Deep Learning 101

Astro Hack Week 2018, Leiden

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Cooking recipe

- Get data (loads of them).
- Get good hardware.
- Define the neural network architecture.
  - A neural network is a composition of differentiable functions.
  - Stick to non-saturating activation function to avoid vanishing gradients.
  - Prefer deep over shallow architectures.
- Optimize with (variants of) stochastic gradient descent.
  - Evaluate gradients with automatic differentiation.

Perceptron

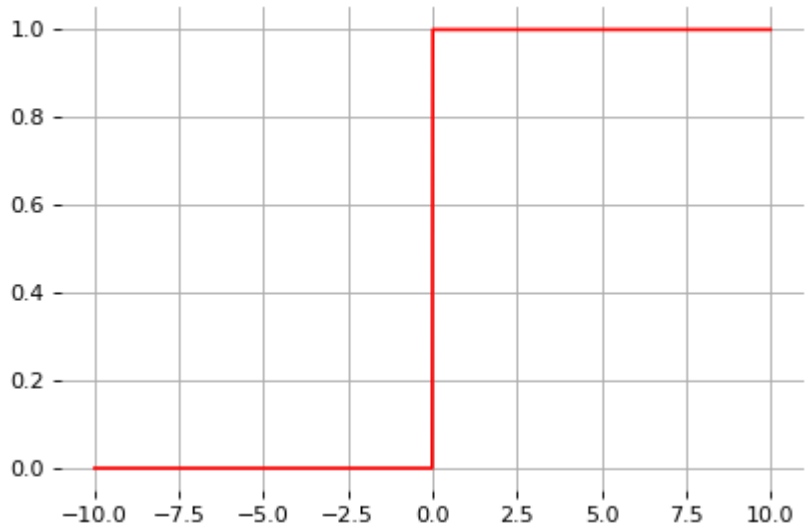
The perceptron (Rosenblatt, 1957) is one of the first mathematical models for a neuron. It is defined as:

$$f(\mathbf{x}) = \begin{cases} 1 & \text{if } \sum_i w_i x_i + b \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

- This model was originally motivated by biology, with w_i being synaptic weights and x_i and f firing rates.
- This is a cartoonesque biological model.

Let us define the activation function:

$$\sigma(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$



Therefore, the perceptron classification rule can be rewritten as

$$f(\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x} + b).$$

Linear discriminant analysis

Consider training data $(\mathbf{x}, y) \sim P(X, Y)$, with

- $\mathbf{x} \in \mathbb{R}^p$,
- $y \in \{0, 1\}$.

Assume class populations are Gaussian, with same covariance matrix Σ (homoscedasticity):

$$P(\mathbf{x}|y) = \frac{1}{\sqrt{(2\pi)^p |\Sigma|}} \exp\left(-\frac{1}{2}(\mathbf{x} - \mu_y)^T \Sigma^{-1} (\mathbf{x} - \mu_y)\right)$$

Using the Bayes' rule, we have:

$$
\begin{aligned}
P(Y=1|\mathbf{x}) &= \frac{P(\mathbf{x}|Y=1)P(Y=1)}{P(\mathbf{x})} \\
&= \frac{P(\mathbf{x}|Y=1)P(Y=1)}{P(\mathbf{x}|Y=0)P(Y=0)+P(\mathbf{x}|Y=1)P(Y=1)} \\
&= \frac{1}{1+\frac{P(\mathbf{x}|Y=0)P(Y=0)}{P(\mathbf{x}|Y=1)P(Y=1)}}.
\end{aligned}
$$

