Optimization

Lecture 5

Sibylle Hess and Mahdi Shafiee

February, 2021

TU/e Technische Universiteit Eindhoven University of Technology

Optimization

Unconstrained Optimization Problem

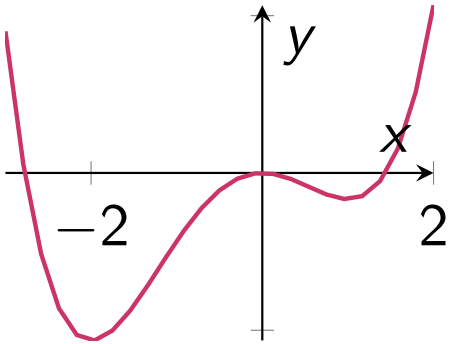
Given an objective function $f : \mathbb{R}^n \to \mathbb{R}$, the objective of an unconstrained optimization problem is:

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

We say that:

- $x^* \in \arg\min_{x \in \mathbb{R}^n} f(x)$ is a minimizer
- $\min_{x \in \mathbb{R}^n} f(x)$ is the minimum

Local and Global Minimizers



global minimizer: $x^* = -2$
local minimizer: $x_3 = 1$

A global minimizer is a vector x^* satisfying

$$f(x^*) \leq f(x) \text{ for all } x \in \mathbb{R}^n$$

A local minimizer is a vector x_0 satisfying

$$f(x_0) \leq f(x) \text{ for all } x \in \mathcal{N}_\epsilon(x_0),$$

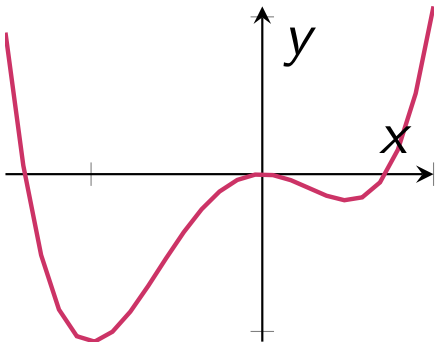
where $\mathcal{N}_\epsilon(x_0) = \{x \in \mathbb{R}^n | \|x - x_0\| \leq \epsilon\}$

How can we solve an unconstrained optimization problem?

With FONC and SONC.

Finding Stationary Points: our Minimizer Candidates

Every local minimizer x_0 is a stationary point: $\frac{d}{dx} f(x_0) = 0$
(a.k.a. 1st order necessary condition)



$$f(x) = \frac{1}{4}x^4 + \frac{1}{3}x^3 - x^2$$

$$\frac{d}{dx} f(x) = x^3 + x^2 - 2x$$

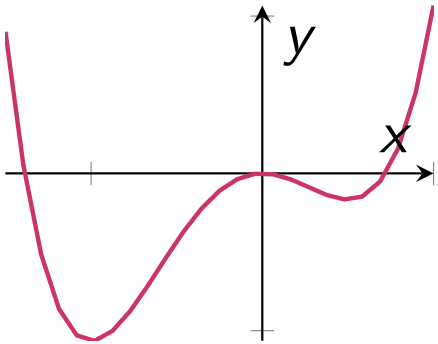
$$\frac{d^2}{dx^2} f(x) = 3x^2 + 2x - 2$$

$$\frac{d}{dx} f(x) = 0 \quad \Leftrightarrow \quad x_1 = -2, x_2 = 0, x_3 = 1$$

Possible local minimizers: $x_1 = -2, x_2 = 0, x_3 = 1$

Identifying Minimizers by the Curvature

Every stationary point x_0 with increasing function values around it is a local minimizer: $\frac{d}{dx}f(x_0) = 0$ & $\frac{d^2}{dx^2}f(x_0) \geq 0$
(a.k.a 2nd order sufficient condition)



$$f(x) = \frac{1}{4}x^4 + \frac{1}{3}x^3 - x^2$$

$$\frac{d}{dx}f(x) = x^3 + x^2 - 2x$$

$$\frac{d^2}{dx^2}f(x) = 3x^2 + 2x - 2$$

$$\frac{d^2}{dx^2}f(-2) = 6 \geq 0, \quad \frac{d^2}{dx^2}f(0) = -2 < 0, \quad \frac{d^2}{dx^2}f(1) = 3 \geq 0$$

We identify the local minimizers $x_1 = -2$ and $x_2 = 3$.

What Happens in Higher Dimensions?

The derivative of a function $f : \mathbb{R}^d \to \mathbb{R}$ is given by its partial derivatives:

$$\frac{\partial f(x)}{\partial x} = \begin{pmatrix} \frac{\partial f(x)}{\partial x_1} & \dots & \frac{\partial f(x)}{\partial x_d} \end{pmatrix} \in \mathbb{R}^{1 \times d} \qquad \text{(Jacobian)}$$

$$\nabla_x f(x) = \begin{pmatrix} \frac{\partial f(x)}{\partial x_1} \\ \vdots \\ \frac{\partial f(x)}{\partial x_d} \end{pmatrix} \in \mathbb{R}^d \qquad \text{(Gradient)}$$

First Order Necessary Condition

FONC

If x is a local minimizer of $f : \mathbb{R}^d \to \mathbb{R}$ and f is continuously differentiable in an open neighborhood of x, then

$$\nabla f(x) = 0$$

A vector x is called stationary point if $\nabla f(x) = 0$.

