

# PV027 Optimization

Tomáš Brázdil

# Resources & Prerequisites

## Resources:

- ▶ Lectures & tutorials (the **main** resources)
- ▶ Books:

Joaquim R. R. A. Martins and Andrew Ning. Engineering Design Optimization. Cambridge University Press, 2021. ISBN: 9781108833417.

Jorge Nocedal and Stephen J. Wright. Numerical optimization. Springer, 2006. ISBN: 0387303030.

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We shall need elementary knowledge and understanding of

- ▶ Linear algebra in  $\mathbb{R}^n$   
Operations with vectors and matrices, bases, diagonalization.
- ▶ Multi-variable calculus (i.e., in  $\mathbb{R}^n$ )  
Partial derivatives, gradients, Hessians, Taylor's theorem.

We will refresh our memories during lectures and tutorials.

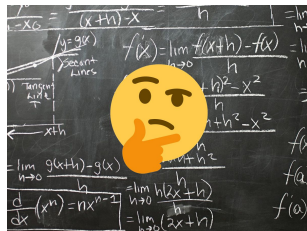
# Evaluation

**Oral exam** - You will get a manual describing the knowledge necessary for **E** and better.

There might be homework assignments that you may discuss at tutorials, but (for this year) there is no mandatory homework.

Please be aware that

This is a **difficult math-based course**.



# What is Optimization

## **Merriam Webster:**

An act, process, or methodology of making something (such as a design, system, or decision) as perfect, functional, or effective as possible.

*specifically*: the mathematical procedures (such as finding the maximum of a function) involved in this.

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## **Britannica**

Collection of mathematical principles and methods for solving quantitative problems in many disciplines, including physics, biology, engineering, economics, and business.

Historically, (mathematical/numerical) optimization is called *mathematical programming*.

# Optimization

People optimize in

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  - ▶ transportation,
  - ▶ education,
  - ▶ ...

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  - ▶ ...
- ▶ machine learning

# Optimization Algorithms

## scipy.optimize.minimize

```
scipy.optimize.minimize(fun, x0, args=(), method=None, jac=None, hess=None,  
hessp=None, bounds=None, constraints=(), tol=None, callback=None, options=None)
```

**method** : *str or callable, optional*

Type of solver. Should be one of

- 'Nelder-Mead' (see here)
- 'Powell' (see here)
- 'CG' (see here)
- 'BFGS' (see here)
- 'Newton-CG' (see here)
- 'L-BFGS-B' (see here)

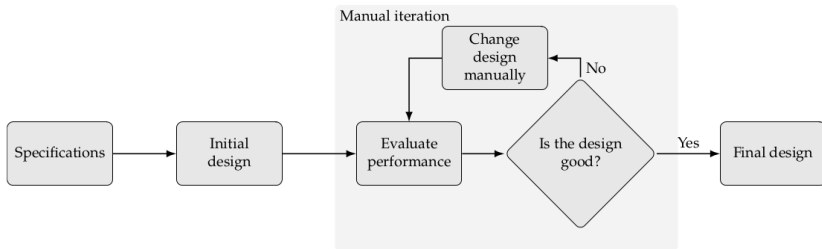
# Optimization Algorithms

## `sklearn.linear_model.LogisticRegression`

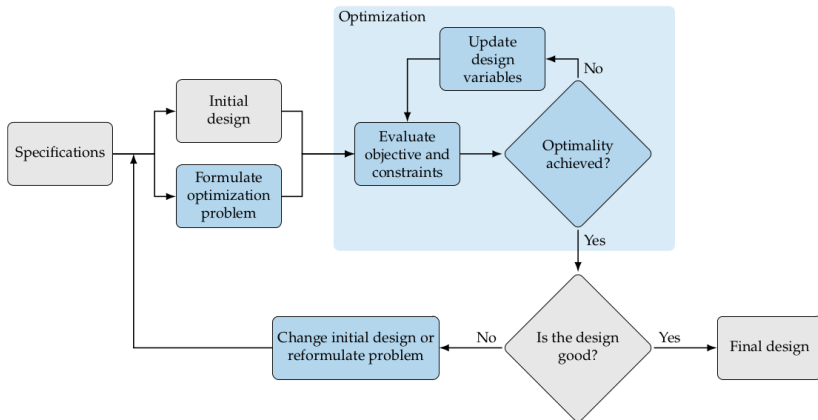
```
class sklearn.linear_model.LogisticRegression(penalty='l2', *, dual=False, tol=0.0001, C=1.0, fit_intercept=True,
intercept_scaling=1, class_weight=None, random_state=None, solver='lbfgs', max_iter=100, multi_class='auto', verbose=0,
warm_start=False, n_jobs=None, l1_ratio=None)
```

**solver** : {'lbfgs', 'liblinear', 'newton-cg', 'newton-cholesky', 'sag', 'saga'}, default='lbfgs'  
Algorithm to use in the optimization problem. Default is 'lbfgs'. To choose a solver,

# Design Optimization Process



# Design Optimization Process



A bit naive example:

- ▶ Consider a company with several plants producing a single product but with different efficiency.
- ▶ The goal is to set the production of each plant so that demand for goods is satisfied, but overproduction is minimized.



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- ▶ Then you notice that all plant employees must work.
- ▶ Then you start solving transportation problems depending on the location of the plants.
- ▶ ...

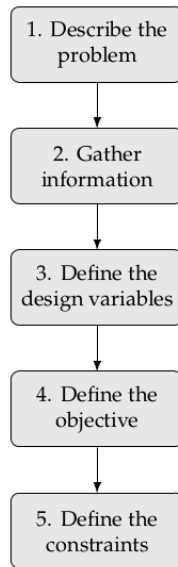
# Optimization Problem Formulation

## 1. Describe the problem

- ▶ Problem formulation is vital since the optimizer exploits any weaknesses in the model formulation.
- ▶ You might get the “right answer to the wrong question.”
- ▶ The problem description is typically informal at the beginning.

## 2. Gather information

- ▶ Identify possible inputs/outputs.
- ▶ Gather data and identify the analysis procedure.



# Optimization Problem Formulation

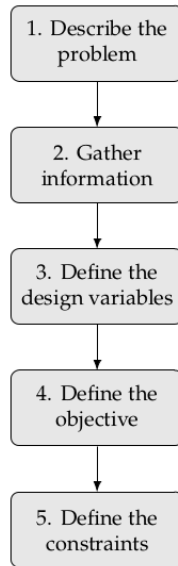
## 3. Define the design **variables**

- Identify the quantities that describe the system:

$$x \in \mathbb{R}^n$$

(i.e., certain characteristics of the system, such as position, investments, etc.)

- The variables are supposed to be independent; the optimizer must be free to choose the components of  $x$  independently.
- The choice of variables is typically not unique (e.g., a square can be described by its side or area).
- The variables may affect the functional form of the objective and constraints (e.g., linear vs non-linear).



# Optimization Problem Formulation

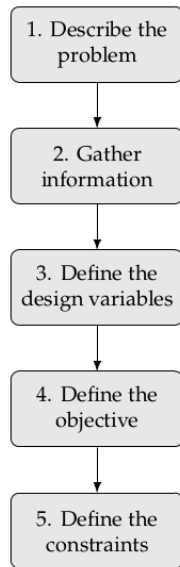
## 4. Define the **objective**

- ▶ The function determines if one design is better than another.
- ▶ Must be a scalar computable from the variables:

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

(e.g., profit, time, potential energy, etc.)

- ▶ The objective function is either maximized or minimized depending on the application.
- ▶ The choice is not always obvious: E.g., minimizing just the weight of a vehicle might result in a vehicle being too expensive to be manufactured.



# Optimization Problem Formulation

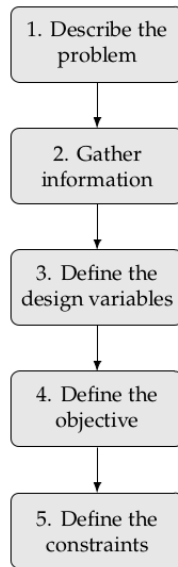
## 5. Define the **constraints**

- ▶ Prescribe allowed values of the variables.
- ▶ May have a general form

$$c(x) \leq 0 \text{ or } c(x) \geq 0 \text{ or } c(x) = 0$$

(e.g., time cannot be negative, bounded amount of money to invest)

Where  $c : \mathbb{R}^n \rightarrow \mathbb{R}$  is a function depending on the variables.



# Modelling and Optimization

The **Optimization Problem** consists of

- ▶ **variables**
- ▶ **objective**
- ▶ **constraints**

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We concentrate on the optimization part but keep in mind that it is intertwined with modeling.

The **Optimization Problem (OP)**: Find settings of variables so that the objective is maximized/minimized while satisfying the constraints.

An **Optimization Algorithm (OA)** solves the above problem and provides a **solution**, some setting of variables satisfying the constraints and minimizing/maximizing the objective.

# Optimization Problems

# Optimization Problem Formally

Denote by

$f : \mathbb{R}^n \rightarrow \mathbb{R}$  an *objective function*,

$x$  a vector of real *variables*,

$g_1, \dots, g_{n_g}$  *inequality constraint functions*  $g_i : \mathbb{R}^n \rightarrow \mathbb{R}$ .

$h_1, \dots, h_{n_h}$  *equality constraint functions*  $h_j : \mathbb{R}^n \rightarrow \mathbb{R}$ .

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The optimization problem is to

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{by varying} & x \\ \text{subject to} & g_i(x) \leq 0 \quad i = 1, \dots, n_g \\ & h_j(x) = 0 \quad j = 1, \dots, n_h \end{array}$$

## Optimization Problem - Example

$$f(x_1, x_2) = (x_1 - 2)^2 + (x_2 - 1)^2$$

$$g_1(x_1, x_2) = x_1^2 - x_2$$

$$g_2(x_1, x_2) = x_1 + x_2 - 2$$

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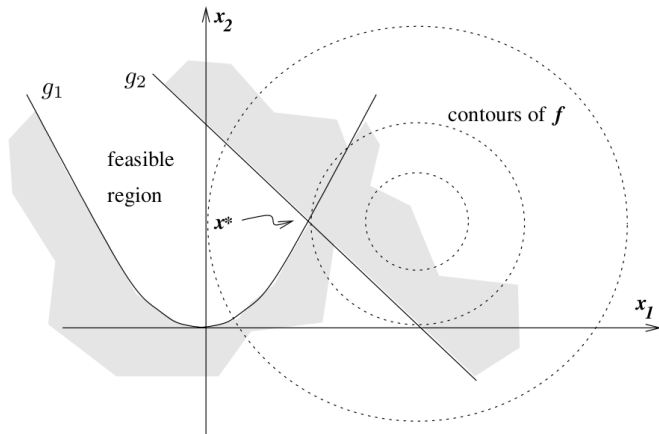
$$\text{minimize } (x_1 - 2)^2 + (x_2 - 1)^2 \quad \text{subject to } \begin{cases} x_1^2 - x_2 \leq 0, \\ x_1 + x_2 - 2 \leq 0. \end{cases}$$

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A *contour* of  $f$  is defined, for some  $c \in \mathbb{R}$ , by  $\{x \in \mathbb{R}^n \mid f(x) = c\}$



# Constraints

Consider the constraints

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Define the *feasibility region* by

$$\mathcal{F} = \{x \mid g_i(x) \leq 0, h_j(x) = 0, i = 1, \dots, n_g, j = 1, \dots, n_h\}$$

$x \in \mathcal{F}$  is *feasible*,  $x \notin \mathcal{F}$  is *infeasible*.

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$x^* \in \mathcal{F}$  is now a *constrained minimizer* if

$$f(x^*) \leq f(x) \quad \text{for all } x \in \mathcal{F}$$

# Constraints

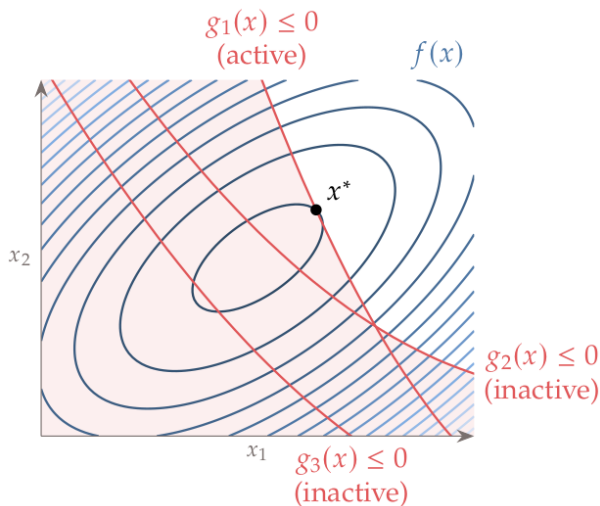
Inequality constraints  $g_i(x) \leq 0$  can be *active* or *inactive*.

*active* at  $x$

$$g_i(x) = 0$$

*inactive* at  $x$

$$g_i(x) < 0$$



## More Practical Example

The problem formulation:

- ▶ A company has two chemical factories  $F_1$  and  $F_2$ , and a dozen retail outlets  $R_1, \dots, R_{12}$ .
- ▶ Each  $F_i$  can produce (maximum of)  $a_i$  tons of a chemical each week.
- ▶ Each retail outlet  $R_j$  demands at least  $b_j$  tons.
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**The problem:** Determine how much each factory should ship to each outlet to satisfy the requirements and minimize cost.

## More Practical Example

Variables:  $x_{ij}$  for  $i = 1, 2$  and  $j = 1, \dots, 12$ . Each  $x_{ij}$  (intuitively) corresponds to tons shipped from  $F_i$  to  $R_j$ .

