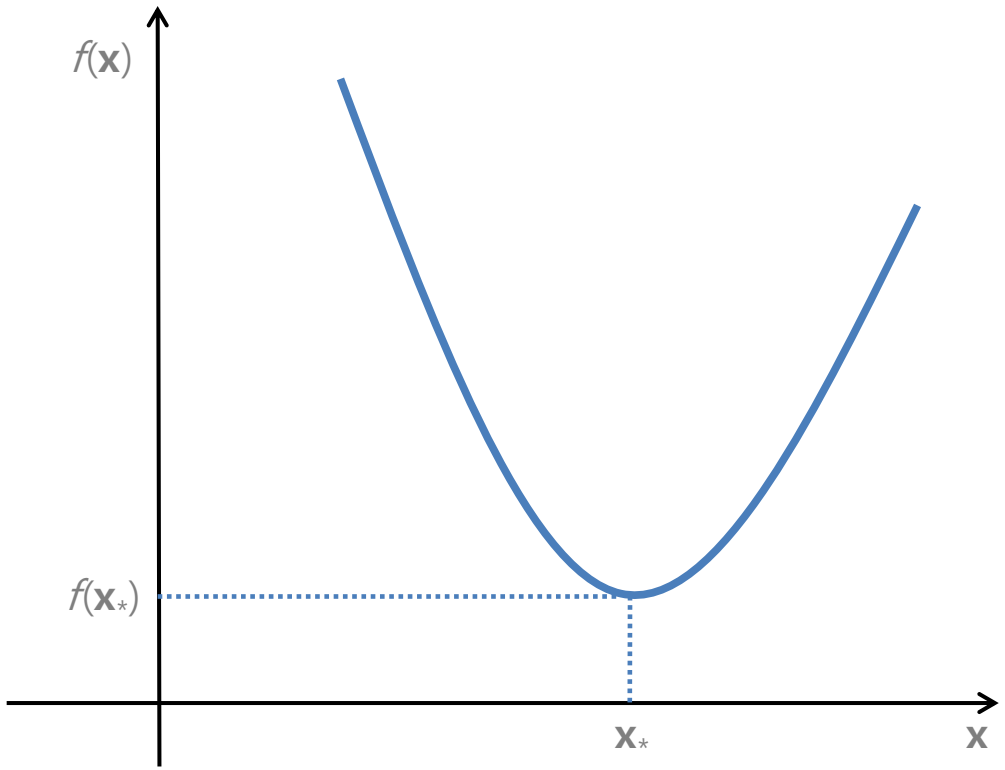


Not good for anisotropic functions.



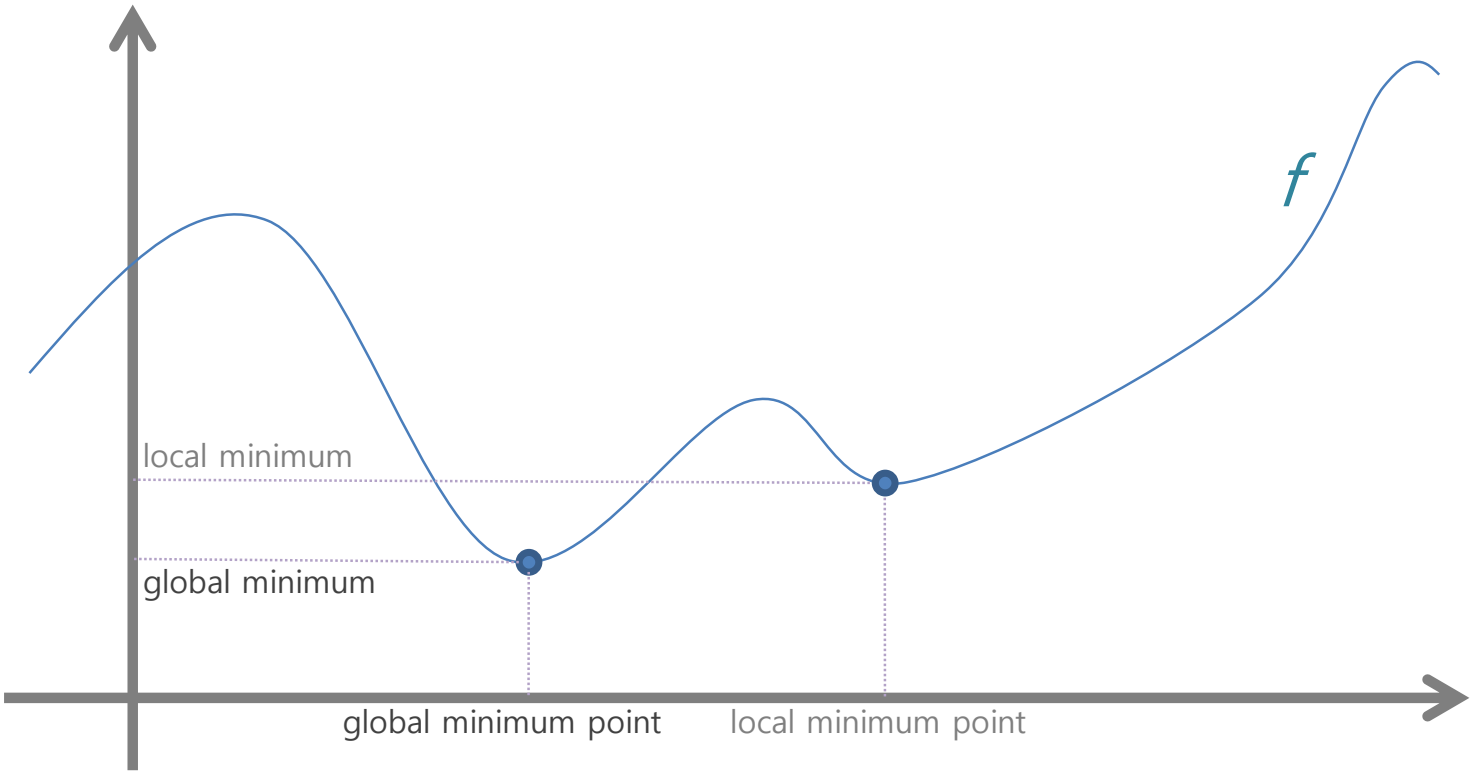
# Steepest descent algorithm

finds the global minimum $\mathbf{x}_*$ for



# Steepest descent algorithm

may not find the global minimum $\mathbf{x}_*$ when $f$ looks like




Finding the global optimum is difficult even in 1D case.

- Global minimum (point) $\mathbf{x}_*$: $f(\mathbf{x}_*) \leq f(\mathbf{x}), \forall \mathbf{x} \in \mathcal{X}$.
- Local minimum (point): a point which becomes a global minimum point when we restrict the domain to a (arbitrary small) neighborhood of itself.