Second Order Necessary Condition

SONC

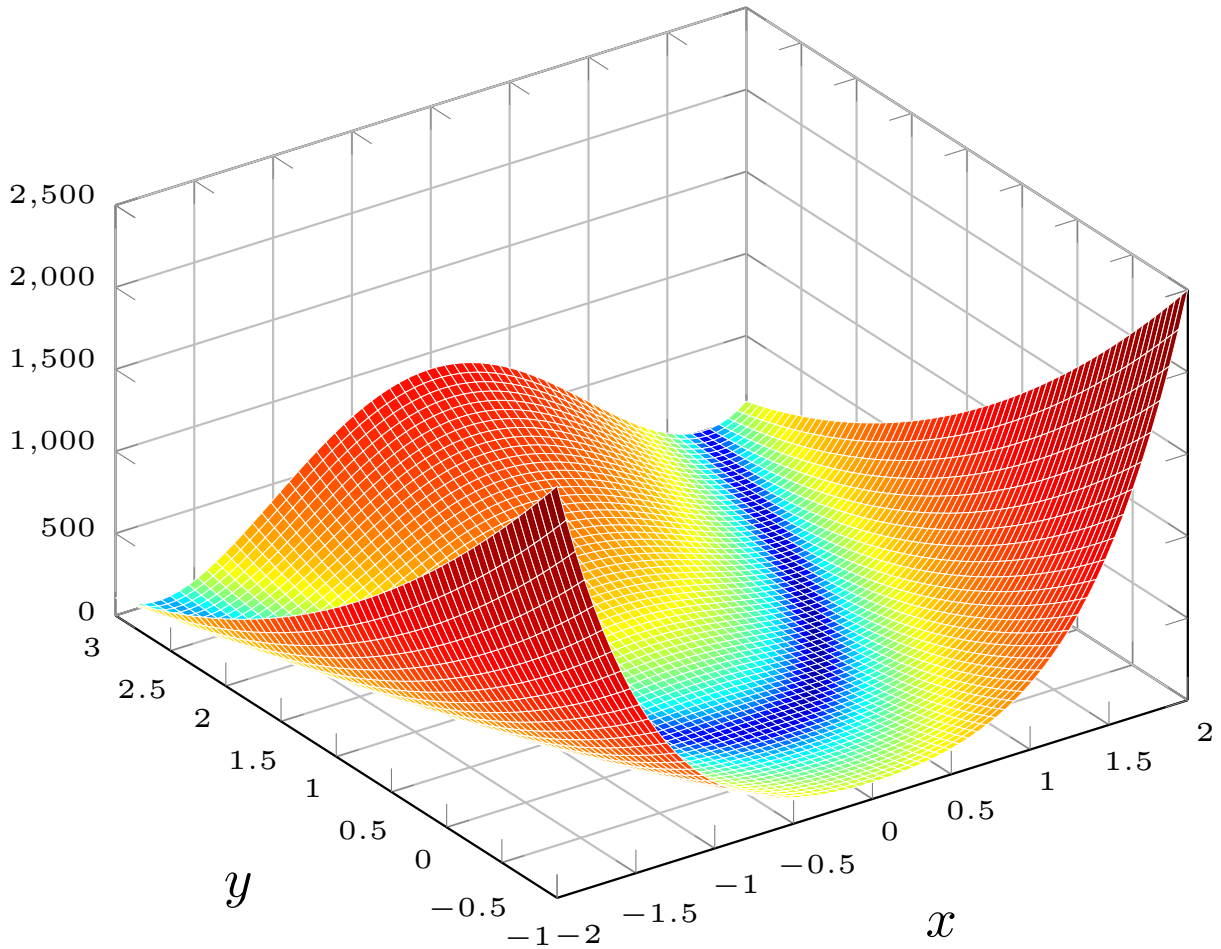
If x is a local minimizer of $f : \mathbb{R}^d \to \mathbb{R}$ and $\nabla^2 f$ is continuous in an open neighborhood of x, then

$$\nabla f(\mathrm{x}) = 0 \text{ and } \nabla^2 f(\mathrm{x}) \text{ is positive semidefinite}$$

A matrix $A \in \mathbb{R}^{d \times d}$ is positive semidefinite if

$$\mathrm{x}^\top A \mathrm{x} \geq 0 \text{ for all } \mathrm{x} \in \mathbb{R}^d$$

Example: the Rosenbrock Function



Candidate Minimizers of the Rosenbrock Function

The Rosenbrock function is given by

$$f(\mathrm{x}) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$

We compute the gradient and set it to zero:

$$\nabla f(\mathrm{x}) = \begin{pmatrix} 400x_1(x_1^2 - x_2) + 2(x_1 - 1) \\ 200(x_2 - x_1^2) \end{pmatrix} = 0,$$
$$\Leftrightarrow \mathrm{x} = (1, 1)$$

According to FONC we have one stationary point, i.e., one local minimizer candidate at $\mathrm{x}_0 = (1, 1)$.

Evaluating the Curvature at the Candidate Minimizer

We compute the Hessian function of f at $x_0 = (1, 1)$:

$$\nabla^2 f(x) = 200 \begin{pmatrix} 1 & -2x_1 \\ -2x_1 & 6x_1^2 - 2x_2 + 0.01 \end{pmatrix}$$

$$\nabla^2 f(x_0) = 200 \begin{pmatrix} 1 & -2 \\ -2 & 4.01 \end{pmatrix}$$

We check now if the Hessian is positive semi-definite at the stationary point. Let $x \in \mathbb{R}^2$, then

$$x^\top \nabla^2 f(x_0) x = (x_1 - 2x_2)^2 + 0.01 x_2^2 \geq 0$$

Hence, $\nabla^2 f(x_0)$ is p.s.d. and $x_0 = (1, 1)$ satisfies the SONC for a local minimizer of f.

Nice, so finding local minimizers is not a big deal

IF we have an unconstrained objective with an objective function which is twice continuously differentiable.