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$$\min \sum_{ij} c_{ij} x_{ij}$$



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subject to

$$\sum_{j=1}^{12} x_{ij} \leq a_i, \quad i = 1, 2$$

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The above is *linear programming* problem since both the objective and constraint functions are linear.

# Discrete Optimization

In our original optimization problem definition, we consider real (continuous) variables.

Sometimes, we need to assume discrete values. For example, in the previous example, the factories may produce tractors. In such a case, it does not make sense to produce 4.6 tractors.

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Usually, an *integer* constraint is added, such as

$$x_i \in \mathbb{Z}$$

It constrains  $x_i$  only to integer values. This leads to so-called *integer programming*.

*Discrete optimization* problems have discrete and finite variables.

## Wing Design Example

Our goal is to design the wing shape of an aircraft.

Assume a rectangular wing.



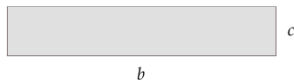
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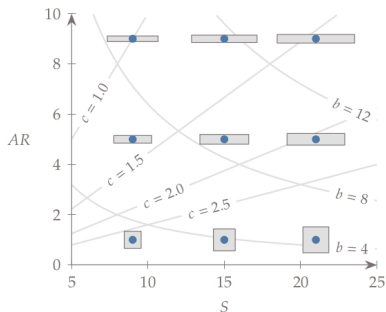
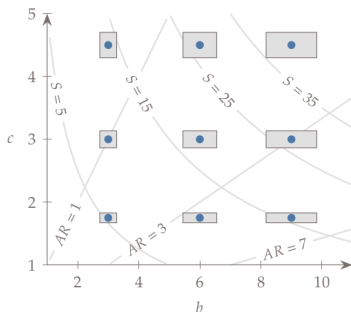
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The parameters are called *span*  $b$  and *chord*  $c$ .

However, two other variables are often used in aircraft design: Wing area  $S$  and wing aspect ratio  $AR$ . It holds that

$$S = bc \quad AR = b^2/S$$



# Wing Design Example

What exactly are the objectives and constraints?

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Our objective function is the power required to keep level flight:

$$f(b, c) = \frac{Dv}{\eta}$$

Here,

- ▶  $D$  is the drag

That is the aerodynamic force that opposes an aircraft's motion through the air.

- ▶  $\eta$  is the propulsive efficiency

That is the efficiency with which the energy contained in a vehicle's fuel is converted into kinetic energy of the vehicle.

- ▶  $v$  is the lift velocity

That is the velocity needed to lift the aircraft, which depends on its weight.



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The lift can be approximated using the following formula.

$$L = q \cdot C_L \cdot S$$

Where  $q = \frac{1}{2} \varrho v^2$  is the fluid dynamic pressure, here  $\varrho$  is the air density,  $C_L$  is a lift coefficient (depending on the wing shape).

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Thus, we may obtain the lift velocity as

$$v = \sqrt{2W / \varrho C_L S} = \sqrt{2(W_0 + W_S bc) / \varrho C_L bc}$$

Similarly, various physics-based arguments provide approximations of the drag  $D$  and the propulsion efficiency  $\eta$ .

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The viscous drag can be approximated by

$$D_f = k C_f q S$$

Here,  $k$  is the form factor (accounts for the pressure drag), and  $C_f$  is the skin friction coefficient that can be approximated by

$$C_f = 0.074 / Re^{0.2}$$

Where  $Re$  is the Reynolds number that somewhat characterizes air flow patterns around the wing and is defined as follows:

$$Re = \rho v c / \mu$$

Here  $\mu$  is the air dynamic viscosity.



# Wing Design Example

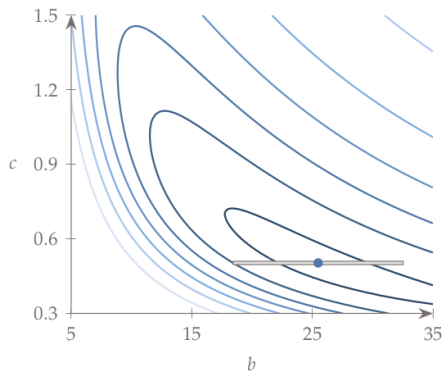
The propulsion efficiency  $\eta$  can be roughly approximated by the Gaussian efficiency curve.

$$\eta = \eta_{\max} \exp\left(\frac{-(v - \bar{v})^2}{2\sigma^2}\right)$$

Here,  $\bar{v}$  is the peak propulsive efficiency velocity, and  $\sigma$  is the std of the efficiency function.

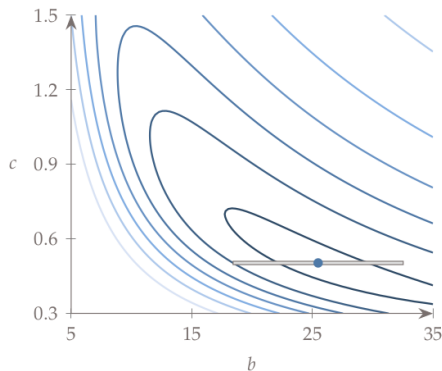
# Wing Design Example

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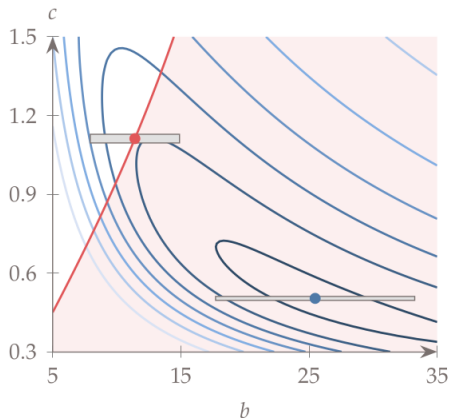
The objective function contours:



The engineers would refuse the solution: The aspect ratio is much higher than typically seen in airplanes. It adversely affects the structural strength. Add constraints!

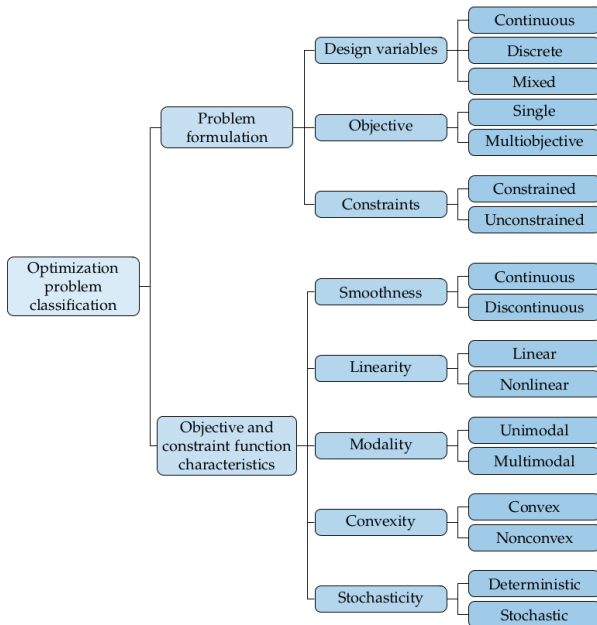
# Wing Design Example

Added a constraint on bending stress at the root of the wing:

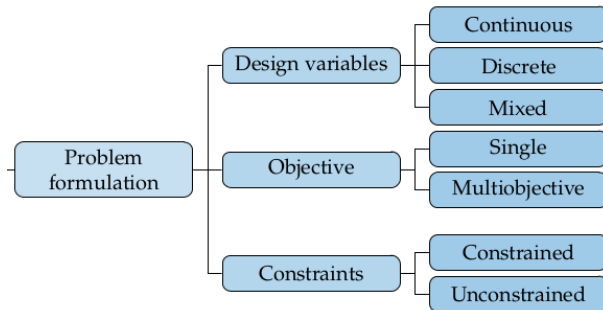


It looks like a reasonable wing ...

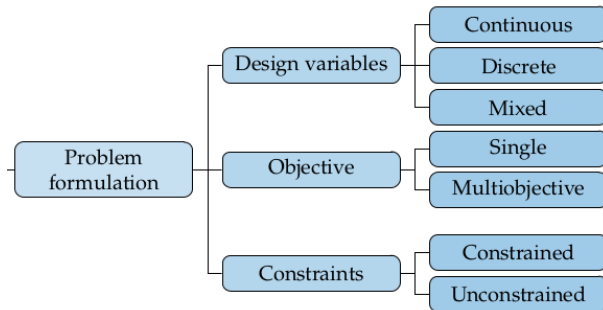
# Optimization Problem Classification



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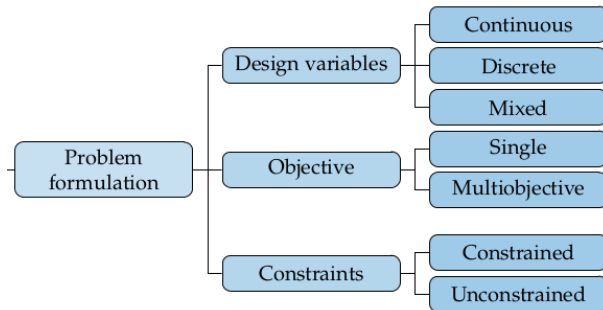


# Optimization Problem Classification



- *Continuous* allows only  $x_i \in \mathbb{R}$ , *discrete* allows only  $x_i \in \mathbb{Z}$ , mixed allows variables of both kinds.

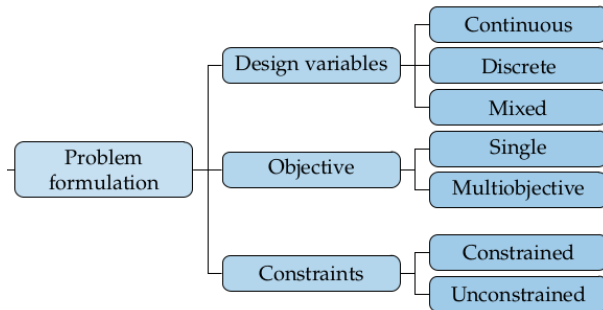
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- ▶ *Single-objective*:  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ , *Multi-objective*:  $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$

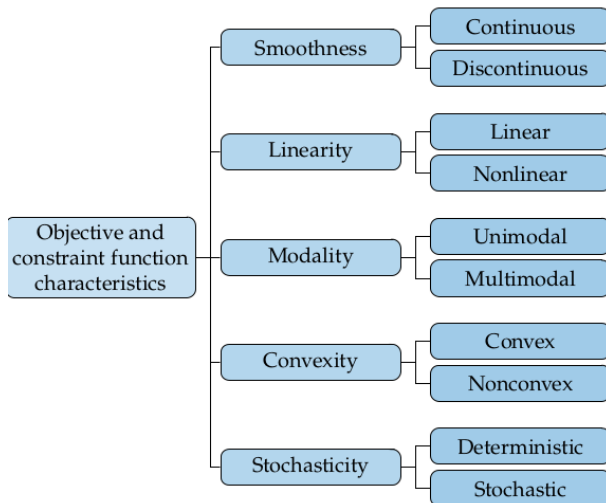


# Optimization Problem Classification



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- ▶ *Single-objective*:  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ , *Multi-objective*:  $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$
- ▶ *Unconstrained*: No constraints, just the objective function.

# Optimization Problem Classification

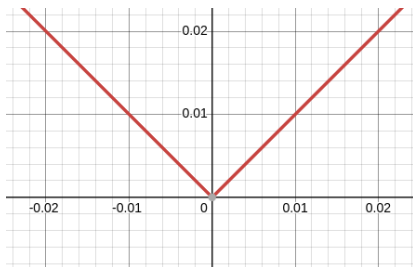


# Smoothness

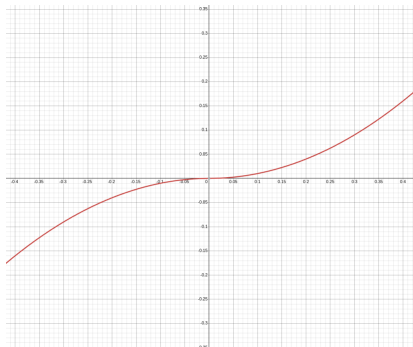
We consider various classes of problems depending on the smoothness properties of the objective/constraint functions:

- ▶  $C^0$ : Continuous function Continuity allows us to estimate value in small neighborhoods.  
Discontinuous functions exist.
- ▶  $C^1$ : Continuous first derivatives  
The derivatives give information on the slope. If continuous, it changes smoothly, allowing us to estimate the slope locally.  
Nondifferentiable continuous functions and differentiable functions with discontinuous derivatives exist.
- ▶  $C^2$ : Continuous second derivatives The second derivatives inform about curvature.  
Continuously differentiable functions without second derivatives and twice differentiable functions with discontinuous second derivatives exist.

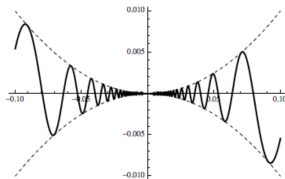
$f(x) = |x|$  is continuous,  $f$  is not differentiable at 0



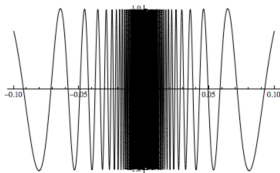
$f(x) = x|x|$  is differentiable on  $\mathbb{R}$ ,  $f'$  has no second derivative at 0



$$f(x) = \begin{cases} x^2 \sin(1/x) & \text{if } x \neq 0 \\ 0 & \text{if } x = 0 \end{cases}$$



$$f'(x) = \begin{cases} 2x \sin(1/x) - \cos(1/x), & x \neq 0 \\ 0, & x = 0 \end{cases}$$



$f$  is differentiable on  $\mathbb{R}$ ,  $f'$  is not continuous at 0

$$f(x) = \begin{cases} x^4 \sin(1/x) & \text{if } x \neq 0 \\ 0 & \text{if } x = 0 \end{cases}$$

$f$  is differentiable on  $\mathbb{R}$ ,

$$f'(x) = \begin{cases} 4x^3 \sin(1/x) - x^2 \cos(1/x), & x \neq 0 \\ 0, & x = 0 \end{cases}$$

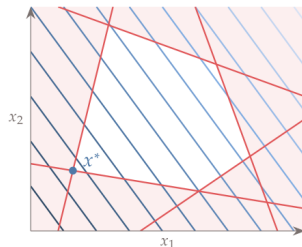
$f'$  is differentiable on  $\mathbb{R}$ ,

$$f''(x) = \begin{cases} 12x^2 \sin(1/x) - 6x \cos(1/x) - \sin(1/x), & x \neq 0 \\ 0, & x = 0 \end{cases}$$

Clearly,  $f''$  does not have a limit at 0 as  $\sin(1/x)$  oscillates between  $-1$  and  $1$  and thus **is not continuous**.