# Linear least-squares regression

Given a set of data points (pairs of input and output)

$$D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\} \subset \mathcal{X} \times \mathcal{Y} \subset \mathbb{R}^n \times \mathbb{R},$$

Least-squares regression finds $f^*$ that minimizes the sum of squared error:

$$f^* = \arg\min_f \sum_{i=1}^{N} (f(\mathbf{x}_i) - y_i)^2.$$

If $f$ is linear (or affine)

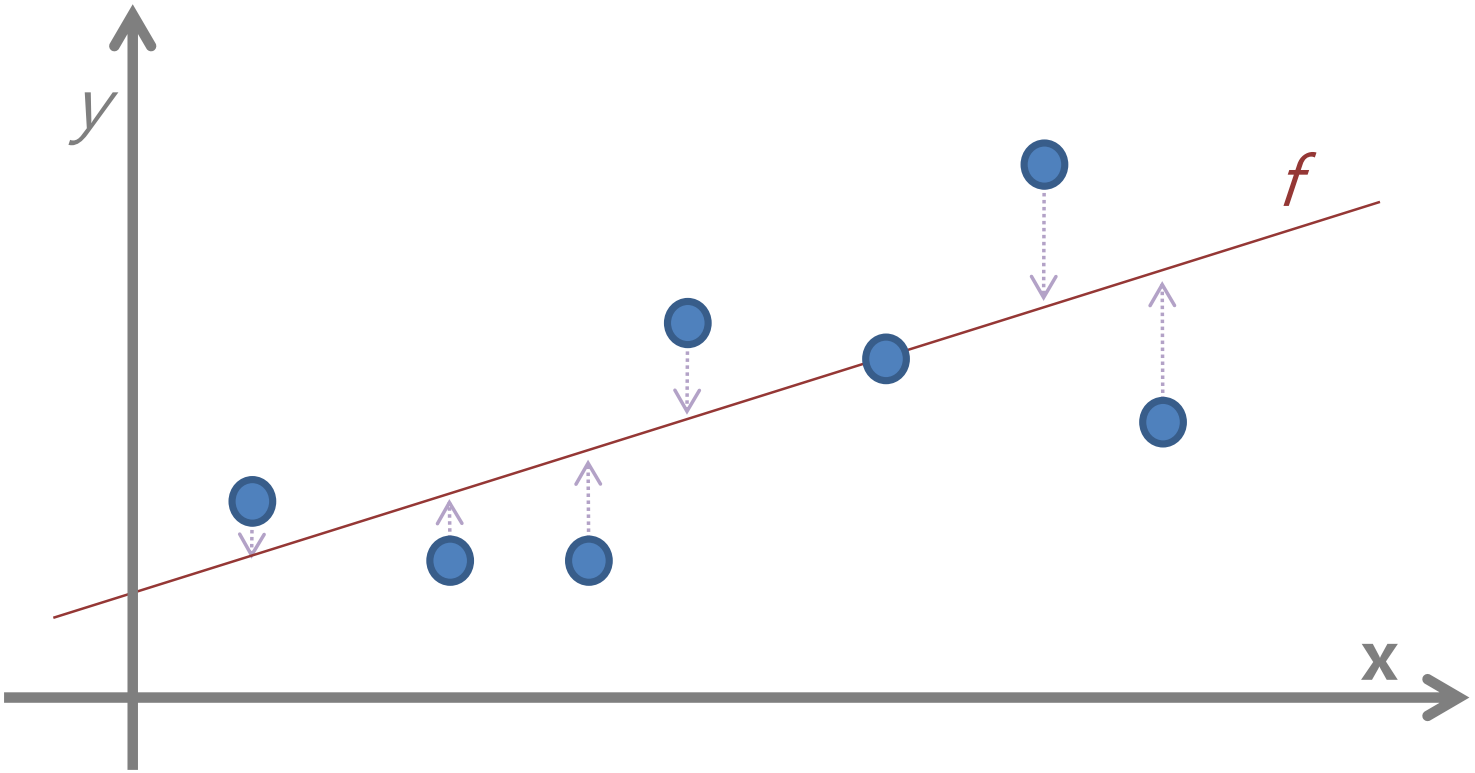
$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + c,$$

finding the optimum $f^*$ is equivalent to finding the optimal parameter $\mathbf{w}_*$.
Offset $c$ can be removed by replacing $\mathbf{x}$ and $\mathbf{w}$ with

$$\begin{pmatrix} \mathbf{x} \\ 1 \end{pmatrix} \text{ and } \begin{pmatrix} \mathbf{w} \\ c \end{pmatrix},$$

respectively.

# One-dimensional example (linear least-squares)



# Linear least-squares regression

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x},$$

$$f^* = \operatorname*{arg\,min}_{\text{Linear } f} \sum_{i=1}^{N} (f(\mathbf{x}_i) - y_i)^2$$

$$\Leftrightarrow \mathbf{w}_* = \operatorname*{arg\,min}_{\mathbf{w}\in\mathbb{R}^n} \sum_{i=1}^{N} (\mathbf{w}^\top \mathbf{x}_i - y_i)^2. \tag{2}$$

With data matrix $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_N)$ and label vector $\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix}$,

problem (2) can be rewritten as

$$\mathbf{w}_* = \operatorname*{arg\,min}_{\mathbf{w}\in\mathbb{R}^n} \|\mathbf{X}^\top \mathbf{w} - \mathbf{y}\|^2.$$

Show that $\|\mathbf{X}^\top \mathbf{w} - \mathbf{y}\|^2 = \sum_{i=1}^{N} (f(\mathbf{x}_i) - y_i)^2$!