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It follows that with

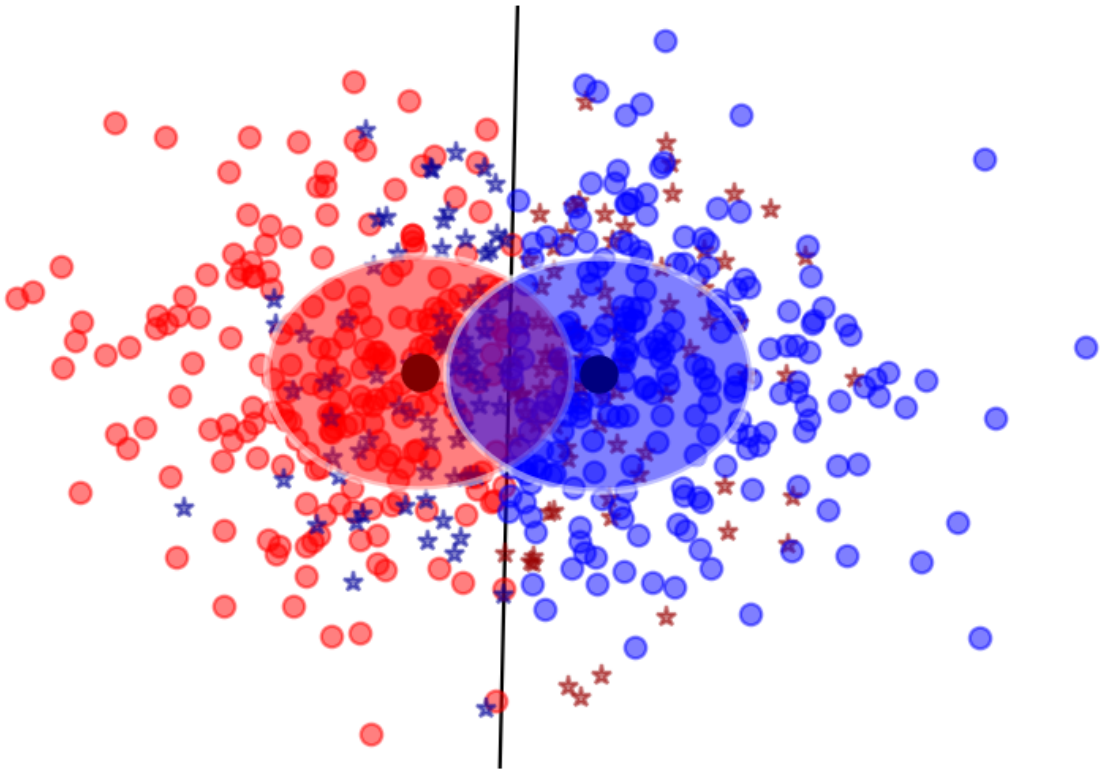
$$\sigma(x) = \frac{1}{1+\exp(-x)},$$

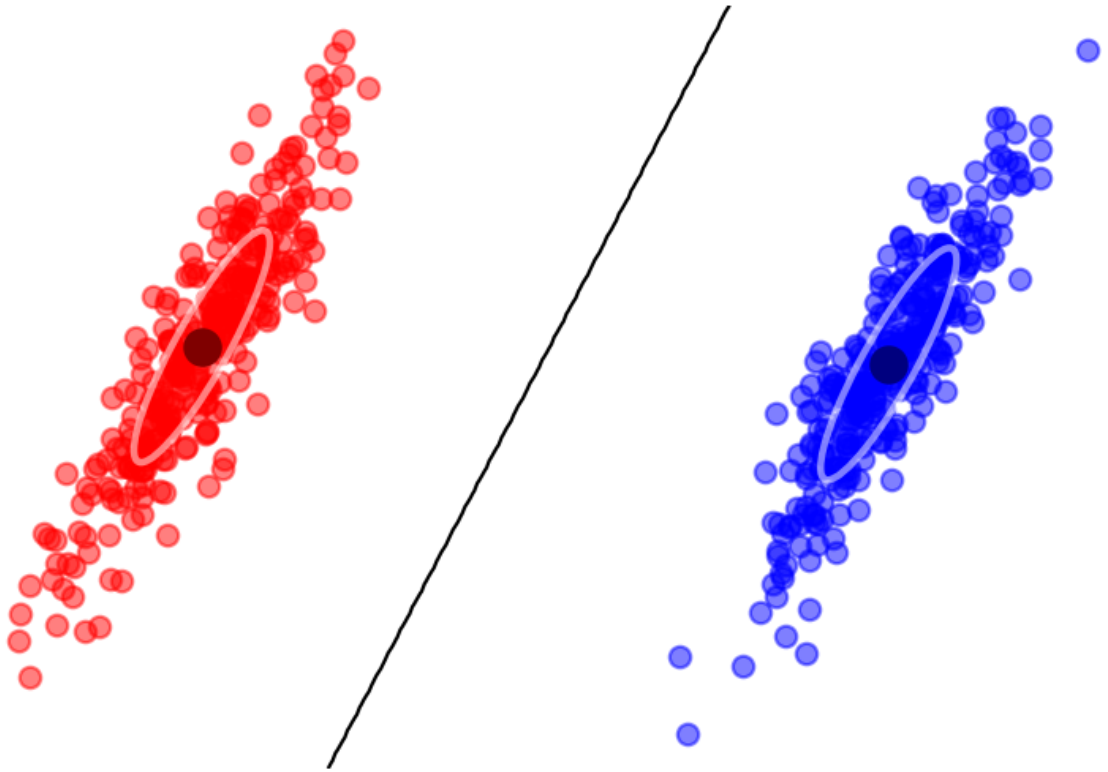
we get

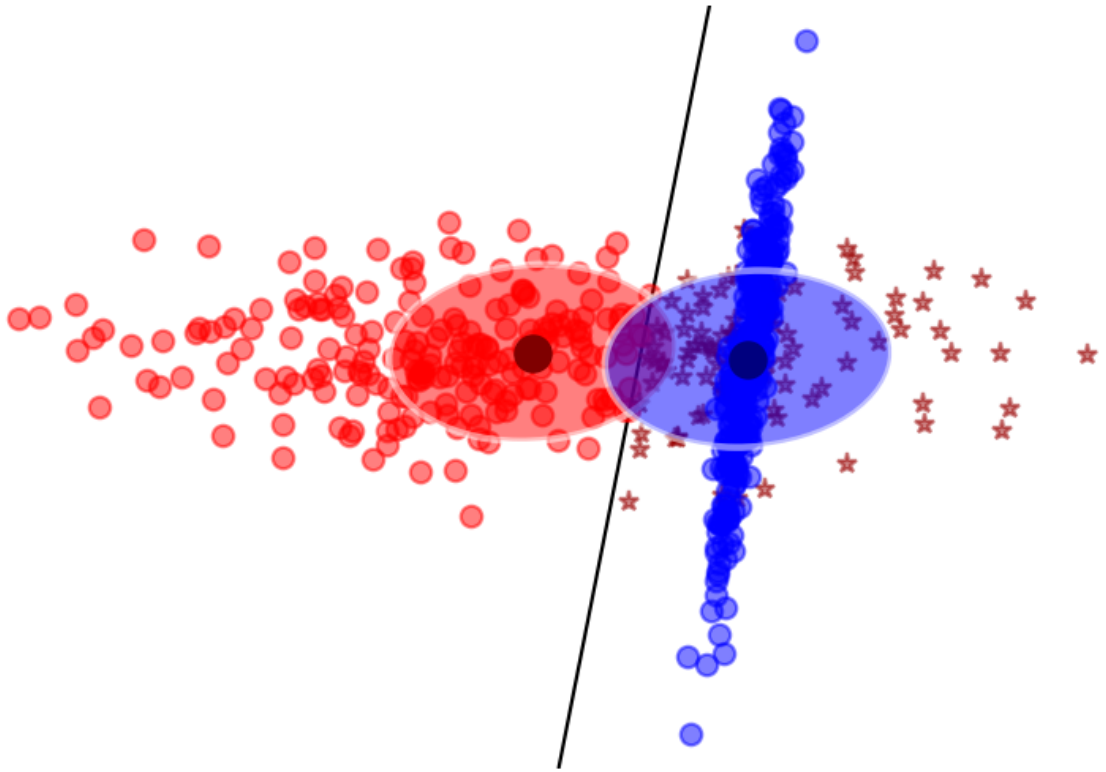
$$P(Y=1|\mathbf{x}) = \sigma\left(\log\frac{P(\mathbf{x}|Y=1)}{P(\mathbf{x}|Y=0)} + \log\frac{P(Y=1)}{P(Y=0)}\right).$$