# Linearity

Linear programming: Both the objective and the constraints are linear.



It is possible to solve precisely, efficiently, and in rational numbers (see the linear programming later).

# Multimodality

Denote by  $\mathcal{F}$  the feasibility set.

$x^*$  is a (weak) *local minimiser* if there is  $\varepsilon > 0$  such that

$$f(x^*) \leq f(x) \text{ for all } x \in \mathcal{F} \text{ satisfying } \|x^* - x\| \leq \varepsilon$$



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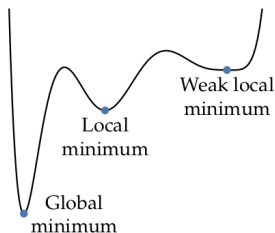
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Global/local minimiser is *strict* if the inequality is strict.



*Unimodal* functions have a single global minimiser in  $\mathcal{F}$ ,  
*multimodal* have multiple local minimisers in  $\mathcal{F}$ .

# Convexity

$S \subseteq \mathbb{R}^n$  is a *convex set* if the straight line segment connecting any two points in  $S$  lies entirely inside  $S$ . Formally, for any two points  $x \in S$  and  $y \in S$ , we have  $\alpha x + (1 - \alpha)y \in S$  for all  $\alpha \in [0, 1]$

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$f$  is a *convex function* if its domain is a convex set and if for any two points  $x$  and  $y$  in this domain, the graph of  $f$  lies below the straight line connecting  $(x, f(x))$  to  $(y, f(y))$  in the space  $\mathbb{R}^{n+1}$ . That is, we have

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A **standard form convex optimization** assumes

- ▶ convex objective  $f$  and convex inequality constraint functions  $g_i$
- ▶ affine equality constraint functions  $h_j$

**Implications:**

- ▶ Every local minimum is a global minimum.
- ▶ If the above inequality is strict for all  $x \neq y$ , then there is a unique minimum.

# Stochasticity

Sometimes, the parameters of a model cannot be specified with certainty.

For example, in the transportation model, customer demand cannot be predicted precisely in practice.

However, such parameters may often be statistically estimated and modeled using an appropriate probability distribution.

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However, such parameters may often be statistically estimated and modeled using an appropriate probability distribution.

*Stochastic optimization* problem is to minimize/maximize the expectation of a statistic parametrized with the variables  $x$ :

Find  $x$  maximizing  $\mathbb{E}f(x; W)$

Here,  $W$  is a vector of random variables, and the expectation is taken using the probability distribution of these variables.

In this course, we stick with *deterministic optimization*.



# Optimization Algorithms

# Optimization Algorithm

An *optimization algorithm* solves the optimization problem, i.e., searches for  $x^*$ , which (in some sense) minimizes the objective  $f$  and satisfies the constraints.

Typically, the algorithm computes a set of candidate solutions  $x_0, x_1, \dots$  and then identifies one resembling a solution.

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The problem is to

- ▶ compute the candidate solutions,  
Complexity of the objective function, difficulties in selection of the candidates, etc.
- ▶ Select the one closest to a minimum.  
It is Hard to decide whether a given point is a minimum (even a local one). Example: Neural networks training.

# Optimization Algorithm Properties

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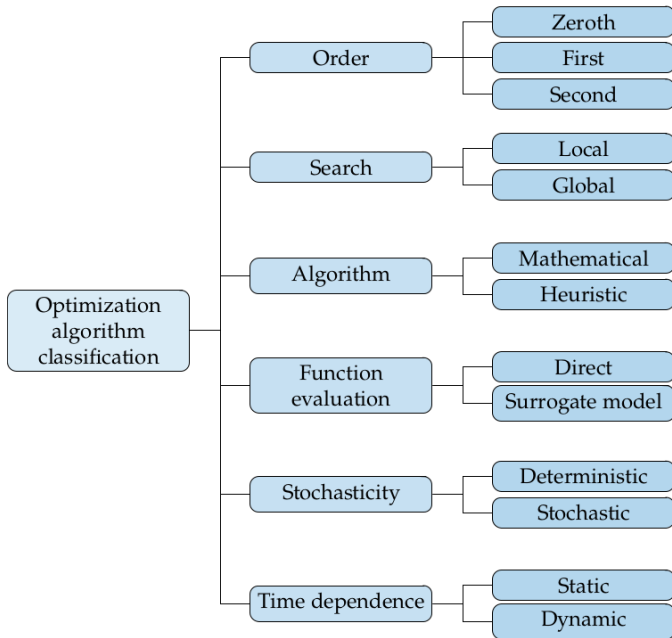
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Typically, we are concerned with the following issues:

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- ▶ *Efficiency*: OA should not require too much computer time or storage.
- ▶ *Accuracy*: OA should be able to identify a solution with precision without being overly sensitive to
  - ▶ errors in the data/model
  - ▶ the arithmetic rounding errors





# Order and Search

## Order

- ▶ Zeroth = *gradient-free*: no info about derivatives is used
- ▶ First = *gradient-based*: use info about first derivatives (e.g., gradient descent)
- ▶ Second = use info about first and second derivatives (e.g., Newton's method)

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## Search

- ▶ *Local search* = start at a point and search for a solution by successively updating the current solution (e.g., gradient descent)
- ▶ *Global search* tries to span the whole space (e.g., grid search)

# Mathematical vs Heuristic

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For example, for linear optimization problems, the simplex algorithm converges to a minimum (or says that there is no minimum) in, at most, exponentially many steps, and we may efficiently decide whether we have reached a minimum.

We may prove only some or none of the properties for some algorithms.

There are (almost) infinitely many heuristic algorithms without provable convergence, often motivated by the behaviors of various animals.

# Deterministic vs Stochastic and Static vs Dynamic

*Stochastic optimization* is based on a random selection of candidate solutions.

Evolutionary algorithms contain some randomness (e.g., in the form of random mutations).

Also, various variants of the gradient-based methods are often randomized (e.g., variants of the stochastic gradient descent).



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---

In this course, we stick to *static* optimization problems where we solve the optimization problem only once.

In contrast, the *dynamic* optimization, a sequence of (usually) dependent optimization problems are solved sequentially.

For example, consider driving a car where the driver must react optimally to changing situations several times per second.

Dynamic optimization problems are usually defined using a kind of (Markov) decision process.

# Summary

The course consists of the following main parts:

- ▶ Unconstrained optimization
  - ▶ Non-linear objectives, (twice) differentiable
  - ▶ Second-order methods (quasi-Newton)
- ▶ Constrained optimization
  - ▶ Non-linear objectives and constraints, (twice) differentiable
  - ▶ Lagrange multipliers, Newton-Lagrange method
  - ▶ Quadratic programming (a little bit)
- ▶ Linear programming
  - ▶ Linear objectives and constraints
  - ▶ Simplex algorithm deep dive (including the degenerate case)
- ▶ Integer linear programming
  - ▶ Linear objectives and mixed integer linear constraints
  - ▶ Branch-and-bound, Gomory cuts algorithms
- ▶ A little bit on non-differentiable algorithms.

You will need to understand: Calculus in  $\mathbb{R}^n$  (gradient, Hessian) and linear algebra in  $\mathbb{R}^n$  (vectors, matrices, geometry)

# Single-variable Objectives

# Unconstrained Single Variable Optimization Problem

An objective function  $f : \mathbb{R} \rightarrow \mathbb{R}$

A variable  $x$

Find  $x^*$  such that

$$f(x^*) \leq \min_{x \in \mathbb{R}} f(x)$$

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Find  $x^*$  such that

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We consider

- ▶  $f$  continuously differentiable
- ▶  $f$  twice continuously differentiable

Present the following methods:

- ▶ Gradient descent
- ▶ Newton's method
- ▶ Secant method

# Gradient Based Methods

An objective function  $f : \mathbb{R} \rightarrow \mathbb{R}$

A variable  $x \in \mathbb{R}$

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# Gradient Based Methods

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A variable  $x \in \mathbb{R}$

Find  $x^*$  such that

$$f(x^*) \leq \min_{x \in \mathbb{R}} f(x)$$

Assume that

$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h} \quad \text{for } x \in \mathbb{R}$$

is continuous on  $\mathbb{R}$ .

Denote by  $\mathcal{C}^1$  the set of all continuously differentiable functions.

# Gradient Descent in Single Variable

Gradient descent algorithm for finding a local minimum of a function  $f$ , using a variable step length.

**Input:** Function  $f$  with first derivative  $f'$ , initial point  $x_0$ , initial step length  $\alpha_0 > 0$ , tolerance  $\epsilon > 0$

**Output:** A point  $x$  that approximately minimizes  $f(x)$

- 1: Set  $k \leftarrow 0$
- 2: **while**  $|f'(x_k)| > \epsilon$  **do**
- 3:     Calculate the derivative:  $y' \leftarrow f'(x_k)$
- 4:     Update  $x_{k+1} \leftarrow x_k - \alpha_k \cdot y'$
- 5:     Update step length  $\alpha_k$  to  $\alpha_{k+1}$  based on a certain strategy
- 6:     Increment  $k$
- 7: **end while**
- 8: **return**  $x_k$



# Convergence of Single Variable Gradient Descent

## Theorem 1

Assume that  $f$  is

- ▶ differentiable, i.e., that  $f'$  exists,
- ▶ bounded below, i.e., there is  $B \in \mathbb{R}$  such that  $f(x) \geq B$  for all  $x \in \mathbb{R}$ ,
- ▶  $L$ -smooth, i.e., there is  $L > 0$  such that  $|f'(x) - f'(x')| \leq L|x - x'|$  for all  $x, x' \in \mathbb{R}$ .

Consider a sequence  $x_0, x_1, \dots$  computed by the gradient descent algorithm for  $f$ . Assume a constant step length  $\alpha \leq \frac{1}{L}$ .

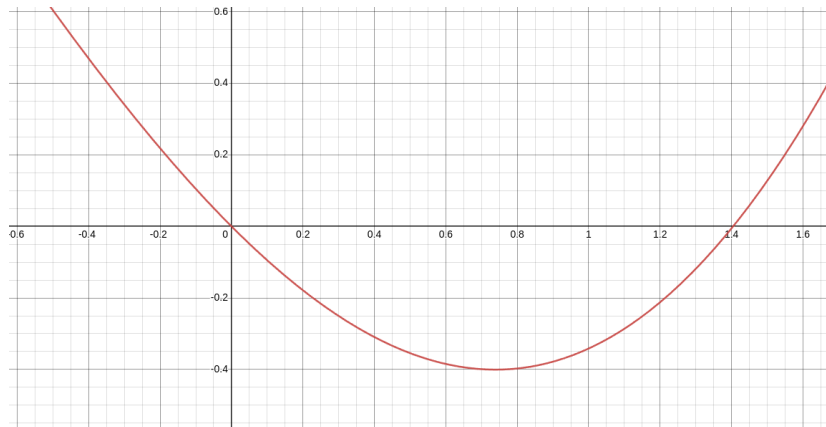
Then  $\lim_{k \rightarrow \infty} |f'(x_k)| = 0$  and, moreover,

$$\min_{0 \leq t < T} |f'(x_t)| \leq \sqrt{\frac{2L(f(x_0) - B)}{T}}$$

## Example

Consider the following objective function  $f$

$$f(x) = \frac{1}{2}x^2 - \sin x$$



## Example

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Assume  $x_0 = 0.5$ , and that the required accuracy is  $\epsilon = 10^{-4}$ , i.e., we stop when  $|x_{k+1} - x_k| < \epsilon$ .

Consider the step length  $\alpha = 1$ .

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Consider the step length  $\alpha = 1$ .

We compute

$$f'(x) = x - \cos x.$$

Then,

$$\begin{aligned}x_1 &= 0.5 - (0.5 - \cos 0.5) \\&= 0.5 - (-0.37758) \\&= 0.87758\end{aligned}$$

## Example

Continuing in the same way:

$$x_1 = 0.87758$$

$$x_2 = 0.63901$$

$$x_3 = 0.80269$$

$$x_4 = 0.69478$$

$$x_5 = 0.76820$$

$$x_6 = 0.71917$$

$$x_7 = 0.75236$$

$$x_8 = 0.73008$$

$$x_9 = 0.74512$$

$$x_{10} = 0.73501$$

$$x_{11} = 0.74183$$

$$x_{12} = 0.73724$$

$$x_{13} = 0.74033$$

$$x_{14} = 0.73825$$

$$x_{15} = 0.73965$$

$$x_{16} = 0.73870$$

$$x_{17} = 0.73934$$

$$x_{18} = 0.73891$$

$$x_{19} = 0.73920$$

$$x_{20} = 0.73901$$

$$x_{21} = 0.73914$$

$$x_{22} = 0.73905$$

Note that  $|x_{22} - x_{21}| < 10^{-4}$ .

