

Foundations of Machine Learning in Python

Moritz Wolter

July 12, 2022

High Performance Computing and Analytics Lab, Uni Bonn

Overview

Derivatives and Gradients

Optimization

Optimization

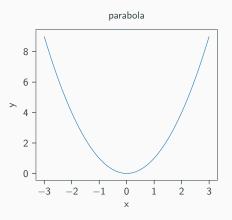
Traditionally, optimization means minimizing using a cost function f(x). Given the cost, we must find the cheapest point x^* on the function, or in other words,

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

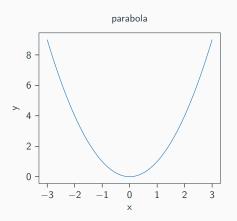
Functions

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

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



Where is the minimum?

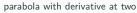


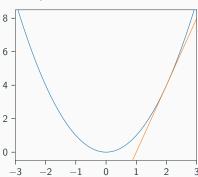
In this case we immediately see it's at zero. Finding it algorithmically requires derivate information.

Derivatives and Gradients

The derivative

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





Derivation of the parabola derivative

$$\lim_{h \to 0} \frac{(x+h)^2 - x^2}{h} \Leftrightarrow \lim_{h \to 0} \frac{x^2 + 2xh + h^2 - x^2}{h} \tag{4}$$

$$\Leftrightarrow \lim_{h \to 0} \frac{2xh + h^2}{h} \tag{5}$$

$$\Leftrightarrow \lim_{h \to 0} \frac{h(2x+h)}{h} \tag{6}$$

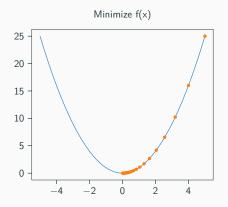
$$\Leftrightarrow \lim_{h \to 0} 2x + h \tag{7}$$

$$\Leftrightarrow 2x$$
 (8)

Steepest descent on the parabola

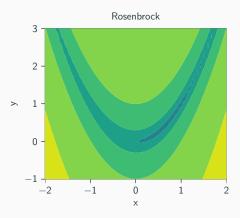
$$x_n = x_{n-1} - \alpha \cdot \frac{df}{dx} \tag{9}$$

Working with $x_0 = 5$ and $\alpha = 0.1$ for 25 steps leads to:



Multidimensional problems

$$f(x,y) = (a-x)^2 + b(y-x^2)^2$$
 (10)



The gradient

$$\nabla f = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$
 (11)

Rosenbrock gradient

$$\nabla f(x,y) = \begin{pmatrix} -2a + 2x - 4byx + 4bx^{3} \\ 2by - 2bx^{2} \end{pmatrix}$$
 (12)

Gradient descent

$$x_0 = [0.1, 3.], \ \alpha = 0.01$$

$$x_n = x_{n-1} - \alpha \cdot \nabla f(x)$$
 (13)

Gradient descent on the Rosenbrock function

Rosenbrock Optimization

Gradient descent with momentum

Rosenbrock Optimization

Optimization

Frame 2

TODO