Optimization for Robotics Summer School

Lecture 1 & 2: Introduction to Optimization

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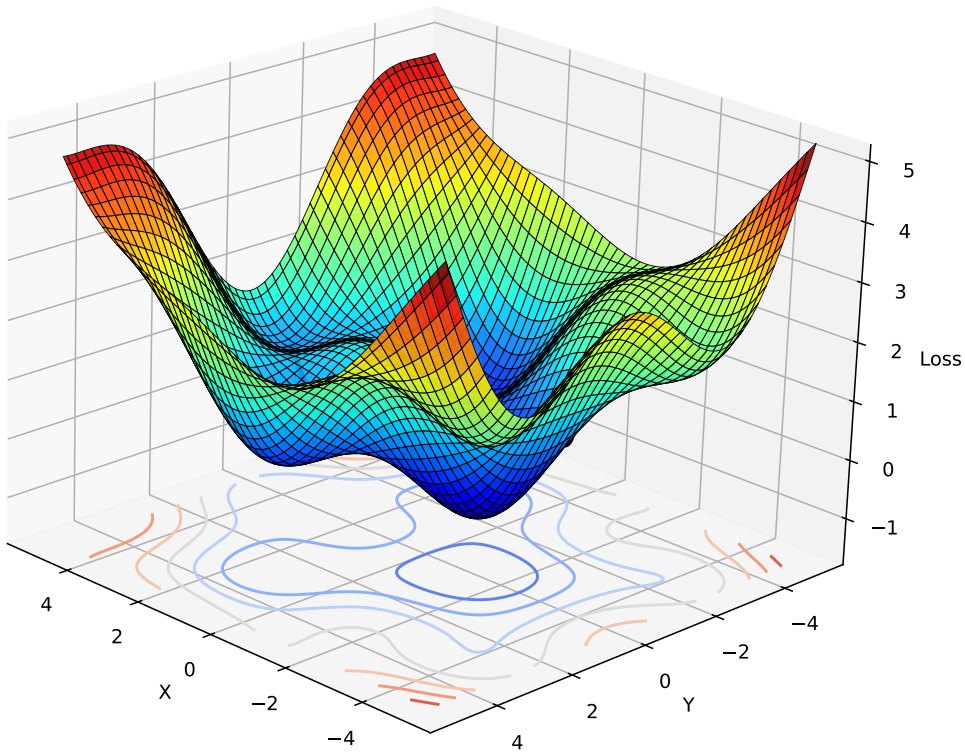
Template made by Panagiotis Papagiannopoulos

What is Optimization?

Optimization is the process of making something as effective or functional as possible.



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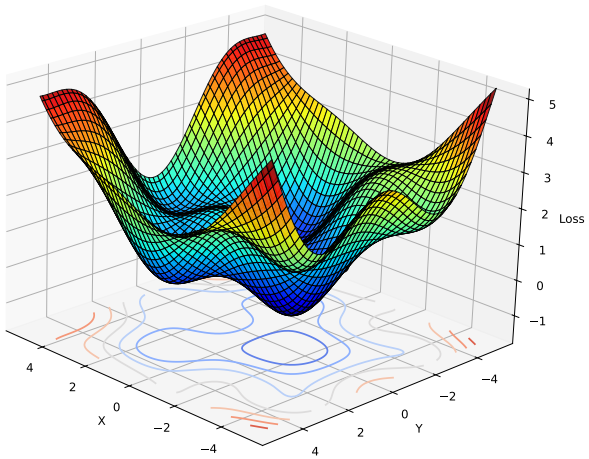
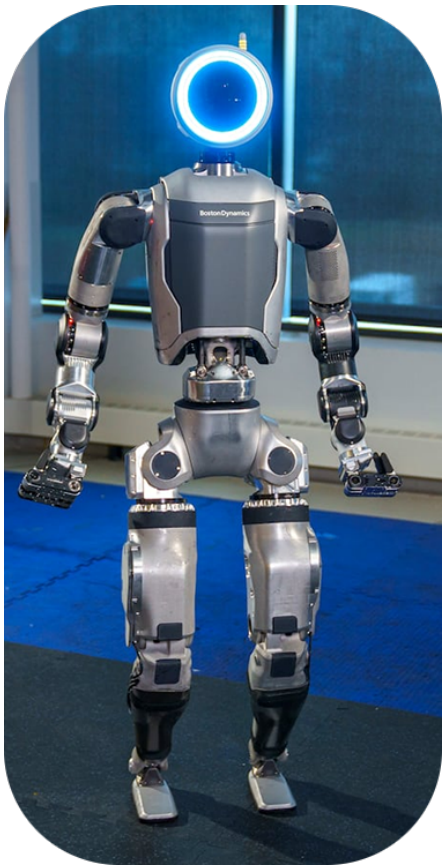


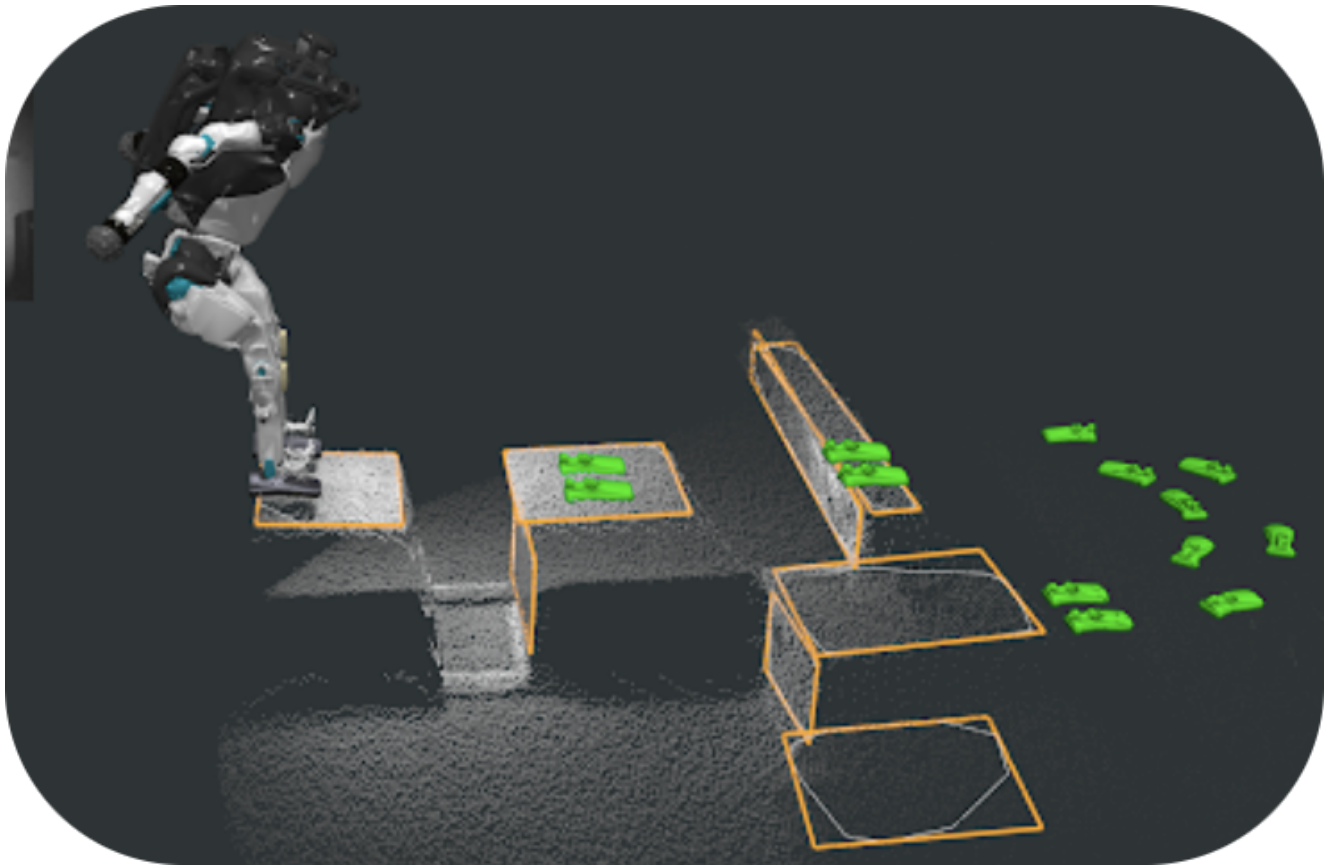
What is the goal of optimization?

- To find the best solution to a problem, which involves minimizing or maximizing a (set of) function(s) (**the objective function(s)**).

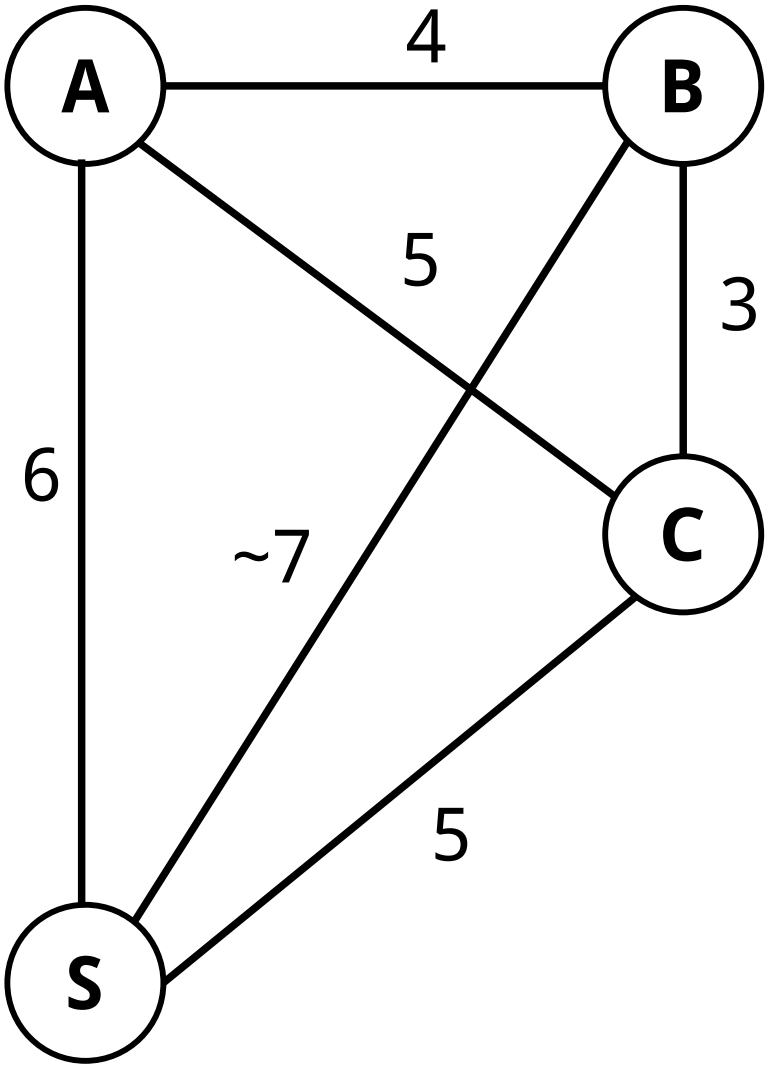
- To find the values of the *unknowns* (**the variables**) that lead to the optimal outcome, subject to certain **constraints**.

Why?





Discrete Optimization Example



Example: A delivery driver needs to drop off packages at 3 different houses, and they want to minimize total travel distance.

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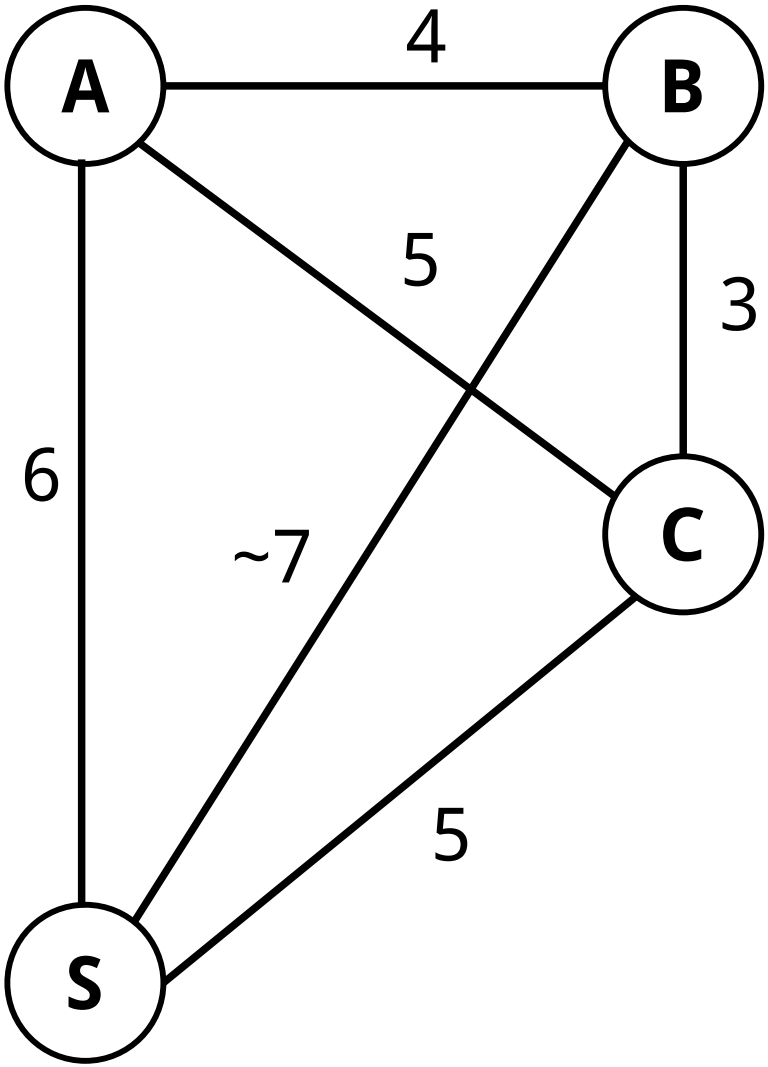

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- We have a set of possible solutions. Can we enumerate them?

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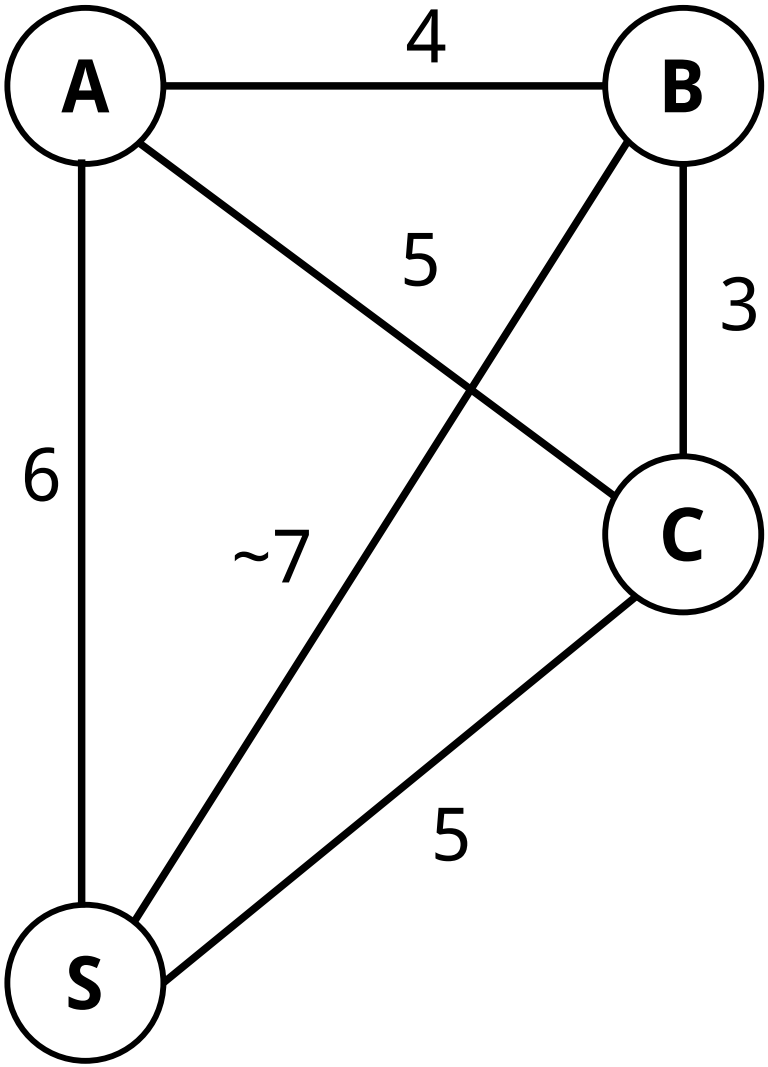

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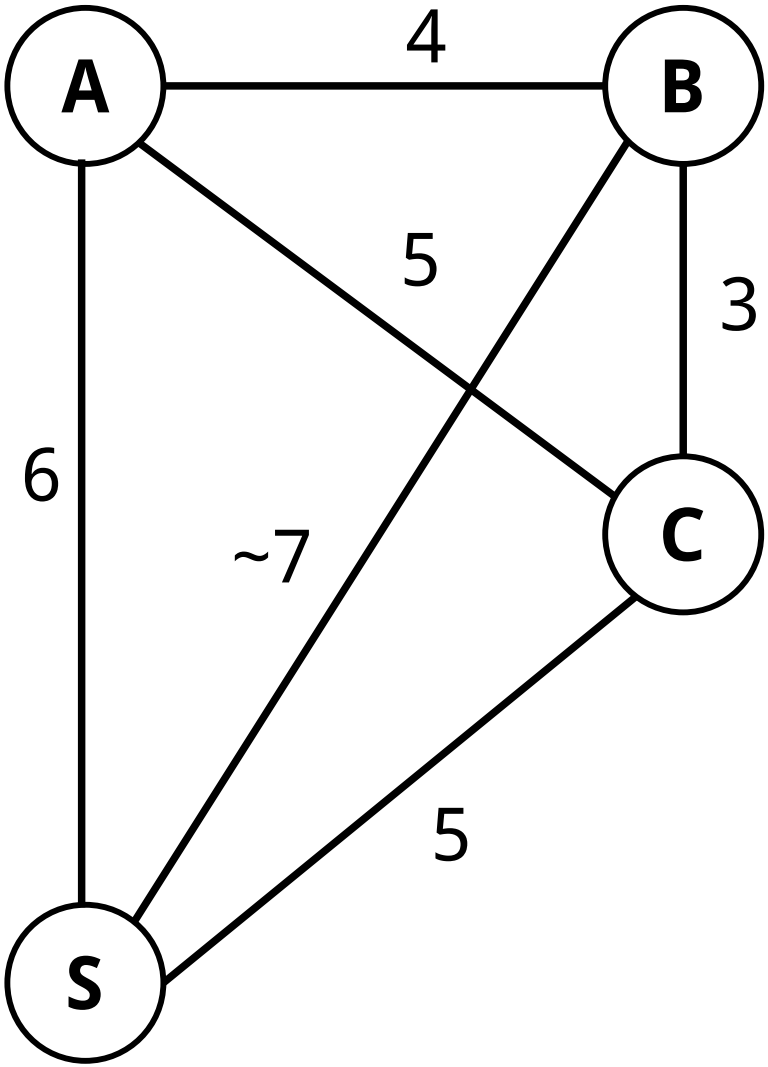

Example: A delivery driver needs to drop off packages at 3 different houses, and they want to minimize total travel distance.