Let's consider a more complex setting:

Introducing Constraints

Constrained Optimization Problem

Given

- an objective function $f : \mathbb{R}^d \to \mathbb{R}$ and
- constraint functions $c_i, g_k : \mathbb{R}^d \to \mathbb{R}$,

then the objective of an constrained optimization problem is

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \; & f(\mathrm{x}) \\ \text{s.t.} \; & c_i(\mathrm{x}) = 0 && \text{for } 1 \leq i \leq m, \\ & g_k(\mathrm{x}) \geq 0 && \text{for } 1 \leq k \leq l \end{aligned}$$

We call the set of vectors satisfying the constraints the feasible set:

$$\mathcal{C} = \{\mathrm{x} \mid c_i(\mathrm{x}) = 0, g_k(\mathrm{x}) \geq 0 \text{ for } 1 \leq i \leq m, 1 \leq k \leq m\}.$$

How can we solve a constrained optimization tasks?

If we have constraints, then FONC and SONC do not help much anymore..

What if I can't compute the minimizers by these approaches?

Do Numerical Optimization

Approximating a Minimizer

If the minimizers can not be computed directly/analytically, then Numerical Optimization can come to the rescue.

The general scheme of numerical optimization methods is:

1: **function** $\textsc{Optimizer}(f)$
2: $\quad x_0 \leftarrow \textsc{Initialize}(x_0)$
3: $\quad$ **for** $t \in \{1, \ldots, t_{max} - 1\}$ **do**
4: $\quad\quad x_{t+1} \leftarrow \textsc{Update}(x_t, f)$
5: $\quad$ **end for**
6: $\quad$ **return** $x_{t_{max}}$
7: **end function**

Coordinate Descent

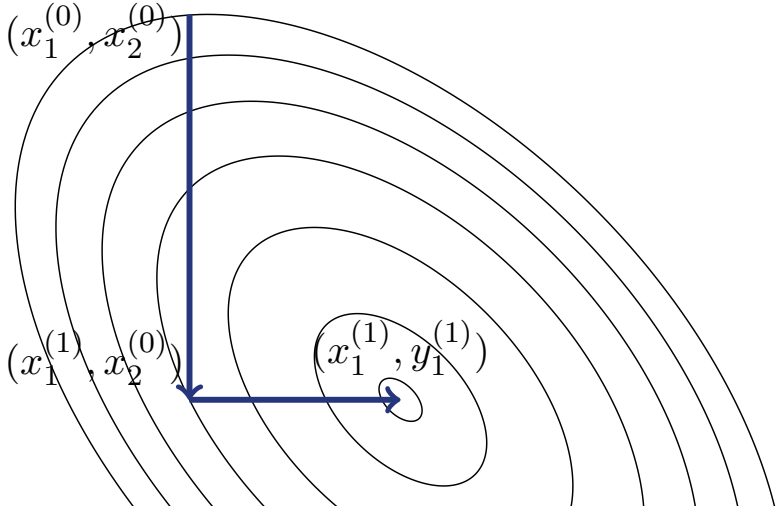
Sometimes, we can not determine the minimum analytically, but the minimum in a coordinate direction.

Coordinate descent update: for $i \in \{1, \dots d\}$ do

$$x_i^{(t+1)} \leftarrow \arg\min_{x_i} f(x_1^{(t+1)}, \dots, x_{i-1}^{(t+1)}, x_i, x_{i+1}^{(t)}, \dots, x_d^{(t)})$$

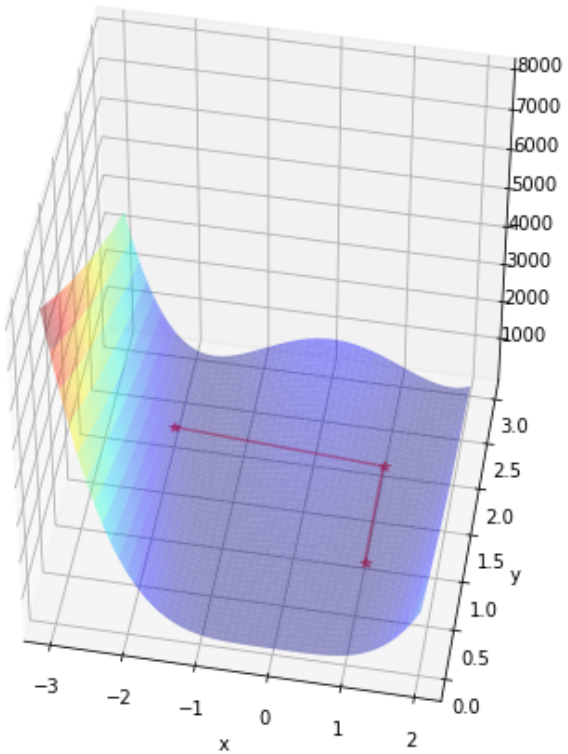
Coordinate descent minimizes in every step, hence