## Example

What if we consider the step length  $1/k$ ? Then

$$x_1 = 0.50000$$

$$x_2 = 0.87758$$

$$x_3 = 0.75830$$

$$x_4 = 0.74753$$

$$x_5 = 0.74399$$

$$x_6 = 0.74235$$

$$x_7 = 0.74144$$

$$x_8 = 0.74087$$

$$x_9 = 0.74050$$

$$x_{10} = 0.74024$$

$$x_{11} = 0.74004$$

$$x_{12} = 0.73990$$

$$x_{13} = 0.73978$$

$$x_{14} = 0.73969$$

Note that  $|x_{14} - x_{13}| < 10^{-4}$  but  $x_{14}$  is far from the solution which is 0.7390....

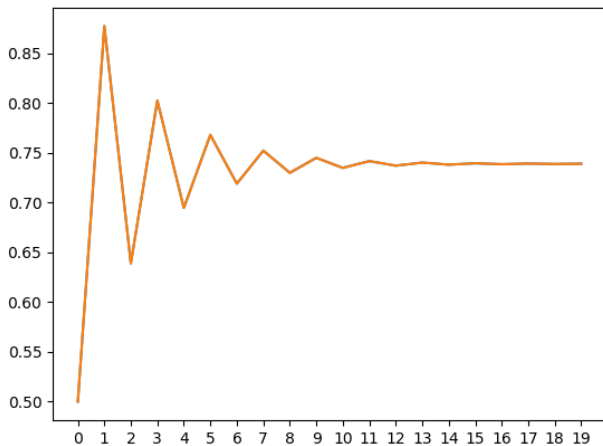
## Example

What if we consider the step length  $1/k$ ? Then

$x_1 = 0.50000$	$x_{115} = 0.739100605$
$x_2 = 0.87758$	$x_{116} = 0.739100379$
$x_3 = 0.75830$	$x_{117} = 0.739100159$
$x_4 = 0.74753$	$x_{118} = 0.739099944$
$x_5 = 0.74399$	$x_{119} = 0.739099734$
$x_6 = 0.74235$	$x_{120} = 0.739099529$
$x_7 = 0.74144$	$x_{121} = 0.739099328$
$x_8 = 0.74087$	$x_{122} = 0.739099132$
$x_9 = 0.74050$	$x_{123} = 0.739098940$
$x_{10} = 0.74024$	$x_{124} = 0.739098752$
$x_{11} = 0.74004$	$x_{125} = 0.739098568$
$x_{12} = 0.73990$	$x_{126} = 0.739098388$
$x_{13} = 0.73978$	$x_{127} = 0.739098212$
$x_{14} = 0.73969$	$x_{128} = 0.739098040$
$\dots$	

## Example

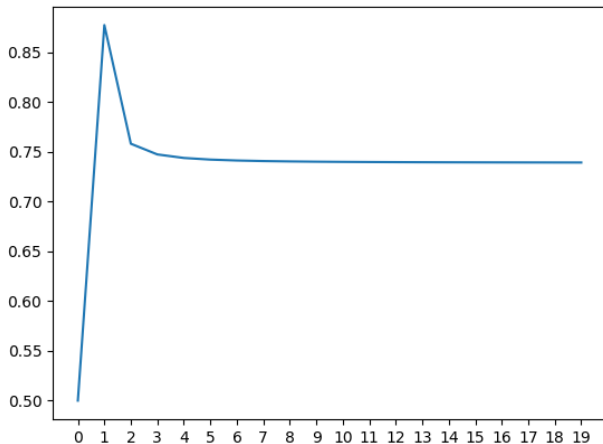
Gradient descent with the step length = 1.0:





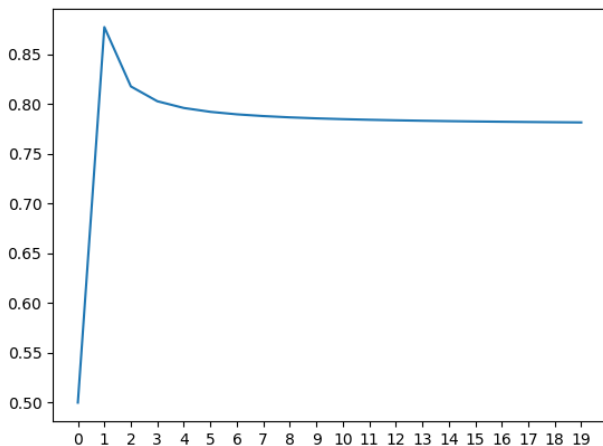
## Example

Gradient descent with the step length  $= 1/k$ :



## Example

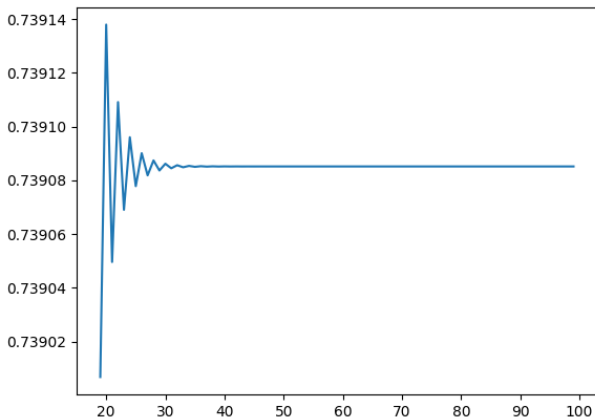
Gradient descent with the step length  $= 1/k^2$ :



It does not seem to converge to the same number as the previous step lengths.

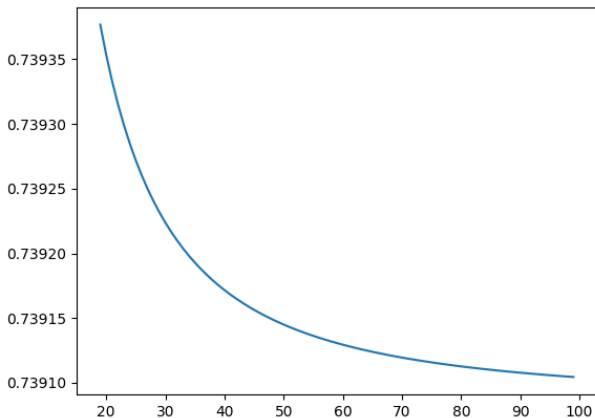
## Example

Gradient descent with the step length = 1.0:



## Example

Gradient descent with the step length  $= 1/k$ :



# Properties of Gradient Descent

- ▶ The objective must be differentiable, however:
  - ▶ Can be extended to functions with few non-linearities by considering differentiable parts or sub-gradients.
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Might be very slow or too fast (even overshoot and diverge).
- ▶ For convex functions, the algorithm converges to a minimum (if it converges).
- ▶ Straightforward to implement if the derivatives are available.

GD is much more interesting in multiple variables, forming the basis for neural network learning (see later).

Better algorithm for unimodal functions using just derivatives?

# Newton's Method

An objective function  $f : \mathbb{R} \rightarrow \mathbb{R}$

A variable  $x \in \mathbb{R}$

Find  $x^*$  such that

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Assume that

$$f''(x) = \lim_{h \rightarrow 0} \frac{f'(x+h) - f'(x)}{h} \quad \text{for } x \in \mathbb{R}$$

is continuous on  $\mathbb{R}$ .

Denote by  $\mathcal{C}^2$  the set of all twice continuously differentiable functions.

## Taylor Series Approximation

We would need the  $o$ -notation: Given functions  $f, g : \mathbb{R} \rightarrow \mathbb{R}$  we write  $f = o(g)$  if

$$\lim_{x \rightarrow 0} \frac{f(x)}{g(x)} = 0$$

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Thus, such  $f$  can be reasonably approximated around  $x_0$  with a quadratic function

$$f(x) \approx q(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2}f''(x_0)(x - x_0)^2$$

## Newton's Method Idea

The method computes successive approximations  $x_0, x_1, \dots, x_k, \dots$  as the GD.

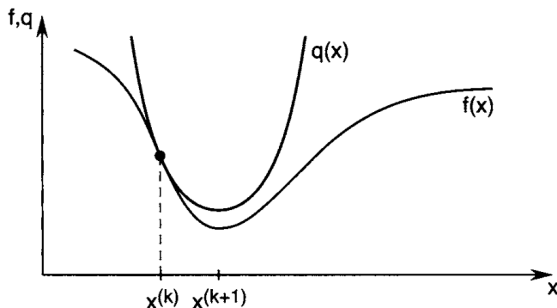
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is considered around  $x_k$ .





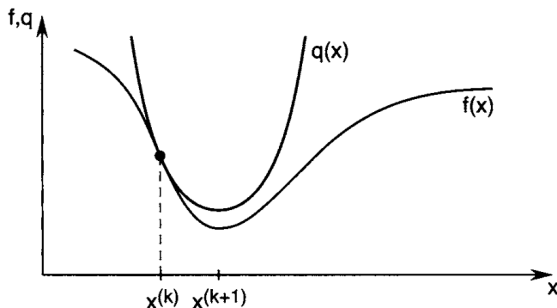
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Then  $x_{k+1}$  is set to the extreme point of  $q(x)$  (i.e.,  $q'(x_{k+1}) = 0$ ).

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$$q'(x) = 0 \text{ iff } x = x_k - \frac{f'(x_k)}{f''(x_k)}$$

Newton's method then sets

$$x_{k+1} := x_k - \frac{f'(x_k)}{f''(x_k)}$$

# Newton's Method Algorithm

**Input:** A function  $f$  with derivative  $f'$  and second derivative  $f''$ ,  
initial point  $x_0$ , tolerance  $\epsilon > 0$

**Output:** A point  $x$  that approximately minimizes  $f(x)$

- 1: Set  $k \leftarrow 0$
- 2: **while**  $|x_{k+1} - x_k| > \epsilon$  **do**
- 3:     Calculate the derivative:  $y' \leftarrow f'(x_k)$
- 4:     Calculate the second derivative :  $y'' \leftarrow f''(x_k)$
- 5:     Update the estimate:  $x_{k+1} \leftarrow x_k - \frac{y'}{y''}$
- 6:     Increment  $k$
- 7: **end while**
- 8: **return**  $x_k$

Note that the method implicitly assumes that  $f''(x_k) \neq 0$  in every iteration.

## Example

Consider the following objective function  $f$

$$f(x) = \frac{1}{2}x^2 - \sin x$$

Assume  $x_0 = 0.5$ , and that the required accuracy is  $\epsilon = 10^{-5}$ , i.e., we stop when  $|x_{k+1} - x_k| \leq \epsilon$ .

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$$f'(x) = x - \cos x, \quad f''(x) = 1 + \sin x.$$

Hence,

$$\begin{aligned} x_1 &= 0.5 - \frac{0.5 - \cos 0.5}{1 + \sin 0.5} \\ &= 0.5 - \frac{-0.3775}{1.479} \\ &= 0.7552 \end{aligned}$$

## Example

Proceeding similarly, we obtain

$$x_2 = x_1 - \frac{f'(x_1)}{f''(x_1)} = x_1 - \frac{0.02710}{1.685} = 0.7391$$

$$x_3 = x_2 - \frac{f'(x_2)}{f''(x_2)} = x_2 - \frac{9.461 \times 10^{-5}}{1.673} = 0.7390851339$$

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Note that

$$|x_4 - x_3| < \epsilon = 10^{-5}$$

$$f'(x_4) = -8.6 \times 10^{-6} \approx 0$$

$$f''(x_4) = 1.673 > 0$$

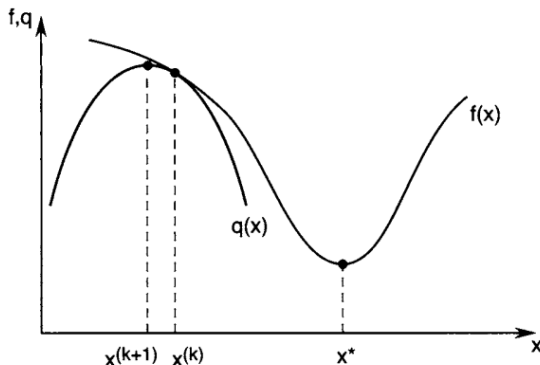
So, we conclude that  $x^* \approx x_4$  is a strict minimizer.

However, remember that the above does not have to be true!

# Convergence

Newton's method works well if  $f''(x) > 0$  everywhere.

However, if  $f''(x) < 0$  for some  $x$ , Newton's method may fail to converge to a minimizer (converges to a point  $x$  where  $f'(x) = 0$ ):



If the method converges to a minimizer, it does so *quadratically*.  
What does this mean?

# Types of Convergence Rates

## Linear Convergence

An algorithm is said to have linear convergence if the error at each step is proportionally reduced by a constant factor:

$$\lim_{k \rightarrow \infty} \frac{|x_{k+1} - x^*|}{|x_k - x^*|} = r, \quad 0 < r < 1$$

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## Superlinear Convergence

Convergence is superlinear if:

$$\lim_{k \rightarrow \infty} \frac{|x_{k+1} - x^*|}{|x_k - x^*|} = 0$$

This often requires an algorithm to utilize second-order information.

# Quadratic Convergence of Newton's Method

## Quadratic Convergence

Quadratic convergence is achieved when the number of accurate digits roughly doubles with each iteration:

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Newton's method is a classic example of an algorithm with quadratic convergence.