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- What is the optimal solution?

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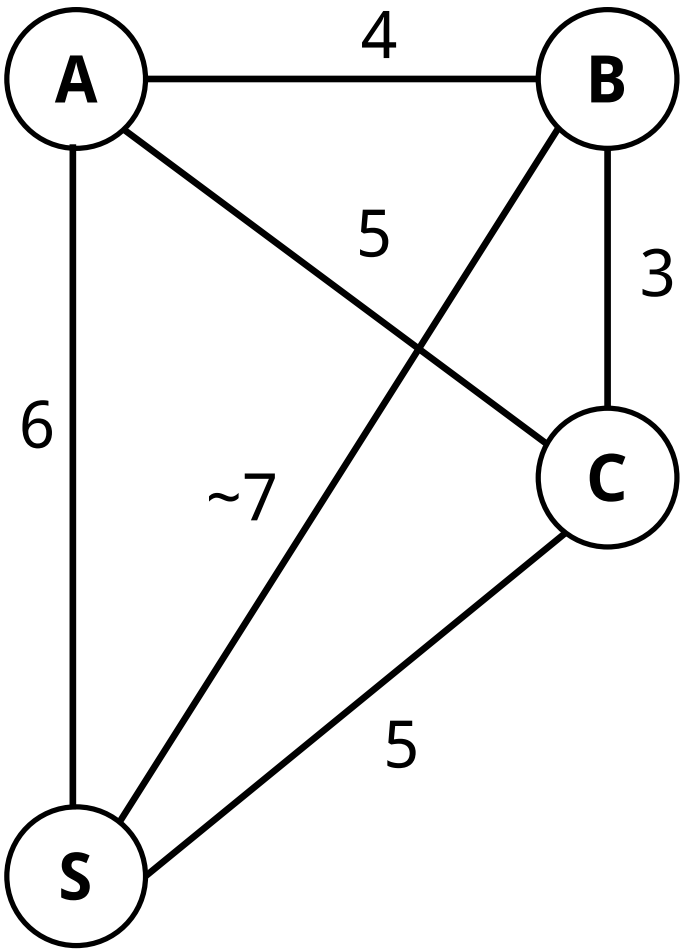

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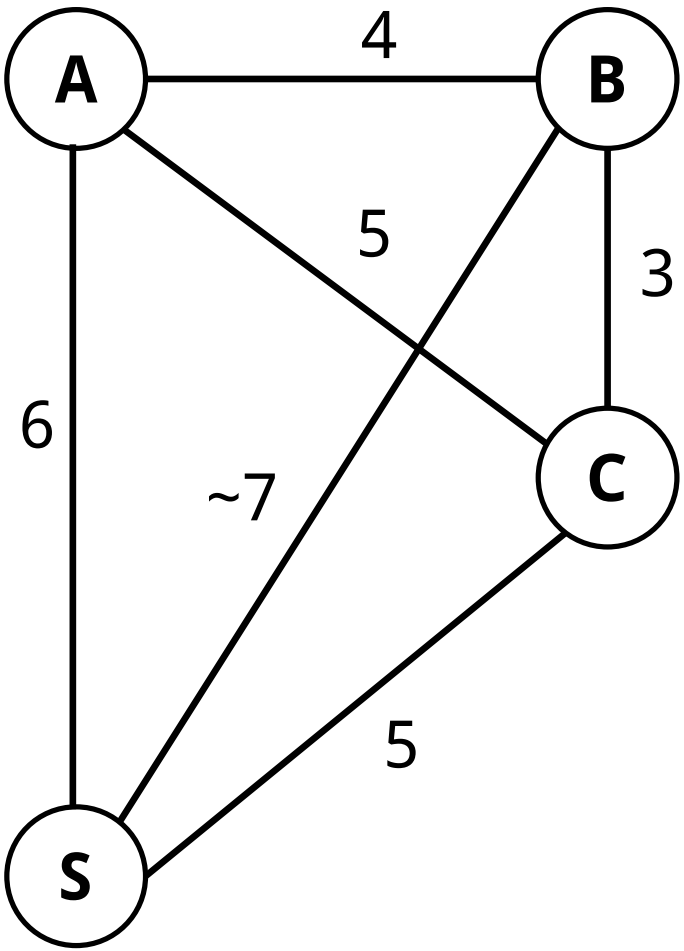

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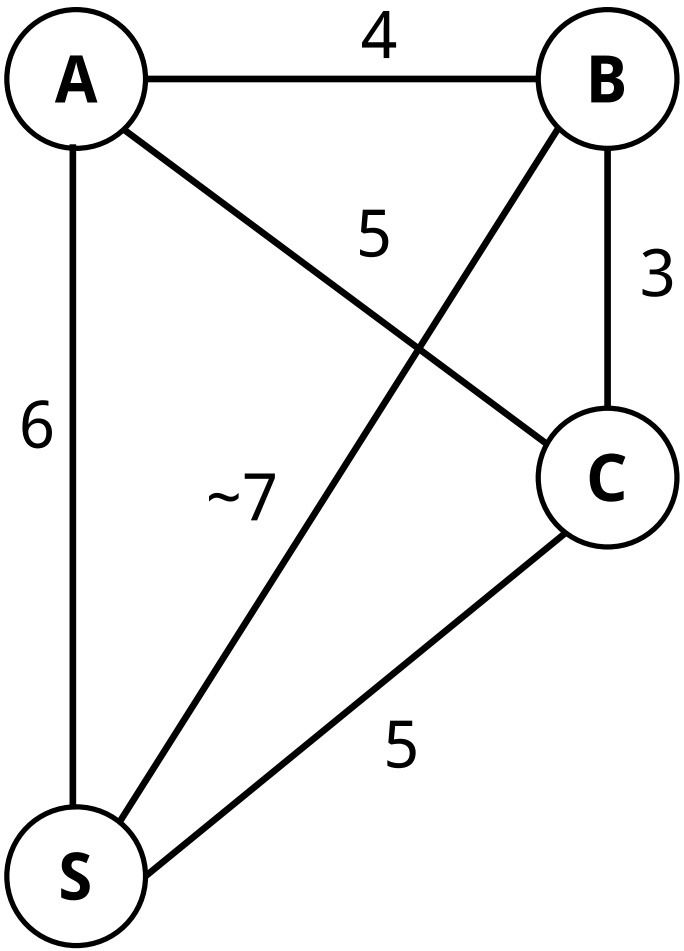

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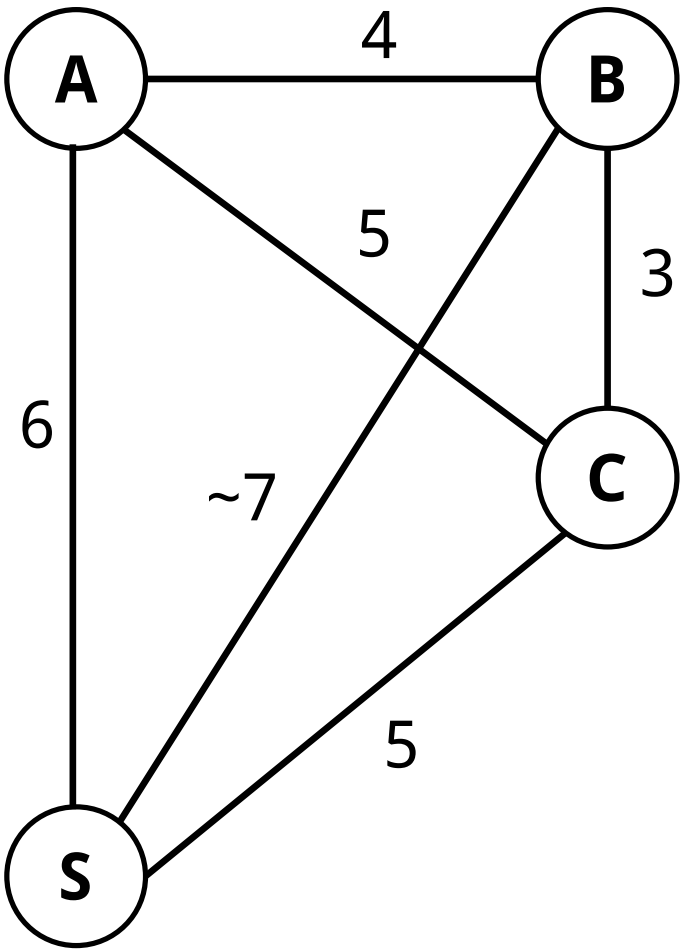

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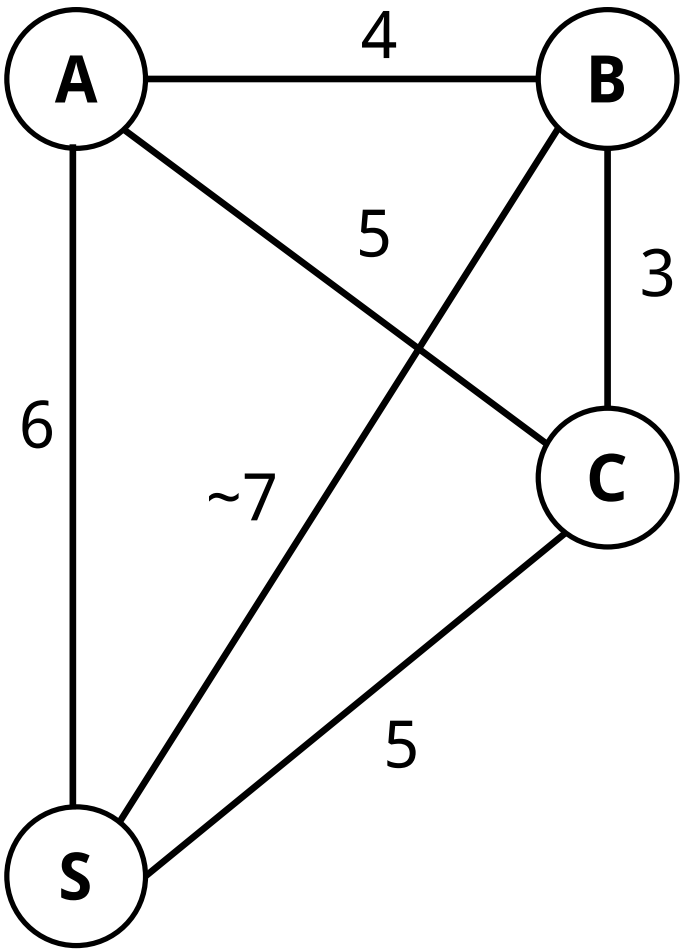

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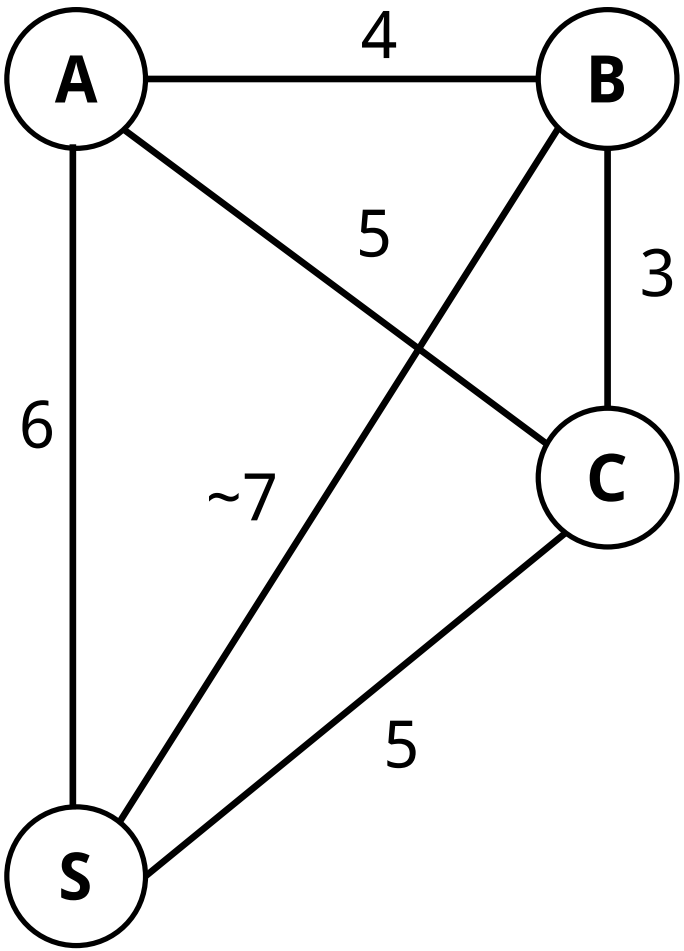

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The optimal solution is? We have two!

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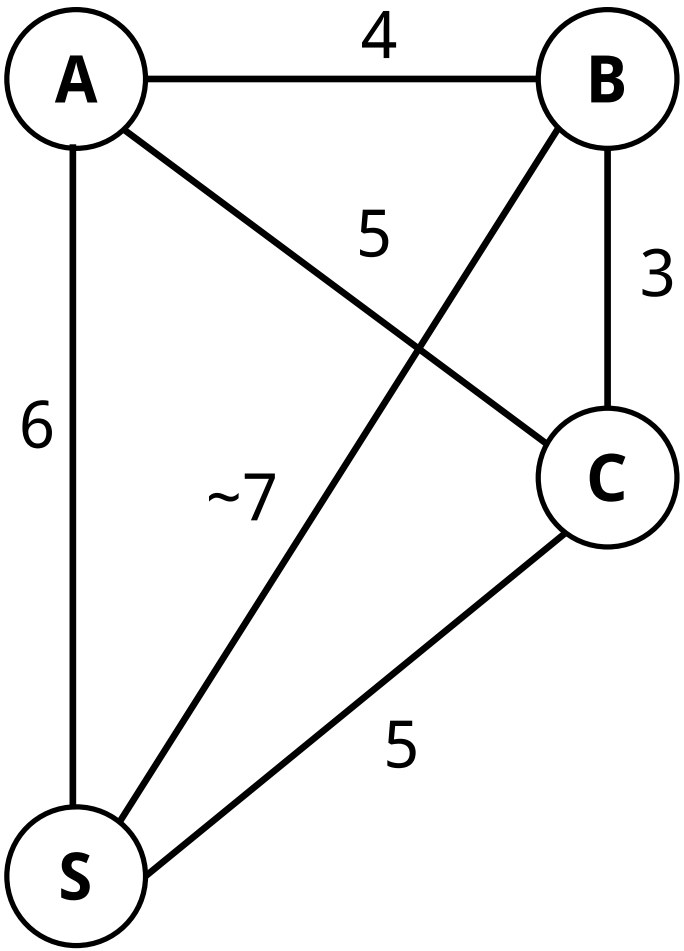

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The optimal solution is? We have two!

In general, we cannot enumerate all possible solutions! What can we do?

Some notation

$$\boldsymbol{y} = f(\boldsymbol{x}) : \mathbb{R}^N \rightarrow \mathbb{R}^M,$$

$\boldsymbol{x} \in \mathbb{R}^N, \boldsymbol{y} \in \mathbb{R}^M$.

What is $\frac{\partial f}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}}$?

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What is $\frac{\partial f}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}}$?

$$\frac{\partial f}{\partial \boldsymbol{x}} = \begin{bmatrix} \frac{\partial \boldsymbol{y}_1}{\partial \boldsymbol{x}_1} & \frac{\partial \boldsymbol{y}_1}{\partial \boldsymbol{x}_2} & \cdots & \frac{\partial \boldsymbol{y}_1}{\partial \boldsymbol{x}_N} \\ \frac{\partial \boldsymbol{y}_2}{\partial \boldsymbol{x}_1} & \frac{\partial \boldsymbol{y}_2}{\partial \boldsymbol{x}_2} & \cdots & \frac{\partial \boldsymbol{y}_2}{\partial \boldsymbol{x}_N} \\ \ddots & \ddots & \ddots & \ddots \\ \frac{\partial \boldsymbol{y}_M}{\partial \boldsymbol{x}_1} & \frac{\partial \boldsymbol{y}_M}{\partial \boldsymbol{x}_2} & \cdots & \frac{\partial \boldsymbol{y}_M}{\partial \boldsymbol{x}_N} \end{bmatrix} \in \mathbb{R}^{M \times N}$$

This is called the **Jacobian**.