# Steepest descent for linear least-squares regression



Objective:

$$\mathcal{O}(\mathbf{w}) = \|\mathbf{X}^\top \mathbf{w} - \mathbf{y}\|^2$$
$$\nabla_{\mathbf{w}} \mathcal{O}(\mathbf{w}) = 2\mathbf{X}(\mathbf{X}^\top \mathbf{w} - \mathbf{y})$$

Optimization algorithm:
Given $T$ and $\alpha$,

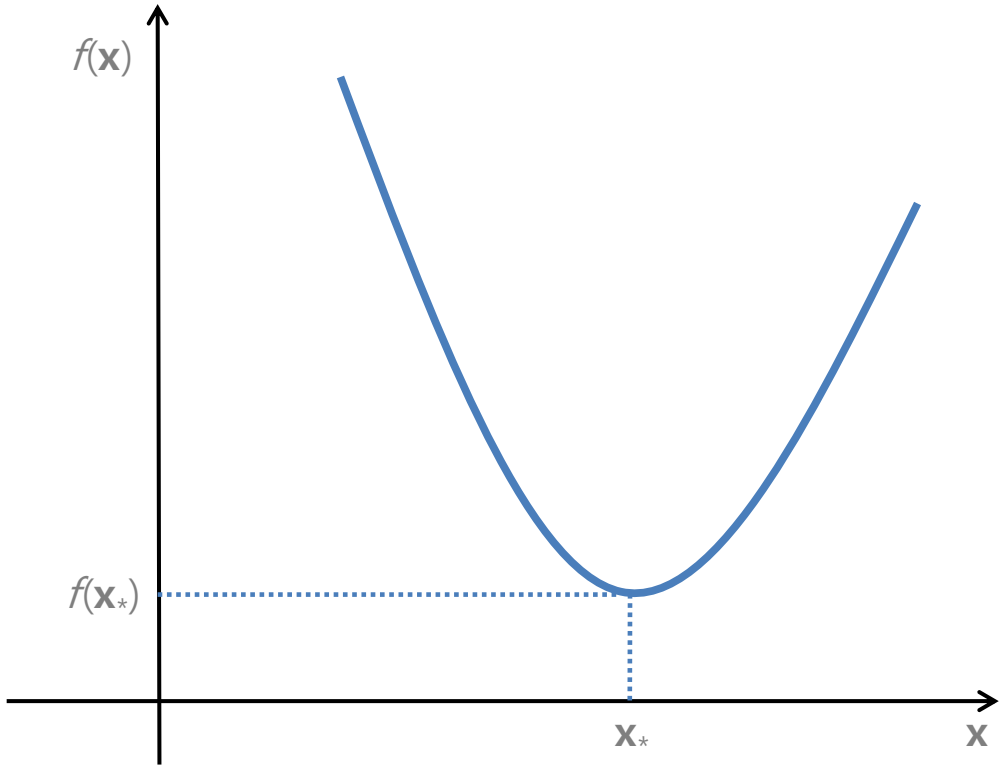
(I) $t = 0$; Make an initial guess $\mathbf{w}_t$;

(II) Iterate until $\frac{\|f(\mathbf{w}_t)\|}{\|f(\mathbf{w}_0)\|} < T$.

(i) $\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \left(2\mathbf{X}(\mathbf{X}^\top \mathbf{w}_t - \mathbf{y})\right)$;

(ii) $t = t + 1$;

# Closed form solution for linear least-squares regression




When our optimization objective $f$ does not have local minima other than the global minimum $\mathbf{x}_*$, $\mathbf{x}_*$ can be identified by setting the gradient $\nabla f$ to zero.

# Closed form solution for linear least-squares regression



Objective:

$$\mathcal{O}(\mathbf{w}) = \|\mathbf{X}^\top \mathbf{w} - \mathbf{y}\|^2$$
$$\nabla_{\mathbf{w}} \mathcal{O}(\mathbf{w}) = 2\mathbf{X}(\mathbf{X}^\top \mathbf{w} - \mathbf{y}).$$

The minimum $\mathbf{w}_*$ satisfies

$$\begin{aligned}\nabla_{\mathbf{w}} \mathcal{O}(\mathbf{w}_*) = 2\mathbf{X}(\mathbf{X}^\top \mathbf{w}_* - \mathbf{y}) = 0 \\ \Leftrightarrow 2\mathbf{X}\mathbf{X}^\top \mathbf{w}_* - 2\mathbf{X}\mathbf{y} = 0 \\ \Leftrightarrow \mathbf{X}\mathbf{X}^\top \mathbf{w}_* = \mathbf{X}\mathbf{y}.\end{aligned}$$

# Two optimization approaches for linear least-squares regression

- Steepest descent:

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \left(2\mathbf{X}\mathbf{X}^\top \mathbf{w}_t - 2\mathbf{X}\mathbf{y}\right).$$

  Complexity: $O(n \times N)$ per iteration (why?).
  $N$: # data points, $n$: data dimensionality.

- Closed form solution:

$$\mathbf{X}\mathbf{X}^\top \mathbf{w}_* = \mathbf{X}\mathbf{y}.$$

  Complexity: $O(n^3 + N \times n^2)$.

# Summary

- Almost all machine learning tasks are formulated as optimization problems.
- Steepest descent: one of the simplest optimization algorithms.
  - requires evaluating gradient.
  - Good for isotropic functions.
  - Remaining questions
    - Alternatives to steepest descent, e.g. when $f$ is anisotropic?
    - How many iterations do we need? Convergence analysis?
- Iterative vs. closed form solution for linear least-squares regression.

## Optimization (minimization) problem

Given a function $f : \mathcal{X} \subset \mathbb{R}^n \mapsto \mathbb{R}$, find an element $\mathbf{x}_*$ such that $f(\mathbf{x}_*) \leq f(\mathbf{x}), \forall \mathbf{x} \in \mathcal{X}$.

- Maximization can be converted to a minimization by multiplying $f$ by $-1$.
- Optimization problem can be accompanied by constraints (constrained optimization problem):

$$\begin{aligned} \mathbf{x}_* = \arg\min_{\mathbf{x}\in\mathcal{X}} & f(\mathbf{x}), \\ \text{s.t. } & g_i(\mathbf{x}) \leq 0, i = \{1, \ldots, k\}, \\ & h_j(\mathbf{x}) = 0, j = \{1, \ldots, l\}. \end{aligned}$$

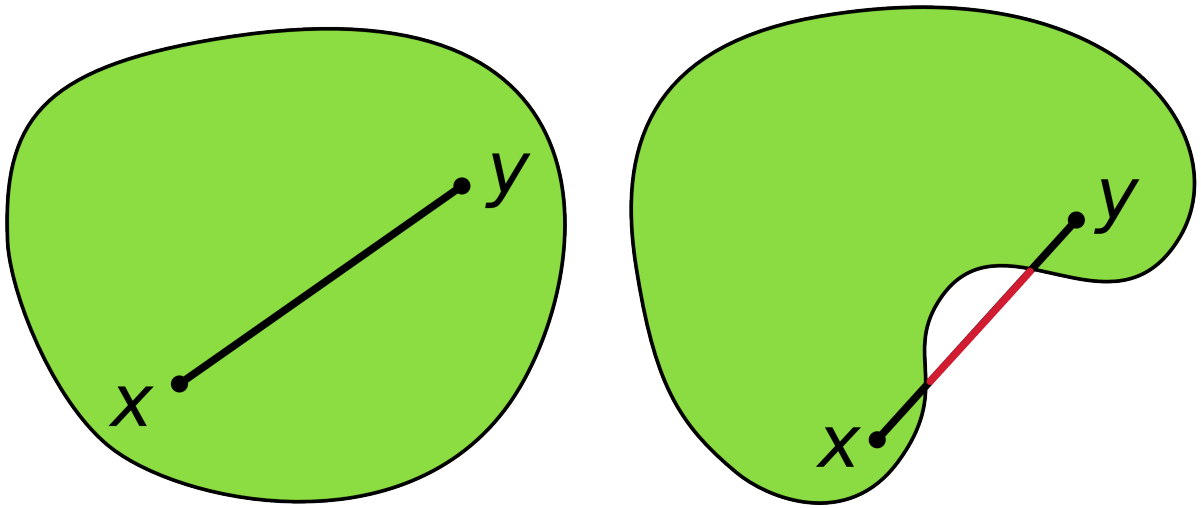
$\{g_i\}$ and $\{h_j\}$ are (inequality & equality) *constraint functions*.