Therefore,

$$
\begin{aligned}
& P(Y=1|\mathbf{x}) \\
&= \sigma\left(\log\frac{P(\mathbf{x}|Y=1)}{P(\mathbf{x}|Y=0)} + \underbrace{\log\frac{P(Y=1)}{P(Y=0)}}_{a}\right) \\
&= \sigma\left(\log P(\mathbf{x}|Y=1) - \log P(\mathbf{x}|Y=0) + a\right) \\
&= \sigma\left(-\frac{1}{2}(\mathbf{x}-\mu_1)^T\Sigma^{-1}(\mathbf{x}-\mu_1) + \frac{1}{2}(\mathbf{x}-\mu_0)^T\Sigma^{-1}(\mathbf{x}-\mu_0) + a\right) \\
&= \sigma\left(\underbrace{(\mu_1-\mu_0)^T\Sigma^{-1}}_{\mathbf{w}^T}\mathbf{x} + \underbrace{\frac{1}{2}(\mu_0^T\Sigma^{-1}\mu_0 - \mu_1^T\Sigma^{-1}\mu_1) + a}_{b}\right) \\
&= \sigma\left(\mathbf{w}^T\mathbf{x} + b\right)
\end{aligned}
$$



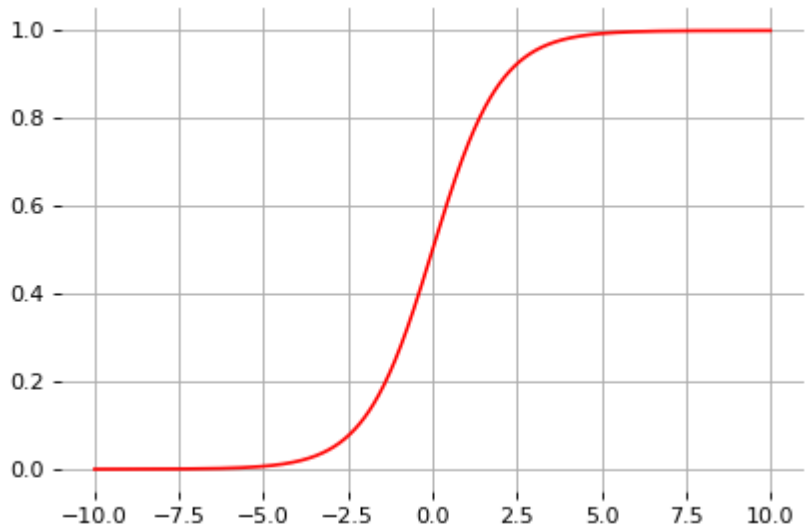




Note that the sigmoid function

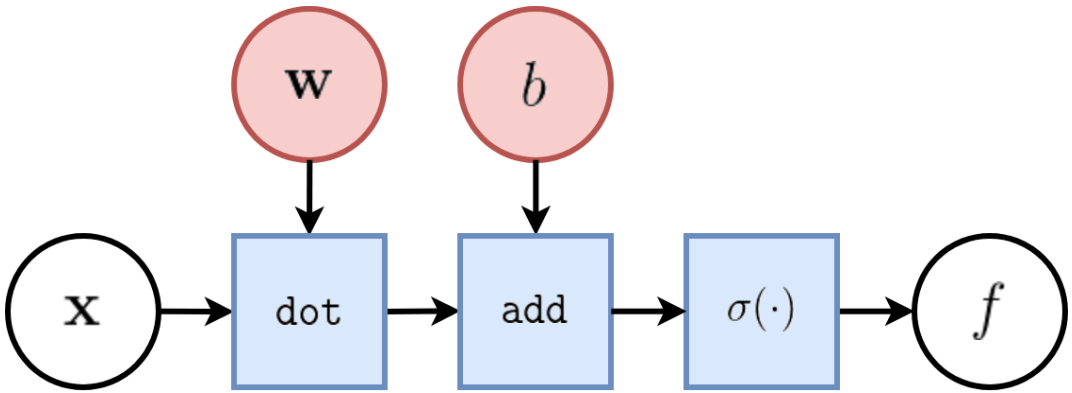
$$\sigma(x) = \frac{1}{1 + \exp(-x)}$$

looks like a soft heavyside:



Therefore, the overall model $f(\mathbf{x}; \mathbf{w}, b) = \sigma(\mathbf{w}^T \mathbf{x} + b)$ is very similar to the perceptron.

In terms of tensor operations, the computational graph of f can be represented as:



where

- white nodes correspond to inputs and outputs;
- red nodes correspond to model parameters;
- blue nodes correspond to intermediate operations, which themselves produce intermediate output values (not represented).