Notation Continued

- When $M = 1$, then $\frac{\partial f}{\partial \boldsymbol{x}} \in \mathbb{R}^{1 \times N}$ (row vector),
- When $M = 1$, we usually denote the **gradient** of f with $\nabla_{\boldsymbol{x}} f$; in other words, $\nabla_{\boldsymbol{x}} f = \frac{\partial f}{\partial \boldsymbol{x}}^T \in \mathbb{R}^{N \times 1}$ (column vector),
- When $M = 1$, the **Hessian** of f is:

$$\nabla^2_{\boldsymbol{xx}} f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_N} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_N} \\ \ddots & \ddots & \ddots & \ddots \\ \frac{\partial^2 f}{\partial x_N \partial x_1} & \frac{\partial^2 f}{\partial x_N \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_N^2} \end{bmatrix}$$

Taylor Series/Linearization

We want to compute the Taylor expansion of f around $\bar{\boldsymbol{x}}$:

$$f(\boldsymbol{x}) \approx f(\bar{\boldsymbol{x}}) + \frac{\partial f}{\partial \boldsymbol{x}}\Big|_{\bar{\boldsymbol{x}}} (\boldsymbol{x} - \bar{\boldsymbol{x}}) + \dots$$

We can write: $\boldsymbol{x} = \bar{\boldsymbol{x}} + \Delta \boldsymbol{x}$, **and thus**:

$$f(\boldsymbol{x}) = f(\bar{\boldsymbol{x}} + \Delta \boldsymbol{x}) \approx f(\bar{\boldsymbol{x}}) + \frac{\partial f}{\partial \boldsymbol{x}}\Big|_{\bar{\boldsymbol{x}}} \Delta \boldsymbol{x} + \dots$$

Unconstrained Continuous Optimization

Unconstrained Optimization (minimization!):

$$\min_{\boldsymbol{x}} f(\boldsymbol{x})$$

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Unconstrained Optimization (minimization!):

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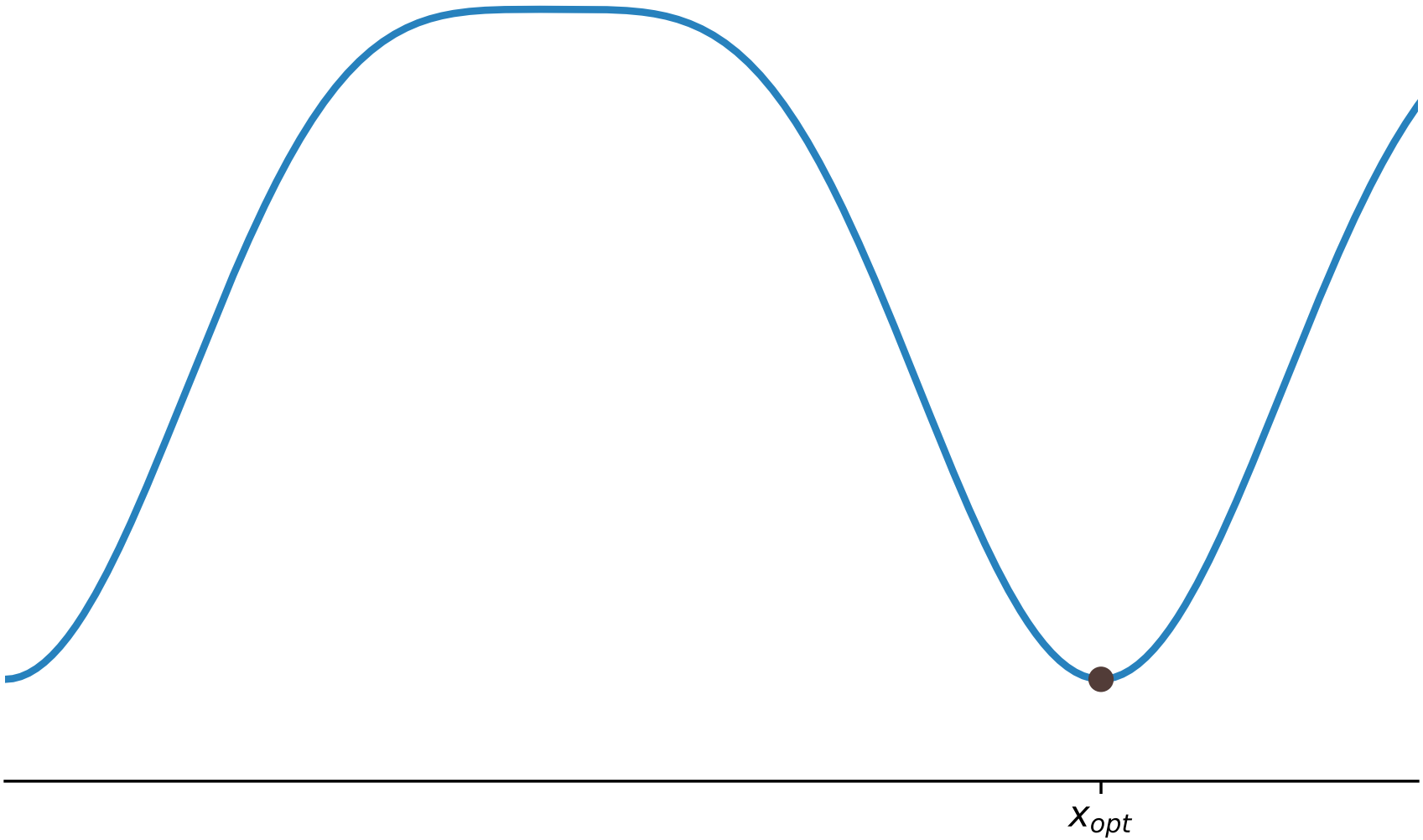
- $\boldsymbol{x} \in \mathbb{R}^N$: **variables**
- $f(\boldsymbol{x}) : \mathbb{R}^N \rightarrow \mathbb{R}$: **objective function**
- $\boldsymbol{x}_*$ is the (global) **optimal solution**, if $f(\boldsymbol{x}_*) \leqslant f(\boldsymbol{x}), \forall \boldsymbol{x}$
- $\boldsymbol{x}_*$ is a **local optimum**, if $f(\boldsymbol{x}_*) \leqslant f(\boldsymbol{x}), \forall \boldsymbol{x} \in \mathcal{N}_{\boldsymbol{x}_*}$ (neighborhood of $\boldsymbol{x}_*$)

How does a solution look like?



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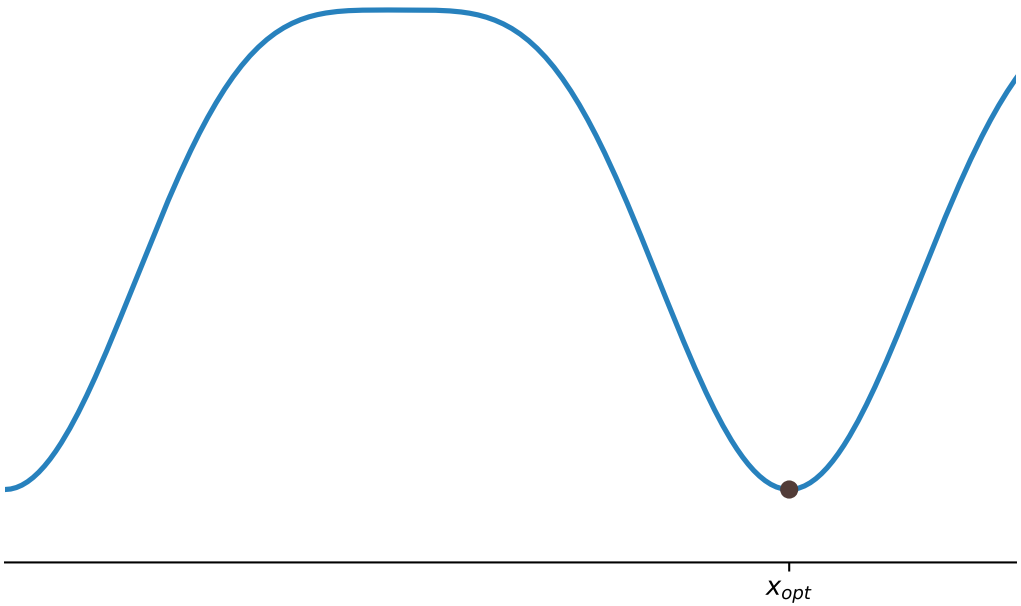

Necessary Condition for a (local) solution (when f is smooth):

$$\left.\frac{\partial f}{\partial \boldsymbol{x}}\right|_{\boldsymbol{x}_*} = 0 \Leftrightarrow \nabla_{\boldsymbol{x}} f(\boldsymbol{x}_*) = 0$$

How does a solution look like? (3)

First Order Necessary Condition for a (local) minimum:

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Second Order Necessary Condition for a (local) minimum:

$$\nabla_{\boldsymbol{x}} f(\boldsymbol{x}_*) = 0$$

$$\nabla^2_{\boldsymbol{x}\boldsymbol{x}} f(\boldsymbol{x}_*) \text{ is psd}$$

Necessary and Sufficient Conditions

- **Necessary conditions** $\rightarrow$ if $\boldsymbol{x}_*$ is a (local) minimum, then these conditions hold;

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- **Sufficient conditions** $\rightarrow$ if these conditions hold for $\boldsymbol{x}_\dagger$, then $\boldsymbol{x}_\dagger$ is a (local) minimum.

Enough of this! Let's see some action!

Problems related to optimization or maybe **useful to optimization**

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Problems related to optimization or maybe **useful to optimization**

- **Root Finding:** Find $\boldsymbol{x}^*$ such that $f(\boldsymbol{x}^*) = 0$,
- **Fixed Point:** Find $\boldsymbol{x}^*$ such that $f(\boldsymbol{x}^*) = \boldsymbol{x}^*$,
- Many ways of solving this:
  - Fixed-Point Iteration
  - ...
  - Newton's Method

Newton's Method

- Linearize around current estimate, $\boldsymbol{x}_k$:

$$f(\boldsymbol{x}_k + \Delta\boldsymbol{x}) \approx f(\boldsymbol{x}_k) + \frac{\partial f}{\partial \boldsymbol{x}}\Big|_{\boldsymbol{x}_k} \Delta\boldsymbol{x}$$

- We then set $f(\boldsymbol{x}_k + \Delta\boldsymbol{x}) = 0$ and solve for $\Delta\boldsymbol{x}$:

$$f(\boldsymbol{x}_k) + \frac{\partial f}{\partial \boldsymbol{x}}\Big|_{\boldsymbol{x}_k} \Delta\boldsymbol{x} = 0$$

$$\Delta\boldsymbol{x} = -\left(\frac{\partial f}{\partial \boldsymbol{x}}\Big|_{\boldsymbol{x}_k}\right)^{-1} f(\boldsymbol{x}_k)$$

- We apply the correction $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \Delta\boldsymbol{x}$

- Repeat until convergence

And so?

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}), f(\boldsymbol{x}) : \mathbb{R}^N \rightarrow \mathbb{R}$$

Necessary Condition for solution (when f is smooth):

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Idea: We can frame optimization as root finding in the gradient!

Optimization via Root Finding

Newton's Method for Optimization:

$$\nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k + \Delta\boldsymbol{x}) \approx \nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k) + \frac{\partial}{\partial \boldsymbol{x}} \Big(\nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k) \Big) \Delta\boldsymbol{x} = 0$$

$$\nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k + \Delta\boldsymbol{x}) \approx \nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k) + \nabla^2_{\boldsymbol{xx}} f(\boldsymbol{x}_k) \Delta\boldsymbol{x} = 0$$

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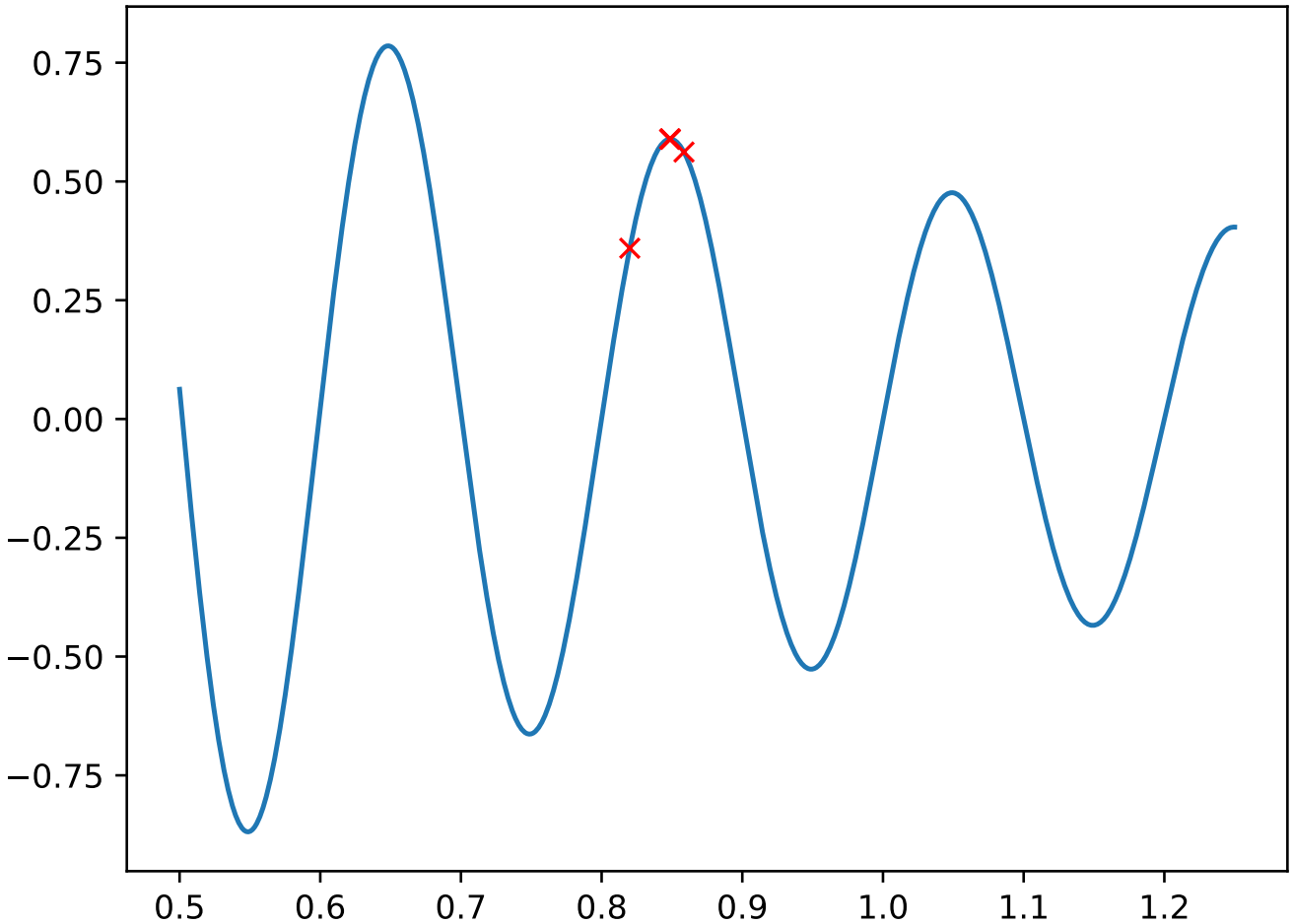
$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \Delta\boldsymbol{x}$$

Optimization via Root Finding - Code Example



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Not sufficient! Let's have a look at the 1D case:

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$$\Delta \boldsymbol{x} = \underbrace{-}_{\text{“descent”}} \underbrace{\left(\nabla^2_{\boldsymbol{xx}} f(\boldsymbol{x}_k)\right)^{-1}}_{\text{“learning rate”}} \underbrace{\nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k)}_{\text{“gradient”}}$$

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- If $\nabla^2_{\boldsymbol{xx}} f(\boldsymbol{x}) > 0$, then **“descent”**,
- If $\nabla^2_{\boldsymbol{xx}} f(\boldsymbol{x}) < 0$, then **“ascent”**!

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In $\mathbb{R}^N$:

- If $\nabla^2_{\boldsymbol{xx}} f(\boldsymbol{x}) \succ 0$ (positive definite), **“descent”**,
- If $\nabla^2_{\boldsymbol{xx}} f(\boldsymbol{x}) \prec 0$ (negative definite), **“ascent”**!

"Damped" Newton's Method

So, how do we solve this?

"Damped" Newton's Method

So, how do we solve this? Many was! Simplest yet effective is to add regularization or "damping":

$$\boldsymbol{H} = \nabla^2_{\boldsymbol{xx}} f(\boldsymbol{x}_k)$$
$$\text{while } \boldsymbol{H} \preceq 0 :$$
$$\quad \boldsymbol{H} = \boldsymbol{H} + \beta \boldsymbol{I}$$
$$\Delta \boldsymbol{x} = -\boldsymbol{H}^{-1} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k)$$
$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \Delta \boldsymbol{x}$$

Backtracking Line Search

- Often $\Delta \boldsymbol{x}$ overshoots the real optimum. Why?

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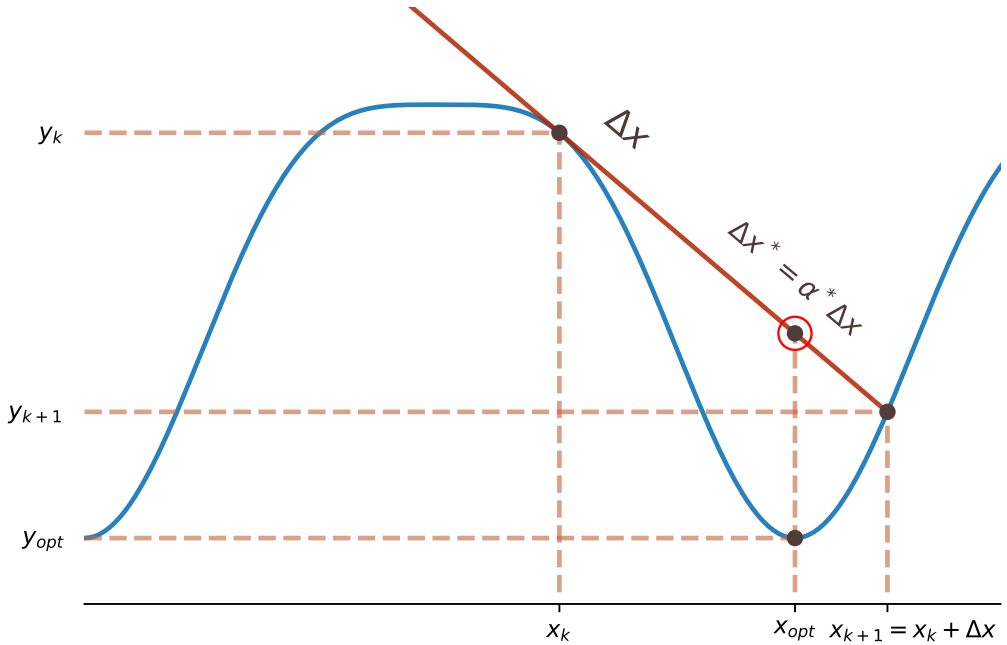

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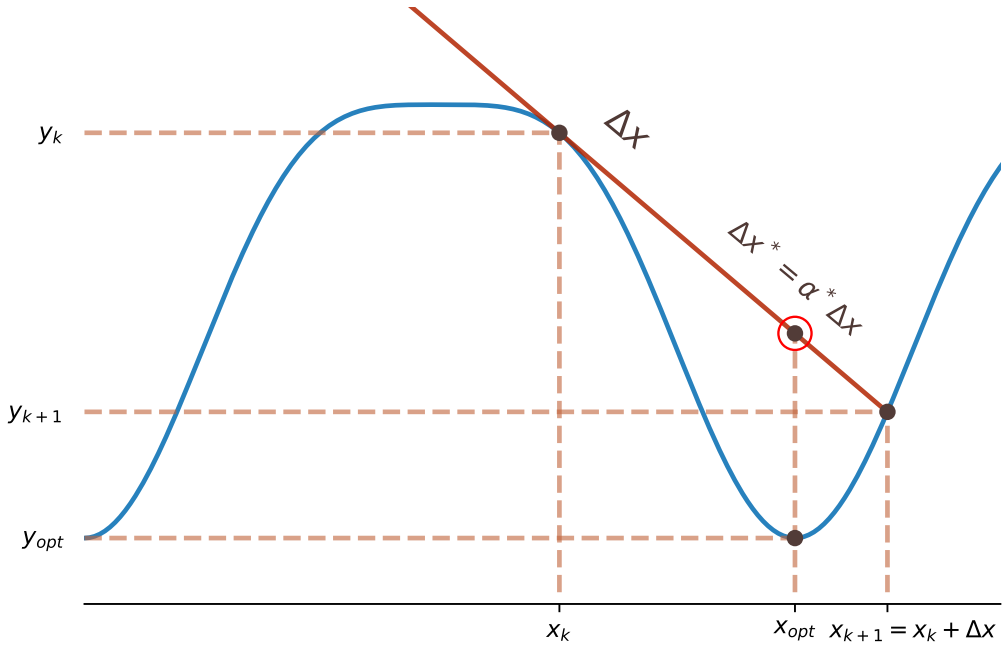

- To fix this issue:
  - We check if $f(\boldsymbol{x}_k + \Delta \boldsymbol{x})$ is good
  - If not, we "backtrack"; aka, we decrease $\Delta \boldsymbol{x}$
  - Repeat until we have a nice reduction

Line Search - Armijo Rule

Armijo Rule:

$$\begin{aligned} \alpha &= 1 \\ \text{while } & f(\boldsymbol{x}_k + \alpha \Delta \boldsymbol{x}) > f(\boldsymbol{x}_k) + b\alpha \nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k)^T \Delta \boldsymbol{x} : \\ & \alpha = c\alpha \\ \boldsymbol{x}_{k+1} &= \boldsymbol{x}_k + \alpha \Delta \boldsymbol{x} \end{aligned}$$

with $0 < c < 1$, α is like a "step-size", and b is the "tolerance". Usually, $c = 0.5$ and b in range from $1e^{-4}$ to 0.1.

