Optimization for Machine Learning in Python

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Overview

Introduction

Optimization

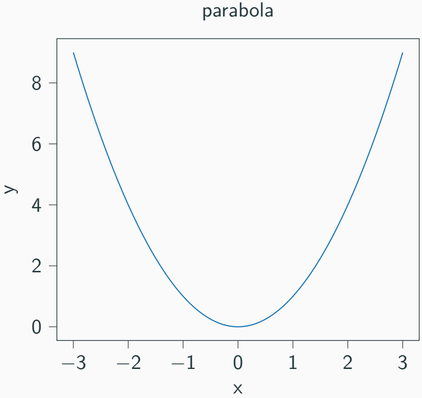
Traditionally, optimization means minimizing using a cost function $f(x)$. Given the cost, we must find the cheapest point x^* on the function, or in other words,

$$x^* = \min_{x \in \mathbb{R}} f(x) \tag{1}$$

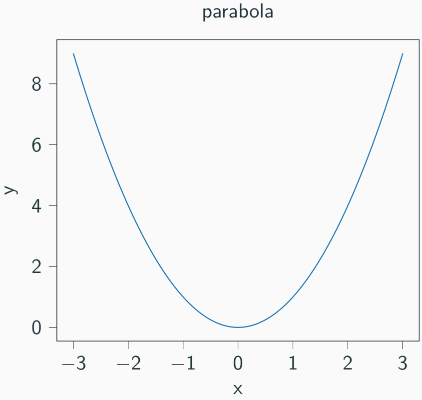
Functions

Functions are mathematical mappings. Consider for example, the quadratic function, $f(x) : \mathbb{R} \to \mathbb{R}$:

$$f(x) = x^2 \tag{2}$$



Where is the minimum?



In this case, we immediately see it's at zero. To find it via an iterative process, we require derivate information.

Summary

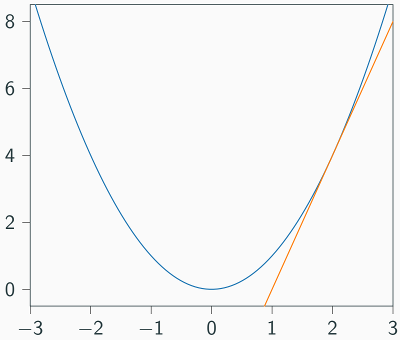
- Functions assign a value to each input.
- We seek an iterative way to find the smallest value.
- Doing so requires derivates.

The derivative

The derivative

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \tag{3}$$

parabola with derivative at two



Derivation of the parabola derivative

$$\begin{aligned}
\lim_{h\to 0} \frac{(x+h)^2 - x^2}{h} &= \lim_{h\to 0} \frac{x^2 + 2xh + h^2 - x^2}{h} && (4)\\
&= \lim_{h\to 0} \frac{2xh + h^2}{h} && (5)\\
&= \lim_{h\to 0} \frac{h(2x+h)}{h} && (6)\\
&= \lim_{h\to 0} 2x + h && (7)\\
&= 2x && (8)
\end{aligned}$$

Derivation of the parabola derivative

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Derive on the board.

Derivate of a parabola:

$$\begin{aligned}
\lim_{h\to 0} \frac{(x+h)^2 - x^2}{h} &= \lim_{h\to 0} \frac{x^2 + 2xh + h^2 - x^2}{h} && (9)\\
&= \lim_{h\to 0} \frac{2xh + h^2}{h} && (10)\\
&= \lim_{h\to 0} \frac{h(2x+h)}{h} && (11)\\
&= \lim_{h\to 0} 2x + h && (12)\\
&= 2x && (13)
\end{aligned}$$

The derivate of a polynomial

What is the derivative of the function $f(x) = x^n$?