## Convex set

A subset $C$ of a vector space is called convex if $\forall \mathbf{x}, \mathbf{y} \in C$ and $\lambda \in [0, 1]$

$$\lambda \mathbf{x} + (1 - \lambda)\mathbf{y} \in C.$$

examples:

- 

- $\mathbb{R}^n$
- a cone in $\mathbb{R}^n$

[Wikipedia]

## Convex function

A function on a convex set $C$ is

- convex if

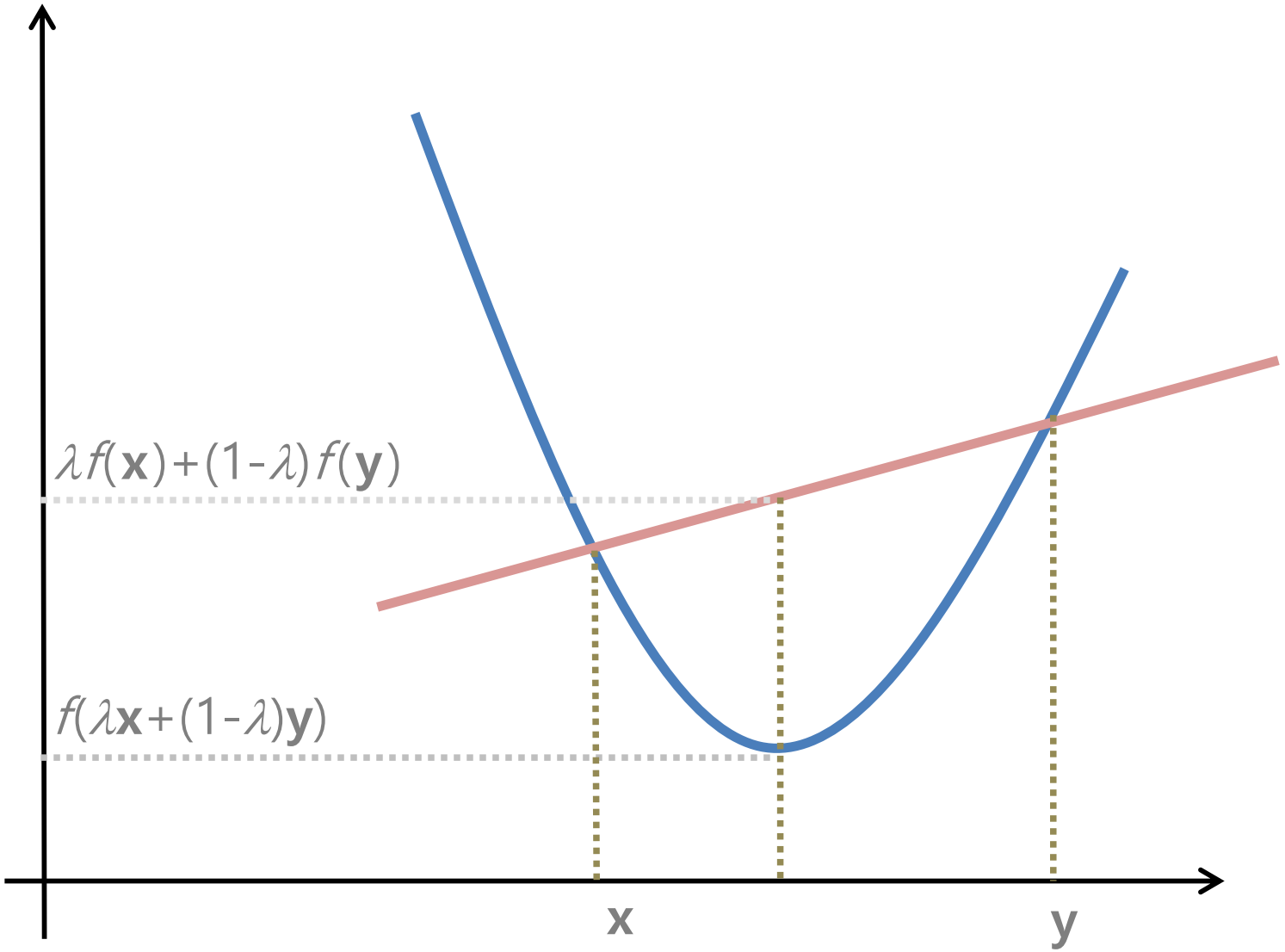
$$f(\lambda \mathbf{x} + (1-\lambda)\mathbf{y}) \leq \lambda f(\mathbf{x}) + (1-\lambda) f(\mathbf{y}),$$

- strictly convex if

$$f(\lambda \mathbf{x} + (1-\lambda)\mathbf{y}) < \lambda f(\mathbf{x}) + (1-\lambda) f(\mathbf{y})$$

$\forall \mathbf{x}, \mathbf{y} \in C$ and $\lambda \in [0, 1]$.

# Convex function



# Convex function

If $f$ is twice continuously differentiable,

- $f : \mathbb{R} \mapsto \mathbb{R}$ is convex if $\frac{d^2 f}{d\mathbf{x}^2}$ is positive everywhere.
- $f : \mathbb{R}^n \mapsto \mathbb{R}$ is convex if the Hessian matrix is positive definite everywhere.

Example: second-order polynomial

$$p(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top \mathbf{A}\mathbf{x} + \mathbf{b}^\top \mathbf{x} + c$$

is convex if $\mathbf{A}$ is (symmetric) positive definite.

The Hessian matrix $\frac{d^2 p}{d\mathbf{x}^2}[\mathbf{x}]$ of $p$ is $A$ for all $\mathbf{x}$.