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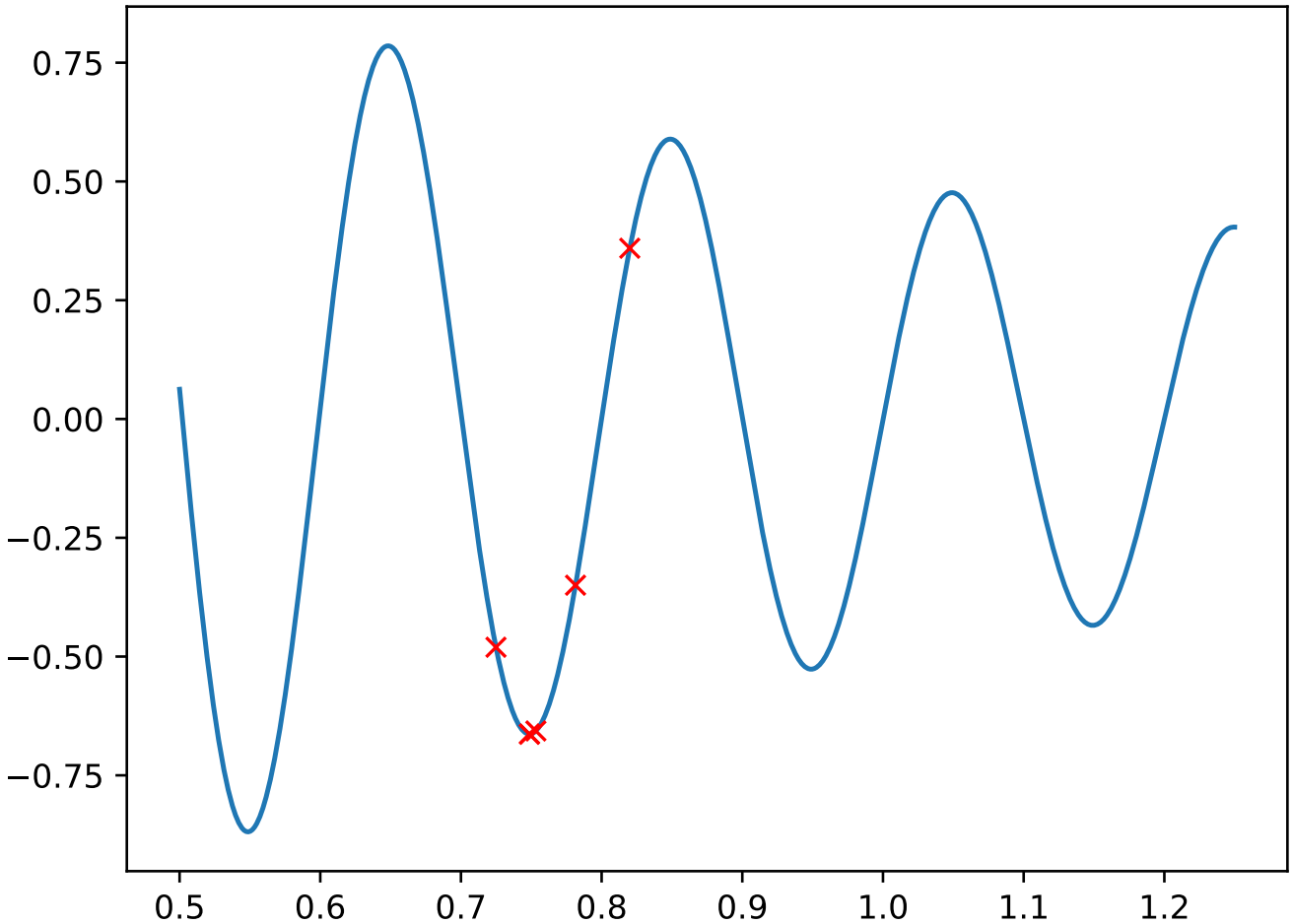
\end{aligned}
$$

with $0 < c < 1$, α is like a "step-size", and b is the "tolerance". Usually, $c = 0.5$ and b in range from $1e^{-4}$ to 0.1.

Intuition: The actual step needs to agree with the Taylor expansion (linearization) up to a tolerance.

Newton's Method with tricks - Code Example



Newton's Method and Optimization

Newton's Method:

- Quadratic Convergence
- Very accurate
- $O(N^3)$ for solving the linear system
  - We can improve this by exploiting the structure of the problem
- **Newton's Method for Optimization:**
  - Local! It will only find the "closest" minimum point
  - **We need to "fix" it in order to optimize!**

Gradient Descent

What if we do not have the Hessian?

- We can approximate it: **Quasi-Newton Methods** (e.g. BFGS)
- We can use the gradient only!

[1] Toussaint, Marc. 2012. Some Notes on Gradient Descent.

Gradient Descent

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Let's go back to our update equation:

$$\Delta \boldsymbol{x} = \underbrace{-}_{\text{"descent"}} \underbrace{\alpha}_{\text{"learning rate"}} \underbrace{\nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k)}_{\text{"gradient"}}$$

How to choose the "learning rate"?

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How to choose the "learning rate"?

1. Initialize $\alpha = \alpha_0$
2. $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \alpha \nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k)$
3. if $f(\boldsymbol{x}_{k+1}) > f(\boldsymbol{x}_k)$ then $\alpha = \alpha\beta$ $(0 < \beta < 1)$ and $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k$
4. if $f(\boldsymbol{x}_{k+1}) < f(\boldsymbol{x}_k)$ then $\alpha = \alpha\zeta$ $(\zeta > 1)$
5. $k = k + 1$ and back to step 2 until we converge

It is guaranteed to always converge to a local minimum[1]! Usually $\beta = 0.5, \zeta = 1.2$.

[1] Toussaint, Marc. 2012. Some Notes on Gradient Descent.

Gradient Descent With Momemtum

$$\Delta \boldsymbol{x} = \underbrace{-}_{\text{“descent”}} \underbrace{\alpha}_{\text{“learning rate”}} \underbrace{\nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k)}_{\text{“gradient”}}$$

How to choose the “learning rate”?

- ...

Gradient Descent With Momemtum

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How to choose the “learning rate”?

- ...
- Momemtum:
  1. Initialize $\boldsymbol{m}_0 = \mathbf{0}, \eta \in [0, 1]$
  2. $\boldsymbol{m}_{k+1} = \eta \boldsymbol{m}_k + (1 - \eta)\alpha \nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k)$
  3. $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \boldsymbol{m}_{k+1}$
  4. $k = k + 1$ and back to step 2 until we converge

Faster convergence and “smooths out” the noise in gradient steps.

Adam Optimizer

$$\Delta \boldsymbol{x} = \underbrace{-}_{\text{“descent”}} \underbrace{\alpha}_{\text{“learning rate”}} \underbrace{\nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k)}_{\text{“gradient”}}$$

How to choose the “learning rate”?

Adam Optimizer

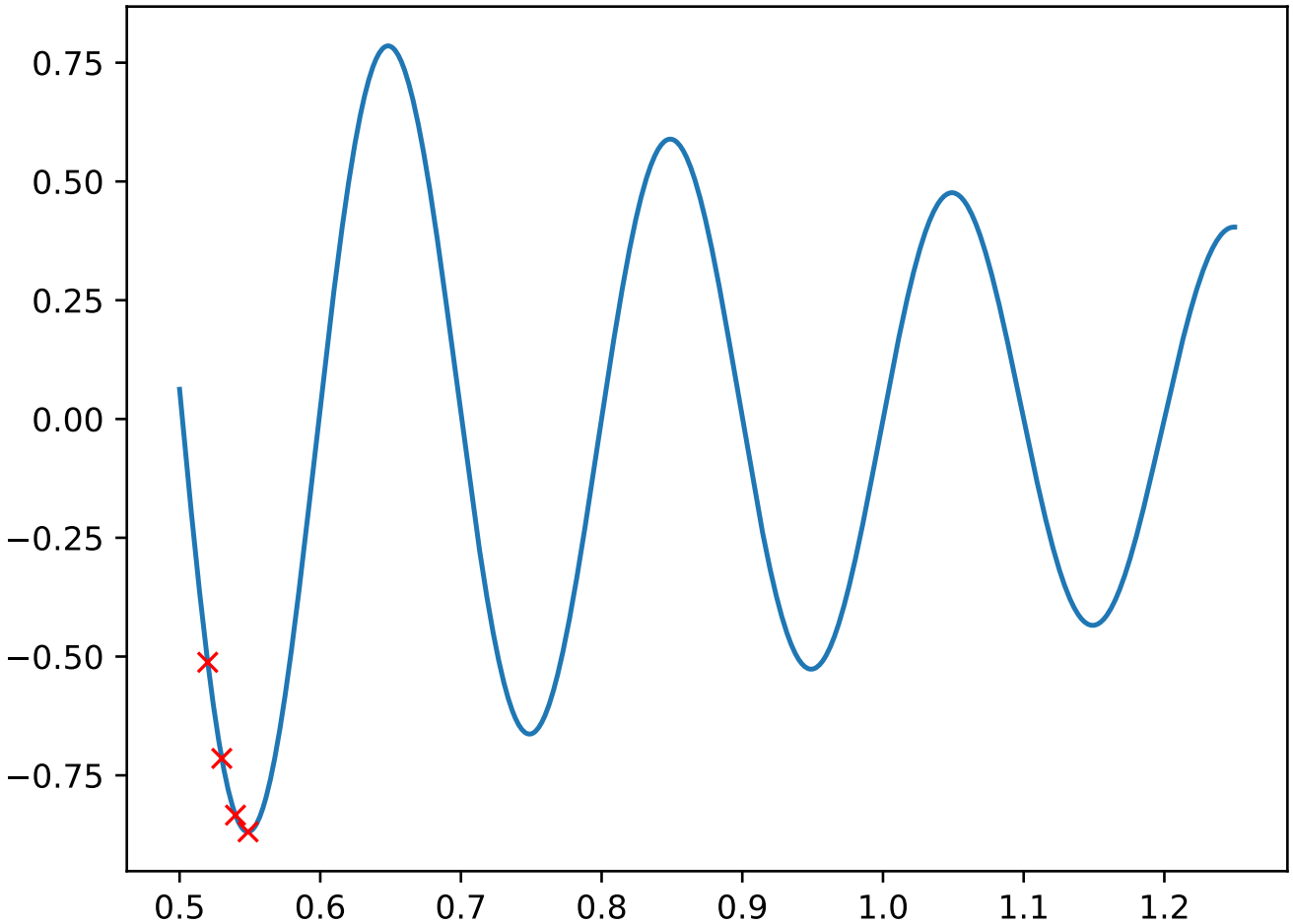
$$\Delta \boldsymbol{x} = \underbrace{-}_{\text{“descent”}} \quad \underbrace{\alpha}_{\text{“learning rate”}} \quad \underbrace{\nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k)}_{\text{“gradient”}}$$

How to choose the “learning rate”?

- **Adam Optimizer**:
  1. Initialize $\boldsymbol{m}_0 = \boldsymbol{v}_0 = \boldsymbol{0}, \beta_1, \beta_2 \in [0, 1), \epsilon > 0$
  2. $\boldsymbol{g}_{k+1} = \nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k)$
  3. $\boldsymbol{m}_{k+1} = \beta_1 \boldsymbol{m}_k + (1 - \beta_1)\boldsymbol{g}_{k+1}$
  4. $\boldsymbol{v}_{k+1} = \beta_2 \boldsymbol{v}_k + (1 - \beta_2)\boldsymbol{g}_{k+1}^2$
  5. $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \alpha \dfrac{\frac{\boldsymbol{m}_{k+1}}{1-\beta_1^{k+1}}}{\sqrt{\frac{\boldsymbol{v}_{k+1}}{1-\beta_2^{k+1}}} + \epsilon}$
  6. $k = k + 1$ and back to step 2 until we converge

One of the most versatile first order optimizers. *Not always the best choice, but surely the first one!* Usually $\beta_1 = 0.9, \beta_2 = 0.999$ and $\epsilon = 10^{-8}$.

Gradient Descent - Code Example



Stochastic Gradient Descent

- We cannot always compute the *exact* $\nabla_{\boldsymbol{x}} f(\boldsymbol{x}_k)$:
  - We do not have access and we approximate it via finite differences
  - Computation limitations: too big of a dataset!
  - Computation limitations: too expensive to compute the actual one, we use an approximated version!
  - ...

Stochastic Gradient Descent

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  - Computation limitations: too big of a dataset!
  - Computation limitations: too expensive to compute the actual one, we use an approximated version!
  - ...
- **Stochastic Gradient Descent** (SGD) is just acknowledging this fact!
- Under assumptions and mitigation measures, we can still theoretically converge to a local optimum

SGD - Verdict

- **Pros:**
  - Can handle large datasets
  - Can handle noisy gradients
  - Can handle non-smooth functions

SGD - Verdict

- **Pros:**
  - Can handle large datasets
  - Can handle noisy gradients
  - Can handle non-smooth functions
- **Cons:**
  - Convergence is not guaranteed
  - May oscillate around the optimum
  - Requires careful tuning of hyperparameters

Gradient Approximation via Finite Differences

- **What if we cannot compute the gradient at all?**

Gradient Approximation via Finite Differences

- **What if we cannot compute the gradient at all?**
- We know that $\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) = \lim_{h \to 0} \frac{f(\boldsymbol{x}+h)-f(\boldsymbol{x})}{h}$

Gradient Approximation via Finite Differences

- **What if we cannot compute the gradient at all?**
- We know that $\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) = \lim_{h \to 0} \frac{f(\boldsymbol{x}+h)-f(\boldsymbol{x})}{h}$
- **Idea:** Let's use $\frac{f(\boldsymbol{x}+h)-f(\boldsymbol{x})}{h}$ as an approximation of the gradient!
- As we make $\boldsymbol{h}$ smaller, we should be getting better approximations! Up to a limit! We have finite precision!
- In N-D, this looks like this:

$$\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) \approx \begin{bmatrix} \frac{f(\boldsymbol{x}+h\boldsymbol{e}_1)-f(\boldsymbol{x})}{h} \\ \vdots \\ \frac{f(\boldsymbol{x}+h\boldsymbol{e}_D)-f(\boldsymbol{x})}{h} \end{bmatrix}$$

where $\boldsymbol{e}_i$ is a direction vector (aka all zeros instead of the i-th component that is equal to 1).