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} = nx^{n-1} \tag{14}$$

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Derivate of a polynomial $f(x) = x^n$ [DFO20]:

$$\begin{aligned}
\frac{\mathrm{d}f(x)}{\mathrm{d}x} &= \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} = \lim_{h \to 0} \frac{(x+h)^n - x^n}{h} && (15)\\
&= \lim_{h \to 0} \frac{\sum_{i=0}^{n} \binom{n}{i} x^{n-1} h^i - x^n}{h} && (16)\\
&= \lim_{h \to 0} \frac{\sum_{i=1}^{n} \binom{n}{i} x^{n-1} h^i}{h} && (17)\\
&= \lim_{h \to 0} \sum_{i=1}^{n} \binom{n}{i} x^{n-1} h^{i-1} && (18)\\
&= \lim_{h \to 0} (\binom{n}{1} x^{n-1}) + \sum i = 2n \binom{n}{i} x^{n-i} h^{i-1} && (19)\\
&= \frac{n!}{1!(n-1)!} x^{n-1} = nx^{n-1}. && (20)
\end{aligned}$$

Summary

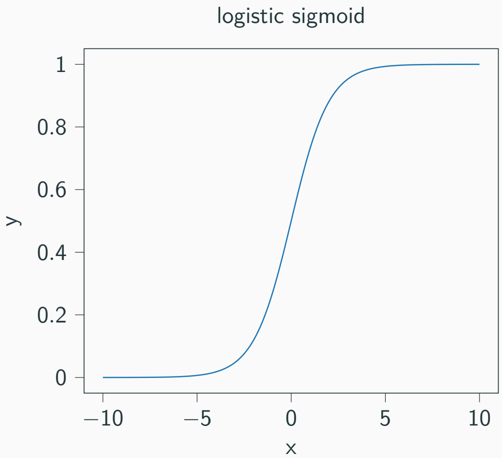
- A function is differentiable if the limit of the difference quotient exists.
- For any point on a differentiable function, the derivative provides a tangent slope.
- We will exclusively work with differentiable functions in this course.

Differentiation Rules [DFO20]

$$
\begin{aligned}
\text{Product Rule: } (f(x)g(x))' \qquad &= f'(x)g(x) + f(x)g'(x) && (21)\\
\text{Quotient Rule: } \left(\frac{f(x)}{g(x)}\right)' \qquad &= \frac{f'(x)g(x) - f(x)g'(x)}{(g(x))^2} && (22)\\
\text{Sum Rule: } (f(x) + g(x))' \qquad &= f'(x) + g'(x) && (23)\\
\text{Chain Rule: } (g(f(x)))' \qquad &= g'(f(x))f'(x) && (24)
\end{aligned}
$$

The logistic sigmoid [GBC16]

$$\sigma(x) = \frac{1}{1 + e^{-x}} \tag{25}$$



The Quotient Rule

TODO

The Chain Rule

How to best differentiate $f(x) = \sigma(2x + 1)$?

Optimization in a single dimension

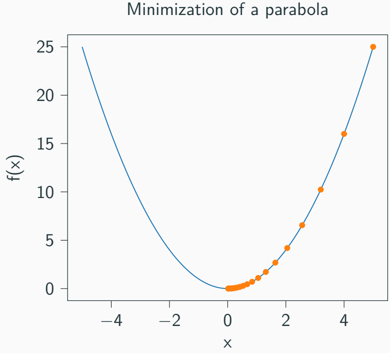
Steepest descent

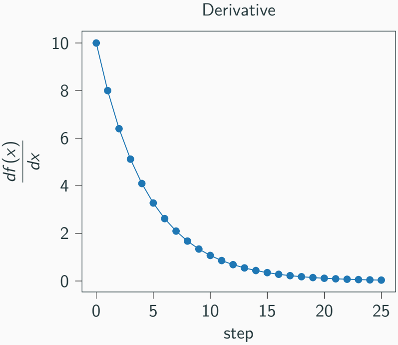
To find a minimum, we descent along the gradient, with n denoting the step number, $\epsilon \in \mathbb{R}$ the step size and $\frac{df}{dx}$ the derivate of f along $x \in \mathbb{R}$:

$$x_n = x_{n-1} - \epsilon \cdot \frac{df}{dx}. \tag{26}$$

Steepest descent on the parabola

Working with the initial position $x_0 = 5$ and a step size of $\epsilon = 0.1$ for 25 steps leads to:





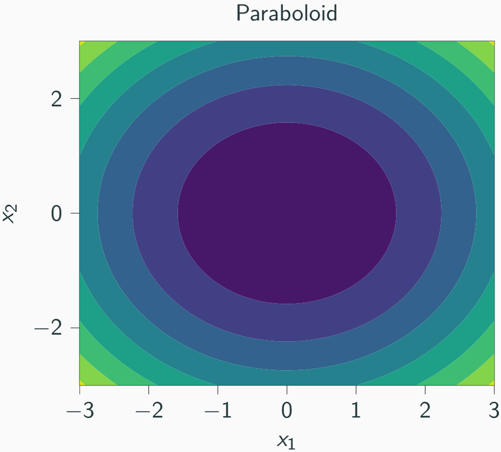
Summary

- Following the negative derivative iteratively got us to the minimum.
- At points of interest, the first derivate is zero.