## Theorem 2 (Quadratic Convergence of Newton's Method)

*Let  $f : \mathbb{R} \rightarrow \mathbb{R}$  satisfy  $f \in \mathcal{C}^2$  and suppose  $x^*$  is a minimizer of  $f$  such that  $f''(x^*) > 0$ . Assume Lipschitz continuity of  $f''$ . If the initial guess  $x_0$  is sufficiently close to  $x^*$ , then the sequence  $\{x_k\}$  computed by the Newton's method converges quadratically to  $x^*$ .*



## Newton's Method of Tangents

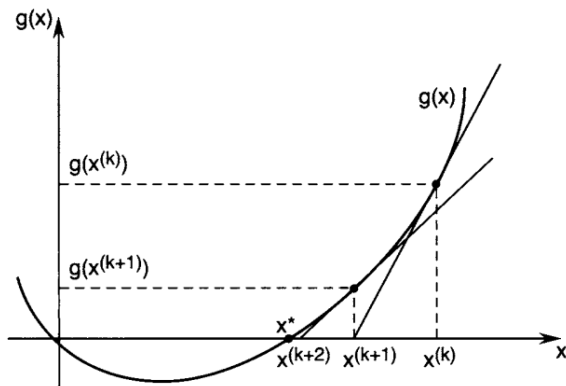
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Newton's method is also a technique for finding roots of functions. In our case, this means finding a root of  $f'$ .

Denote  $g = f'$ . Then Newton's approximation goes like this:

$$x_{k+1} = x_k - \frac{g(x_k)}{g'(x_k)}$$



## Secant Method

What if  $f''$  is unavailable, but we want to use something like Newton's method (with its superlinear convergence)?

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Assume  $f \in \mathcal{C}^1$  and try to approximate  $f''$  around  $x_{k-1}$  with

$$f''(x) \approx \frac{f'(x) - f'(x_{k-1})}{x - x_{k-1}}$$

Substituting  $x$  with  $x_k$ , we obtain

$$\frac{1}{f''(x_k)} \approx \frac{x_k - x_{k-1}}{f'(x_k) - f'(x_{k-1})}$$

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$$\frac{1}{f''(x_k)} \approx \frac{x_k - x_{k-1}}{f'(x_k) - f'(x_{k-1})}$$

Then, we may try to use Newton's step with this approximation:

$$x_{k+1} = x_k - \frac{x_k - x_{k-1}}{f'(x_k) - f'(x_{k-1})} \cdot f'(x_k)$$

Is the rate of convergence superlinear?

## Example

Consider the following objective function  $f$

$$f(x) = \frac{1}{2}x^2 - \sin x$$

Assume  $x_0 = 0.5$  and  $x_1 = 1.0$ .

Now, we need to initialize the first two values.

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We have  $f'(x) = x - \cos x$

Hence,

$$\begin{aligned}x_2 &= 1.0 - \frac{1.0 - 0.5}{(1.0 - \cos 1.0) - (0.5 - \cos 0.5)}(0.5 - \cos 0.5) \\&= 0.7254\end{aligned}$$

## Example

Continuing, we obtain:

$$x_0 = 0.5$$

$$x_1 = 1.0$$

$$x_2 = 0.72548$$

$$x_3 = 0.73839$$

$$x_4 = 0.739087$$

$$x_5 = 0.739085132$$

$$x_6 = 0.739085133$$



## Example

Start the secant method with the approximation given by Newton's method:

$$x_0 = 0.5$$

$$x_1 = 0.7552$$

$$x_2 = 0.7381$$

$$x_3 = 0.739081$$

$$x_5 = 0.7390851339$$

$$x_6 = 0.7390851332$$

...

Compare with Newton's method:

$$x_0 = 0.5$$

$$x_1 = 0.7552$$

$$x_2 = 0.7391$$

$$x_3 = 0.7390851339$$

$$x_4 = 0.73908513321516067229$$

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# Superlinear Convergence of Secant Method

## Theorem 3 (Superlinear Convergence of Secant Method)

*Assume  $f : \mathbb{R} \rightarrow \mathbb{R}$  twice continuously differentiable and  $x^*$  a minimizer of  $f$ . Assume  $f''$  Lipschitz continuous and  $f''(x^*) > 0$ . The sequence  $\{x_k\}$  generated by the Secant method converges to  $x^*$  superlinearly if  $x_0$  and  $x_1$  are sufficiently close to  $x^*$ .*

The rate of convergence  $p$  of the Secant method is given by the positive root of the equation  $p^2 - p - 1 = 0$ , which is  $p = \frac{1+\sqrt{5}}{2} \approx 1.618$  (the golden ratio). Formally,

$$\lim_{k \rightarrow \infty} \frac{|x_{k+1} - x^*|}{|x_k - x^*|^{\frac{1+\sqrt{5}}{2}}} = C, \quad C > 0$$

## Secant Method for Root Finding

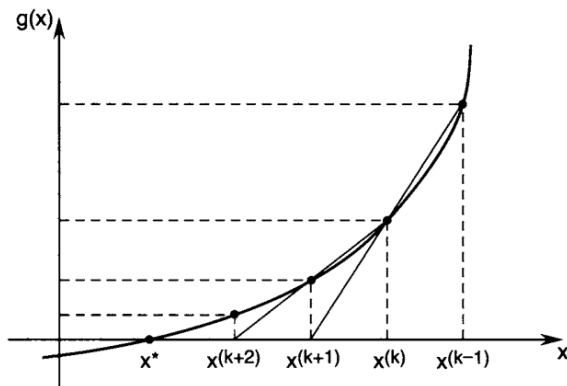
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Denote  $g = f'$ . Then the secant method approximation is

$$x_{k+1} = x_k - \frac{x_k - x_{k-1}}{g(x_k) - g(x_{k-1})} \cdot g(x_k)$$



# General Form

Note that all methods have similar update formula:

$$x_{k+1} = x_k - \frac{f'(x_k)}{a_k}$$

Different choice of  $a_k$  produce different algorithm:

- ▶  $a_k = 1$  gives the **gradient descent**,
- ▶  $a_k = f''(x_k)$  gives **Newton's method**,
- ▶  $a_k = \frac{f'(x_k) - f'(x_{k-1})}{x_k - x_{k-1}}$  gives the **secant method**,
- ▶  $a_k = f''(x_m)$  where  $m = \lfloor k/p \rfloor p$  gives **Shamanskii method**.

# Summary

- ▶ Newton's method
  - ▶ Converges quickly to an extremum under rather strict conditions (see Theorem 2)
  - ▶ The choice of the initial point is critical; the method may diverge to a stationary point, which is not a minimizer. The method may also cycle.
  - ▶ If the second derivative is very small, close to the minimizer, the method can be very slow (the quadratic convergence is guaranteed only if the second derivative is non-zero at the minimizer and the constants depend on the second derivative).

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  - ▶ If the second derivative is very small, close to the minimizer, the method can be very slow (the quadratic convergence is guaranteed only if the second derivative is non-zero at the minimizer and the constants depend on the second derivative).
- ▶ Secant method
  - ▶ The second derivative is not needed.
  - ▶ Superlinear (but not quadratic) convergence for an initial point close to a minimum (under rather strict conditions Theorem 3)

# Constrained Single Variable Optimization Problem

An objective function  $f : \mathbb{R} \rightarrow \mathbb{R}$

A variable  $x$

A constraint

$$a_0 \leq x \leq b_0$$

Consider the following cases:

- ▶  $f$  continuously differentiable on  $[a_0, b_0]$
- ▶  $f$  twice continuously differentiable on  $[a_0, b_0]$

**Homework:** Modify the gradient descent and Newton's method to work on the bounded interval (the above definitions guarantee continuous differentiability at  $a_0$  and  $b_0$ ).



# Unconstrained Optimization Overview

## Notation

In what follows, we will work with vectors in  $\mathbb{R}^n$ .

The vectors will be (usually) denoted by  $x \in \mathbb{R}^n$ .

We often consider sequences of vectors,  $x_0, x_1, \dots, x_k, \dots$

The index  $k$  will usually indicate that  $x_k$  is the  $k$ -th vector in a sequence.

When we talk (relatively rarely) about components of vectors, we use  $i$  as an index, i.e.,  $x_i$  will be the  $i$ -th component of  $x \in \mathbb{R}^n$ .

We denote by  $\|x\|$  the Euclidean norm of  $x$ .

We denote by  $\|x\|_\infty$  the  $\mathcal{L}^\infty$  norm giving the maximum of absolute values of components of  $x$ .

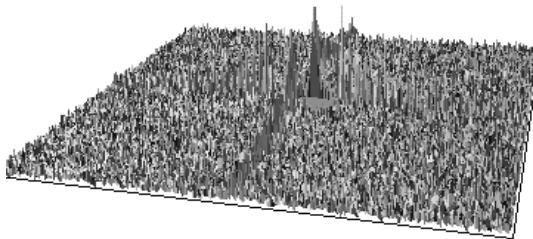
We occasionally use the matrix norm  $\|A\|$ , consistent with the Euclidean norm, defined by

$$\|A\| = \sup_{\|x\|=1} \|Ax\| = \sqrt{\lambda_1}$$

Here  $\lambda_1$  is the largest eigenvalue of  $A^\top A$ .

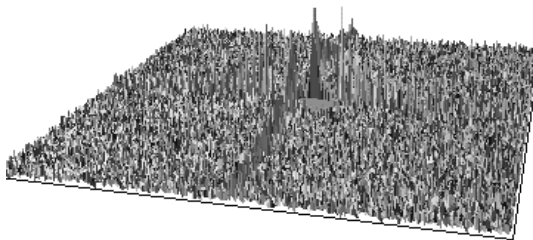
# How to Recognize (Local) Minimum

How do we verify that  $x^* \in \mathbb{R}^n$  is a minimizer of  $f$ ?



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How do we verify that  $x^* \in \mathbb{R}^n$  is a minimizer of  $f$ ?



Technically, we should examine *all* points in the immediate vicinity if one has a smaller value (impractical).

Assuming the smoothness of  $f$ , we may benefit from the “stable” behavior of  $f$  around  $x^*$ .

# Derivatives and Gradients

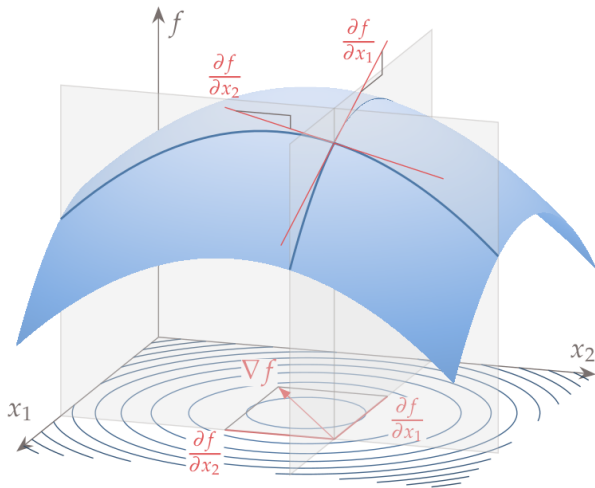
The gradient of  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ , denoted by  $\nabla f(x)$ , is a column vector of first-order partial derivatives of the function concerning each variable:

$$\nabla f(x) = \left[ \frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots, \frac{\partial f}{\partial x_n} \right]^\top,$$

Where each partial derivative is defined as the following limit:

$$\frac{\partial f}{\partial x_i} = \lim_{\varepsilon \rightarrow 0} \frac{f(x_1, \dots, x_i + \varepsilon, \dots, x_n) - f(x_1, \dots, x_i, \dots, x_n)}{\varepsilon}$$

# Gradient



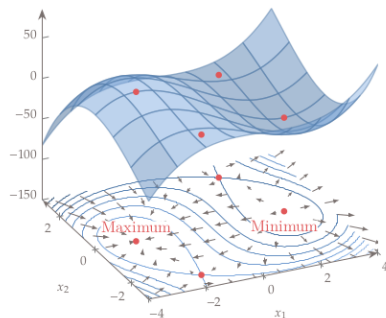
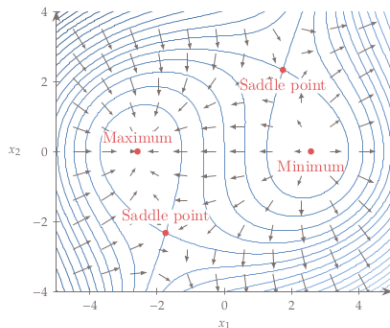
The gradient is a vector pointing in the direction of the most significant function increase from the current point.

# Gradient

Consider the following function of two variables:

$$f(x_1, x_2) = x_1^3 + 2x_1x_2^2 - x_2^3 - 20x_1.$$

$$\nabla f(x_1, x_2) = \begin{bmatrix} 3x_1^2 + 2x_2^2 - 20 \\ 4x_1x_2 - 3x_2^2 \end{bmatrix}$$

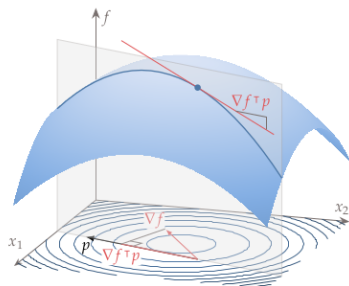
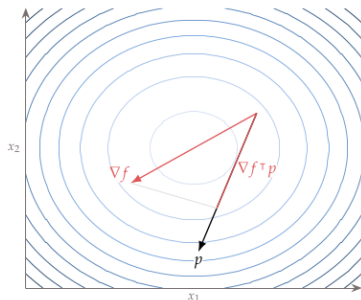


## Directional Derivatives vs Gradient

The rate of change in a direction  $p$  is quantified by a directional derivative, defined as

$$\nabla_p f(x) = \lim_{\varepsilon \rightarrow 0} \frac{f(x + \varepsilon p) - f(x)}{\varepsilon}.$$

We can find this derivative by projecting the gradient onto the desired direction  $p$  using the dot product  $\nabla_p f(x) = (\nabla f(x))^\top p$



(Here, we assume continuous partial derivatives.)



## Geometry of Gradient

Consider the geometric interpretation of the dot product:

$$\nabla_p f(x) = (\nabla f(x))^{\top} p = \|\nabla f\| \|p\| \cos \theta$$

Here  $\theta$  is the angle between  $\nabla f$  and  $p$ .