Gradient Approximation via Finite Differences (2)

- In practice we use $\frac{f(\boldsymbol{x}+h)-f(\boldsymbol{x}-h)}{2h}$
- This has an error $O(h^2)$
- Numerically more stable (aka we can use smaller h)
- In N-D, this looks like this:

$$\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) \approx \begin{bmatrix} \frac{f(\boldsymbol{x}+h\boldsymbol{e}_1)-f(\boldsymbol{x}-h\boldsymbol{e}_1)}{2h} \\ \vdots \\ \frac{f(\boldsymbol{x}+h\boldsymbol{e}_D)-f(\boldsymbol{x}-h\boldsymbol{e}_D)}{2h} \end{bmatrix}$$

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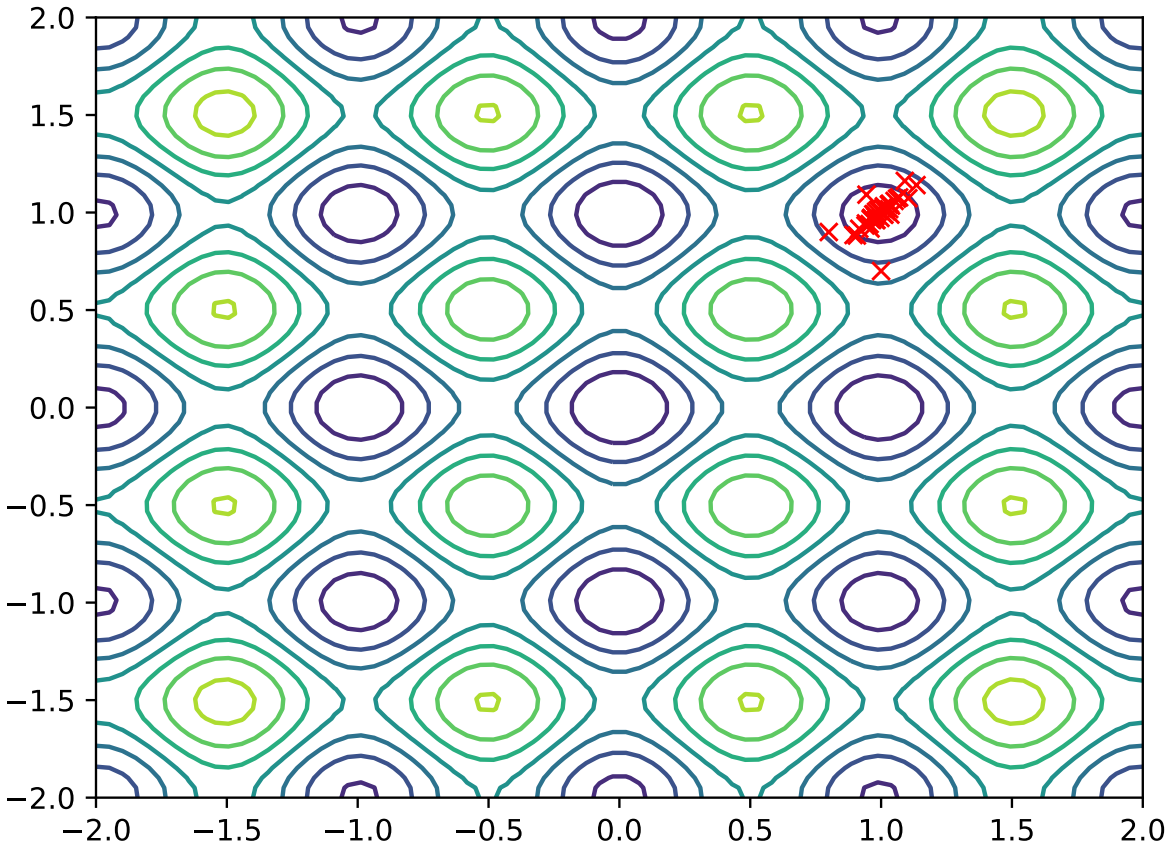
Gradient Approximation - Code Example (2)



Gradient Approximation via Finite Differences (3)

Pros:

- Simple
- Easy to implement
- Accurate results for small h

Cons:

- We need $2D$ function calls for one gradient approximation
- If your function is "expensive", this is a bad way of approximating the gradient
- Many numerical errors can arise

Gradient Approximation with Random Samples

- How can we use the finite difference idea and random sampling to approximate more efficiently high-dimensional gradients?
- **Simple idea:**

$$\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) \approx \sum_{i=1}^{N} \frac{(f(\boldsymbol{x}+\sigma\boldsymbol{\epsilon}_i) - f(\boldsymbol{x}-\sigma\boldsymbol{\epsilon}_i))}{2N\sigma}\boldsymbol{\epsilon}_i$$

where $\boldsymbol{\epsilon}_i \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$.

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- **Why is this efficient?**

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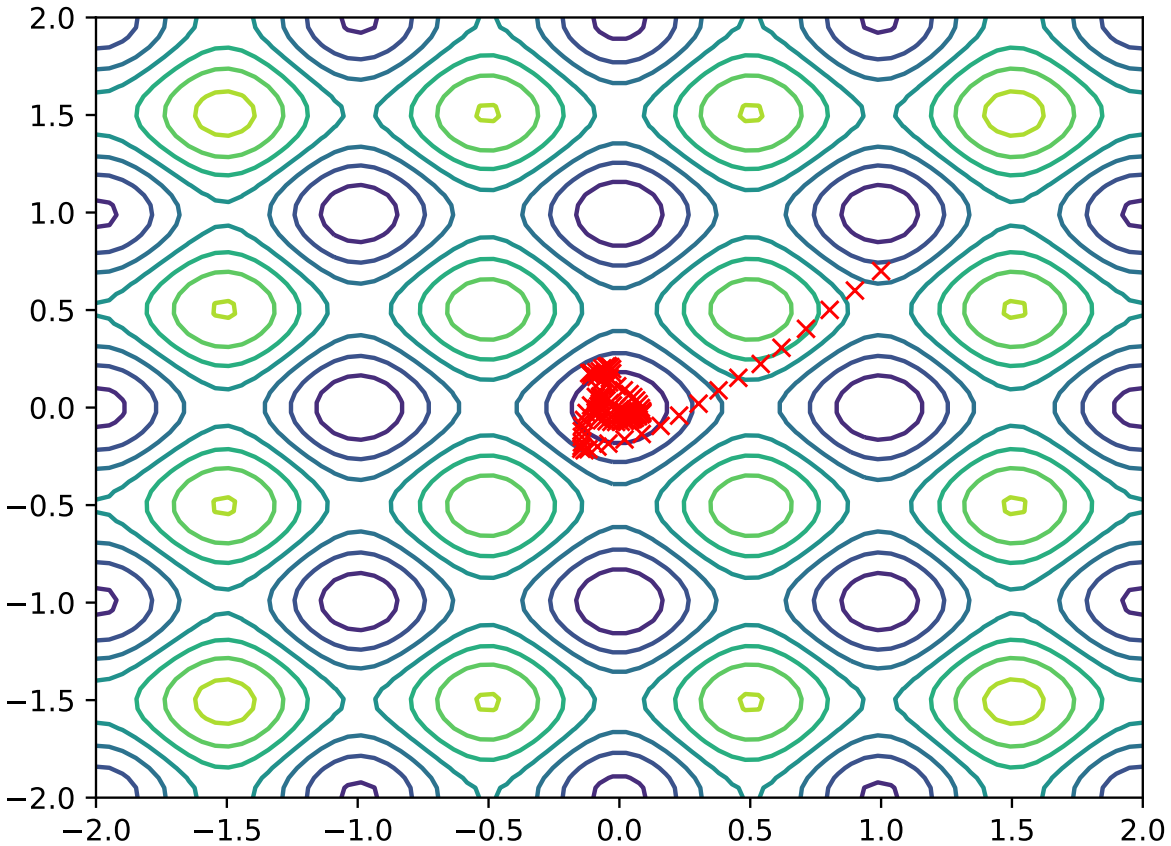
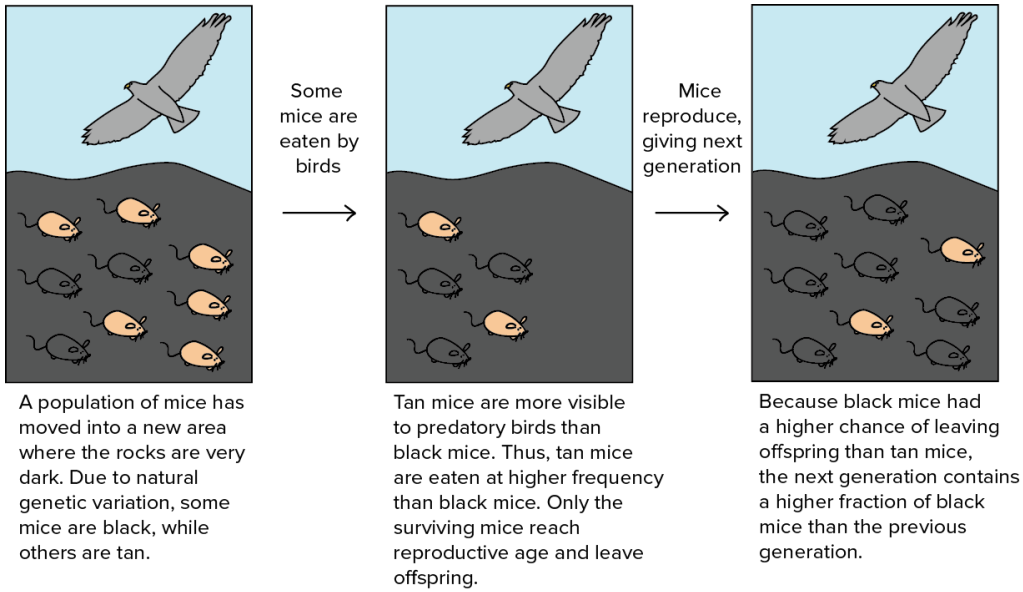
  where $\boldsymbol{\epsilon}_i \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$.
- **Why is this efficient?**
- **Why is this effective?**

Gradient with Random Samples - Code Example



Evolutionary Algorithms



Source: Khan Academy "Darwin, evolution, & natural selection"

- The previous approximation is part of an *evolutionary algorithm* called **Antithetic Evolution Strategies**!!
- **Evolutionary Algorithms** (EAs) are inspired by the natural evolution of fittest.
- **Evolution Strategies** are EAs that model the population as a parameteric distribution (e.g. Gaussian) and optimize its parameters.

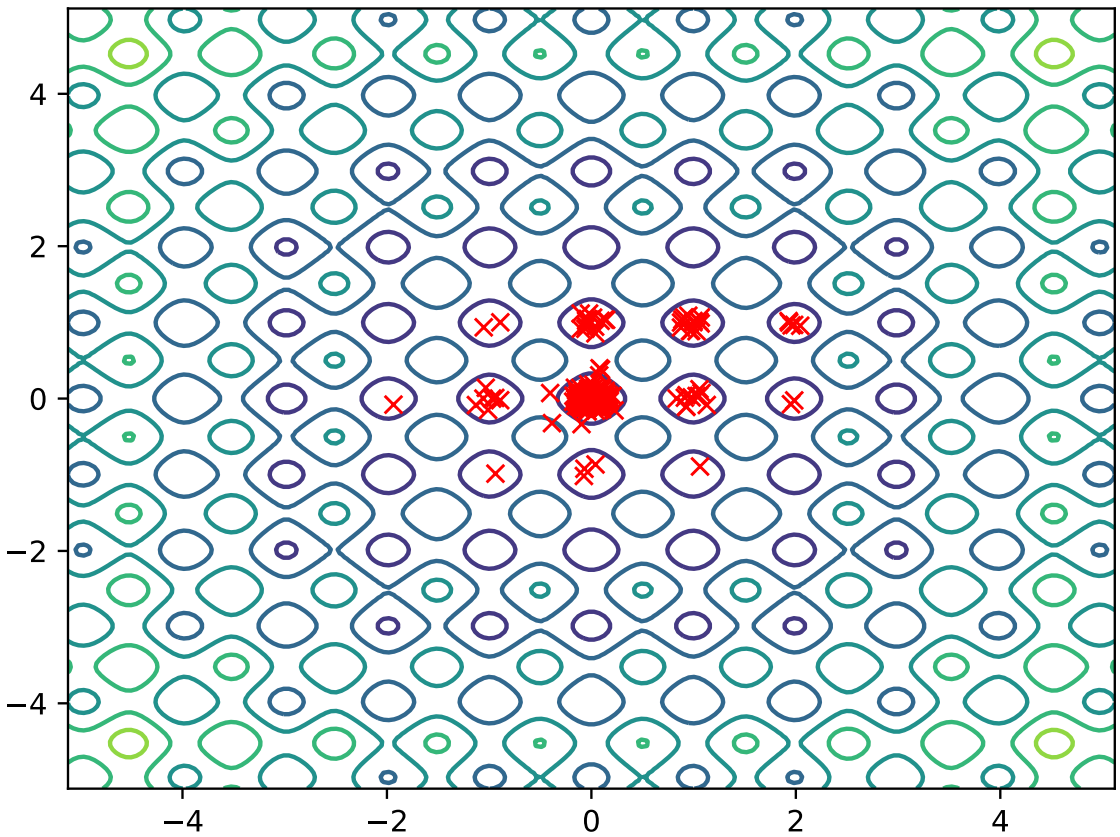
Evolutionary Algorithms - General Structure

1. Generate or set the initial population
2. Evaluate each individual in the population
3. Select individuals for reproduction (*parents*)
4. Breed new individuals (*offspring*) or update existing individuals through crossover and mutation operations
5. Discard the least-fit individuals or replace them with new individuals
6. Possibly re-generate the population
7. Go back to step 2 (repeat until convergence/stopping criteria)

A Simple Genetic Algorithm

1. Generate or set the initial population of size N, $\mathcal{P} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$
2. Evaluate each individual in the population, $\mathcal{F} = \{f(\boldsymbol{x}_1), \ldots, f(\boldsymbol{x}_N)\}$
3. Sort $\mathcal{F}$ and select the best $M < N$ individuals for reproduction, $\mathcal{P}_{\text{elite}} = \{\boldsymbol{x}_1^{\text{elite}}, \ldots, \boldsymbol{x}_M^{\text{elite}}\}$
4. Set $\mathcal{O} = \varnothing$
5. For each $\boldsymbol{x}_i^{\text{elite}} \in \mathcal{P}_{\text{elite}}$:
   1. Select randomly another $\boldsymbol{x}_j^{\text{elite}} \in \mathcal{P}_{\text{elite}}$ $(i \neq j)$
   2. Compute: $\boldsymbol{x}_i^{\text{offspring}} = \boldsymbol{x}_i^{\text{elite}} + \underbrace{\epsilon_1}_{\text{mutation}} + \underbrace{\epsilon_2(\boldsymbol{x}_j^{\text{elite}} - \boldsymbol{x}_i^{\text{elite}})}_{\text{crossover}}$, where $\epsilon_1 \sim \mathcal{N}(\mathbf{0}, \sigma_1 \boldsymbol{I}), \epsilon_2 \sim \mathcal{N}(\mathbf{0}, \sigma_2 \boldsymbol{I})$.
   3. Add $\boldsymbol{x}_i^{\text{offspring}}$ to $\mathcal{O}$
6. Replace the lowest scoring individuals of $\mathcal{P}$ with $\mathcal{O}$
7. Go back to step 2 (repeat until convergence/stopping criteria)

Genetic Algorithm - Code Example

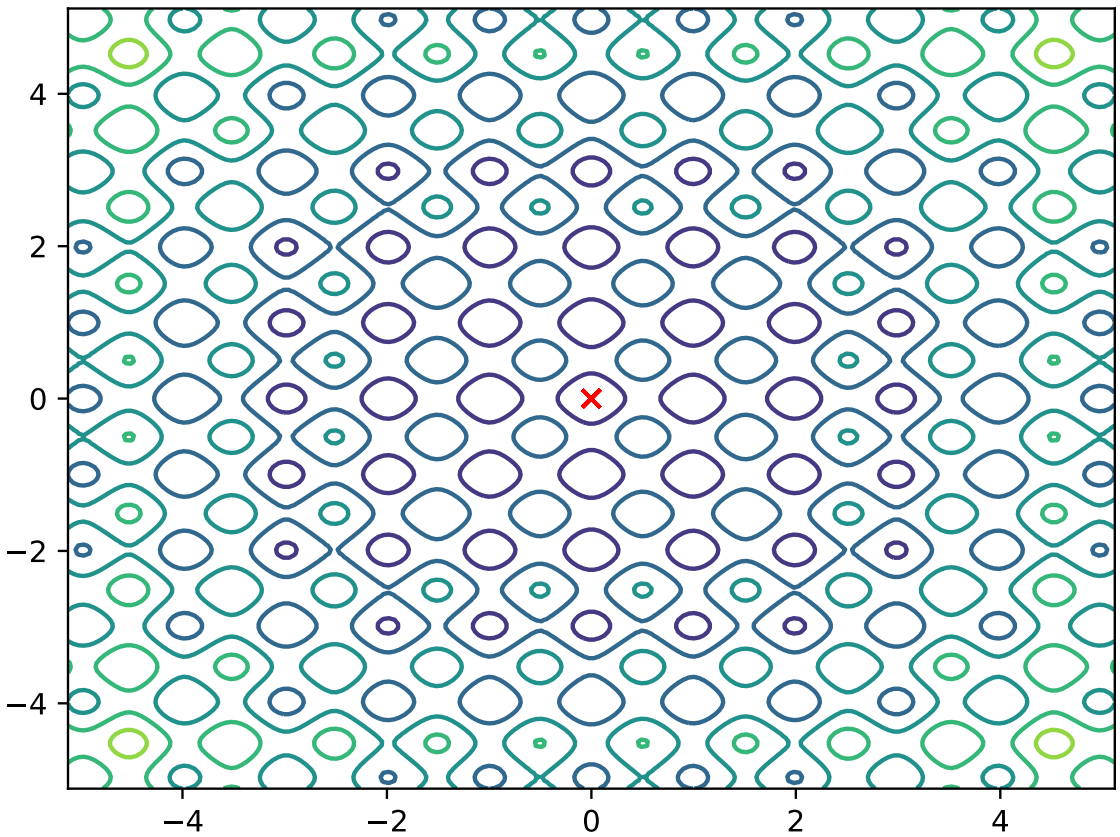


Cross Entropy Method (CEM)

Cross Entropy Method (CEM) or Simple Evolution Strategies:

1. The population is a Gaussian distribution: $\mathcal{N}(\boldsymbol{\mu}, \text{diag}(\boldsymbol{\sigma}^2))$
2. Generate a population of size N, $\mathcal{P} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$, where $\boldsymbol{x}_i \sim \mathcal{N}(\boldsymbol{\mu}_k, \text{diag}(\boldsymbol{\sigma}_k^2))$
3. Evaluate each individual in the population, $\mathcal{F} = \{f(\boldsymbol{x}_1), \ldots, f(\boldsymbol{x}_N)\}$
4. Select the best $M < N$ individuals from $\mathcal{F}$: $\mathcal{P}_{\text{elite}} = \{\boldsymbol{x}_1^{\text{elite}}, \ldots, \boldsymbol{x}_M^{\text{elite}}\}$
5. $\boldsymbol{\mu}_{k+1} = \frac{1}{M} \sum_{\boldsymbol{x}_i^{\text{elite}} \in \mathcal{P}_{\text{elite}}} \boldsymbol{x}_i^{\text{elite}}$ (Sample mean)
6. $\boldsymbol{\sigma}_{k+1}^2 = \frac{1}{M} \sum_{\boldsymbol{x}_i^{\text{elite}} \in \mathcal{P}_{\text{elite}}} (\boldsymbol{x}_i^{\text{elite}} - \boldsymbol{\mu}_k)^2$ (Sample variance)
7. Go back to step 2 (repeat until convergence/stopping criteria)

Cross Entropy Method - Code Example



Covariance Matrix Adaptation ES (CMA-ES)

- Similar to CEM
- We use a full Covariance matrix, not just a diagonal
- Effective heuristics for adapting the Covariance matrix
- Versatile black-box optimizer!
- Very good performance with small populations!

Zero-Order-Optimization - Verdict

- **Pros:**
  - No need for gradients
  - Can handle non-smooth functions
  - Can handle noisy functions
  - Global optimization

Zero-Order-Optimization - Verdict

- **Pros:**
  - No need for gradients
  - Can handle non-smooth functions
  - Can handle noisy functions
  - Global optimization
- **Cons:**
  - Slow convergence
  - Requires many function evaluations
  - Tricky to scale to high dimensions

Constrained Optimization: Equality Constraints

$$\min_{\boldsymbol{x}} f(\boldsymbol{x})$$
$$\text{s.t. } h(\boldsymbol{x}) = 0$$

where $f(\boldsymbol{x}) : \mathbb{R}^N \rightarrow \mathbb{R}, h(\boldsymbol{x}) : \mathbb{R}^N \rightarrow \mathbb{R}^M$.