This unit is the core component all neural networks!

Logistic regression

Same model

$$P(Y = 1|\mathbf{x}) = \sigma\left(\mathbf{w}^T\mathbf{x} + b\right)$$

as for linear discriminant analysis.

But,

- ignore model assumptions (Gaussian class populations, homoscedasticity);
- instead, find $\mathbf{w}, b$ that maximizes the likelihood of the data.

We have,

$$
\begin{aligned}
&\arg\max_{\mathbf{w},b} P(\mathbf{d}|\mathbf{w},b) \\
&= \arg\max_{\mathbf{w},b} \prod_{\mathbf{x}_i,y_i\in\mathbf{d}} P(Y=y_i|\mathbf{x}_i,\mathbf{w},b) \\
&= \arg\max_{\mathbf{w},b} \prod_{\mathbf{x}_i,y_i\in\mathbf{d}} \sigma(\mathbf{w}^T\mathbf{x}_i+b)^{y_i}\left(1-\sigma(\mathbf{w}^T\mathbf{x}_i+b)\right)^{1-y_i} \\
&= \arg\min_{\mathbf{w},b} \underbrace{\sum_{\mathbf{x}_i,y_i\in\mathbf{d}} -y_i\log\sigma(\mathbf{w}^T\mathbf{x}_i+b)-(1-y_i)\log(1-\sigma(\mathbf{w}^T\mathbf{x}_i+b))}_{\mathcal{L}(\mathbf{w},b)=\sum_i \ell(y_i,\hat{y}(\mathbf{x}_i;\mathbf{w},b))}
\end{aligned}
$$

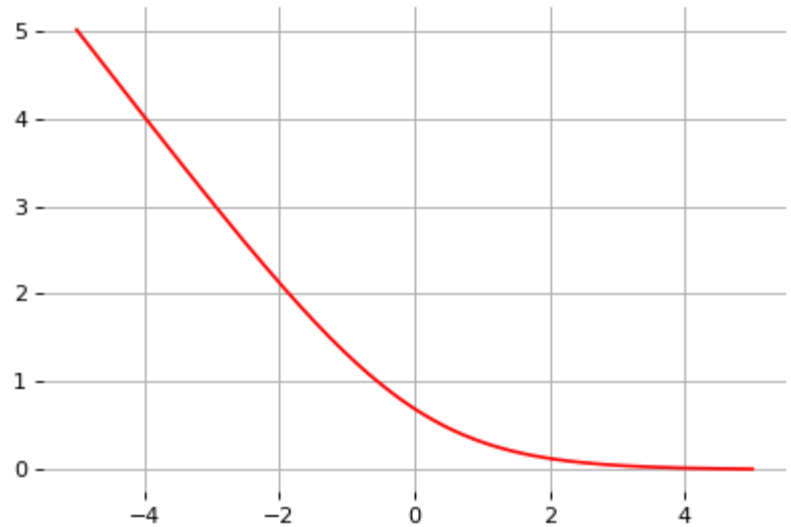
This loss is an instance of the cross-entropy

$$H(p,q)=\mathbb{E}_p[-\log q]$$

for $p=Y|\mathbf{x}_i$ and $q=\hat{Y}|\mathbf{x}_i$.

When Y takes values in $\{-1, 1\}$, a similar derivation yields the logistic loss

$$\mathcal{L}(\mathbf{w}, b) = -\sum_{\mathbf{x}_i, y_i \in \mathbf{d}} \log \sigma\left(y_i(\mathbf{w}^T \mathbf{x}_i + b)\right).$$



- In general, the cross-entropy and the logistic losses do not admit a minimizer that can be expressed analytically in closed form.
- However, a minimizer can be found numerically, using a general minimization technique such as gradient descent.

Gradient descent

Let $\mathcal{L}(\theta)$ denote a loss function defined over model parameters θ (e.g., $\mathbf{w}$ and b).

To minimize $\mathcal{L}(\theta)$, gradient descent uses local linear information to iteratively move towards a (local) minimum.

For $\theta_0 \in \mathbb{R}^d$, a first-order approximation around θ_0 can be defined as

$$\hat{\mathcal{L}}(\theta_0 + \epsilon) = \mathcal{L}(\theta_0) + \epsilon^T \nabla_\theta \mathcal{L}(\theta_0) + \frac{1}{2\gamma} ||\epsilon||^2.$$

A minimizer of the approximation $\hat{\mathcal{L}}(\theta_0 + \epsilon)$ is given for

$$\begin{aligned}\nabla_\epsilon \hat{\mathcal{L}}(\theta_0 + \epsilon) &= 0 \\ &= \nabla_\theta \mathcal{L}(\theta_0) + \frac{1}{\gamma}\epsilon,\end{aligned}$$

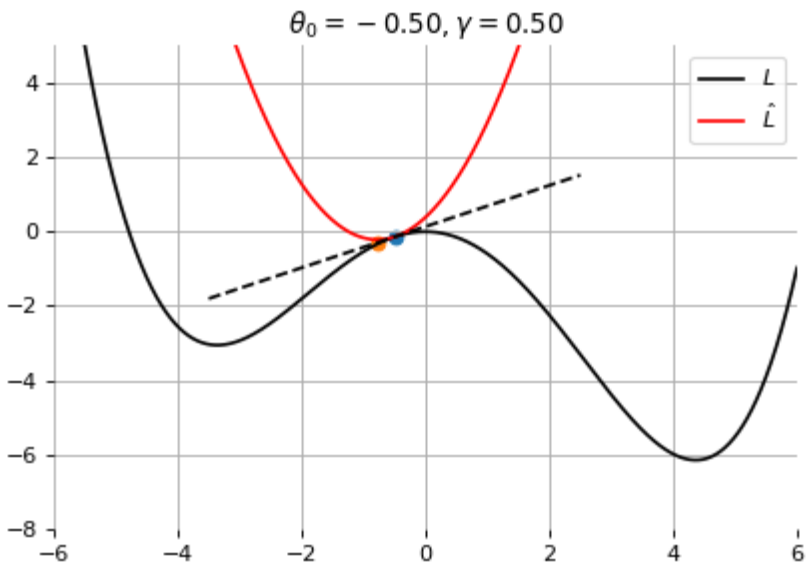
which results in the best improvement for the step $\epsilon = -\gamma \nabla_\theta \mathcal{L}(\theta_0)$.