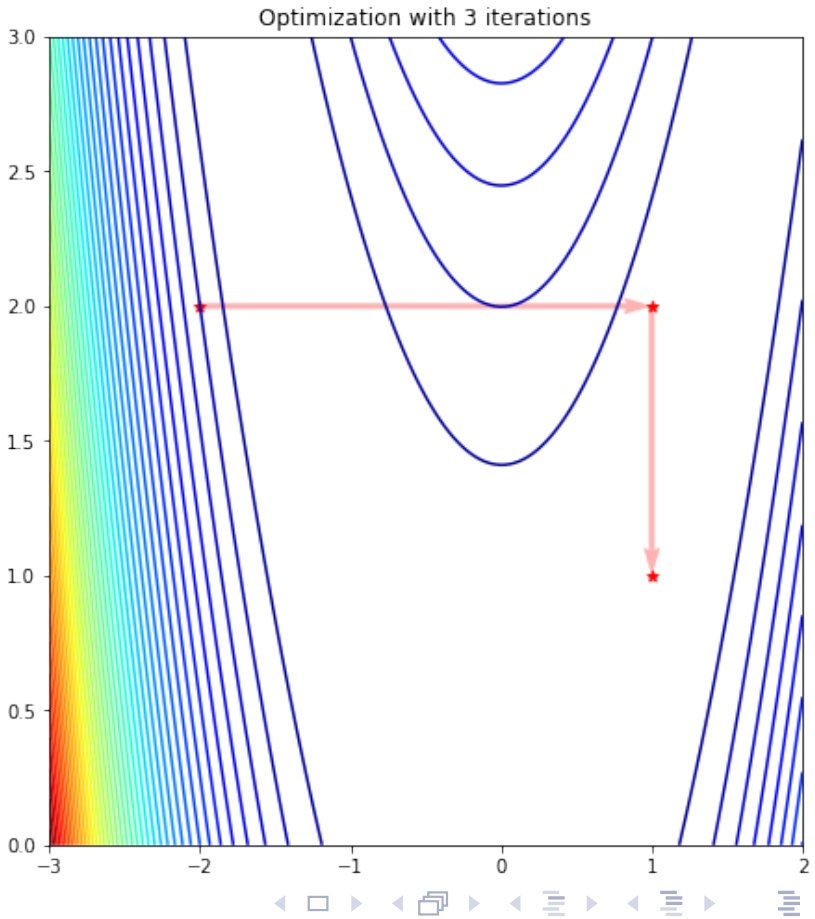
$$f(\mathrm{x}^{(0)}) \geq f(\mathrm{x}^{(1)}) \geq f(\mathrm{x}^{(2)}) \geq \dots$$



Example: Coordinate Descent on the Rosenbrock Function

$$\arg\min_{x_1 \in \mathbb{R}} f(x_1, x_2) = 1 \qquad \arg\min_{x_2 \in \mathbb{R}} f(x_1, x_2) = x_1^2$$





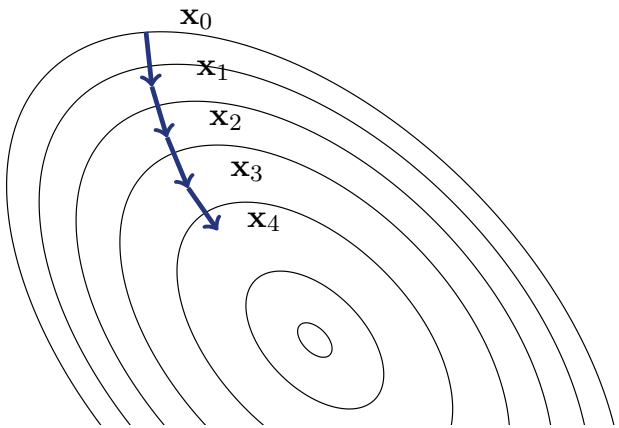
Gradient Descent

If we do not know much but a gradient, we can apply gradient descent.

Gradient descent update:

$$x_{t+1} \leftarrow x_t - \eta \nabla f(x_t)$$

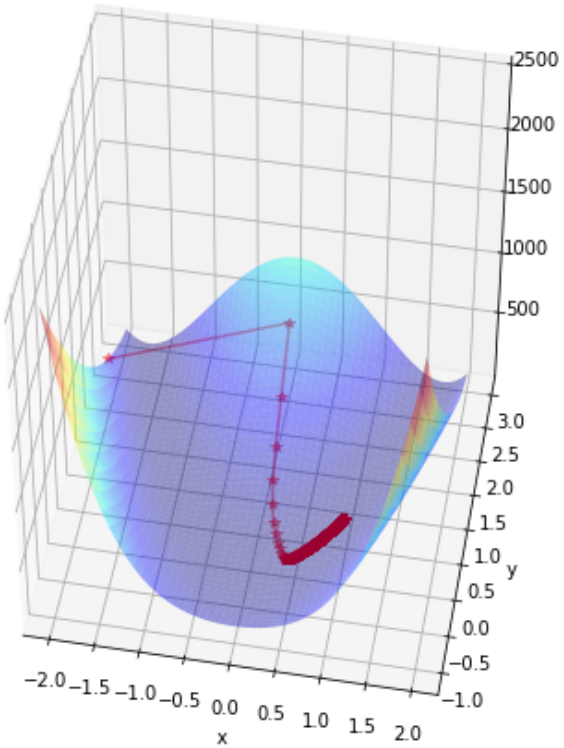
where η is the step size.

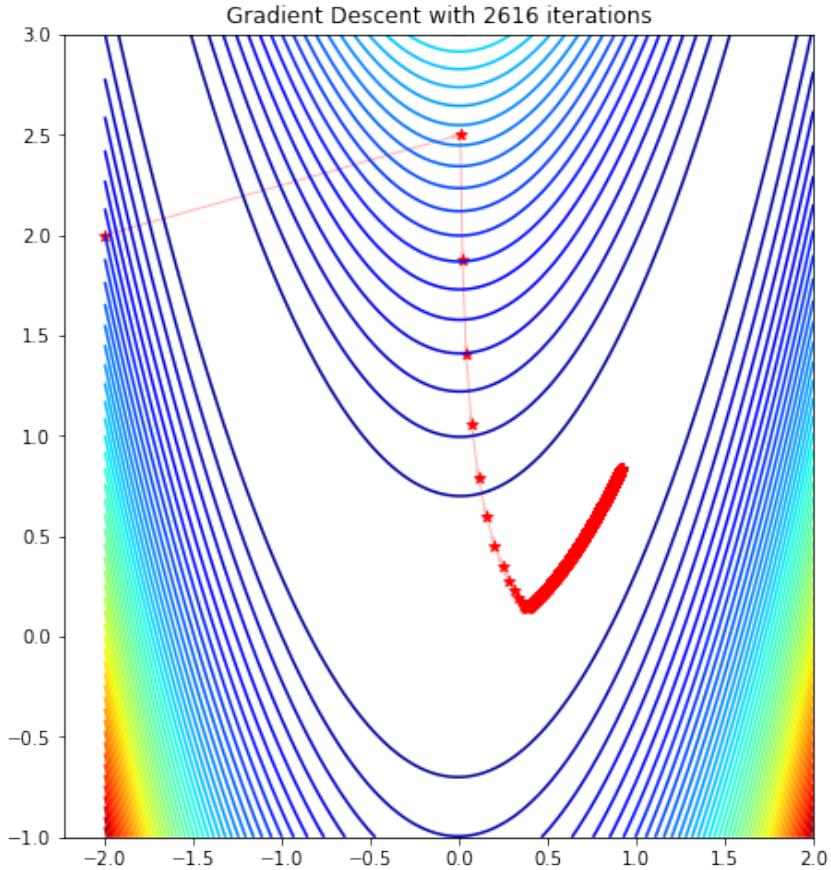


The negative gradient points into the direction of steepest descent. Hence, for a small enough step size we obtain a sequence