First Order Necessary Conditions:

$$1)\ \frac{\partial f}{\partial \boldsymbol{x}} + \boldsymbol{\lambda}^T \frac{\partial h}{\partial \boldsymbol{x}} = 0$$
$$2)\ h(\boldsymbol{x}) = 0$$

$\boldsymbol{\lambda} \in \mathbb{R}^M$

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$$2)\ h(\boldsymbol{x}) = 0$$

$\boldsymbol{\lambda} \in \mathbb{R}^M$ and $\boldsymbol{\lambda}$ is called the **"Lagrange multiplier"** or **"dual variable"**.

Constrained Optimization: Equality Constraints (2)

$$\min_{x,y} \; (x-1)^2 + (y-2)^2$$

$$\text{s.t. } \; x + y - 2 = 0$$

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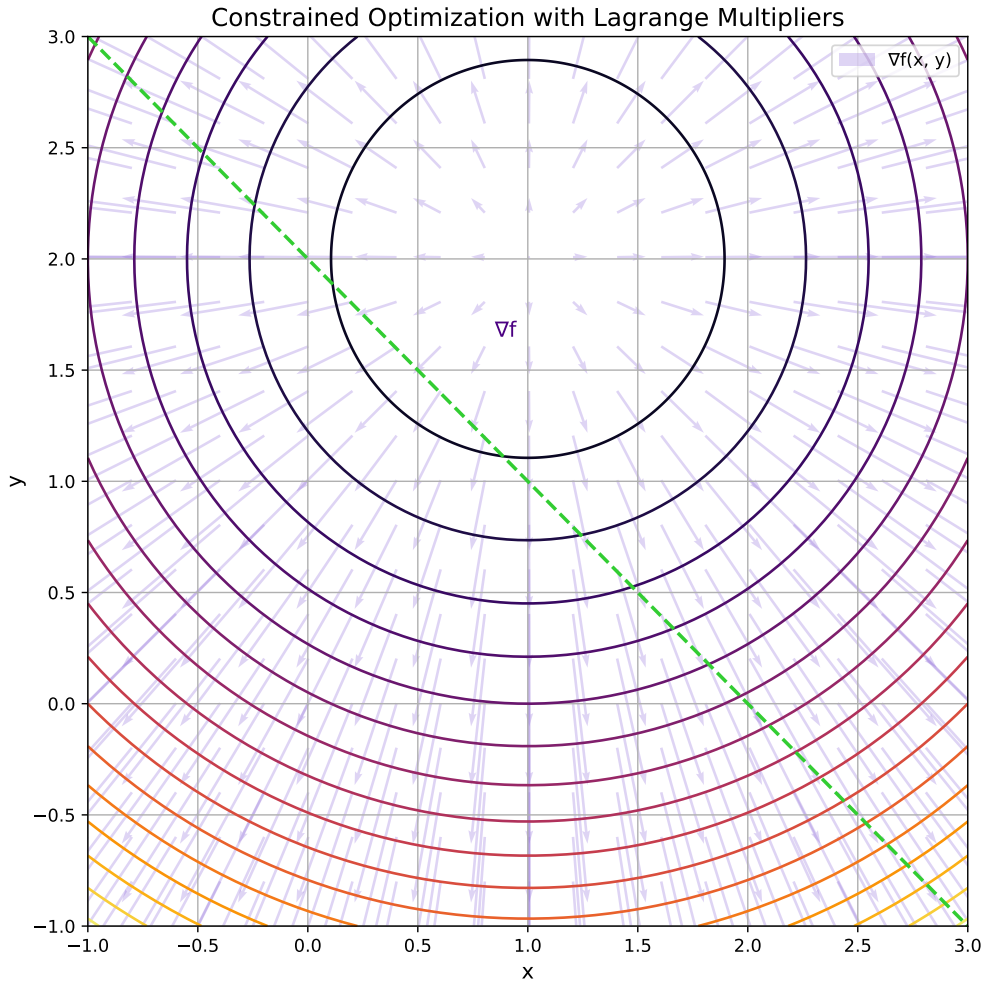
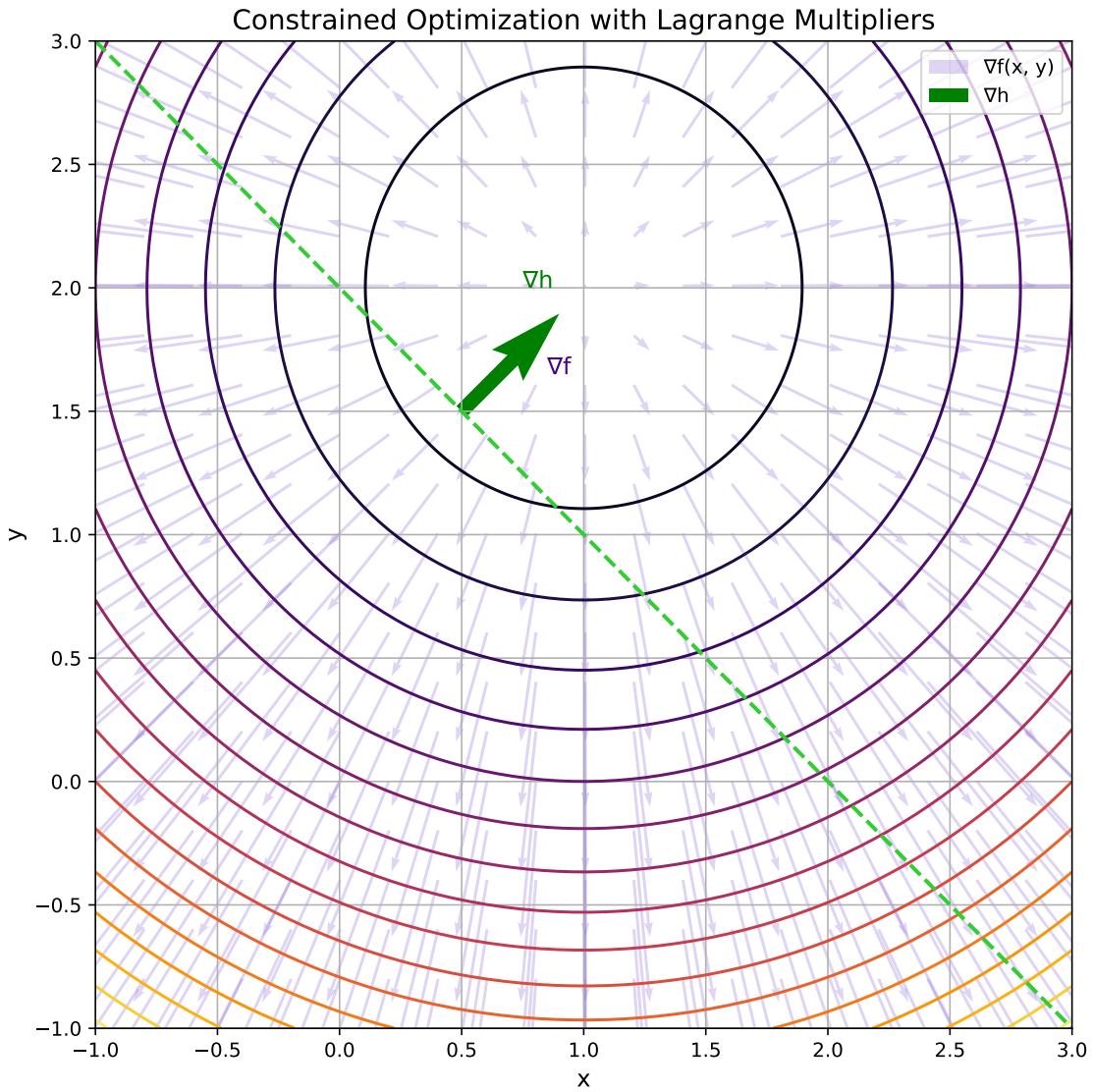
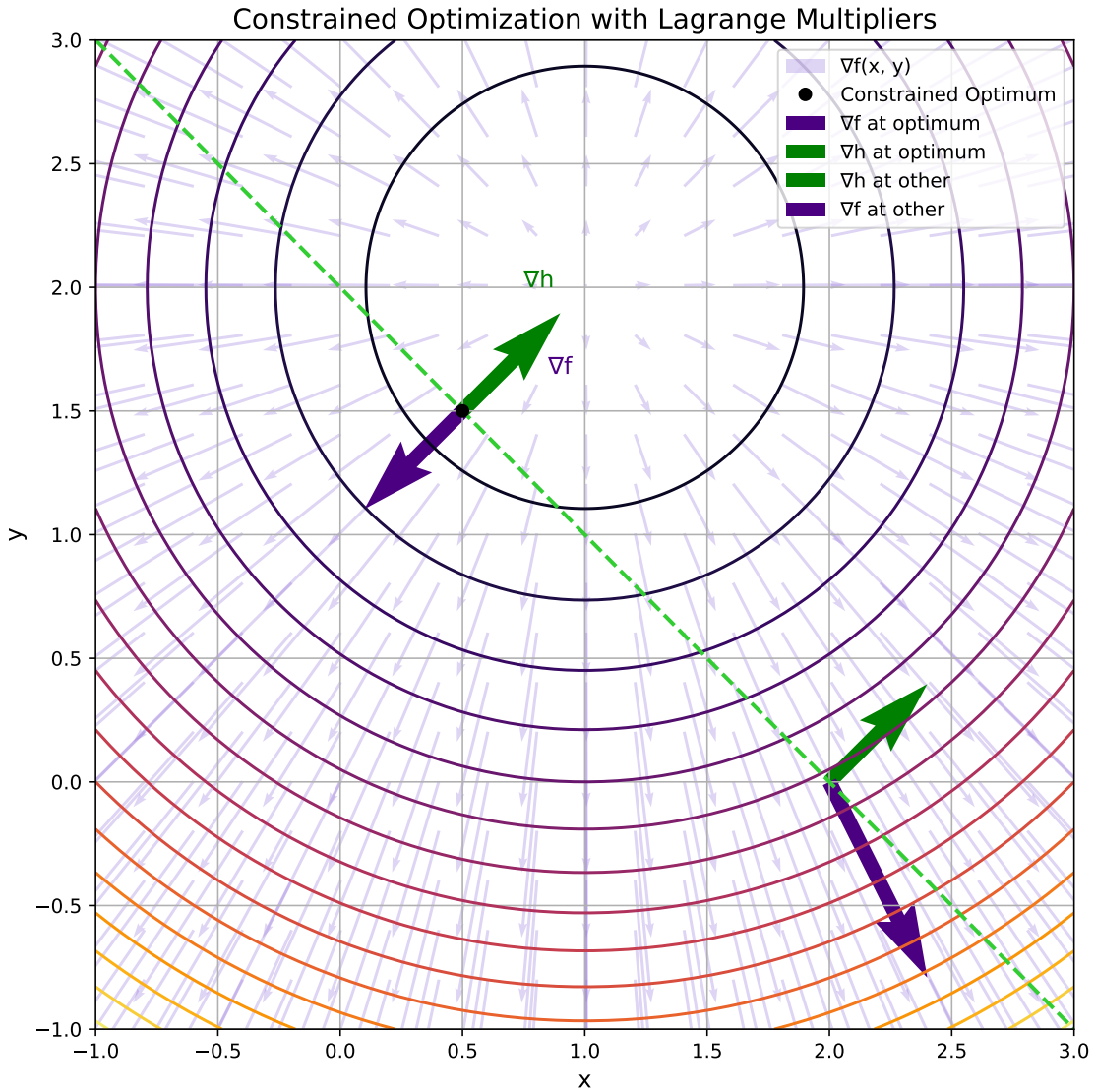


Constrained Optimization: Equality Constraints (3)



Constrained Optimization: Equality Constraints (4)



Lagrangian for Equality Constraints

We define the **Lagrangian** as follows:

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) + \boldsymbol{\lambda}^T h(\boldsymbol{x})$$

Now we can say:

$$1)\ \nabla_{\boldsymbol{x}} \mathcal{L} = \nabla_{\boldsymbol{x}} f(\boldsymbol{x}) + \left(\frac{\partial h}{\partial \boldsymbol{x}}\right)^T \boldsymbol{\lambda} = 0$$

$$2)\ \nabla_{\boldsymbol{\lambda}} \mathcal{L} = h(\boldsymbol{x}) = 0$$

We have recovered the original conditions! We call these conditions **"KKT Conditions"**.

Optimization with Equality Constraints

OK! How can we find the solution to this?

OK! How can we find the solution to this?

Idea! Let's use Newton's method!

$$\nabla_{\boldsymbol{x}}\mathcal{L}(\boldsymbol{x}_k+\Delta\boldsymbol{x},\boldsymbol{\lambda}_k+\Delta\boldsymbol{\lambda})=\nabla_{\boldsymbol{x}}\mathcal{L}(\boldsymbol{x}_k,\boldsymbol{\lambda}_k)+\frac{\partial^2\mathcal{L}}{\partial\boldsymbol{x}^2}\Big|_{\boldsymbol{x}_k,\boldsymbol{\lambda}_k}\Delta\boldsymbol{x}+\underbrace{\frac{\partial^2\mathcal{L}}{\partial\boldsymbol{x}\partial\boldsymbol{\lambda}}\Big|_{\boldsymbol{x}_k,\boldsymbol{\lambda}_k}}_{\left(\frac{\partial h}{\partial\boldsymbol{x}}\Big|_{\boldsymbol{x}_k}\right)^T}\Delta\boldsymbol{\lambda}=0$$

$$\nabla_{\boldsymbol{\lambda}}\mathcal{L}(\boldsymbol{x}_k+\Delta\boldsymbol{x},\boldsymbol{\lambda}_k+\Delta\boldsymbol{\lambda})=h(\boldsymbol{x}_k)+\frac{\partial h}{\partial\boldsymbol{x}}\Big|_{\boldsymbol{x}_k}\Delta\boldsymbol{x}=0$$

Optimization with Equality Constraints (2)

$$\nabla_{\boldsymbol{x}}\mathcal{L}(\boldsymbol{x}_k+\Delta\boldsymbol{x},\boldsymbol{\lambda}_k+\Delta\boldsymbol{\lambda})=\nabla_{\boldsymbol{x}}\mathcal{L}(\boldsymbol{x}_k,\boldsymbol{\lambda}_k)+\frac{\partial^2\mathcal{L}}{\partial\boldsymbol{x}^2}\Big|_{\boldsymbol{x}_k,\boldsymbol{\lambda}_k}\Delta\boldsymbol{x}+\left(\frac{\partial h}{\partial\boldsymbol{x}}\Big|_{\boldsymbol{x}_k}\right)^T\Delta\boldsymbol{\lambda}=0$$

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This is a linear system in $\boldsymbol{z}=\begin{bmatrix}\Delta\boldsymbol{x}\\ \Delta\boldsymbol{\lambda}\end{bmatrix}$:

$$\begin{bmatrix}\frac{\partial^2\mathcal{L}}{\partial\boldsymbol{x}^2}\Big|_{\boldsymbol{x}_k,\boldsymbol{\lambda}_k} & \left(\frac{\partial h}{\partial\boldsymbol{x}}\Big|_{\boldsymbol{x}_k}\right)^T\\ \frac{\partial h}{\partial\boldsymbol{x}}\Big|_{\boldsymbol{x}_k} & \mathbf{0}\end{bmatrix}\begin{bmatrix}\Delta\boldsymbol{x}\\ \Delta\boldsymbol{\lambda}\end{bmatrix}=\begin{bmatrix}-\nabla_{\boldsymbol{x}}\mathcal{L}(\boldsymbol{x}_k,\boldsymbol{\lambda}_k)\\ -h(\boldsymbol{x}_k)\end{bmatrix}$$

This is often called the **"KKT System"**.

Gauss-Netwon Method

$$\frac{\partial^2 \mathcal{L}}{\partial \boldsymbol{x}^2} = \nabla^2_{\boldsymbol{xx}} f + \frac{\partial}{\partial \boldsymbol{x}} \Big[(\frac{\partial h}{\partial \boldsymbol{x}})^T \boldsymbol{\lambda} \Big]$$

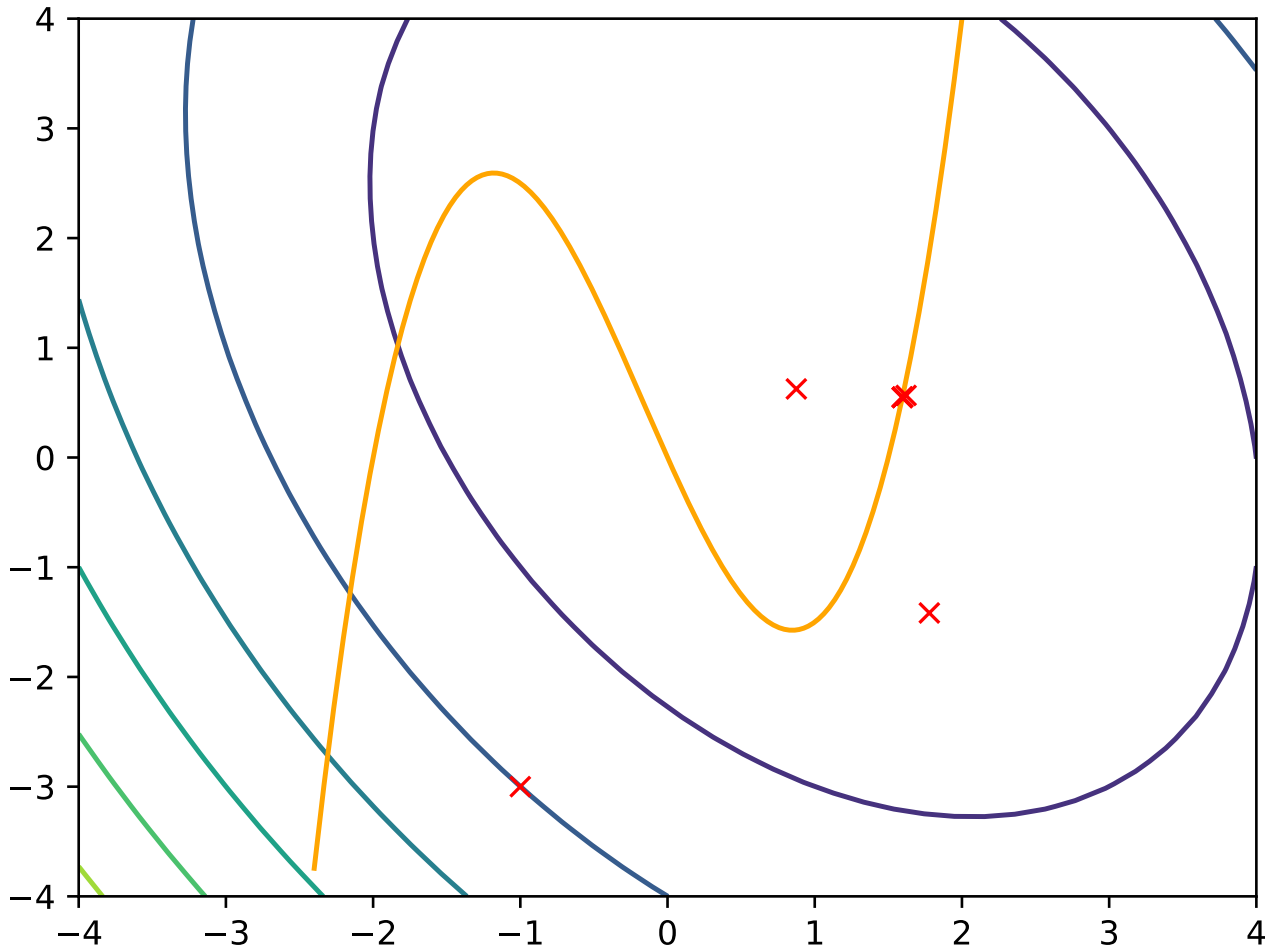
The second term here is:

- A third rank tensor
- Expensive to compute (there are "complicated" ways to compute this faster, e.g. pullback and auto-diff)
- Can be "ugly"/ill-conditioned

In practice, we often remove this term:

- The algorithm is now called "Gauss-Newton"
- In theory it has slower convergence
- In practice it takes more iterations, but each iteration is faster!

