Machine learning from scratch

Lecture 2: Convex optimization

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Optimization: Derivatives

The **derivative** is an important concept in optimization and in machine learning. Mathematical definition: Let $f : \mathbb{R} \mapsto \mathbb{R}$ be a function. Its derivative f' is defined by:

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

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$$\begin{aligned} f'(x) > 0 &\iff \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} > 0 \\ &\iff f(x+h) < f(x) \\ &\iff f \text{ is increasing (because } x + h < x) \end{aligned}$$

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Conclusion: f is increasing $\iff f' > 0$

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\lim_{h \to 0} \frac{f(x+h) - f(x)}{h} < 0 &\iff f(x+h) - f(x) = 0 \\
&\iff f(x+h) = f(x)
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Conclusion: f is decreasing $\iff f' < 0$

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Summary:

- f is increasing $\iff f'(x) > 0$
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What do we do with this?

If we want to find f's minimum, a strategy could be:

1. Start at a random point $x_0 \in \mathbb{R}$
2. Compute $f'(x_0)$ and then
   - if $f'(x_0) > 0$ then move to the left (because f is increasing)
   - if $f'(x_0) < 0$ then move to the right (because f is decreasing)
   - if $f'(x_0) = 0$ then we stop

Derivatives: How to compute them?

There are several ways to compute the derivatives.

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- By **applying the definition**

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

  with a small h (*e.g.* $h = 0.01$). This is called the **finite difference approximation**.

- By using **closed-form derivatives**, *e.g.*

$$\text{if } f(x) = x^2 \text{, then } f'(x) = 2x$$

  How do we know that? By using the formula!

Derivative: Practical example

Recall the definition:

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Exercice: Apply this formula for $f(x) = x^2$. What is $f'(x)$?

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$$\begin{aligned}
f'(x) &= \lim_{h \to 0} \frac{(x+h)^2 - x^2}{h} \\
&= \lim_{h \to 0} \frac{x^2 + 2hx + h^2 - x^2}{h} \\
&= \lim_{h \to 0} \frac{2hx + h^2}{h} \\
&= \lim_{h \to 0} 2x + h = 2x
\end{aligned}$$

We can apply this logic to the usual functions (log, cos, sin, ...) and obtain what we call **closed-form solutions**.

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We can apply this logic to the usual functions (log, cos, sin, ...) and obtain what we call **closed-form solutions**.
Exercise: Do the same for $f(x) = \frac{1}{x}$.

Derivatives: Finite difference approximation

Recall: The **finite difference approximation** consists in applying the following formula

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

with h close enough to 0.

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There's a symmetric and more stable formula, called the **centered finite difference approximation**.

$$f'(x) = \frac{df}{dx}(x) = \lim_{h \to 0} \frac{f(x+h) - f(x-h)}{2h}$$

Chain rule

Another important rule concerning derivatives is the **chain rule**:

$$(f(g(x)))' = g'(x)f'(g(x)) \tag{1}$$

or, equivalently:

$$\frac{df(g(x))}{dx} = \frac{df(g)}{dg}\frac{dg(x)}{dx} \tag{2}$$

Gradient: Generalizing the derivatives

Derivatives look like a practical way to get the minimum of a function, which is what we want to achieve (minimizing $J(\theta)$).

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However, the definition we've seen only applies to function from $\mathbb{R}$ to $\mathbb{R}$. The **gradient** is a generalization of the derivative for functions from $\mathbb{R}^d$ to $\mathbb{R}$, like J.

Beyond derivatives: Gradient

Let's consider a function of f 2 real variables x and y, *e.g.*

$$f(x, y) = xy$$

The gradient of f is a 2-dimensional vector noted ∇f defined by:

$$\nabla f(x, y) = \left[\frac{\partial f(x, y)}{\partial x}, \frac{\partial f(x, y)}{\partial y}\right]$$

where

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is the **partial derivative** of f with respect to x (considering y as a constant), and

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Exercise: What is $\nabla f(x, y)$ for $f(x, y) = xy$ and $f(x, y) = x + y$?

Beyond derivatives: Gradient

Interpretation of the gradient: Direction of **steepest descent** of f

Back to least squares: context reminder

living area (m^2)	# bedrooms	intercept	price (1000's BGN)
50	1	1	30
76	2	1	48
26	1	1	12
102	3	1	90

$$h(\boldsymbol{x}) = \sum_{j=0}^{d} \theta_j x_j = \theta^T \boldsymbol{x}$$

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Suppose we chose the following loss function:

$$\ell\left(y, \hat{y}\right) = \frac{1}{2}\left(y - \hat{y}\right)^2$$

This leads to the following least squares *cost function*:

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{n}\left(h\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)^2$$

This problem the **ordinary least squares** (OLS) regression model.

Least Mean Squares (LMS) update rule

To apply the LMS update rule, we need to compute the gradient of J. Let's compute it for a single $(\boldsymbol{x}, y)$ sample:

$$\begin{aligned} \frac{\partial}{\partial \theta_j} J(\theta) &= \frac{\partial}{\partial \theta_j} \frac{1}{2} \left(h\left(\boldsymbol{x}\right) - y \right)^2 \\ &= ? \end{aligned}$$

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Exercise: Compute the gradient and find the update rule.

Least Mean Squares (LMS) update rule

Solution:

$$\begin{aligned}
\frac{\partial}{\partial \theta_j} J(\theta) &= \frac{\partial}{\partial \theta_j} \frac{1}{2} \left(h\left(\boldsymbol{x}\right) - y\right)^2 \\
&= 2\frac{1}{2} \left(h\left(\boldsymbol{x}\right) - y\right) \frac{\partial}{\partial \theta_j} \left(h\left(\boldsymbol{x}\right) - y\right) \\
&= \left(h\left(\boldsymbol{x}\right) - y\right) \frac{\partial}{\partial \theta_j} \left(\sum_{k=0}^{d} \theta_k x_k - y\right) \\
&= \left(h\left(\boldsymbol{x}\right) - y\right) x_j
\end{aligned}$$

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&= \left(h(\boldsymbol{x}) - y \right) x_j
\end{aligned}$$

So the gradient descent update becomes

$$\begin{aligned}
\theta_j &:= \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \\
&:= \theta_j + \alpha \left(y - h(\boldsymbol{x}) \right) x_j
\end{aligned}$$

Conclusion

We had an overview of the optimization techniques.

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Next Thursday, we will review what needs to be reviewed (tell me by email so that I can adapt or when the class starts) and start implementing:

- The loss function for the least-squares problem
- Its gradient
- The Gradient descent weight upgrade
- Run it on a toy example

Thank you! Questions?

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https://github.com/azubiolo/itstep