Therefore, model parameters can be updated iteratively using the update rule:

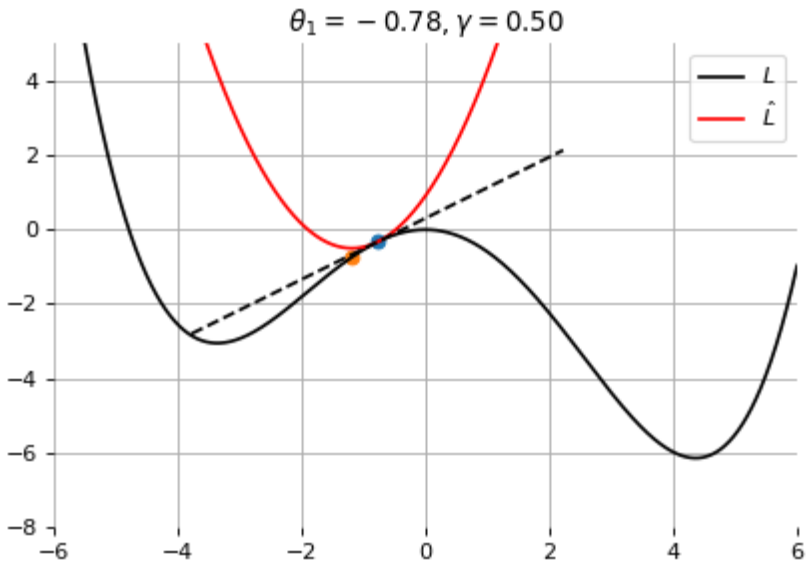
$$\theta_{t+1} = \theta_t - \gamma \nabla_\theta \mathcal{L}(\theta_t)$$

Notes:

- θ_0 are the initial parameters of the model;
- γ is the learning rate;
- both are critical for the convergence of the update rule.



Example 1: Convergence to a local minima



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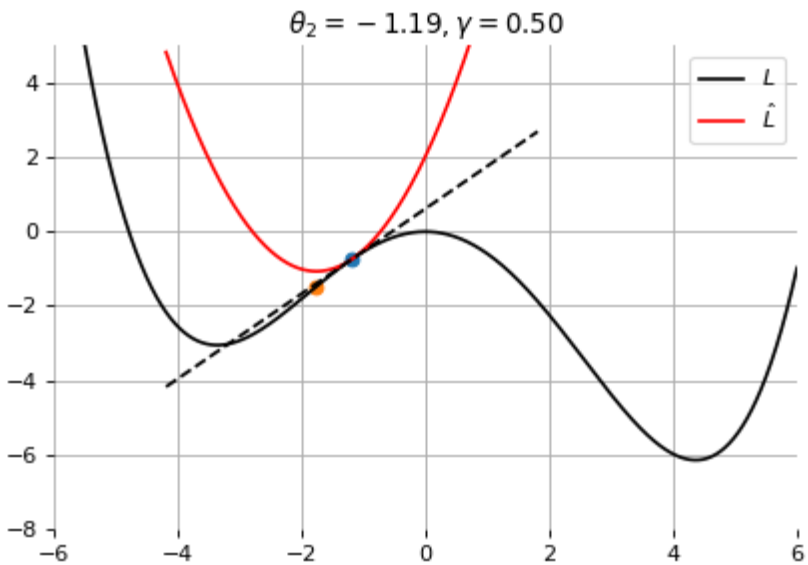

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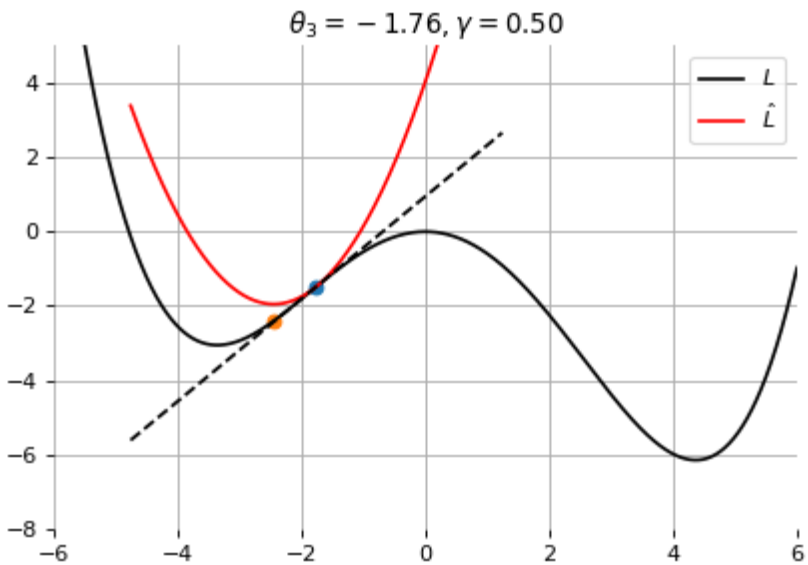