# (symmetric) Positive definite matrix

$$\mathbf{x}^\top \mathbf{A}\mathbf{x} > 0, \forall \mathbf{x} \neq 0$$

- $\mathbf{A}$ is invertible and $\mathbf{A}^{-1}$ is positive definite.
- Eigenvalues of $\mathbf{A}$ are positive:

$$\mathbf{x}^\top \mathbf{A}\mathbf{x} = \mathbf{x}^\top (\mathbf{E}\Lambda\mathbf{E}^{-1})\mathbf{x} = \mathbf{x}^\top (\mathbf{E}\Lambda\mathbf{E}^\top)\mathbf{x} = (\mathbf{E}^\top \mathbf{x})^\top \Lambda (\mathbf{E}^\top \mathbf{x}).$$

$$\Rightarrow \mathbf{x}^\top \mathbf{A}\mathbf{x} > 0 \text{ if elements of } \Lambda \text{ are positive.}$$

# Optimization problem types

$$\mathbf{x}_* = \arg\min_{\mathbf{x}\in\mathcal{X}} f(\mathbf{x}),$$
$$\text{s.t. } g_i(\mathbf{x}) \leq 0, i = \{1,\ldots,k\},$$
$$h_j(\mathbf{x}) = 0, j = \{1,\ldots,l\}.$$

- Constrained vs. unconstrained optimization.
- Discrete vs. continuous optimization.
- Deterministic vs. stochastic optimization.

# Linear programming

$$\mathbf{x}_* = \arg\min_{\mathbf{x}\in\mathbb{R}^n} \mathbf{c}^\top \mathbf{x},$$
$$\text{s.t. } A\mathbf{x} = \mathbf{b},$$
$$\mathbf{x} \geq 0.$$

Example: a company manufactures two types of boxes, A and B.

- The boxes undergo two major processes: cutting and pinning operations.
- The profits per unit are 6 for A and 4 for B.
- A requires 2 minutes for cutting and 3 minutes for pinning.
- B requires 2 minutes for cutting and 1 minutes for pinning.
- Available operating time is 120 minutes and 60 minutes for cutting and pinning machines.
- We have to decide the optimum A and B quantities to maximize the profits.

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$$\mathbf{x} = [x^A, x^B]^\top$$

$$\mathbf{x}_* = \underset{\mathbf{x}\in\mathbb{R}^2}{\arg\max} f(\mathbf{x}) = 6x^A + 4x^B \text{ (objective function)}$$

$$\text{s.t. } 2x^A + 3x^B \leq 120 \text{ (cutting constraint)}$$

$$2x^A + x^B \leq 60 \text{ (pinning constraint)}$$

$$x^A, x^B \geq 0 \text{ (box quantities cannot be negative) .}$$

# Integer programming

$$\mathbf{x} = [x^A, x^B]^\top$$

$$\mathbf{x}_* = \arg\max_{\mathbf{x}\in\mathbb{R}^2} f(\mathbf{x}) = 6x^A + 4x^B \text{ (objective function)}$$

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$$2x^A + x^B \leq 60 \text{ (pinning constraint)}$$

$$x^A, x^B \geq 0 \text{ (box quantities cannot be negative) .}$$

If box quantities need to be integers ...

$$\mathbf{x}_* = \arg\max_{\mathbf{x}\in\mathbb{Z}^2} \; 6x^A + 4x^B,$$

$$\text{s.t. } 2x^A + 3x^B \leq 120,$$

$$2x^A + x^B \leq 60$$

$$x^A, x^B \geq 0.$$

- Quadratic programming:

$$\mathbf{x}_* = \arg\min_{\mathbf{x}\in\mathbb{R}^n} f(\mathbf{x}) = \mathbf{x}^\top Q\mathbf{x} + \mathbf{c}^\top \mathbf{x},$$
$$\text{s.t. } A\mathbf{x} \leq \mathbf{b},$$

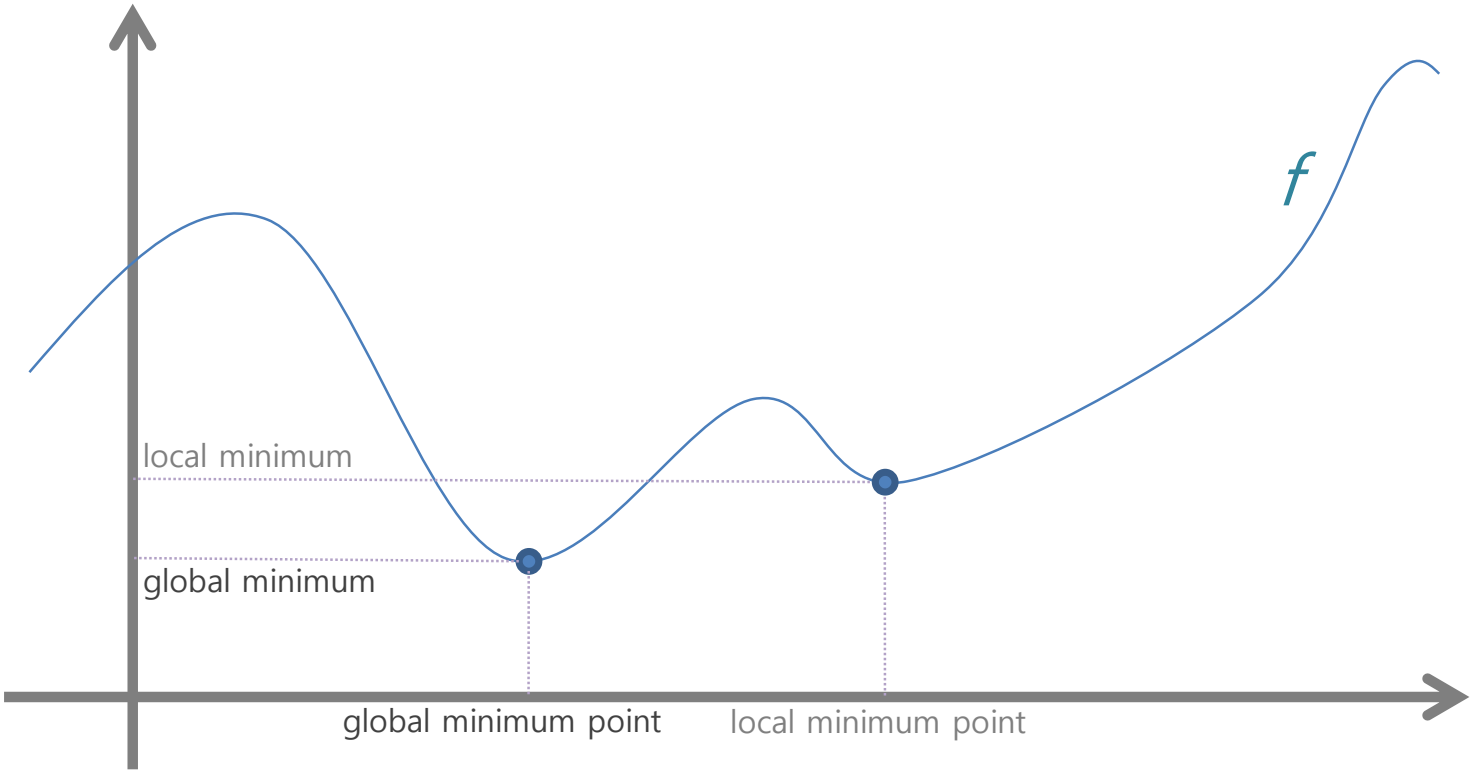
  where $Q$ is a real symmetric matrix.

