Optimization for Machine Learning in Python

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September 12, 2022

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Overview

Introduction

Optimization

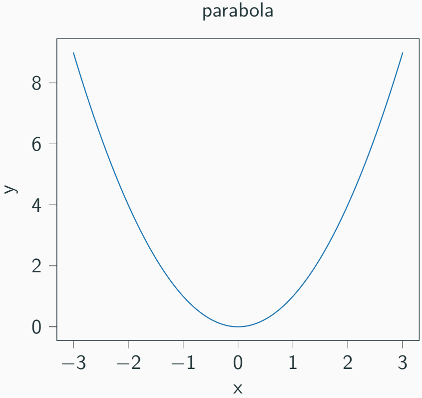
Traditionally, optimization means minimizing using a cost function $f(x)$. Given the cost, we must find the cheapest point x^* on the function, or in other words,

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

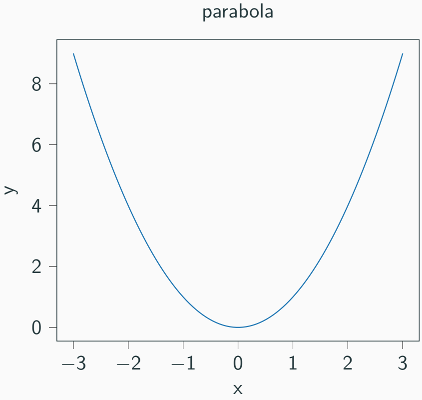
Functions

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

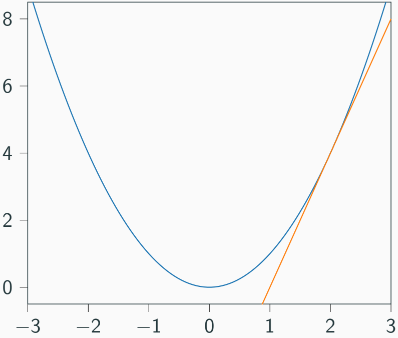
- Functions assign a value to each input.
- We seek an iterative way to find the smallest value.
- Doing so requires derivates.

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

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

The derivate of a polynomial

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

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} = nx^{n-1} \tag{9}$$

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]

$$\text{Product Rule: } (g(x)h(x))' = g'(x)h(x) + g(x)h'(x) \tag{10}$$

$$\text{Quotient Rule: } \left(\frac{g(x)}{h(x)}\right)' = \frac{g'(x)h(x) - g(x)h'(x)}{(h(x))^2} \tag{11}$$

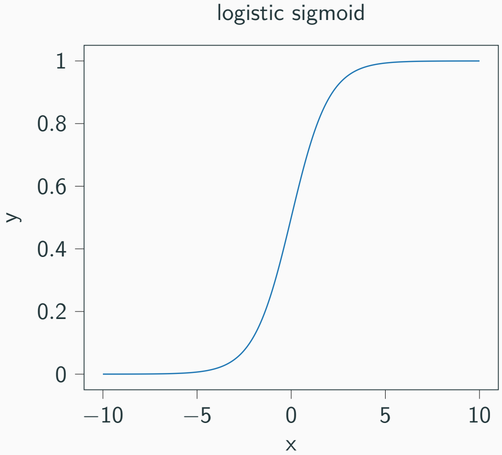
$$\text{Sum Rule: } (g(x) + h(x))' = g'(x) + h'(x) \tag{12}$$

$$\text{Chain Rule: } (g(h(x)))' = g'(h(x))h'(x) \tag{13}$$

The logistic sigmoid [GBC16]

The sigmoid function $\sigma(x)$ is a common activation function.

$$\sigma(x) = \frac{1}{1 + e^{-x}} \tag{14}$$



Using the Quotient Rule i

$$\frac{\mathrm{d}\sigma(x)}{\mathrm{dx}} = \frac{\mathrm{d}}{\mathrm{dx}} \frac{1}{1+e^{-x}} \tag{15}$$

$$= \frac{\mathrm{d}}{\mathrm{dx}} \frac{1}{1+e^{-x}} \cdot 1 \tag{16}$$

$$= \frac{\mathrm{d}}{\mathrm{dx}} \frac{1}{1+e^{-x}} \cdot \frac{e^x}{e^x} \tag{17}$$