Optimization in many dimensions

The two-dimensional paraboloid

$$f(x_1, x_2) = x_1^2 + x_2^2 \tag{27}$$



The gradient

The gradient lists partial derivatives with respect to all inputs in a vector. For a function $f : \mathbb{R}^n \to \mathbb{R}$ of n variables the gradient $\nabla f : \mathbb{R}^n \to \mathbb{R}^n$ is defined as

$$\nabla f = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}. \tag{28}$$

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- Gradients point in the steepest ascent direction.
- To find the gradient, we must compute the partial derivate with respect to every input.
- A vector collects all derivates.

Computing the gradient of the paraboloid

$$\nabla f(x_1, x_2) = \nabla(x_1^2 + x_2^2) \tag{29}$$

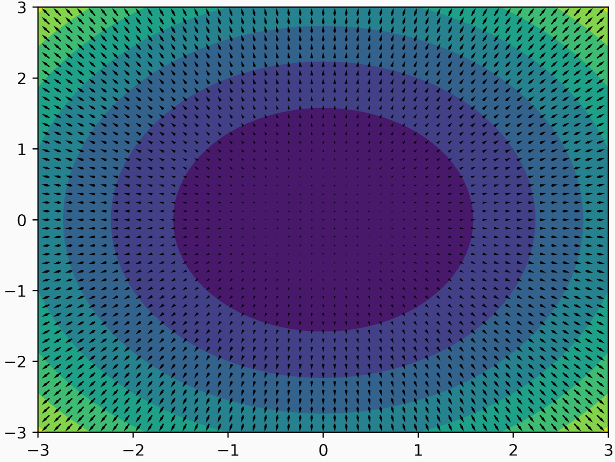
$$= \begin{pmatrix} 2x_1 \\ 2x_2 \end{pmatrix} \tag{30}$$

Gradients at points

For every point $\mathbf{p} = (x_1, x_2, \ldots, x_n)$ we can write

$$\nabla f(\mathbf{p}) = \begin{pmatrix} \frac{\partial f}{\partial x_1}(\mathbf{p}) \\ \frac{\partial f}{\partial x_2}(\mathbf{p}) \\ \vdots \\ \frac{\partial f}{\partial x_n}(\mathbf{p}) \end{pmatrix}. \tag{31}$$

Gradients on the Paraboloid



Gradient descent

Initial position: $x_0 = [2.9, -2.9]$,
Gradient step size: $\epsilon = 0.025$

$$x_n = x_{n-1} - \epsilon \cdot \nabla f(\mathbf{x}) \tag{32}$$

n denotes the step number, ∇ the gradient operator, and $f(\mathbf{x})$ a vector valued function.

Gradient descent on the Paraboloid

Paraboloid Optimization

The Rosenbrock test function

$$f(x_1, x_2) = (a - x_1)^2 + b(x_2 - x_1^2)^2 \tag{33}$$

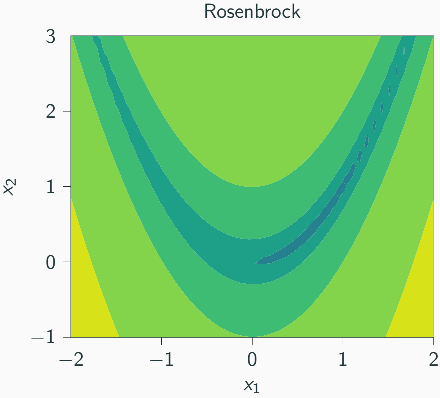


Figure: Rosenbrock function with a=1 and b=100 .