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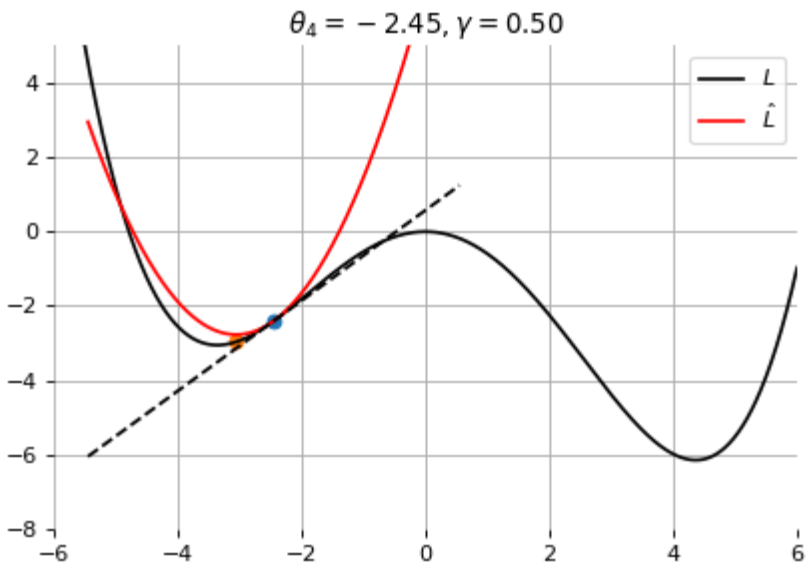

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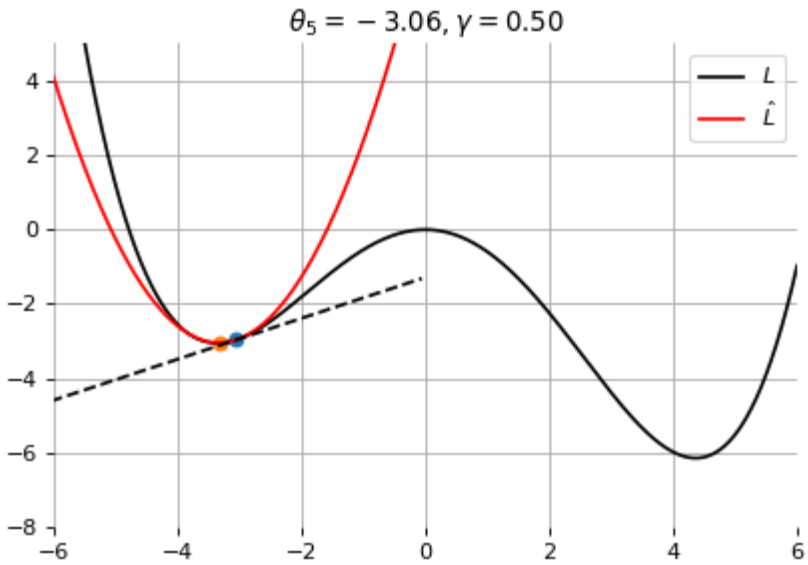

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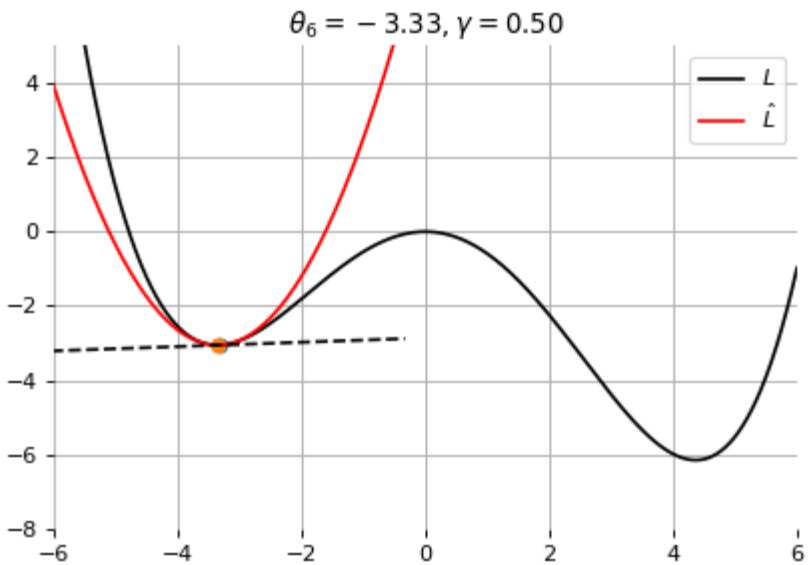

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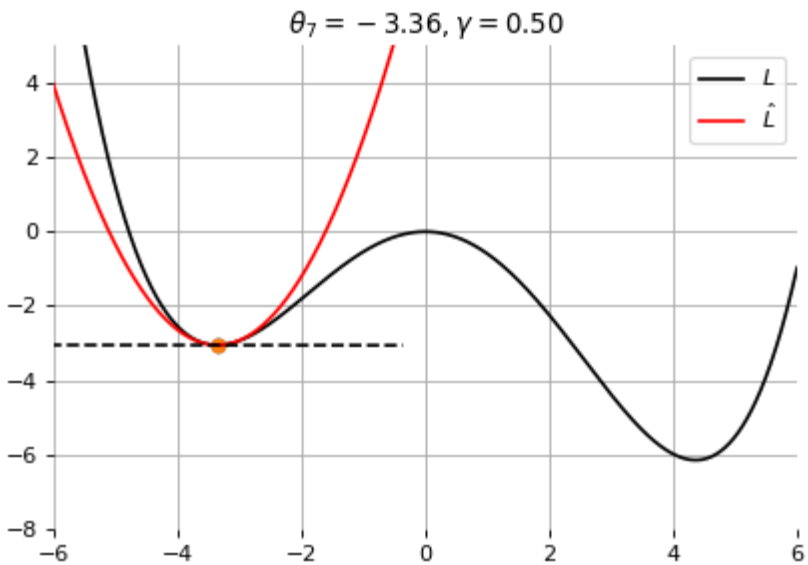