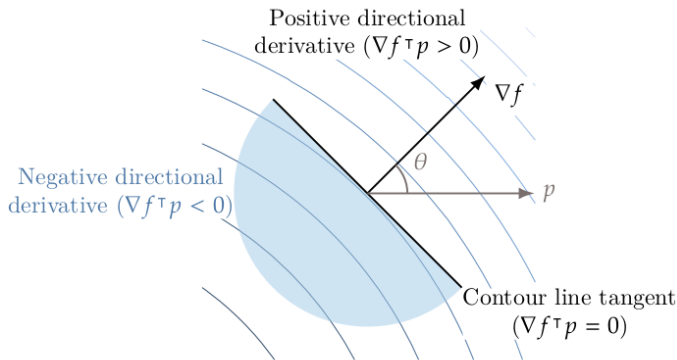
## Geometry of Gradient

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Here  $\theta$  is the angle between  $\nabla f$  and  $p$ .

The directional derivative is maximized by  $\theta = 0$ , i.e., when  $\nabla f$  and  $p$  point in the same direction.



## Hessian

Taking derivative twice, possibly w.r.t. different variables, gives the *Hessian* of  $f$

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

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We have

$$H_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}.$$

If  $f$  has continuous second partial derivatives, then  $H$  is symmetric, i.e.,  $H_{ij} = H_{ji}$ .

## Geometry of Hessian

Let  $x$  be fixed and let  $g(t) = f(x + tp)$ .

What exactly are  $g'(0)$  and  $g''(0)$ ?

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Thus, for our fixed  $x$  we have

$$\begin{aligned} g''(t) &= (g'(t))' \\ &= (\nabla_p f(x + tp))' = [\nabla(\nabla_p f(x + tp))]^\top p \\ &= (H(x + tp)p)^\top p = p^\top H(x + tp)p \end{aligned}$$



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Thus  $g''(0) = p^\top H(x)p$ .

## Principal Curvature Directions

Fix  $x$  and consider  $H = H(x)$ . Consider unit eigenvectors  $\hat{v}_k$  of  $H$ :

$$H\hat{v}_k = \kappa_k \hat{v}_k$$

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# Principal Curvature Directions

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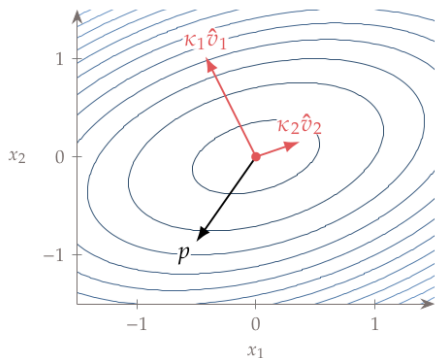
$$H\hat{v}_k = \kappa_k \hat{v}_k$$

For symmetric  $H$ , the unit eigenvectors form an orthonormal basis, and there is a rotation matrix  $R$  such that

$$H = RDR^{-1} = RDR^T$$

Here  $D$  is diagonal with  $\kappa_1, \dots, \kappa_n$  on the diagonal.

If  $\kappa_1 \geq \dots \geq \kappa_n$ , the direction of  $\hat{v}_1$  is the maximum curvature direction of  $f$  at  $x$ .



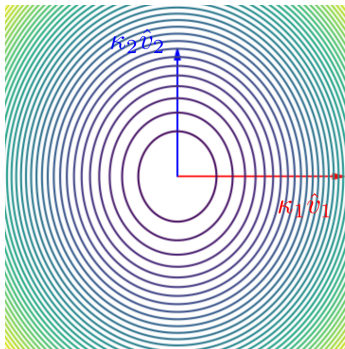
Consider  $f(x) = x^\top Hx$  where

$$H = \begin{pmatrix} 4/3 & 0 \\ 0 & 1 \end{pmatrix}$$

The eigenvalues are

$$\kappa_1 = 4/3 \quad \kappa_2 = 1$$

Their corresponding eigenvectors are  $(1, 0)^\top$  and  $(0, 1)^\top$ .



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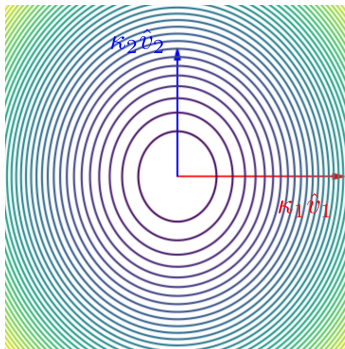
Note that

$$f(x) = \kappa_1 x_1^2 + \kappa_2 x_2^2$$

Considering a direction vector  $p$  and  $x = (0, 0)^\top$  we get

$$g(t) = f(x + tp) = f(tp) = t^2 (\kappa_1 p_1^2 + \kappa_2 p_2^2)$$

which is a parabola with  $g'' = 2 (\kappa_1 p_1^2 + \kappa_2 p_2^2)$ .



Consider  $f(x) = x^\top Hx$  where

$$H = \begin{pmatrix} 4/3 & 1/3 \\ 1/3 & 3/3 \end{pmatrix}$$

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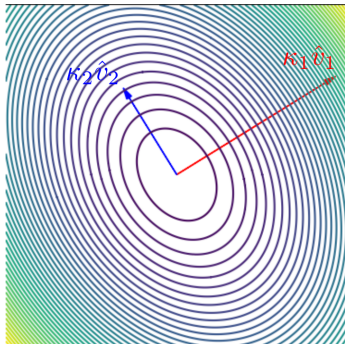
$$H = \begin{pmatrix} 4/3 & 1/3 \\ 1/3 & 3/3 \end{pmatrix}$$

The eigenvalues are

$$\kappa_1 = \frac{1}{6}(7 + \sqrt{5}) \quad \kappa_2 = \frac{1}{6}(7 - \sqrt{5})$$

Their corresponding eigenvectors are

$$\hat{v}_1 = \left( \frac{1}{2}(1 + \sqrt{5}), 1 \right) \quad \hat{v}_2 = \left( \frac{1}{2}(1 - \sqrt{5}), 1 \right)$$



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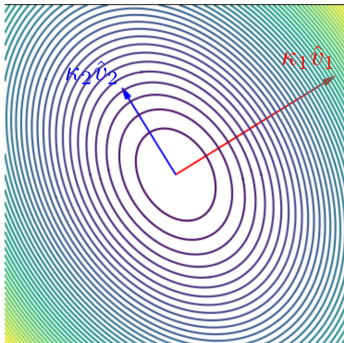
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Note that

$$H = (\hat{v}_1 \ \hat{v}_2) \begin{pmatrix} \kappa_1 & 0 \\ 0 & \kappa_2 \end{pmatrix} (\hat{v}_1 \ \hat{v}_2)^T$$

Here  $(\hat{v}_1 \ \hat{v}_2)$  is a  $2 \times 2$  matrix whose columns are  $\hat{v}_1, \hat{v}_2$ .





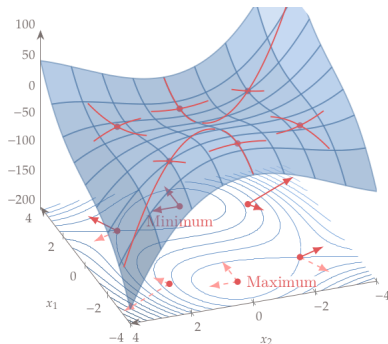
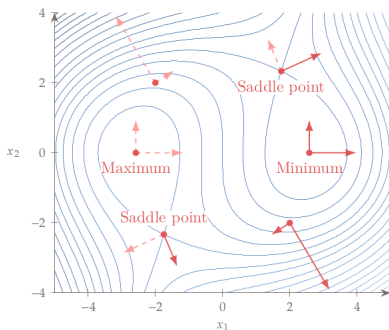
# Hessian Visualization Example

Consider

$$f(x_1, x_2) = x_1^3 + 2x_1x_2^2 - x_2^3 - 20x_1.$$

And it's Hessian.

$$H(x_1, x_2) = \begin{bmatrix} 6x_1 & 4x_2 \\ 4x_2 & 4x_1 - 6x_2 \end{bmatrix}.$$



# Taylor's Theorem

## Theorem 4 (Taylor)

*Suppose that  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is twice continuously differentiable and that  $p \in \mathbb{R}^n$ . Then, we have*

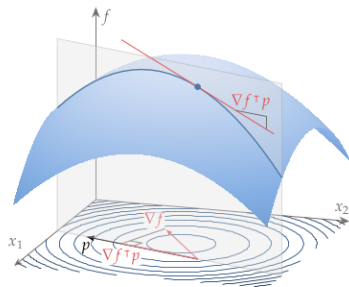
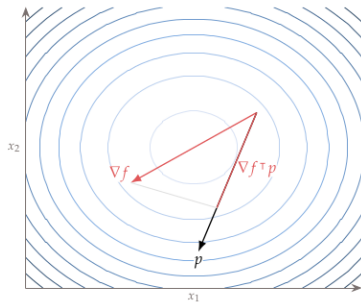
$$f(x + p) = f(x) + \nabla f(x)^T p + \frac{1}{2} p^T H(x) p + o(\|p\|^2).$$

*Here  $H = \nabla^2 f$  is the Hessian of  $f$ .*

# First-Order Necessary Conditions

## Theorem 5

*If  $x^*$  is a local minimizer and  $f$  is continuously differentiable in an open neighborhood of  $x^*$ , then  $\nabla f(x^*) = 0$ .*



## Second-Order Conditions

Note that  $\nabla f(x^*) = 0$  does not tell us whether  $x^*$  is a minimizer, maximizer, or a saddle point.

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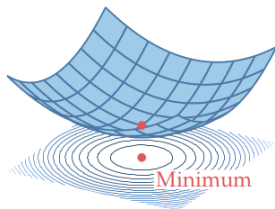
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However, knowing the curvature in all directions from  $x^*$  might tell us what  $x^*$  is, right?

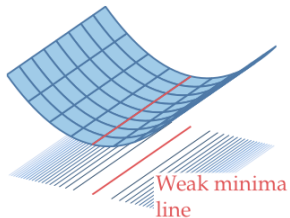
All comes down to the *definiteness* of  $H := H(x^*)$ .

- ▶  $H$  is **positive definite** if  $p^\top H p > 0$  for all  $p$   
iff all eigenvalues of  $H$  are positive
- ▶  $H$  is **positive semi-definite** if  $p^\top H p \geq 0$  for all  $p$   
iff all eigenvalues of  $H$  are nonnegative
- ▶  $H$  is **negative semi-definite** if  $p^\top H p \leq 0$  for all  $p$   
iff all eigenvalues of  $H$  are nonpositive
- ▶  $H$  is **negative definite** if  $p^\top H p < 0$  for all  $p$   
iff all eigenvalues of  $H$  are negative
- ▶  $H$  is **indefinite** if it is not definite in the above sense  
iff  $H$  has at least one positive and one negative eigenvalue.

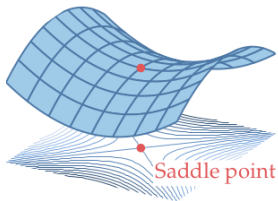
# Definiteness



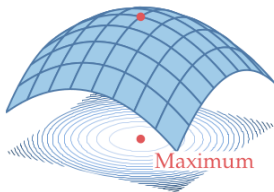
Positive definite



Positive semidefinite



Indefinite



Negative definite



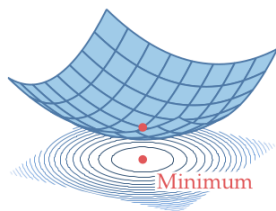
# Second-Order Necessary Condition

## Theorem 6 (Second-Order Necessary Conditions)

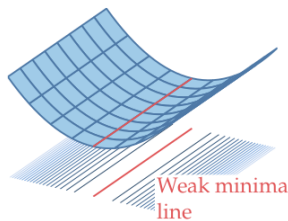
*If  $x^*$  is a local minimizer of  $f$  and  $\nabla^2 f$  is continuous in a neighborhood of  $x^*$ , then  $\nabla f(x^*) = 0$  and  $\nabla^2 f(x^*)$  is positive semidefinite.*

## Theorem 7 (Second-Order Sufficient Conditions)

*Suppose that  $\nabla^2 f$  is continuous in a neighborhood of  $x^*$  and that  $\nabla f(x^*) = 0$  and  $\nabla^2 f(x^*)$  is positive definite. Then  $x^*$  is a strict local minimizer of  $f$ .*



Positive definite



Positive semidefinite

## Example

Consider the following function of two variables:

$$f(x_1, x_2) = 0.5x_1^4 + 2x_1^3 + 1.5x_1^2 + x_2^2 - 2x_1x_2.$$

## Example

Consider the following function of two variables:

$$f(x_1, x_2) = 0.5x_1^4 + 2x_1^3 + 1.5x_1^2 + x_2^2 - 2x_1x_2.$$

Consider the gradient equal to zero:

$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1^3 + 6x_1^2 + 3x_1 - 2x_2 \\ 2x_2 - 2x_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

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From the second equation, we have that  $x_2 = x_1$ . Substituting this into the first equation yields

$$x_1 (2x_1^2 + 6x_1 + 1) = 0.$$

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The solution of this equation yields three points:

$$x_A = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad x_B = \begin{bmatrix} -\frac{3}{2} - \frac{\sqrt{7}}{2} \\ -\frac{3}{2} - \frac{\sqrt{7}}{2} \end{bmatrix}, \quad x_C = \begin{bmatrix} \frac{\sqrt{7}}{2} - \frac{3}{2} \\ \frac{\sqrt{7}}{2} - \frac{3}{2} \end{bmatrix}.$$

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Consider the following function of two variables:

$$f(x_1, x_2) = 0.5x_1^4 + 2x_1^3 + 1.5x_1^2 + x_2^2 - 2x_1x_2.$$

To classify  $x_A, x_B, x_C$ , we need to compute the Hessian matrix:

$$H(x_1, x_2) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix} = \begin{bmatrix} 6x_1^2 + 12x_1 + 3 & -2 \\ -2 & 2 \end{bmatrix}.$$

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The Hessian, at the first point, is

$$H(x_A) = \begin{bmatrix} 3 & -2 \\ -2 & 2 \end{bmatrix},$$

whose eigenvalues are  $\kappa_1 \approx 0.438$  and  $\kappa_2 \approx 4.561$ . Because both eigenvalues are positive, this point is a local minimum.