- Nonlinear programming:

$$\mathbf{x}_* = \arg\min_{\mathbf{x}\in\mathbb{R}^n} f(\mathbf{x}),$$
$$\text{s.t. } g(\mathbf{x}) \leq 0,$$
$$h(\mathbf{x}) = 0,$$

  where $f, g, h$ are nonlinear.

# Optimization

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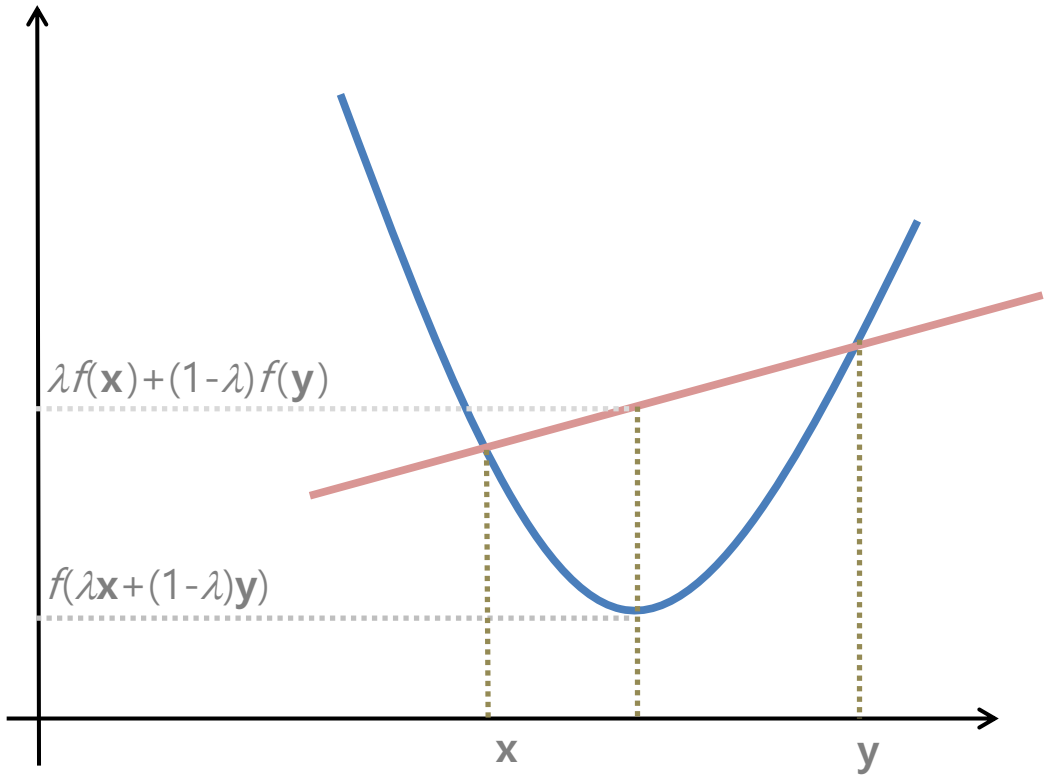
# Convex optimization




$$\mathbf{x}_* = \arg\min_{\mathbf{x}\in\mathbb{R}^n} f(\mathbf{x}),$$
$$\text{s.t. } g(\mathbf{x}) \leq 0,$$

where $f, g : \mathbb{R}^n \to \mathbb{R}$ are convex.

# Convex function

- If $f$ is twice continuously differentiable, $f : \mathbb{R} \mapsto \mathbb{R}$ is convex if $\frac{d^2 f}{d\mathbf{x}^2}$ is positive everywhere.
- If $f$ is twice continuously differentiable, $f : \mathbb{R}^n \mapsto \mathbb{R}$ is convex if the Hessian matrix $Hf|_{\mathbf{x}}$ is positive definite everywhere.
- The second order polynomial

$$p(\mathbf{x}) = \mathbf{x}^\top \mathbf{A}\mathbf{x} + \mathbf{b}^\top \mathbf{x} + c$$

  is convex if $\mathbf{A}$ is positive definite.
- An increasing function of a convex function is convex, e.g. if $f(\cdot)$ is convex, $\log(f(\cdot))$ and $\exp(f(\cdot))$ are convex.
- If $f$ and $g$ are convex, $f + g$ is convex.
- If a local optimum exists for a convex function $f$, it is a global minimum.
- A point $\mathbf{x}_*$ is a local minimum if $\nabla_f(\mathbf{x}_*) = 0$.

# Positive definite matrix



$$\mathbf{x}^\top \mathbf{A}\mathbf{x} > 0, \forall \mathbf{x} \neq 0$$

- $\mathbf{A}$ is invertible and $\mathbf{A}^{-1}$ is positive definite.
- Eigenvalues of $\mathbf{A}$ are positive:

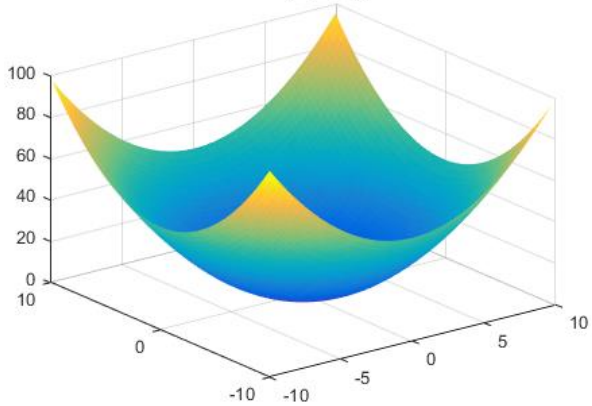
$$\mathbf{x}^\top \mathbf{A}\mathbf{x} = \mathbf{x}^\top (\mathbf{E}\Lambda\mathbf{E}^{-1})\mathbf{x} = \mathbf{x}^\top (\mathbf{E}\Lambda\mathbf{E}^\top)\mathbf{x} = (\mathbf{E}^\top \mathbf{x})^\top \Lambda (\mathbf{E}^\top \mathbf{x}).$$

$$\Rightarrow \mathbf{x}^\top \mathbf{A}\mathbf{x} > 0 \text{ if elements of } \Lambda \text{ are positive.}$$