$$= \frac{\mathrm{d}}{\mathrm{dx}} \frac{e^x}{e^x+1} \tag{18}$$

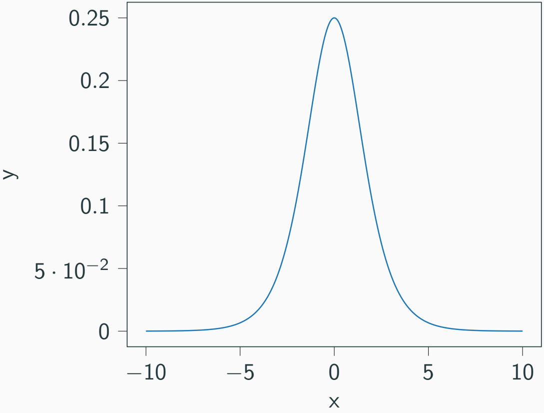
$$g(x) = e^x, h(x) = e^x + 1 \tag{19}$$

Using the Quotient Rule ii

$$
\begin{aligned}
\frac{\mathrm{d}\sigma(x)}{\mathrm{dx}} &= \frac{e^x \cdot (e^x + 1) - e^x \cdot e^x}{(e^x + 1)^2} && (20) \\
&= \frac{e^x \cdot e^x + e^x - e^x \cdot e^x}{(e^x + 1)^2} && (21) \\
&= \frac{e^x}{(e^x + 1)^2} && (22) \\
&= \frac{e^x}{(e^x + 1)} \frac{1}{(e^x + 1)} && (23) \\
&= \frac{e^x}{(e^x + 1)} \left(\frac{1 + e^x - e^x}{(e^x + 1)}\right) && (24) \\
&= \frac{e^x}{(e^x + 1)} \left(\frac{1 + e^x}{(e^x + 1)} - \frac{e^x}{(e^x + 1)}\right) && (25) \\
&= \frac{e^x}{(e^x + 1)} \left(1 - \frac{e^x}{(e^x + 1)}\right) && (26) \\
&= \sigma(x)(1 - \sigma(x)) && (27)
\end{aligned}
$$

The derivative of the sigmoidal function

$$\frac{\mathrm{d}\sigma(x)}{\mathrm{dx}} = \sigma(x) \cdot (1 - \sigma(x)) \tag{28}$$



Using the Chain Rule

How do we best differentiate $f(x) = \sigma(ax + b)$?

$$\frac{\mathrm{d}f(x)}{\mathrm{dx}} = \frac{\mathrm{d}\sigma(ax+b)}{\mathrm{dx}} \tag{29}$$

$$\tag{30}$$

Chain Rule: $(g(h(x)))' = g'(h(x))h'(x)$

$$g(x) = \sigma(x), h(x) = ax + b \tag{31}$$

$$\Rightarrow \sigma(ax+b)(1-\sigma(ax+b))(a) \tag{32}$$

Optimization in a single dimension

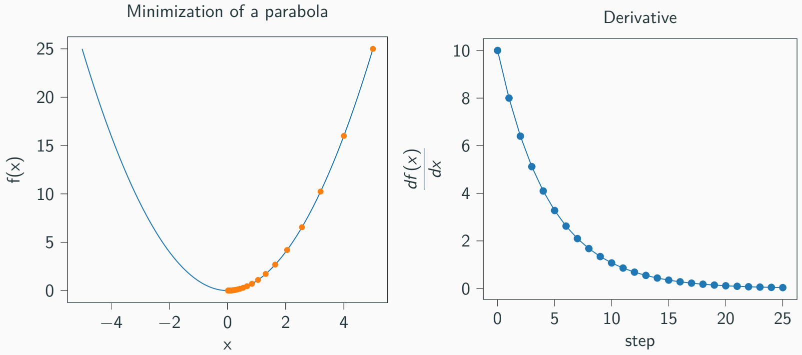
Steepest descent

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 $x \in \mathbb{R}$:

$$x_n = x_{n-1} - \epsilon \cdot \frac{df}{dx}. \tag{33}$$

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:



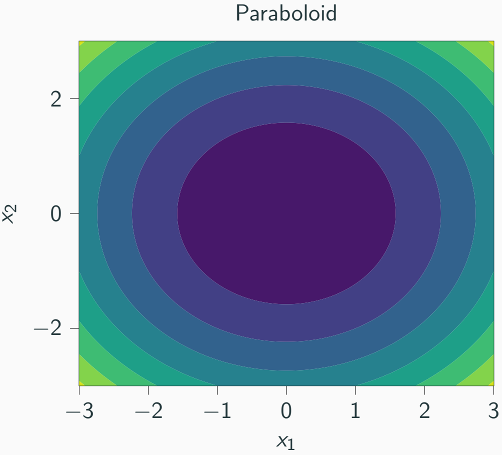
Summary

- 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

$$f(x_1, x_2) = x_1^2 + x_2^2 \tag{34}$$



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

$$\nabla f = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}. \tag{35}$$

Computing the gradient of the paraboloid

$$\nabla f(x_1, x_2) = \nabla(x_1^2 + x_2^2) \tag{36}$$

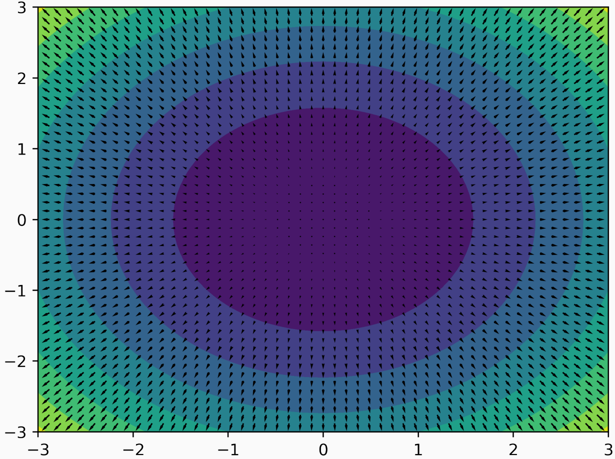
$$= \begin{pmatrix} 2x_1 \\ 2x_2 \end{pmatrix} \tag{37}$$

Gradients at points

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

$$\nabla f(\mathbf{p}) = \begin{pmatrix} \frac{\partial f}{\partial x_1}(\mathbf{p}) \\ \frac{\partial f}{\partial x_2}(\mathbf{p}) \\ \vdots \\ \frac{\partial f}{\partial x_n}(\mathbf{p}) \end{pmatrix}. \tag{38}$$

Gradients on the Paraboloid



Gradient descent

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

$$x_n = x_{n-1} - \epsilon \cdot \nabla f(\mathbf{x}) \tag{39}$$

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

$$f(x_1, x_2) = (a - x_1)^2 + b(x_2 - x_1^2)^2 \tag{40}$$

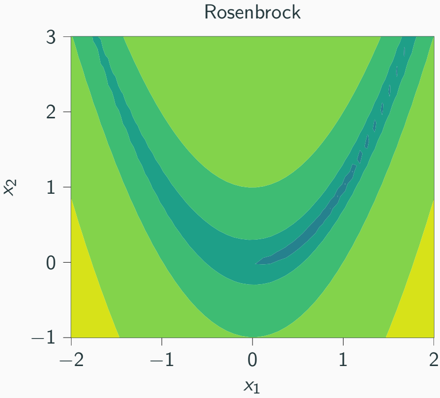


Figure: Rosenbrock function with a=1 and b=100 .

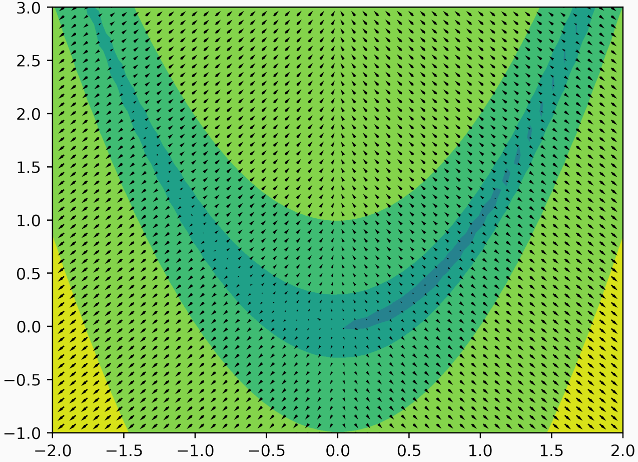
The gradient of the Rosenbrock function

Recall the Rosenbrock function:

$$f(x, y) = (a - x)^2 + b(y - x^2)^2 \tag{41}$$

$$\nabla f(x, y) = \begin{pmatrix} -2a + 2x - 4byx + 4bx^3 \\ 2by - 2bx^2 \end{pmatrix} \tag{42}$$

Gradients on the Rosenbrock function



Gradient descent

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

$$\mathbf{x}_n = \mathbf{x}_{n-1} - \epsilon \cdot \nabla f(\mathbf{x}) \tag{43}$$

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: $\alpha = 0.8$

$$\mathbf{v} = \alpha \mathbf{v}_{n-1} - \epsilon \cdot \nabla f(\mathbf{x}) \tag{44}$$

$$\mathbf{x}_n = \mathbf{x}_{n-1} + \mathbf{v} \tag{45}$$

$\mathbf{v}$ 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.

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.