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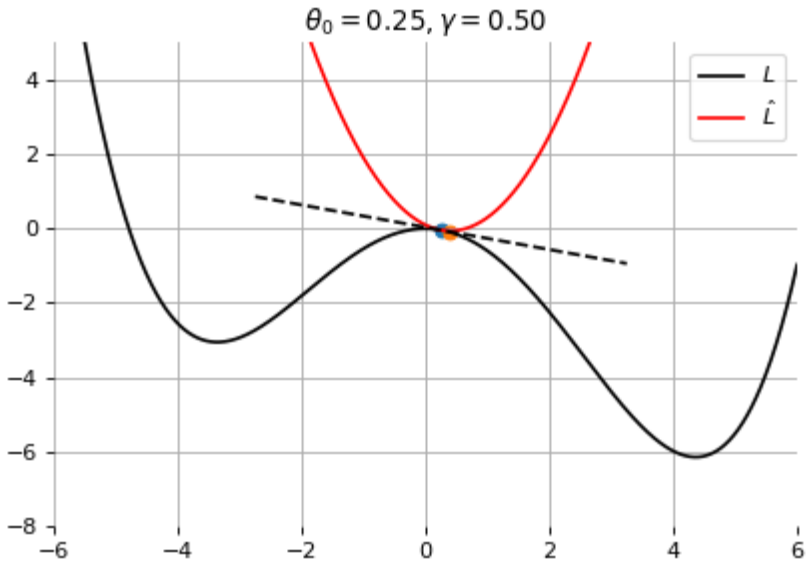

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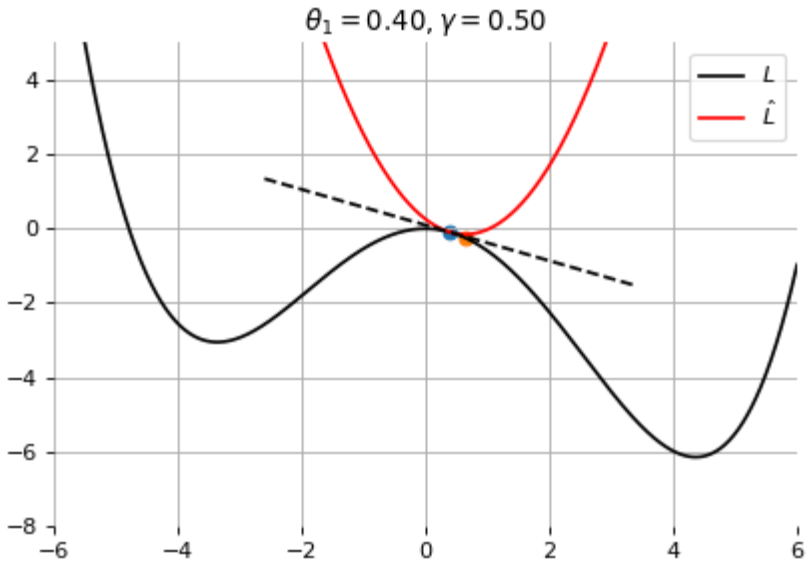

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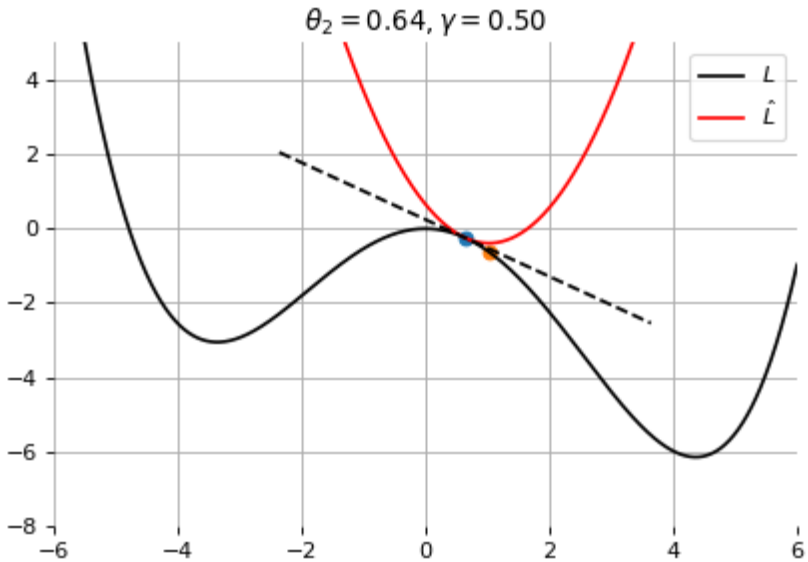