The gradient of the Rosenbrock function

Recall the Rosenbrock function:

$$f(x, y) = (a - x)^2 + b(y - x^2)^2 \tag{34}$$

$$\nabla f(x, y) = \begin{pmatrix} -2a + 2x - 4byx + 4bx^3 \\ 2by - 2bx^2 \end{pmatrix} \tag{35}$$

The gradient of the Rosenbrock function

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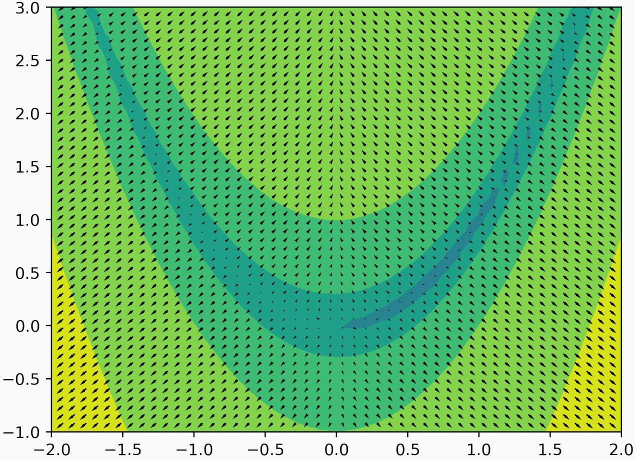
On the board, derive:

$$\begin{aligned} f(x,y) &= (a-x)^2 + b(y-x^2)^2 && (36) \\ &= a^2 - 2ax + x^2 + b(y^2 - 2yx^2 + x^4) && (37) \\ &= a^2 - 2ax + x^2 + by^2 - 2byx^2 + bx^4 && (38) \\ \Rightarrow \frac{\partial f(x,y)}{\partial x} &= -2a + 2x - 4byx + 4bx^3 && (39) \\ \Rightarrow \frac{\partial f(x,y)}{\partial y} &= 2by - 2bx^2 && (40) \end{aligned}$$

Gradients on the Rosenbrock function



Gradient descent

Initial position: $x_0 = [0.1, 3.]$,
Gradient step size: $\epsilon = 0.01$

$$\mathbf{x}_n = \mathbf{x}_{n-1} - \epsilon \cdot \nabla f(\mathbf{x}) \tag{41}$$

n denotes the step number, ∇ the gradient operator, and $f(\mathbf{x})$ a vector valued function.

Gradient descent on the Rosenbrock function

Rosenbrock Optimization

Motivating Momentum

- The standard gradient descent approach gets stuck.
- What if we could somehow use a history of recent gradient information?

Gradient descent with momentum

Initial position: $x_0 = [0.1, 3.]$,
Gradient step size: $\epsilon = 0.01$,
Momentum parameter: $\alpha = 0.8$

$$\mathbf{v} = \alpha \mathbf{v}_{n-1} - \epsilon \cdot \nabla f(\mathbf{x}) \tag{42}$$

$$\mathbf{x}_n = \mathbf{x}_{n-1} + \mathbf{v} \tag{43}$$

$\mathbf{v}$ denotes the velocity vector, n the step number, ∇ the gradient operator, and $f(\mathbf{x})$ a vector-valued function.

Gradient descent with momentum

Rosenbrock Optimization

Summary

- Gradient descent works in high-dimensional spaces!
- On the Rosenbrock function, we required momentum to find the minimum.
- Momentum adds the notion of inertia, which can help overcome local minima in some cases.
- Just like in the 1d case, the gradient equals zero at local minima and saddle points.

Optimization for deep learning

The chain rule

Optional reading

- Mathematics for machine learning, [DFO20, Chapter 5, Vector Calculus]
- Deep learning, [WN+99, Chapter 8.2, Automatic Differentiation]
- Numerical optimization, [GBC16, Chapter 8, Optimization for Training Deep Models]

References

[DFO20] Marc Peter Deisenroth, A Aldo Faisal, and Cheng Soon Ong. *Mathematics for machine learning*. Cambridge University Press, 2020.

[GBC16] Ian Goodfellow, Yoshua Bengio, and Aaron Courville. *Deep learning*. MIT press, 2016.

[WN+99] Stephen Wright, Jorge Nocedal, et al. "Numerical optimization." In: *Springer Science* 35.67-68 (1999), p. 7.