## Example

Consider the following function of two variables:

$$f(x_1, x_2) = 0.5x_1^4 + 2x_1^3 + 1.5x_1^2 + x_2^2 - 2x_1x_2.$$

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For the second point,

$$H(x_B) = \begin{bmatrix} 3(3 + \sqrt{7}) & -2 \\ -2 & 2 \end{bmatrix}.$$

The eigenvalues are  $\kappa_1 \approx 1.737$  and  $\kappa_2 \approx 17.200$ , so this point is another local minimum.

## Example

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To classify  $x_A, x_B, x_C$ , we need to compute the Hessian matrix:

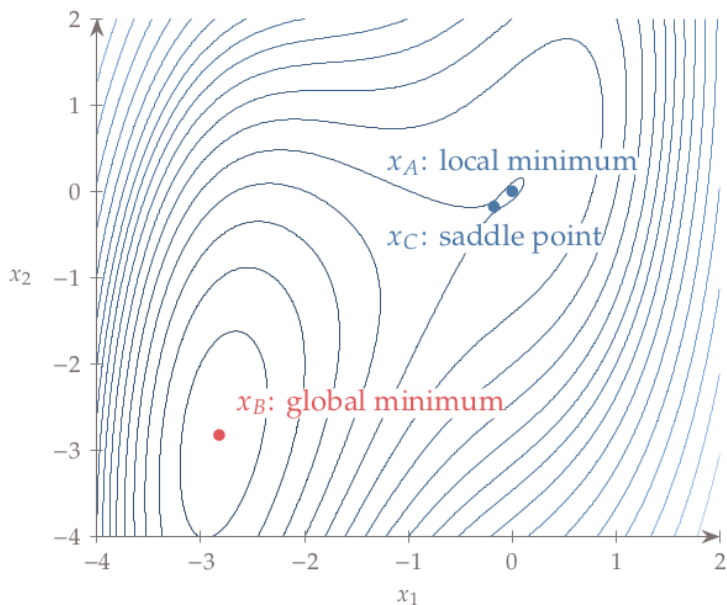
$$H(x_1, x_2) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix} = \begin{bmatrix} 6x_1^2 + 12x_1 + 3 & -2 \\ -2 & 2 \end{bmatrix}.$$

For the third point,

$$H(x_C) = \begin{bmatrix} 9 - 3\sqrt{7} & -2 \\ -2 & 2 \end{bmatrix}.$$

The eigenvalues for this Hessian are  $\kappa_1 \approx -0.523$  and  $\kappa_2 \approx 3.586$ , so this point is a saddle point.

## Example



# Proofs of Some Theorems

## Optional

# Taylor's Theorem

To prove the theorems characterizing minima/maxima, we need the following form of Taylor's theorem:

## Theorem 8 (Taylor)

*Suppose that  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is continuously differentiable and that  $p \in \mathbb{R}^n$ . Then we have that.*

$$f(x + p) = f(x) + \nabla f(x + tp)^T p,$$

*for some  $t \in (0, 1)$ . Moreover, if  $f$  is twice continuously differentiable, we have that*

$$f(x + p) = f(x) + \nabla f(x)^T p + \frac{1}{2} p^T \nabla^2 f(x + tp) p,$$

*for some  $t \in (0, 1)$ .*

## Proof of Theorem 5 (Optional)

We prove that if  $x^*$  is a local minimizer and  $f$  is continuously differentiable in an open neighborhood of  $x^*$ , then  $\nabla f(x^*) = 0$ .

Suppose for contradiction that  $\nabla f(x^*) \neq 0$ . Define the vector  $p = -\nabla f(x^*)$  and note that  $p^T \nabla f(x^*) = -\|\nabla f(x^*)\|^2 < 0$ . Because  $\nabla f$  is continuous near  $x^*$ , there is a scalar  $T > 0$  such that

$$p^T \nabla f(x^* + tp) < 0, \quad \text{for all } t \in [0, T]$$

For any  $\bar{t} \in (0, T]$ , we have by Taylor's theorem that

$$f(x^* + \bar{t}p) = f(x^*) + \bar{t}p^T \nabla f(x^* + tp), \quad \text{for some } t \in (0, \bar{t}).$$

Therefore,  $f(x^* + \bar{t}p) < f(x^*)$  for all  $\bar{t} \in (0, T]$ . We have found a direction leading away from  $x^*$  along which  $f$  decreases, so  $x^*$  is not a local minimizer, and we have a contradiction.  $\square$

## Proof of Theorem 6 (Optional)

We prove that if  $x^*$  is a local minimizer of  $f$  and  $\nabla^2 f$  is continuous in an open neighborhood of  $x^*$ , then  $\nabla f(x^*) = 0$  and  $\nabla^2 f(x^*)$  is positive semidefinite.

We know that  $\nabla f(x^*) = 0$ . For contradiction, assume that  $\nabla^2 f(x^*)$  is not positive semidefinite.

Then we can choose a vector  $p$  such that  $p^T \nabla^2 f(x^*) p < 0$ .

As  $\nabla^2 f$  is continuous near  $x^*$ ,  $p^T \nabla^2 f(x^* + tp) p < 0$  for all  $t \in [0, T]$  where  $T > 0$ .

By Taylor we have for all  $\bar{t} \in (0, T]$  and some  $t \in (0, \bar{t})$

$$f(x^* + \bar{t}p) = f(x^*) + \bar{t}p^T \nabla f(x^*) + \frac{1}{2}\bar{t}^2 p^T \nabla^2 f(x^* + tp) p < f(x^*).$$

Thus,  $x^*$  is not a local minimizer. □

## Proof of Theorem 7 (Optional)

We prove the following: Suppose that  $\nabla^2 f$  is continuous in an open neighborhood of  $x^*$  and that  $\nabla f(x^*) = 0$  and  $\nabla^2 f(x^*)$  is positive definite. Then  $x^*$  is a strict local minimizer of  $f$ .

Because the Hessian is continuous and positive definite at  $x^*$ , we can choose a radius  $r > 0$  so that  $\nabla^2 f(x)$  remains positive definite for all  $x$  in the open ball  $\mathcal{D} = \{z \mid \|z - x^*\| < r\}$ . Taking any nonzero vector  $p$  with  $\|p\| < r$ , we have  $x^* + p \in \mathcal{D}$  and so

$$\begin{aligned} f(x^* + p) &= f(x^*) + p^T \nabla f(x^*) + \frac{1}{2} p^T \nabla^2 f(z) p \\ &= f(x^*) + \frac{1}{2} p^T \nabla^2 f(z) p, \end{aligned}$$

where  $z = x^* + tp$  for some  $t \in (0, 1)$ . Since  $z \in \mathcal{D}$ , we have  $p^T \nabla^2 f(z) p > 0$ , and therefore  $f(x^* + p) > f(x^*)$ , giving the result. □



# Unconstrained Optimization Algorithms

# Search Algorithms

We consider algorithms that

- ▶ Start with an initial guess  $x_0$
- ▶ Generate a sequence of points  $x_0, x_1, \dots$
- ▶ Stop when no progress can be made or when a minimizer seems approximated with sufficient accuracy.

To compute  $x_{k+1}$  the algorithms use the information about  $f$  at the previous iterates  $x_0, x_1, \dots, x_k$ .

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There are two overall strategies:

- ▶ Line search
- ▶ Trust region

## Line Search Overview

To compute  $x_{k+1}$ , a line search algorithm chooses

- ▶ *direction*  $p_k$
- ▶ *step size*  $\alpha_k$

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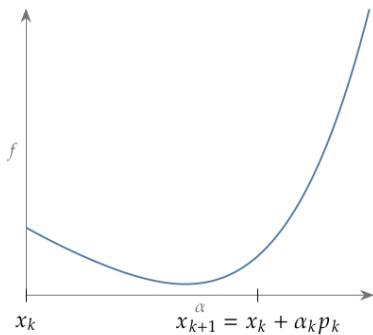
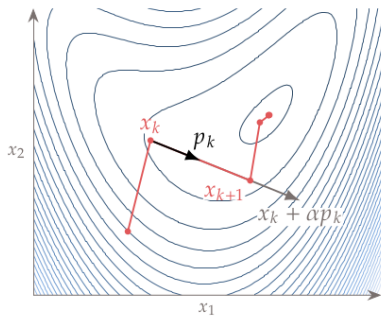
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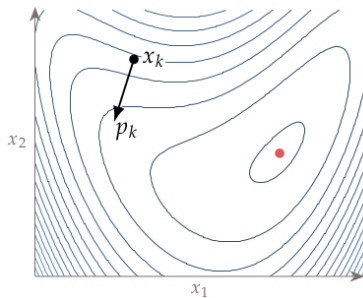
$\alpha_k$  is selected to approximately solve

$$\min_{\alpha > 0} f(x_k + \alpha p_k)$$

However, typically, an exact solution is expensive and unnecessary. Instead, line search algorithms inspect a limited number of trial step lengths and find one that decreases  $f$  appropriately (see later).



A descent direction does not have to be followed to the minimum.





## Trust Region

To compute  $x_{k+1}$ , a trust region algorithm chooses

- ▶ *model function*  $m_k$  whose behavior near  $x_k$  is similar to  $f$
- ▶ a *trust region*  $R \subseteq \mathbb{R}^n$  around  $x_k$ . Usually  $R$  is the ball defined by  $\|x - x_k\| \leq \Delta$  where  $\Delta > 0$  is *trust region radius*.

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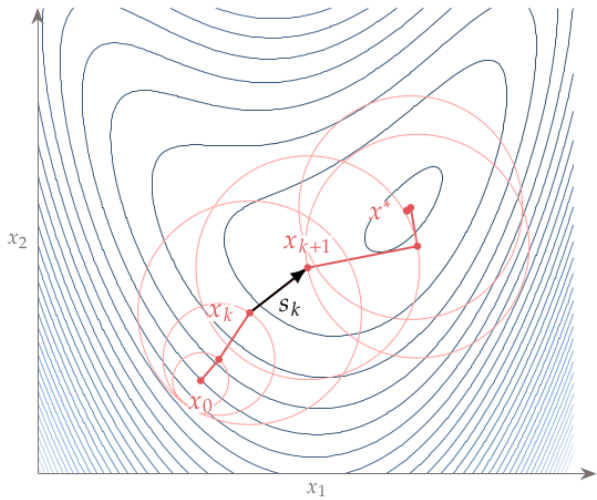
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The model  $m_k$  is usually derived from the Taylor's theorem.

$$m_k(x_k + p) = f_k + p^T \nabla f_k + \frac{1}{2} p^T B_k p$$

Where  $B_k$  approximates the Hessian of  $f$  at  $x_k$ .



# Line Search Methods

# Line Search

For setting the step size, we consider

- ▶ Armijo condition and backtracking algorithm
- ▶ strong Wolfe conditions and bracketing & zooming

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For setting the direction, we consider

- ▶ Gradient descent
- ▶ Newton's method
- ▶ quasi-Newton methods (BFGS)
- ▶ (Conjugate gradients)

We start with the step size.

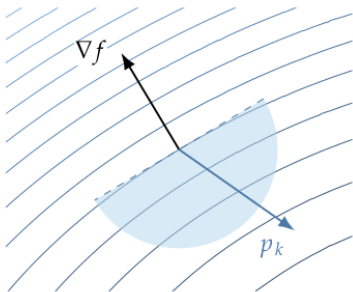
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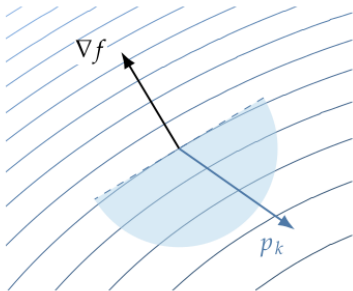
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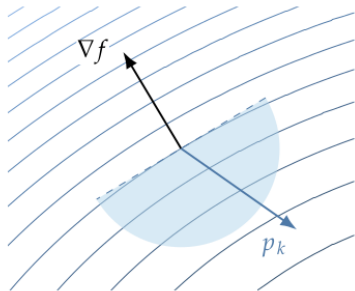
Define

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We know that

$$\phi'(\alpha) = \nabla f(x_k + \alpha p_k)^\top p_k \quad \text{which means} \quad \phi'(0) = \nabla f_k^\top p_k$$

Note that  $\phi'(0)$  must be negative as  $p_k$  is a descent direction.

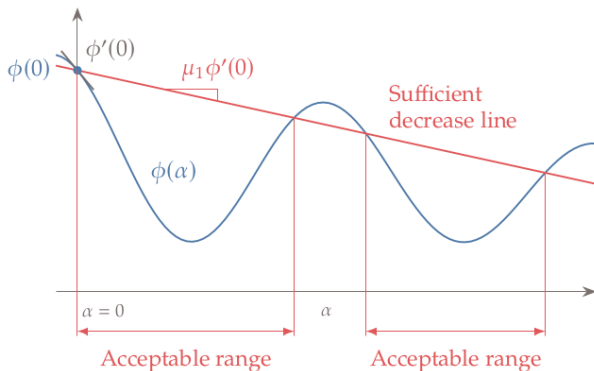


# Armijo Condition

The *sufficient decrease condition* (aka *Armijo condition*)

$$\phi(\alpha) \leq \phi(0) + \alpha (\mu_1 \phi'(0))$$

where  $\mu_1$  is a constant such that  $0 < \mu_1 \leq 1$



In practice,  $\mu_1$  is several orders smaller than 1, typically  $\mu_1 = 10^{-4}$ .