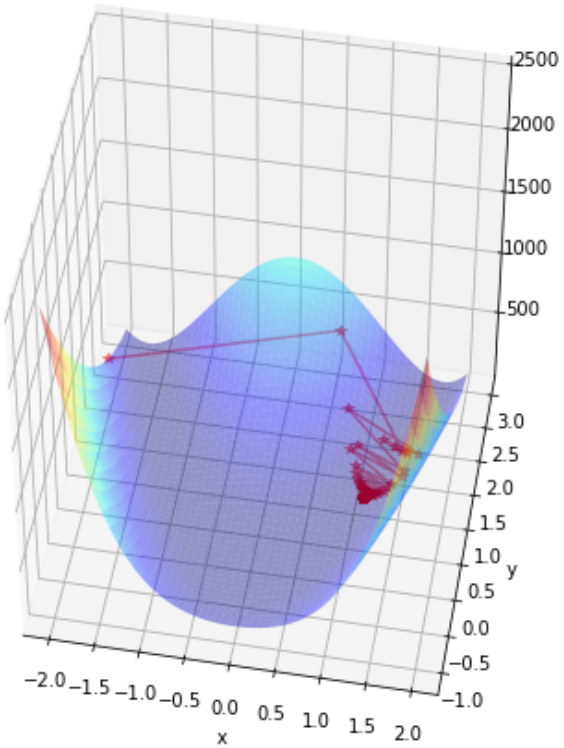
$$f(x_0) \geq f(x_1) \geq f(x_2) \geq \dots$$

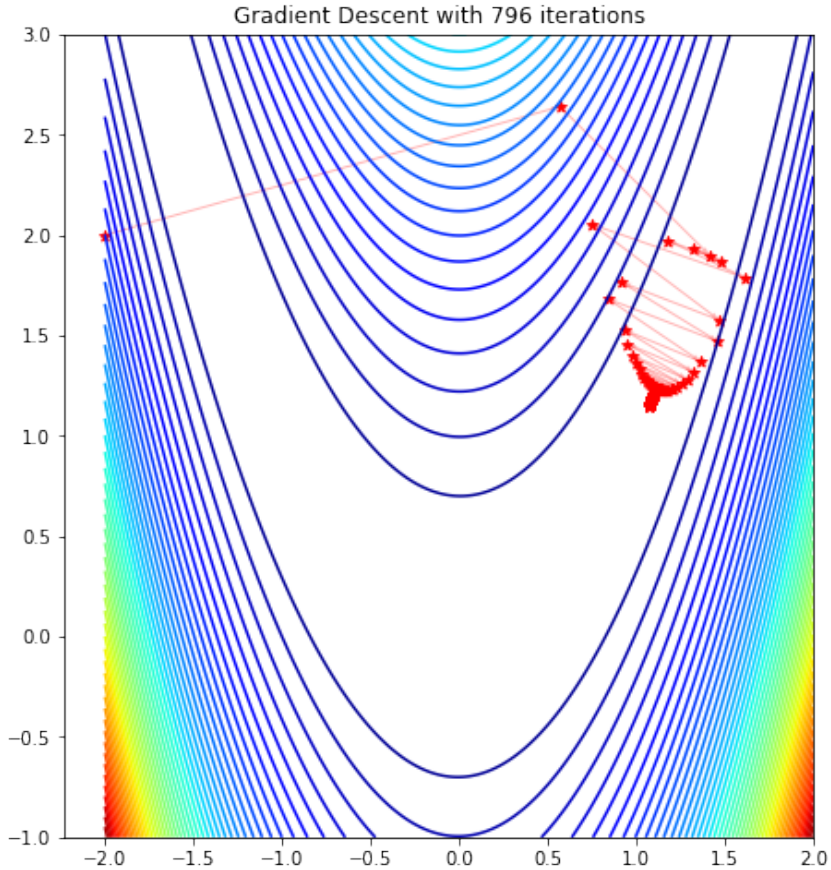
Example: Gradient Descent with $\eta = 0.00125$ on the Rosenbrock Function