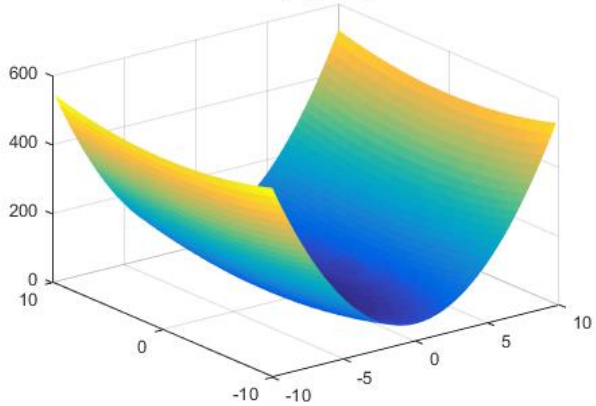
# 2D examples

$$p(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top \mathbf{A}\mathbf{x}.$$

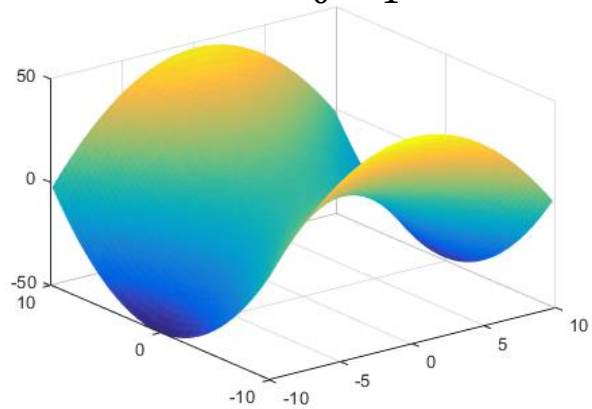
$\mathbf{A} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$



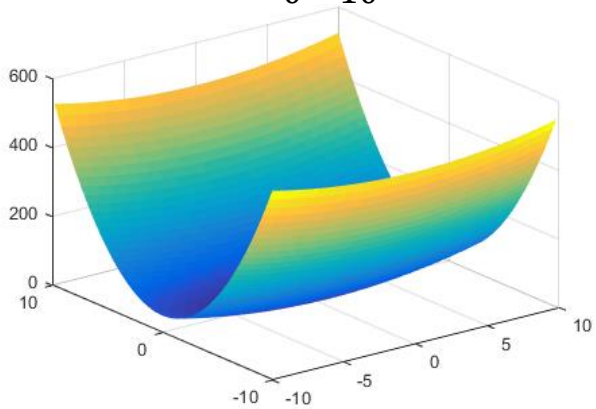

$\mathbf{A} = \begin{pmatrix} 10 & 0 \\ 0 & 1 \end{pmatrix}$




$\mathbf{A} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$




$\mathbf{A} = \begin{pmatrix} 1 & 0 \\ 0 & 10 \end{pmatrix}$



# 2D example 1

Eigen-decomposition of the diagonal matrix $\mathbf{A} = \begin{pmatrix} 10 & 0 \\ 0 & 1 \end{pmatrix}$:

$$\begin{aligned}
\mathbf{A} &= \mathbf{E}\Lambda\mathbf{E}^{-1} = \mathbf{E}\Lambda\mathbf{E}^{\top} \\
&= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 10 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\
&= (\mathbf{e}_1, \mathbf{e}_2) \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} (\mathbf{e}_1, \mathbf{e}_2)^{\top} \\
&= \lambda_1 \mathbf{e}_1 \mathbf{e}_1{}^{\top} + \lambda_2 \mathbf{e}_2 \mathbf{e}_2{}^{\top},
\end{aligned}$$

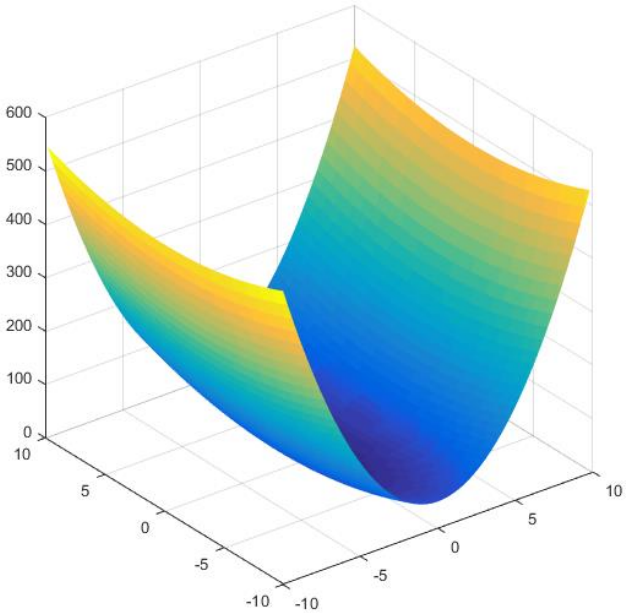
where

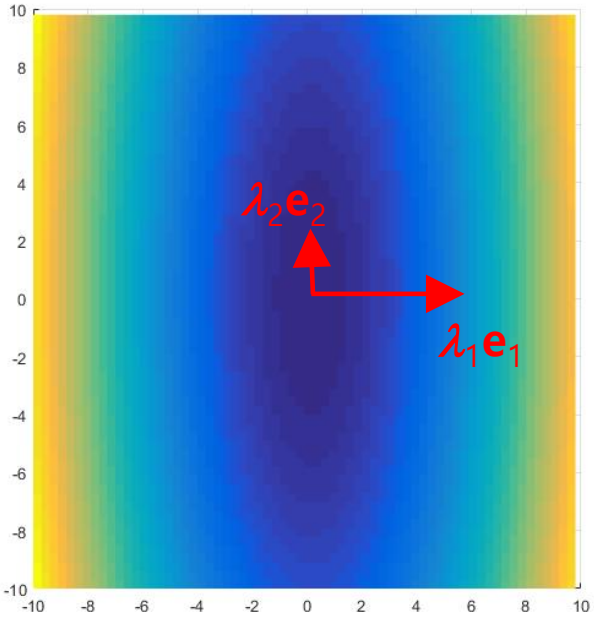
$$\mathbf{e}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \mathbf{e}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \lambda_1 = 10, \lambda_2 = 1.$$

Note: Eigenvectors of $\mathbf{A}$ form a basis.