Gauss-Netwon Method - Code Example



Constrained Optimization: Inequality Constraints

$$\min_{\boldsymbol{x}} \; f(\boldsymbol{x})$$
$$\text{s.t. } \; g(\boldsymbol{x}) \leqslant 0$$

where $f(\boldsymbol{x}) : \mathbb{R}^N \rightarrow \mathbb{R}, g(\boldsymbol{x}) : \mathbb{R}^N \rightarrow \mathbb{R}^M$. We define the **Lagrangian** as follows:

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\mu}) = f(\boldsymbol{x}) + \boldsymbol{\mu}^T g(\boldsymbol{x})$$

First Order Necessary (KKT) Conditions:

$$1) \; \nabla_{\boldsymbol{x}} f(\boldsymbol{x}) + \left(\frac{\partial g}{\partial \boldsymbol{x}}\right)^T \boldsymbol{\mu} = 0, \qquad \text{“stationarity”}$$

$$2) \; g(\boldsymbol{x}) \leqslant 0, \qquad \text{“primal feasibility”}$$

$$3) \; \boldsymbol{\mu} \geqslant 0, \qquad \text{“dual feasibility”}$$

$$4) \; \boldsymbol{\mu}^T g(\boldsymbol{x}) = 0, \qquad \text{“complementarity”}$$

Constrained Optimization: Inequality Constraints (2)

We cannot solve the above in closed form as in the equality case!!

Many methods to solve this:

- Augmented Lagrangian Method (ALM)
- Sequential Quadratic Programming (SQP)
- Interior Point Methods
- ...

Augmented Lagrangian Method

We define the **Augmented Lagrangian** as:

$$\mathcal{L}_\rho(\boldsymbol{x}, \boldsymbol{\mu}) = f(\boldsymbol{x}) + \boldsymbol{\mu}^T g(\boldsymbol{x}) + \frac{\rho}{2}\|\max(0, g(\boldsymbol{x}))\|^2$$

$\frac{\rho}{2}\|\max(0, g(\boldsymbol{x}))\|^2$ is called the **penalty** term.

Pseudocode:

$$1)\ \boldsymbol{x}_{k+1} = \min_{\boldsymbol{x}} \mathcal{L}_\rho(\boldsymbol{x}, \boldsymbol{\mu}_k)$$

$$2)\ \boldsymbol{\mu}_{k+1} = \max\Big(\mathbf{0}, \boldsymbol{\mu}_k + \rho g(\boldsymbol{x}_{k+1})\Big)$$

$$3)\ \rho = \alpha\rho, \text{ with } \alpha \in \mathbb{R}^+$$

Usually $\alpha \approx 10$ and we use (2) only when the constraints are violated. The method comes with strong convergence guarantees.

How can we solve (1)?

Augmented Lagrangian Method - Minimizing $\mathcal{L}_\rho$

- We need to solve $\min_{\boldsymbol{x}} \mathcal{L}_\rho(\boldsymbol{x}, \boldsymbol{\mu})$
- Important to note that $\boldsymbol{\mu}$ and ρ are constants!

Augmented Lagrangian Method - Minimizing $\mathcal{L}_\rho$

- We need to solve $\min_{\boldsymbol{x}} \mathcal{L}_\rho(\boldsymbol{x}, \boldsymbol{\mu})$
- Important to note that $\boldsymbol{\mu}$ and ρ are constants!
- Let's apply Newton's Method:

$$\nabla_{\boldsymbol{x}} \mathcal{L}_\rho(\boldsymbol{x}_k + \Delta \boldsymbol{x}, \boldsymbol{\mu}_k) \approx$$

$$\nabla_{\boldsymbol{x}} \mathcal{L}_\rho(\boldsymbol{x}_k, \boldsymbol{\mu}_k) + \frac{\partial}{\partial \boldsymbol{x}} \Big(\nabla_{\boldsymbol{x}} \mathcal{L}_\rho(\boldsymbol{x}_k, \boldsymbol{\mu}_k) \Big) \Delta \boldsymbol{x} = 0$$

- We need the gradient of $\mathcal{L}_\rho$:

$$\begin{aligned} \nabla_{\boldsymbol{x}} \mathcal{L}_\rho((\boldsymbol{x}, \boldsymbol{\mu})) &= \left(\frac{\partial f}{\partial \boldsymbol{x}} + \boldsymbol{\mu}^T \frac{\partial g}{\partial \boldsymbol{x}} + \rho g(\boldsymbol{x})^T \frac{\partial g}{\partial \boldsymbol{x}} \right)^T \\ &= \left(\frac{\partial f}{\partial \boldsymbol{x}} + \Big(\boldsymbol{\mu} + \rho g(\boldsymbol{x}) \Big)^T \frac{\partial g}{\partial \boldsymbol{x}} \right)^T = 0 \end{aligned}$$

Augmented Lagrangian Method - Minimizing $\mathcal{L}_\rho$ (2)

$$\nabla_{\boldsymbol{x}} \mathcal{L}_\rho(\boldsymbol{x}_k + \Delta\boldsymbol{x}, \boldsymbol{\mu}_k) \approx$$

$$\nabla_{\boldsymbol{x}} \mathcal{L}_\rho(\boldsymbol{x}_k, \boldsymbol{\mu}_k) + \frac{\partial}{\partial \boldsymbol{x}} \Big(\nabla_{\boldsymbol{x}} \mathcal{L}_\rho(\boldsymbol{x}_k, \boldsymbol{\mu}_k) \Big) \Delta\boldsymbol{x} = 0$$

We can use the Gauss-Newton version and:

$$\frac{\partial}{\partial \boldsymbol{x}} \Big(\nabla_{\boldsymbol{x}} \mathcal{L}_\rho(\boldsymbol{x}_k, \boldsymbol{\mu}_k) \Big) \approx \nabla^2_{\boldsymbol{xx}} f(\boldsymbol{x}_k) + \rho \Big(\frac{\partial g}{\partial \boldsymbol{x}}\Big|_{\boldsymbol{x}_k} \Big)^T \frac{\partial g}{\partial \boldsymbol{x}}\Big|_{\boldsymbol{x}_k}$$

$$\Delta\boldsymbol{x} = -\Big(\nabla^2_{\boldsymbol{xx}} f(\boldsymbol{x}_k) + \rho \Big(\frac{\partial g}{\partial \boldsymbol{x}}\Big|_{\boldsymbol{x}_k} \Big)^T \frac{\partial g}{\partial \boldsymbol{x}}\Big|_{\boldsymbol{x}_k} \Big)^{-1} \nabla_{\boldsymbol{x}} \mathcal{L}_\rho(\boldsymbol{x}_k, \boldsymbol{\mu}_k)$$

Merit Functions

- **How can we apply line search in the constrained case?**

Merit Functions

- **How can we apply line search in the constrained case?**
- We define a **merit function**, $P(\boldsymbol{x})$
- Then we apply the Armijo rule to it

$$
\begin{aligned}
\alpha &= 1 \\
\text{while } P(\boldsymbol{x}_k + \alpha \Delta \boldsymbol{x}) &> P(\boldsymbol{x}_k) + b\alpha \nabla_{\boldsymbol{x}} P(\boldsymbol{x}_k)^T \Delta \boldsymbol{x} : \\
\alpha &= c\alpha \\
\boldsymbol{x}_{k+1} &= \boldsymbol{x}_k + \alpha \Delta \boldsymbol{x}
\end{aligned}
$$

Constrained Minimization

Full constrained minimization:

$$\begin{aligned} \min_{\boldsymbol{x}} \; & f(\boldsymbol{x}) \\ \text{s.t.} \; & g(\boldsymbol{x}) \leqslant 0 \\ & h(\boldsymbol{x}) = 0 \end{aligned}$$

The **Lagrangian** is given:

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = f(\boldsymbol{x}) + \boldsymbol{\lambda}^T h(\boldsymbol{x}) + \boldsymbol{\mu}^T g(\boldsymbol{x})$$

First Order Necessary (KKT) Conditions:

1) $\nabla_{\boldsymbol{x}} f(\boldsymbol{x}) + \left(\frac{\partial h}{\partial \boldsymbol{x}}\right)^T \boldsymbol{\lambda} + \left(\frac{\partial g}{\partial \boldsymbol{x}}\right)^T \boldsymbol{\mu} = 0,$ "stationarity"

2) $g(\boldsymbol{x}) \leqslant 0$ and $h(\boldsymbol{x}) = 0,$ "primal feasibility"

3) $\boldsymbol{\mu} \geqslant 0,$ "dual feasibility"

4) $\boldsymbol{\mu}^T g(\boldsymbol{x}) = 0,$ "complementarity"

Usual Merit Functions

- KKT residual

$$P(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = \frac{1}{2} \| \begin{bmatrix} \nabla_{\boldsymbol{x}} \mathcal{L} \\ h(\boldsymbol{x}) \\ \min(0, g(\boldsymbol{x})) \end{bmatrix} \|^2$$

- Weighted Sum

$$P(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = f(\boldsymbol{x}) + \frac{1}{2} w \| \begin{bmatrix} h(\boldsymbol{x}) \\ \min(0, g(\boldsymbol{x})) \end{bmatrix} \|^2$$

- Augmented Lagrangian

$$P(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = \mathcal{L}_{\rho}(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\mu})$$

Quadratic Programming (QP)

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{Q}\boldsymbol{x} + \boldsymbol{q}^T\boldsymbol{x}$$
$$\text{s.t. } \boldsymbol{A}\boldsymbol{x} - \boldsymbol{b} = \boldsymbol{0}$$
$$\boldsymbol{C}\boldsymbol{x} - \boldsymbol{d} \leqslant \boldsymbol{0}$$

where $\boldsymbol{x}, \boldsymbol{q} \in \mathbb{R}^N$, $\boldsymbol{Q} \succ 0 \in \mathbb{R}^{N \times N}$. Let's solve this with the **Augmented Lagrangian Method:**

Quadratic Programming (QP)

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where $\boldsymbol{x}, \boldsymbol{q} \in \mathbb{R}^N$, $\boldsymbol{Q} \succ 0 \in \mathbb{R}^{N\times N}$. Let's solve this with the **Augmented Lagrangian Method:**

$$\mathcal{L}_\rho(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = f(\boldsymbol{x}) + \boldsymbol{\lambda}^T(\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}) + \boldsymbol{\mu}^T(\boldsymbol{C}\boldsymbol{x} - \boldsymbol{d}) + \frac{\rho}{2}\|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\|^2 + \frac{\rho}{2}\|\max(\boldsymbol{0}, \boldsymbol{C}\boldsymbol{x} - \boldsymbol{d})\|^2$$

KKT Conditions:

1) $\boldsymbol{Q}\boldsymbol{x} + \boldsymbol{q} + \boldsymbol{A}^T\boldsymbol{\lambda} + \boldsymbol{C}^T\boldsymbol{\mu} = 0$
2) $\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b} = \boldsymbol{0}$ and $\boldsymbol{C}\boldsymbol{x} - \boldsymbol{d} \leqslant \boldsymbol{0}$
3) $\boldsymbol{\mu} \geqslant \boldsymbol{0}$
4) $\boldsymbol{\mu}^T(\boldsymbol{C}\boldsymbol{x} - \boldsymbol{d}) = \boldsymbol{0}$

General Constrained Optimization

What other methods are there?

- **Active Set Methods**:
  - Try to guess which constraints are active (equal to zero) or not
  - Solve equality constrained optimization only with active constraints
  - Need good heuristic for identifying potentially active constraints
- **Barrier/Interior Point (IP) Methods:**
  - Add inequality constraints as "barriers"/penalties in the cost function. For example, $f'(\boldsymbol{x}) = f(\boldsymbol{x}) - \frac{1}{\rho}\log(-g(\boldsymbol{x}))$
  - Very good for convex problems

General Constrained Optimization (2)

What other methods are there?

- **Penalty Methods:**
  - Add constraint violation into the cost function. For example, $f'(\boldsymbol{x}) = f(\boldsymbol{x}) + \frac{\rho}{2}\|\max(\mathbf{0}, g(\boldsymbol{x}))\|^2$
  - Similar to IP methods, but there is a key difference: IP methods blow up at the boundary, penalty methods start pushing only if there is a violation!
  - Can easily get ill-conditions
  - Cannot get good accuracy
- **Sequential Quadratic Programming (SQP):**
  - Sequential QP problems
  - General idea:
    - Fit a quadratic approximation of the cost function
    - Linearize the constraints
    - Solve the produced QP with slack variables for feasibility
    - Iterate until convergence

Final Verdict on Optimization

- Newton's Method is very effective; Gauss-Newton the one used mostly in practice
- Transforming your problem into well known forms (e.g. QP) can greatly help
- Stochastic Gradient Descent is very effective for large scale or noisy problems
- Evolutionary Algorithms are very effective for non-smooth problems, but do not scale easily on large scale problems
- A lot of good libraries

Deterministic Optimal Control

Continuous Time:

$$\underset{\boldsymbol{x}(t),\boldsymbol{u}(t)}{\operatorname{argmin}} \mathcal{J}(\boldsymbol{x}(t),\boldsymbol{u}(t)) = \int_{t_0}^{t_f} \ell(\boldsymbol{x}(t),\boldsymbol{u}(t))dt + \ell_F(\boldsymbol{x}(t_f))$$

$$\text{s.t.} \qquad \dot{\boldsymbol{x}}(t) = f(\boldsymbol{x}(t),\boldsymbol{u}(t))$$

where

- $\boldsymbol{x}(t) \in \mathbb{R}^N, \boldsymbol{u}(t) \in \mathbb{R}^M$ are the state and control trajectories
- $\mathcal{J}(\boldsymbol{x}(t),\boldsymbol{u}(t))$ is the "cost function"
- $\ell(\boldsymbol{x}(t),\boldsymbol{u}(t))$ is the "stage cost"
- $\ell_F(\boldsymbol{x}(t_f))$ is the "terminal cost"
- $\dot{\boldsymbol{x}}(t) = f(\boldsymbol{x}(t),\boldsymbol{u}(t))$ are the "dynamics constraints"
- We can potentially add more constraints (e.g. torque limits)

Deterministic Optimal Control (2)

- The continuous version is **“infinite dimensional”**

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- The continuous version is **"infinite dimensional"**
- The solution is open loop control trajectories!
- Only very few problems can be solved analytically
- Let's discretize!

Deterministic Optimal Control - Discrete

Discrete Time:

$$\underset{\boldsymbol{x}_{1:K},\boldsymbol{u}_{1:K-1}}{\text{argmin}} \; \mathcal{J}(\boldsymbol{x}_{1:K},\boldsymbol{u}_{1:K-1}) = \sum_{k=1}^{K-1} \ell(\boldsymbol{x}_k,\boldsymbol{u}_k) + \ell_F(\boldsymbol{x}_K)$$

$$\text{s.t.} \qquad \boldsymbol{x}_{k+1} = f_{\text{discrete}}(\boldsymbol{x}_k,\boldsymbol{u}_k)$$

- $\boldsymbol{x}_k \in \mathbb{R}^N$ and $\boldsymbol{u}_k \in \mathbb{R}^M$ are vectors
- The is now **"finite dimensional"**
- The solution is open loop control trajectories!
- We usually call $\boldsymbol{x}_k, \boldsymbol{u}_k$ **"knot points"**

Linear Quadratic Regulator (LQR)

What is the Linear Quadratic Regulator (LQR) problem?

Linear Quadratic Regulator (LQR)

What is the Linear Quadratic Regulator (LQR) problem?

$$\underset{\boldsymbol{x}_{1:K},\boldsymbol{u}_{1:K-1}}{\text{argmin}} \; \mathcal{J}(\boldsymbol{x}_{1:K},\boldsymbol{u}_{1:K-1}) = \sum_{k=1}^{K-1}\left(\frac{1}{2}\boldsymbol{x}_k^T\boldsymbol{Q}_k\boldsymbol{x}_k + \frac{1}{2}\boldsymbol{u}_k^T\boldsymbol{R}_k\boldsymbol{u}_k\right) + \frac{1}{2}\boldsymbol{x}_K^T\boldsymbol{Q}_K\boldsymbol{x}_K$$

$$\text{s.t.} \quad \boldsymbol{x}_{k+1} = \boldsymbol{A}_k\boldsymbol{x}_k + \boldsymbol{B}_k\boldsymbol{u}_k$$

$$\boldsymbol{Q}_k \succeq 0$$

$$\boldsymbol{R}_k \succ 0$$

- Widely used in many real applications
- The "workhorse" of optimal control
- We know "everything" about it!
- Infinite variations and extensions!
- **Time Invariant** if: $\boldsymbol{A}_k = \boldsymbol{A}, \boldsymbol{B}_k = \boldsymbol{B}, \boldsymbol{Q}_k = \boldsymbol{Q}, \boldsymbol{R}_k = \boldsymbol{R}, \forall k$

LQR as a Quadratic Programming Problem

Looking at the LQR problem, it really looks like a QP. Can we write it like one?