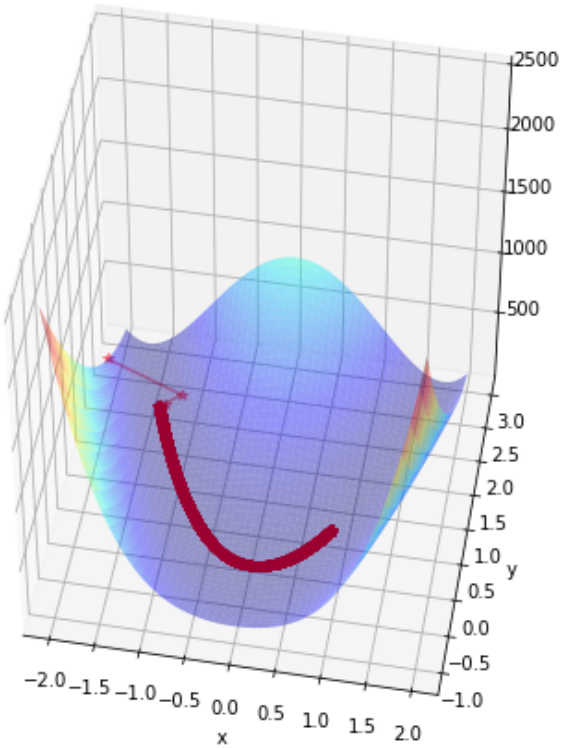


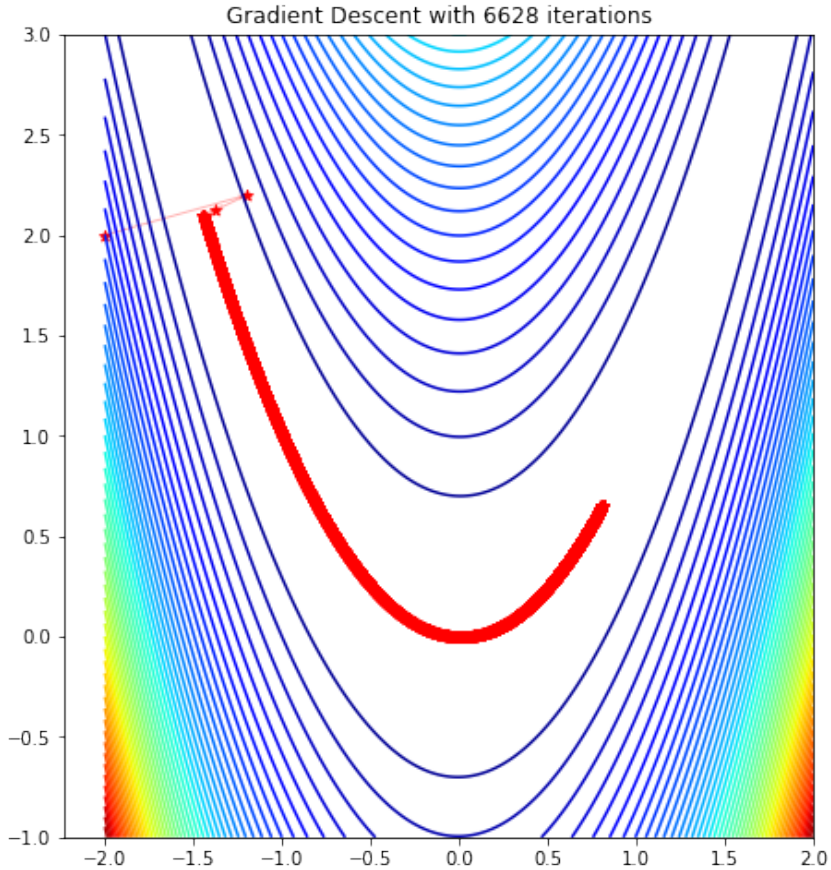
Example: Gradient Descent with $\eta = 0.0016$ on the Rosenbrock Function





Example: Gradient Descent with $\eta = 0.0005$ on the Rosenbrock Function





With every run of numerical optimization I get one minimizer candidate. How do I know if I can do bettter?

Analyze the optimization problem!

When every local minimizer is a global minimizer:

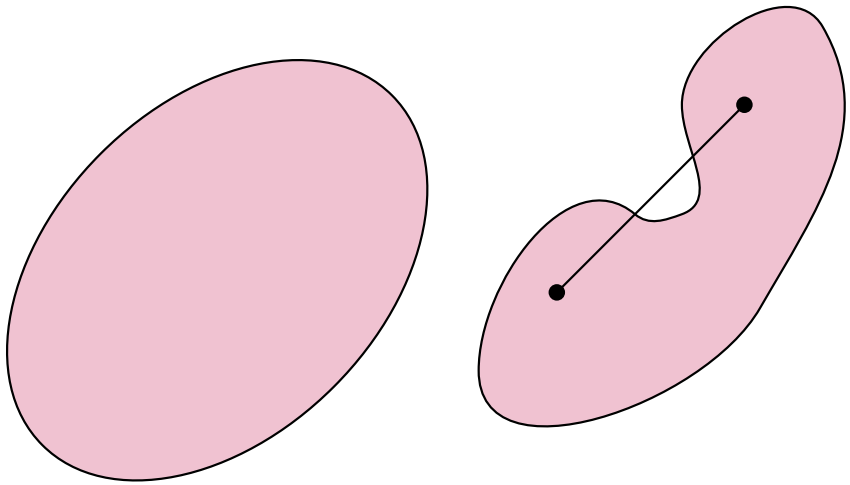
Convex Optimization

Convex Sets

A set $\mathcal{X} \subseteq \mathbb{R}^d$ is convex if and only if the line segment between every pair of points in the set is in the set.