# Backtracking Line Search Algorithm

---

**Algorithm 1** Backtracking Line Search

---

**Input:**  $\alpha_{\text{init}} > 0$ ,  $0 < \mu_1 < 1$ ,  $0 < \rho < 1$

**Output:**  $\alpha^*$  satisfying sufficient decrease condition

- 1:  $\alpha \leftarrow \alpha_{\text{init}}$
  - 2: **while**  $\phi(\alpha) > \phi(0) + \alpha\mu_1\phi'(0)$  **do**
  - 3:      $\alpha \leftarrow \rho\alpha$
  - 4: **end while**
- 

The parameter  $\rho$  is typically set to 0.5. It can also be a variable set by a more sophisticated method (interpolation).

The  $\alpha_{\text{init}}$  depends on the method for setting the descent direction  $p_k$ . For Newton and quasi-Newton, it is 1.0, but for other methods, it might be different.

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There are two scenarios where the method does not perform well:

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Even if our original step size is not too far from an acceptable one, the basic backtracking algorithm ignores any information we have about the function values and gradients. It blindly takes a reduced step based on a preselected ratio  $\rho$ .

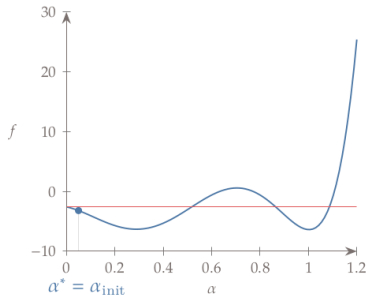
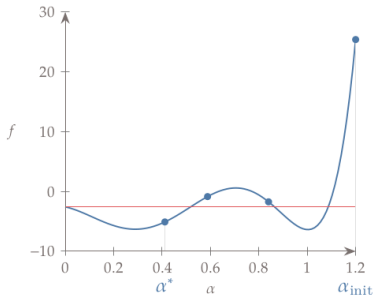
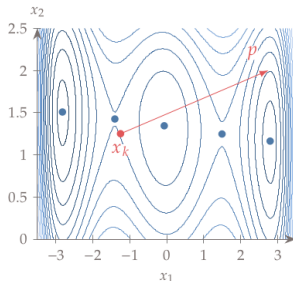


# Backtracking Example

$$f(x_1, x_2) =$$

$$0.1x_1^6 - 1.5x_1^4 + 5x_1^2 \\ + 0.1x_2^4 + 3x_2^2 - 9x_2 + 0.5x_1x_2$$

$$\mu_1 = 10^{-4} \text{ and } \rho = 0.7.$$



## Sufficient Curvature Condition

We want to prevent too short of steps and to “motivate” the search to move closer to the minimum.

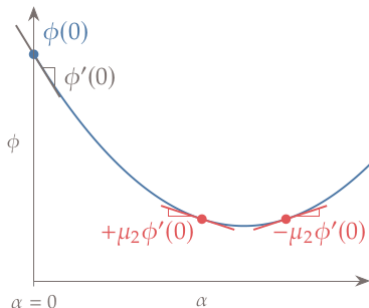
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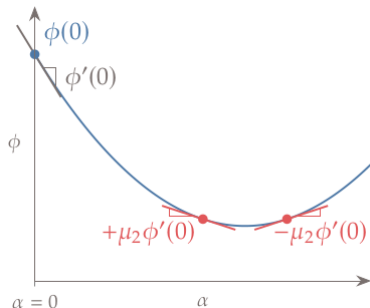
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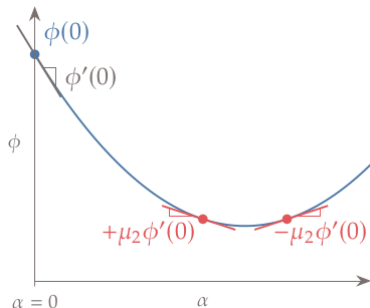
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As  $\mu_2$  tends to 0, the condition enforces  $\phi'(\alpha) = 0$ , which would yield an exact line search.

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Putting together Armijo and sufficient curvature conditions, we obtain *strong Wolfe conditions*

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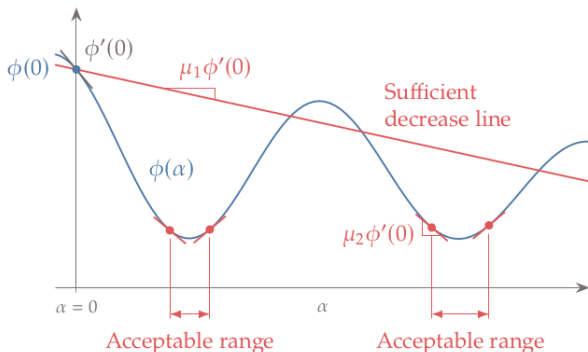
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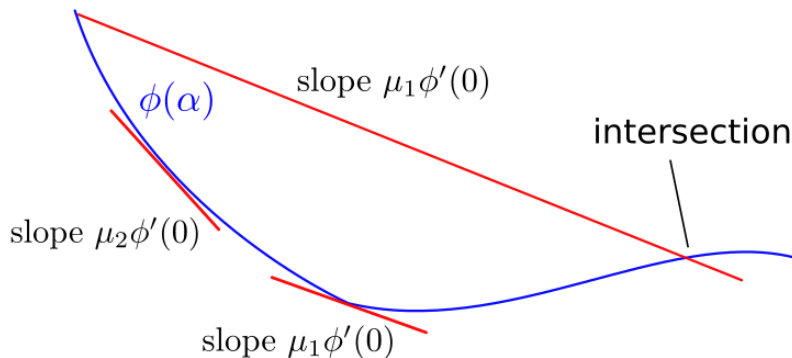




# Satisfiability of Strong Wolfe Conditions

## Theorem 9

Suppose  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is continuously differentiable. Let  $p_k$  be a descent direction at  $x_k$ , and assume that  $f$  is bounded below along the ray  $\{x_k + \alpha p_k \mid \alpha > 0\}$ . Then, if  $0 < \mu_1 < \mu_2 < 1$ , step length intervals exist that satisfy the strong Wolfe conditions.



## Convergence of Line Search

Denote by  $\theta_k$  the angle between  $p_k$  and  $-\nabla f_k$ , i.e., satisfying

$$\cos \theta_k = \frac{-\nabla f_k^T p_k}{\|\nabla f_k\| \|p_k\|}$$

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Recall that  $f$  is  $L$ -smooth for some  $L > 0$  if

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### Theorem 10 (Zoutendijk)

Consider  $x_{k+1} = x_k + \alpha_k p_k$ , where  $p_k$  is a descent direction and  $\alpha_k$  satisfies the strong Wolfe conditions. Suppose that  $f$  is bounded below, continuously differentiable, and  $L$ -smooth. Then

$$\sum_{k \geq 0} \cos^2 \theta_k \|\nabla f_k\|^2 < \infty.$$

## Line Search Algorithm

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1. The bracketing phase finds an interval within which we are certain to find a point that satisfies the strong Wolfe conditions.
2. The zooming phase finds a point that satisfies the strong Wolfe conditions within the interval provided by the bracketing phase.



---

## Algorithm 2 Bracketing

---

**Input:**  $\alpha_1 > 0$  and  $\alpha_{\max}$

- 1: Set  $\alpha_0 \leftarrow 0$
- 2:  $i \leftarrow 1$
- 3: **repeat**
- 4:     Evaluate  $\phi(\alpha_i)$
- 5:     **if**  $\phi(\alpha_i) > \phi(0) + \alpha_i \mu_1 \phi'(0)$  or  $[\phi(\alpha_i) \geq \phi(\alpha_{i-1})$  and  $i > 1]$   
      **then**
- 6:          $\alpha^* \leftarrow \mathbf{zoom}(\alpha_{i-1}, \alpha_i)$  and stop
- 7:     **end if**
- 8:     Evaluate  $\phi'(\alpha_i)$
- 9:     **if**  $|\phi'(\alpha_i)| \leq \mu_2 |\phi'(0)|$  **then**
- 10:        set  $\alpha^* \leftarrow \alpha_i$  and stop
- 11:     **else if**  $\phi'(\alpha_i) \geq 0$  **then**
- 12:        set  $\alpha^* \leftarrow \mathbf{zoom}(\alpha_i, \alpha_{i-1})$  and stop
- 13:     **end if**
- 14:     Choose  $\alpha_{i+1} \in (\alpha_i, \alpha_{\max})$
- 15:      $i \leftarrow i + 1$
- 16: **until** a condition is met

## Explanation of Bracketing

Note that the sequence of trial steps  $\alpha_j$  is monotonically increasing.

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Note that **zoom** is called when one of the following conditions is satisfied:

- ▶  $\alpha_i$  violates the sufficient decrease condition (lines 5 and 6)
- ▶  $\phi(\alpha_i) \geq \phi(\alpha_{i-1})$  (also lines 5 and 6)
- ▶  $\phi'(\alpha_i) \geq 0$  (lines 11 and 12)

The last step increases the  $\alpha_i$ . May use, e.g., a constant multiple.

## Zoom

The following algorithm keeps two step lengths:  $\alpha_{lo}$  and  $\alpha_{hi}$

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The following invariants are being preserved:

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That is,  $\phi$  always slopes down from  $\alpha_{lo}$  to  $\alpha_{hi}$ .

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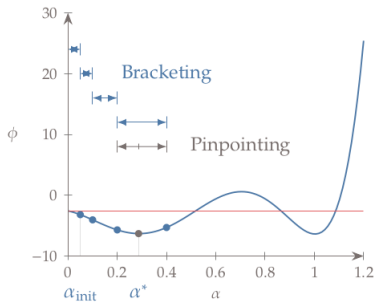
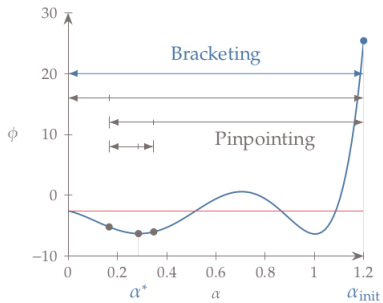
1: function ZOOM( $\alpha_{lo}, \alpha_{hi}$ )
2:   repeat
3:     Set  $\alpha$  between  $\alpha_{lo}$  and  $\alpha_{hi}$  using interpolation
      (bisection, quadratic, etc.)
4:     Evaluate  $\phi(\alpha)$ 
5:     if  $\phi(\alpha) > \phi(0) + \alpha\mu_1\phi'(0)$  or  $\phi(\alpha) \geq \phi(\alpha_{lo})$  then
6:        $\alpha_{hi} \leftarrow \alpha$ 
7:     else
8:       Evaluate  $\phi'(\alpha)$ 
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10:        Set  $\alpha^* \leftarrow \alpha$  and stop
11:      end if
12:      if  $\phi'(\alpha)(\alpha_{hi} - \alpha_{lo}) \geq 0$  then
13:         $\alpha_{hi} \leftarrow \alpha_{lo}$ 
14:      end if
15:       $\alpha_{lo} \leftarrow \alpha$ 
16:    end if
17:  until a condition is met
18: end function

```



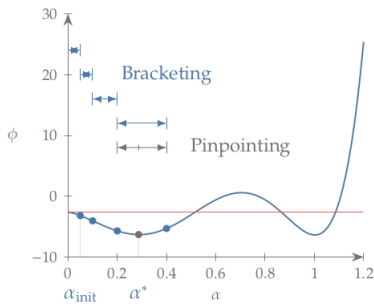
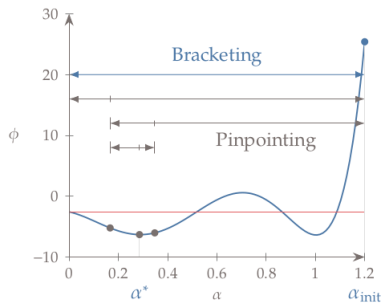
## Bracketing & Zooming Example

We use quadratic interpolation; the bracketing chooses  $\alpha_{i+1} = 2\alpha_i$ , and the sufficient curvature factor is  $\mu_2 = 0.9$ .



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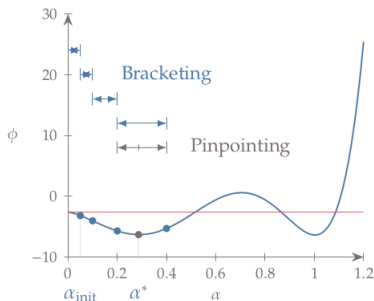
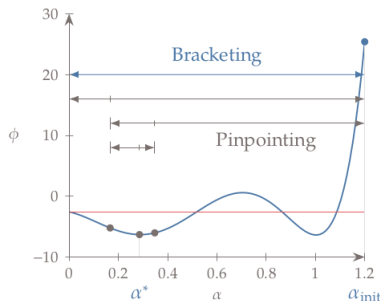
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Bracketing is achieved in the first iteration by using a significant initial step of  $\alpha_{\text{init}} = 1.2$  (left). Then, zooming finds an improved point through interpolation.

The small initial step of  $\alpha_{\text{init}} = 0.05$  (right) does not satisfy the strong Wolfe conditions, and the bracketing phase moves forward toward a flatter part of the function.

## Comments on Line Search

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- ▶ The presented algorithm is implemented in [https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.line\\_search.html](https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.line_search.html)