LQR as a Quadratic Programming Problem

Looking at the LQR problem, it really looks like a QP. Can we write it like one? Yes we can! We assume that $\boldsymbol{x}_1$ (initial conditions) is given, and define:

$$\boldsymbol{z} = \begin{bmatrix} \boldsymbol{u}_1 \\ \boldsymbol{x}_2 \\ \boldsymbol{u}_2 \\ \vdots \\ \boldsymbol{x}_K \end{bmatrix}, \boldsymbol{H} = \begin{bmatrix} \boldsymbol{R}_1 & & & & \\ & \boldsymbol{Q}_2 & & & \\ & & \boldsymbol{R}_2 & & \\ & & & \ddots & \\ & & & & \boldsymbol{Q}_K \end{bmatrix}$$

Now we can define:

$$\begin{aligned} \underset{\boldsymbol{z}}{\text{argmin}} \mathcal{J}(\boldsymbol{z}) &= \frac{1}{2}\boldsymbol{z}^T \boldsymbol{H} \boldsymbol{z} \\ \text{s.t.} \quad & \text{“dynamics constraints”} \end{aligned}$$

LQR as a Quadratic Programming Problem (2)

For the dynamics constraints we have:

$$\underbrace{\begin{bmatrix} \boldsymbol{B}_1 & -\boldsymbol{I} & \boldsymbol{0} & \dots & & & \\ \boldsymbol{0} & \boldsymbol{A}_2 & \boldsymbol{B}_2 & -\boldsymbol{I} & \boldsymbol{0} & \dots & \\ & & & \ddots & & & \\ & & & & \boldsymbol{A}_{K-1} & \boldsymbol{B}_{K-1} & -\boldsymbol{I} \end{bmatrix}}_{\boldsymbol{G}} \begin{bmatrix} \boldsymbol{u}_1 \\ \boldsymbol{x}_2 \\ \boldsymbol{u}_2 \\ \vdots \\ \boldsymbol{x}_K \end{bmatrix} = \underbrace{\begin{bmatrix} -\boldsymbol{A}_1\boldsymbol{x}_1 \\ \boldsymbol{0} \\ \boldsymbol{0} \\ \vdots \\ \boldsymbol{0} \end{bmatrix}}_{\boldsymbol{d}}$$

Now we have a full QP:

$$\underset{\boldsymbol{z}}{\text{argmin}} \mathcal{J}(\boldsymbol{z}) = \frac{1}{2}\boldsymbol{z}^T\boldsymbol{H}\boldsymbol{z}$$

$$\text{s.t.} \qquad \boldsymbol{G}\boldsymbol{z} - \boldsymbol{d} = \boldsymbol{0}$$

LQR as a Quadratic Programming Problem (2)

$$\underset{\boldsymbol{z}}{\text{argmin}} \mathcal{J}(\boldsymbol{z}) = \frac{1}{2}\boldsymbol{z}^T \boldsymbol{H}\boldsymbol{z}$$

$$\text{s.t.} \qquad \boldsymbol{G}\boldsymbol{z} - \boldsymbol{d} = \boldsymbol{0}$$

Can we solve this?

LQR as a Quadratic Programming Problem (2)

$$\underset{\boldsymbol{z}}{\text{argmin}} \mathcal{J}(\boldsymbol{z}) = \frac{1}{2}\boldsymbol{z}^T \boldsymbol{H}\boldsymbol{z}$$
$$\text{s.t.} \qquad \boldsymbol{G}\boldsymbol{z} - \boldsymbol{d} = \boldsymbol{0}$$

Can we solve this? Of course we can! The Lagrangian is:

$$\mathcal{L}(\boldsymbol{z}, \boldsymbol{\lambda}) = \frac{1}{2}\boldsymbol{z}^T \boldsymbol{H}\boldsymbol{z} + \boldsymbol{\lambda}^T(\boldsymbol{G}\boldsymbol{z} - \boldsymbol{d})$$

LQR as a Quadratic Programming Problem (2)

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KKT Conditions:

$$\nabla_{\boldsymbol{z}}\mathcal{L} = \boldsymbol{H}\boldsymbol{z} + \boldsymbol{G}^T\boldsymbol{\lambda} = \boldsymbol{0}$$
$$\nabla_{\boldsymbol{\lambda}}\mathcal{L} = \boldsymbol{G}\boldsymbol{z} - \boldsymbol{d} = \boldsymbol{0}$$

LQR as a Quadratic Programming Problem (2)

$$\underset{\boldsymbol{z}}{\text{argmin}} \mathcal{J}(\boldsymbol{z}) = \frac{1}{2}\boldsymbol{z}^T\boldsymbol{H}\boldsymbol{z}$$
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KKT Conditions:

$$\nabla_{\boldsymbol{z}}\mathcal{L} = \boldsymbol{H}\boldsymbol{z} + \boldsymbol{G}^T\boldsymbol{\lambda} = \boldsymbol{0}$$
$$\nabla_{\boldsymbol{\lambda}}\mathcal{L} = \boldsymbol{G}\boldsymbol{z} - \boldsymbol{d} = \boldsymbol{0}$$

KKT System:

$$\begin{bmatrix} \boldsymbol{H} & \boldsymbol{G}^T \\ \boldsymbol{G} & \boldsymbol{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{z} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \boldsymbol{0} \\ \boldsymbol{d} \end{bmatrix}$$

LQR as a Quadratic Programming Problem (2)

$$\underset{z}{\text{argmin}} \mathcal{J}(z) = \frac{1}{2} z^T H z$$
$$\text{s.t.} \qquad Gz - d = 0$$

Can we solve this? Of course we can! The Lagrangian is:

$$\mathcal{L}(z, \lambda) = \frac{1}{2} z^T H z + \lambda^T (Gz - d)$$

KKT Conditions:

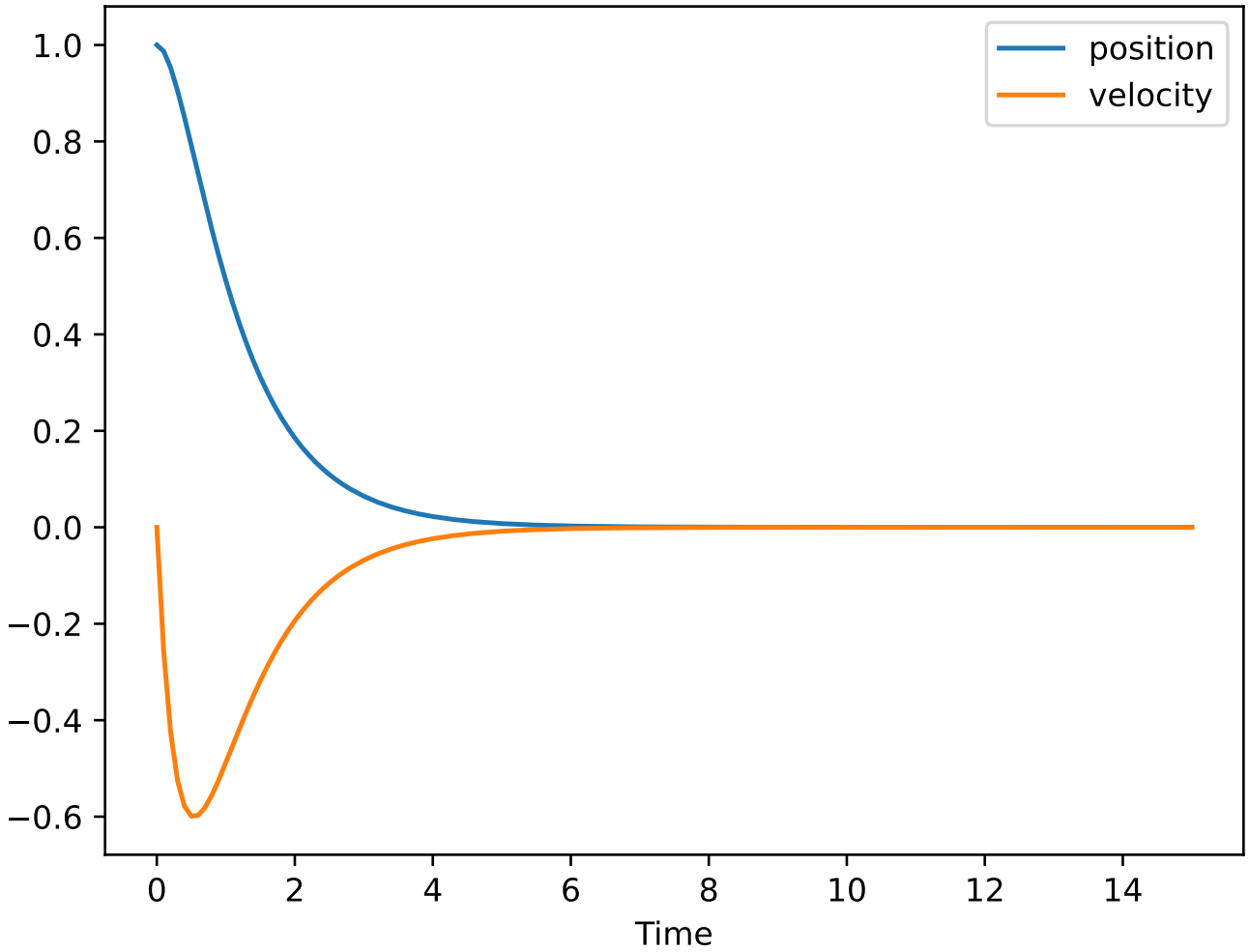
$$\nabla_z \mathcal{L} = Hz + G^T \lambda = 0$$
$$\nabla_\lambda \mathcal{L} = Gz - d = 0$$

KKT System:

$$\begin{bmatrix} H & G^T \\ G & 0 \end{bmatrix} \begin{bmatrix} z \\ \lambda \end{bmatrix} = \begin{bmatrix} 0 \\ d \end{bmatrix}$$

We have the exact solution by solving ONE linear system!

LQR as a QP - Code Example



LQR via Riccati Recursion

Let's write the KKT System in "detail" (for $K = 4$):

$$
\left[\begin{array}{cccccccc}
R_1 & 0 & \cdots & & 0 & B_1^T & \cdots & 0 \\
0 & Q_2 & 0 & \cdots & 0 & -I & A_2^T & \vdots \\
\vdots & 0 & R_2 & 0 & \cdots & 0 & B_2^T & \\
 & \vdots & 0 & Q_3 & 0 & \cdots & -I & A_3^T \\
 & & \vdots & 0 & R_3 & 0 & \cdots & B_3^T \\
0 & 0 & & \vdots & 0 & Q_4 & & -I \\
\hdashline
B_1 & -I & 0 & 0 & \vdots & 0 & \ddots & \vdots \\
\vdots & A_2 & B_2 & -I & 0 & \vdots & & \\
0 & \cdots & & A_3 & B_3 & -I & \cdots & 0
\end{array}\right]
\left[\begin{array}{c} u_1 \\ x_2 \\ u_2 \\ x_3 \\ u_3 \\ x_4 \\ \hdashline \lambda_2 \\ \lambda_3 \\ \lambda_4 \end{array}\right]
=
\left[\begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \hdashline -A_1 x_1 \\ 0 \\ 0 \end{array}\right]
$$

LQR via Riccati Recursion (2)

We first solve the last line of the upper block:

$$\boldsymbol{Q}_4\boldsymbol{x}_4 - \boldsymbol{\lambda}_4 = \boldsymbol{0} \Rightarrow \boldsymbol{\lambda}_4 = \boldsymbol{Q}_K\boldsymbol{x}_4$$

Then we move one line up:

$$\boldsymbol{R}_3\boldsymbol{u}_3 + \boldsymbol{B}_3^T\boldsymbol{\lambda}_4 = \boldsymbol{R}_3\boldsymbol{u}_3 + \boldsymbol{B}_3^T\boldsymbol{Q}_K\boldsymbol{x}_4 = \boldsymbol{0}$$

$$\Rightarrow \boldsymbol{R}_3\boldsymbol{u}_3 + \boldsymbol{B}_3^T\boldsymbol{Q}_K(\boldsymbol{A}_3\boldsymbol{x}_3 + \boldsymbol{B}_3\boldsymbol{u}_3) = \boldsymbol{0}$$

$$\Rightarrow \boldsymbol{u}_3 = -\underbrace{(\boldsymbol{R}_3 + \boldsymbol{B}_3^T\boldsymbol{Q}_K\boldsymbol{B}_3)^{-1}\boldsymbol{B}_3^T\boldsymbol{Q}_K\boldsymbol{A}_3}_{\boldsymbol{K}_3}\boldsymbol{x}_3$$

One more line:

$$\boldsymbol{Q}_3\boldsymbol{x}_3 - \boldsymbol{\lambda}_3 + \boldsymbol{A}_3^T\boldsymbol{\lambda}_4 = \boldsymbol{0} \Rightarrow \boldsymbol{Q}_3\boldsymbol{x}_3 - \boldsymbol{\lambda}_3 + \boldsymbol{A}_3^T\boldsymbol{Q}_K\boldsymbol{x}_4 = \boldsymbol{0}$$

$$\Rightarrow \boldsymbol{Q}_3\boldsymbol{x}_3 - \boldsymbol{\lambda}_3 + \boldsymbol{A}_3^T\boldsymbol{Q}_K(\boldsymbol{A}_3\boldsymbol{x}_3 + \boldsymbol{B}_3\boldsymbol{u}_3) = \boldsymbol{0}$$

$$\Rightarrow \boldsymbol{\lambda}_3 = \underbrace{\left(\boldsymbol{Q}_3 + \boldsymbol{A}_3^T\boldsymbol{Q}_K(\boldsymbol{A}_3 - \boldsymbol{B}_3\boldsymbol{K}_3)\right)}_{\boldsymbol{P}_3}\boldsymbol{x}_3$$

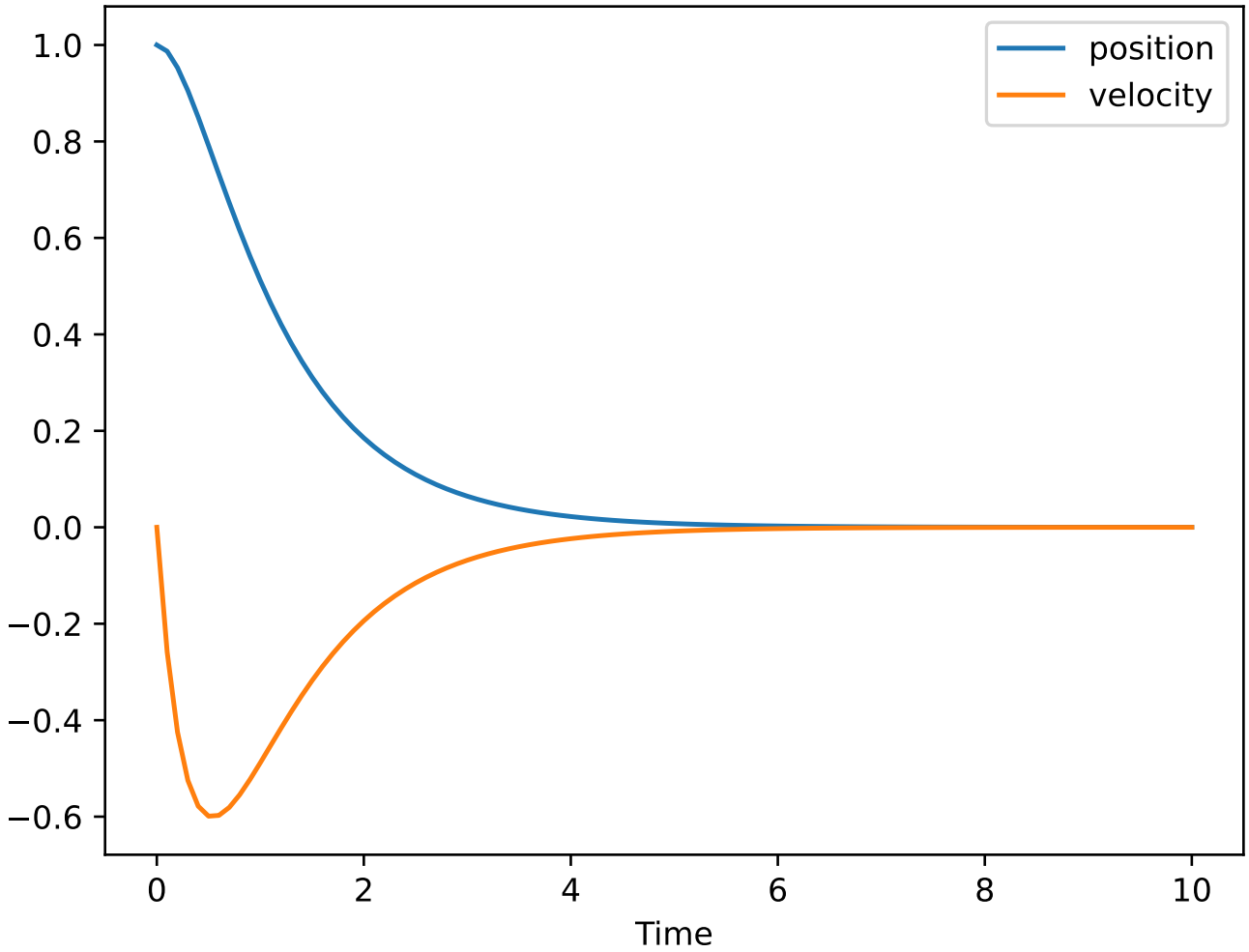
LQR via Riccati Recursion (3)

The recursion is now revealed:

$$\boldsymbol{P}_K = \boldsymbol{Q}_K$$
$$\boldsymbol{K}_k = (\boldsymbol{R}_k + \boldsymbol{B}_k^T \boldsymbol{P}_{k+1} \boldsymbol{B}_k)^{-1} \boldsymbol{B}_k^T \boldsymbol{P}_{k+1} \boldsymbol{A}_k$$
$$\boldsymbol{P}_k = \boldsymbol{Q}_k + \boldsymbol{A}_k^T \boldsymbol{P}_{k+1} (\boldsymbol{A}_k - \boldsymbol{B}_k \boldsymbol{K}_k)$$

- QP has complexity $O(K^3(N+M)^3)$
- Riccati recursion has complexity $O(K(N+M)^3)$
- The Riccati recursion is the optimal exploitation of the sparsity of the KKT system!
- **We also get for free a feedback policy: $\boldsymbol{u} = -\boldsymbol{K}\boldsymbol{x}$!**

LQR via Riccati Recursion - Code Example



Thank you

Any Questions?