That is, for all $x, y \in \mathcal{X}$ and $\alpha \in [0, 1]$

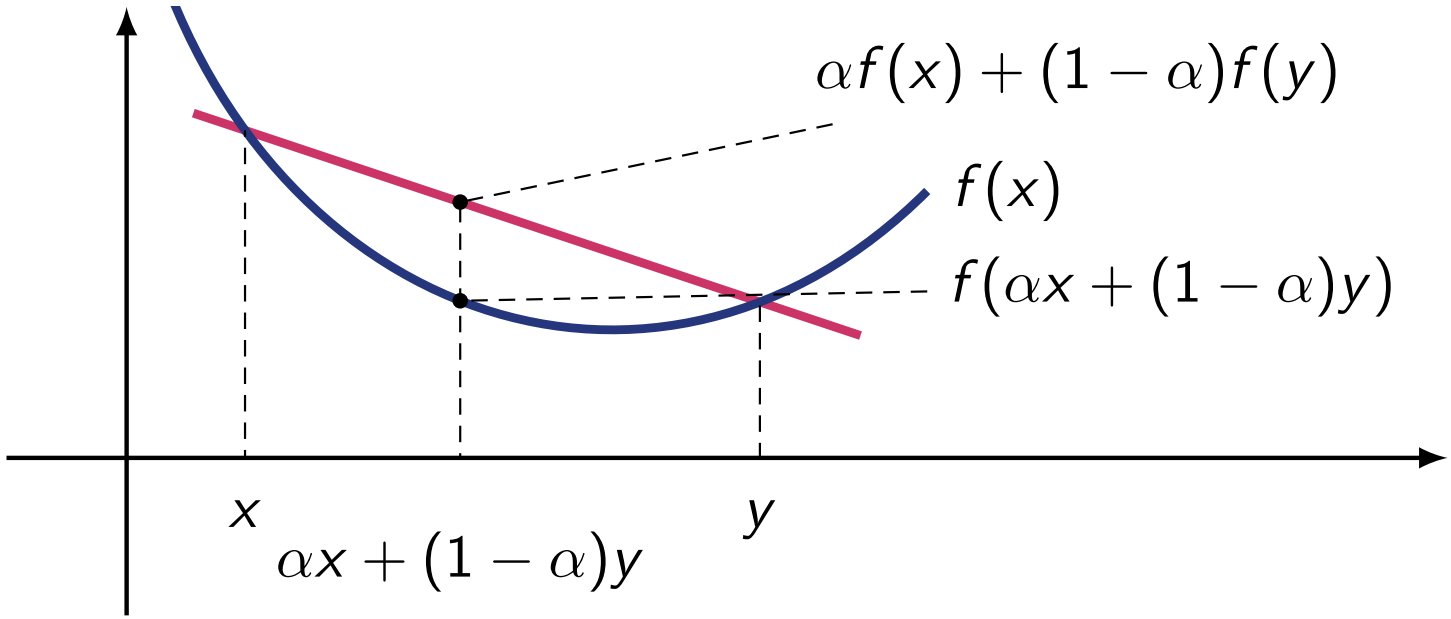
$$\alpha \mathrm{x} + (1 - \alpha)\mathrm{y} \in \mathcal{X}.$$



Convex Functions

A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if and only if for every $\alpha \in [0, 1]$, and $x, y \in \mathbb{R}^d$:

$$f(\alpha x + (1 - \alpha)y) \leq \alpha f(x) + (1 - \alpha)f(y)$$



Convex Optimization Problem

Given

- a convex objective function $f : \mathbb{R}^d \to \mathbb{R}$ and
- a convex feasible set $\mathcal{C} \subseteq \mathbb{R}^d$

then the objective of a convex optimization problem is

$$\min_{x \in \mathbb{R}^d} f(x)$$
$$\text{s.t. } x \in \mathcal{C}$$

Properties of Convex Functions

Theorem

If f is convex, then every local minimizer x^* is a global minimizer.

Note: not every function with one global and local minimum is convex (cf. Rosenbrock function).

Proof (Sketch): Assume that a convex function f has a local minimizer x_{loc} which is not a global minimizer: $f(x_{loc}) > f(x^*)$. Then going towards x^* from x_{loc} minimizes the function value, hence x_{loc} is not a local minimizer.

Properties of Convex Functions

- Nonnegative weighted sums of convex functions are convex: for all $\lambda_1, \ldots, \lambda_k \geq 0$ and $f_1, \ldots, f_k$ convex, then the function

$$f(\mathrm{x}) = \lambda_1 f_1(\mathrm{x}) + \ldots + \lambda_k f_k(\mathrm{x})$$

  is convex.

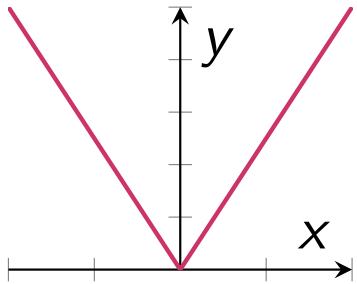
- If $g : \mathbb{R}^d \to \mathbb{R}^k$, $g(\mathrm{x}) = A\mathrm{x} + \mathrm{b}$ is an affine map, and $f : \mathbb{R}^k \to \mathbb{R}$ is a convex function, then the composition

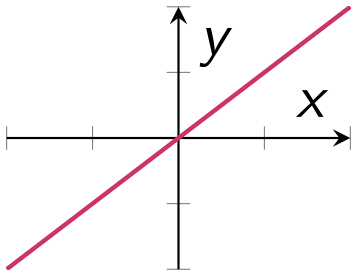
$$f(g(\mathrm{x})) = f(A\mathrm{x} + \mathrm{b})$$

  is a convex function.

Proof: Exercise

Examples of Convex Functions





Every norm is a convex function: for any $x, y \in \mathbb{R}^d$ and $\alpha \in [0, 1]$ we have:

$$\begin{aligned} \|\alpha x + (1-\alpha)y\| &\leq \|\alpha x\| + \|(1-\alpha)y\| \\ &\leq |\alpha|\|x\| + |1-\alpha|\|y\| \\ &= \alpha\|x\| + (1-\alpha)\|y\| \end{aligned}$$

Every linear function f is convex and concave ($-f$ is convex): for any $x, y \in \mathbb{R}^d$ and $\alpha \in [0, 1]$ we have:

$$f(\alpha x + (1-\alpha)y) = \alpha f(x) + (1-\alpha) f(y)$$

Okay nice, so if my optimization problem is convex then I *only* need to find a local minimium (for example by gradient descent).

How do I compute the gradient? Do I always have to compute the partial derivatives?

No, use the chain rule whenever you can!