# 2D example 1

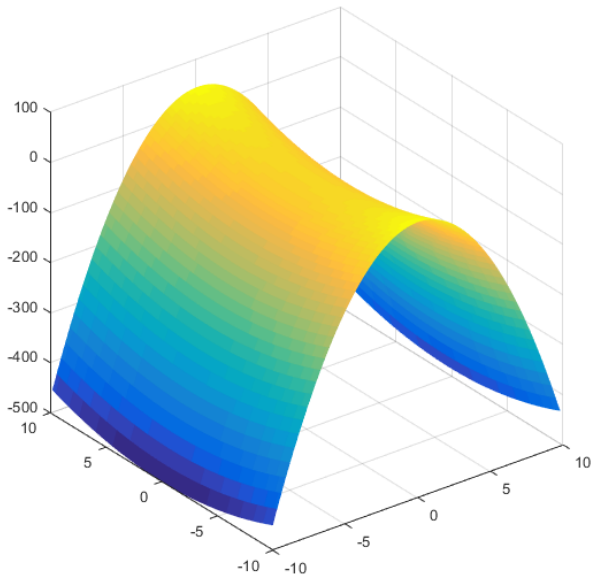
$$p(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top \mathbf{A}\mathbf{x}, \mathbf{A} = \begin{pmatrix} 10 & 0 \\ 0 & 1 \end{pmatrix} = \lambda_1 \mathbf{e}_1 \mathbf{e}_1{}^\top + \lambda_2 \mathbf{e}_2 \mathbf{e}_2{}^\top.$$

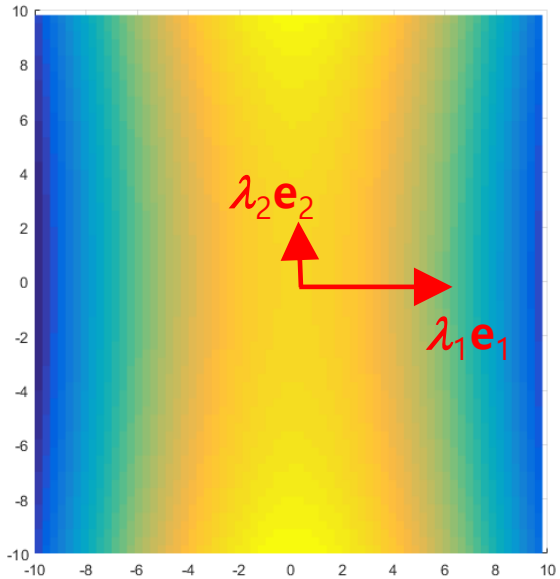


# 2D example 2

$$p(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top \mathbf{A}\mathbf{x}, \mathbf{A} = \begin{pmatrix} -10 & 0 \\ 0 & 1 \end{pmatrix} = \lambda_1 \mathbf{e}_1 \mathbf{e}_1{}^\top + \lambda_2 \mathbf{e}_2 \mathbf{e}_2{}^\top.$$



# 2D example 3

Eigen-decomposition of symmetric matrix $\mathbf{A} = \begin{pmatrix} 5.5 & 4.5 \\ 4.5 & 5.5 \end{pmatrix}$:

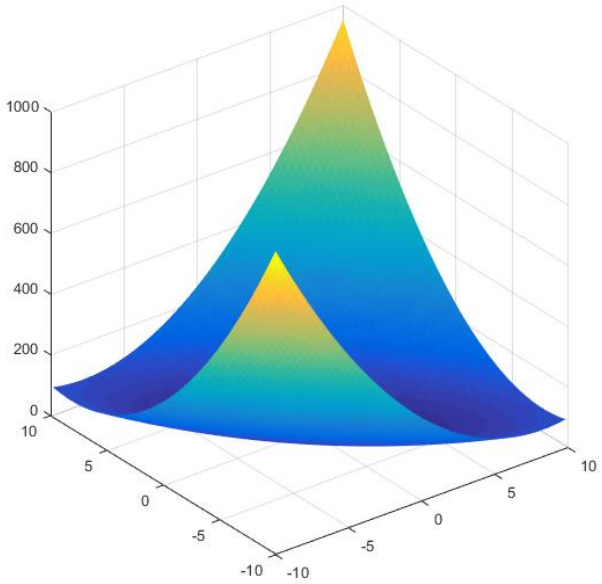
$$\begin{aligned}
\mathbf{A} &= \mathbf{E}\Lambda\mathbf{E}^{-1} = \mathbf{E}\Lambda\mathbf{E}^{\top} \\
&= \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 10 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \\
&= (\mathbf{e}_1, \mathbf{e}_2) \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} (\mathbf{e}_1, \mathbf{e}_2)^{\top} \\
&= \lambda_1 \mathbf{e}_1 \mathbf{e}_1{}^{\top} + \lambda_2 \mathbf{e}_2 \mathbf{e}_2{}^{\top},
\end{aligned}$$

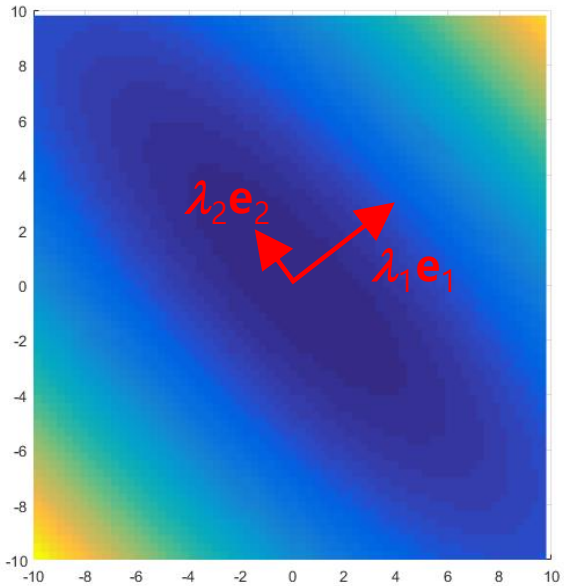
where

$$\mathbf{e}_1 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \mathbf{e}_2 = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \lambda_1 = 10, \lambda_2 = 1.$$

# 2D example 3

$$p(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top \mathbf{A}\mathbf{x}, \mathbf{A} = \begin{pmatrix} 5.5 & 4.5 \\ 4.5 & 5.5 \end{pmatrix} = \lambda_1 \mathbf{e}_1 \mathbf{e}_1{}^\top + \lambda_2 \mathbf{e}_2 \mathbf{e}_2{}^\top.$$



# References


Noc J. Nocedal and S. J. Wright, *Numerical Optimization*, Springer (second edition).

Ber D. P. Bertsekas, *Nonlinear Programming*, Athena Scientific (second edition).

Teu Teukolsky, Vetterling, and Flannery, *Numerical Recipes: The Art of Scientific Computing*, Cambridge University Press (any edition). `http://www.nr.com/`

Pet K. B. Petersen and M. S. Pedersen, *The Matrix Cookbook*.