Gradient Descent needs a Gradient

There are two ways to define the derivative of a function

$$f : \mathbb{R}^{n \times d} \to \mathbb{R}.$$

$$\frac{\partial f(X)}{\partial X} = \begin{pmatrix} \frac{\partial f(X)}{\partial X_{11}} & \cdots & \frac{\partial f(X)}{\partial X_{n1}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f(X)}{\partial X_{1d}} & \cdots & \frac{\partial f(X)}{\partial X_{nd}} \end{pmatrix} \in \mathbb{R}^{d \times n} \qquad \text{(Jacobian)}$$

$$\nabla f(X) = \begin{pmatrix} \frac{\partial f(X)}{\partial X_{11}} & \cdots & \frac{\partial f(X)}{\partial X_{1d}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f(X)}{\partial X_{n1}} & \cdots & \frac{\partial f(X)}{\partial X_{nd}} \end{pmatrix} \in \mathbb{R}^{n \times d} \qquad \text{(Gradient)}$$

Be careful!

This notation is not used by all authors!

The Jacobian of f

$$f : \mathbb{R}^d \to \mathbb{R} \qquad \frac{\partial f(\mathrm{x})}{\partial \mathrm{x}} = \begin{pmatrix} \frac{\partial f(\mathrm{x})}{\partial x_1} & \cdots & \frac{\partial f(\mathrm{x})}{\partial x_d} \end{pmatrix} \in \mathbb{R}^{1 \times d}$$

$$f : \mathbb{R}^{n \times d} \to \mathbb{R} \qquad \frac{\partial f(X)}{\partial X} = \begin{pmatrix} \frac{\partial f(X)}{\partial X_{11}} & \cdots & \frac{\partial f(X)}{\partial X_{n1}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f(X)}{\partial X_{1d}} & \cdots & \frac{\partial f(X)}{\partial X_{nd}} \end{pmatrix} \in \mathbb{R}^{d \times n}$$

$$\mathrm{f} : \mathbb{R} \to \mathbb{R}^c \qquad \frac{\partial \mathrm{f}(x)}{\partial x} = \begin{pmatrix} \frac{\partial f_1(x)}{\partial x} \\ \vdots \\ \frac{\partial f_c(x)}{\partial x} \end{pmatrix} \in \mathbb{R}^c$$

$$\mathrm{f} : \mathbb{R}^d \to \mathbb{R}^c \qquad \frac{\partial \mathrm{f}(\mathrm{x})}{\partial \mathrm{x}} = \begin{pmatrix} \frac{\partial f_1(x)}{\partial x_1} & \cdots & \frac{\partial f_1(x)}{\partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_c(x)}{\partial x_1} & \cdots & \frac{\partial f_c(x)}{\partial x_d} \end{pmatrix} \in \mathbb{R}^{c \times d}$$

The Gradient of f

$$f : \mathbb{R}^d \to \mathbb{R} \qquad \nabla_x f(x) = \begin{pmatrix} \frac{\partial f(x)}{\partial x_1} \\ \vdots \\ \frac{\partial f(x)}{\partial x_d} \end{pmatrix} \in \mathbb{R}^d$$

$$f : \mathbb{R}^{n \times d} \to \mathbb{R} \qquad \nabla_X f(X) = \begin{pmatrix} \frac{\partial f(X)}{\partial X_{11}} & \cdots & \frac{\partial f(X)}{\partial X_{1d}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f(X)}{\partial X_{n1}} & \cdots & \frac{\partial f(X)}{\partial X_{nd}} \end{pmatrix} \in \mathbb{R}^{n \times d}$$

$$\mathrm{f} : \mathbb{R} \to \mathbb{R}^c \qquad \nabla_x \mathrm{f}(x) = \begin{pmatrix} \frac{\partial f_1(x)}{\partial x} & \cdots & \frac{\partial f_c(x)}{\partial x} \end{pmatrix} \in \mathbb{R}^{1 \times c}$$

$$\mathrm{f} : \mathbb{R}^d \to \mathbb{R}^c \qquad \nabla_x \mathrm{f}(x) = \begin{pmatrix} \frac{\partial f_1(x)}{\partial x_1} & \cdots & \frac{\partial f_c(x)}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_1(x)}{\partial x_d} & \cdots & \frac{\partial f_c(x)}{\partial x_d} \end{pmatrix} \in \mathbb{R}^{d \times c}$$

Most Important Derivation Rules

$$\nabla_x f(x) = \left(\frac{\partial f(x)}{\partial x}\right)^\top$$

$$\frac{\partial \alpha f(x) + g(x)}{\partial x} = \alpha \frac{\partial f(x)}{\partial x} + \frac{\partial g(x)}{\partial x} \qquad \text{(linearity)}$$

$$\frac{\partial f(g(x))}{\partial x} = \frac{\partial f(g)}{\partial g}\frac{\partial g(x)}{\partial x} \qquad \text{(chain rule)}$$

Exercise: Derive the following equations:

$$\frac{\partial \|x\|^2}{\partial x}, \frac{\partial b - ax}{\partial x}, \frac{\partial b - Ax}{\partial x}, \nabla_x \|b - Ax\|^2, \nabla_X \|D - YX^\top\|^2$$

Most Important Derivation Rules

$$\nabla_x f(x) = \left(\frac{\partial f(x)}{\partial x}\right)^\top$$

$$\frac{\partial \alpha f(x) + g(x)}{\partial x} = \alpha \frac{\partial f(x)}{\partial x} + \frac{\partial g(x)}{\partial x} \qquad \text{(linearity)}$$

$$\frac{\partial f(g(x))}{\partial x} = \frac{\partial f(g)}{\partial g}\frac{\partial g(x)}{\partial x} \qquad \text{(chain rule)}$$

Exercise: Derive the following equations:

$$\frac{\partial \|x\|^2}{\partial x}, \frac{\partial b - ax}{\partial x}, \frac{\partial b - Ax}{\partial x}, \nabla_x \|b - Ax\|^2, \nabla_X \|D - YX^\top\|^2$$