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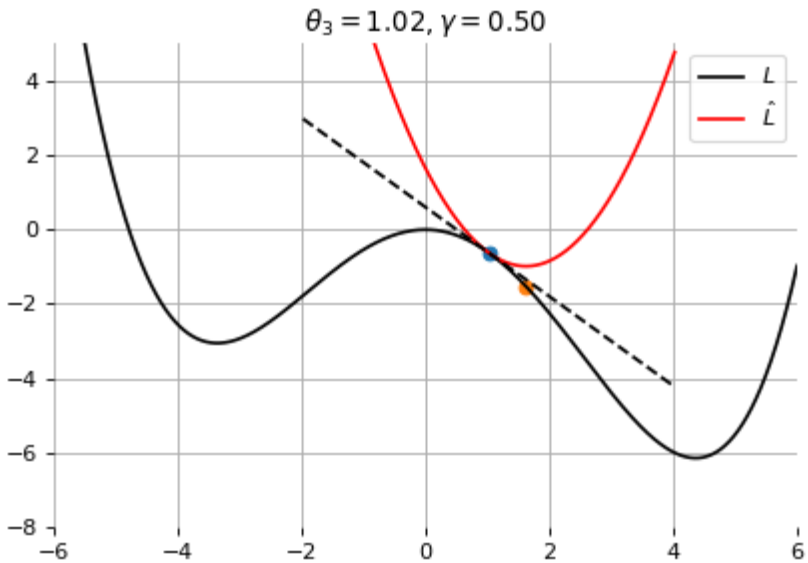

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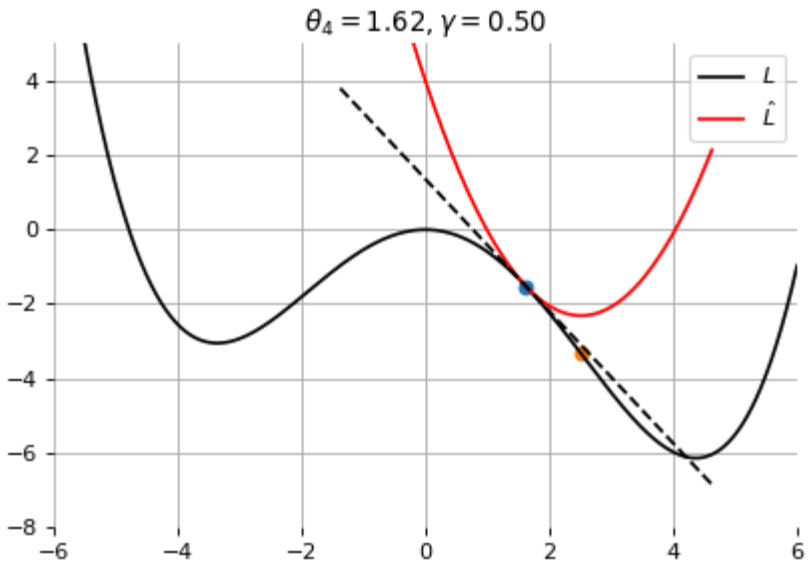

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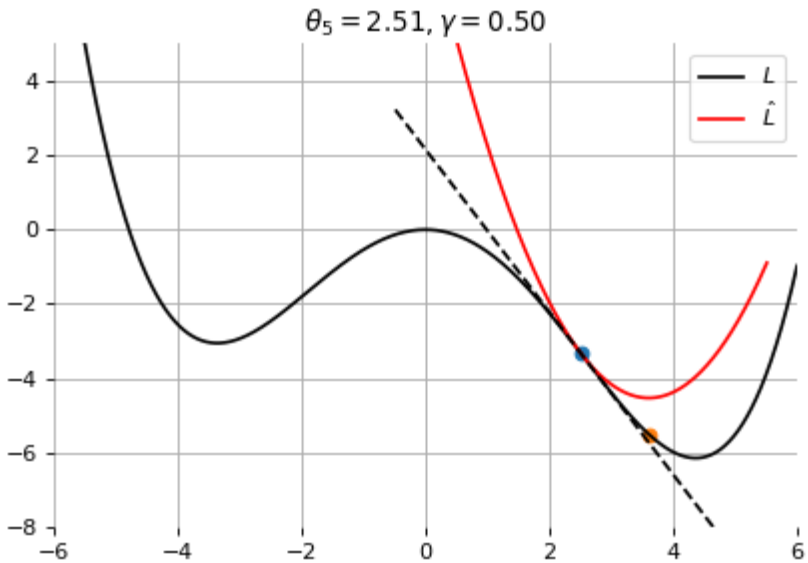

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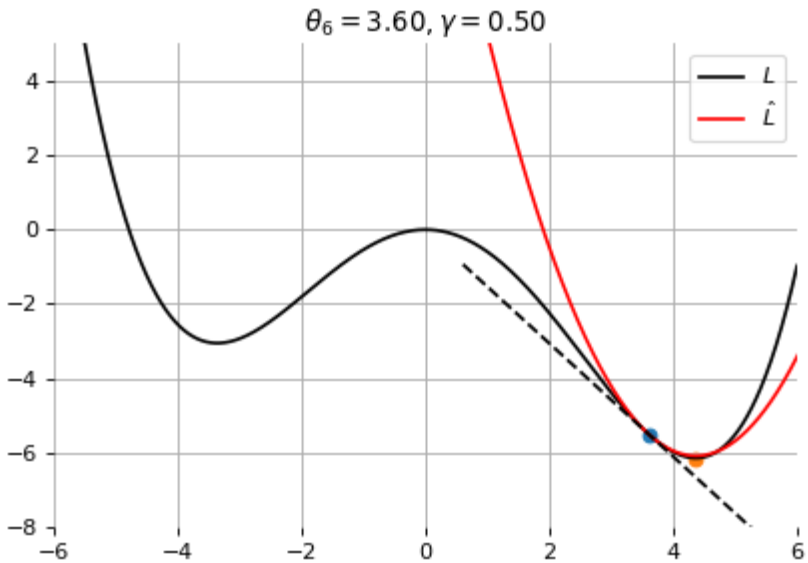

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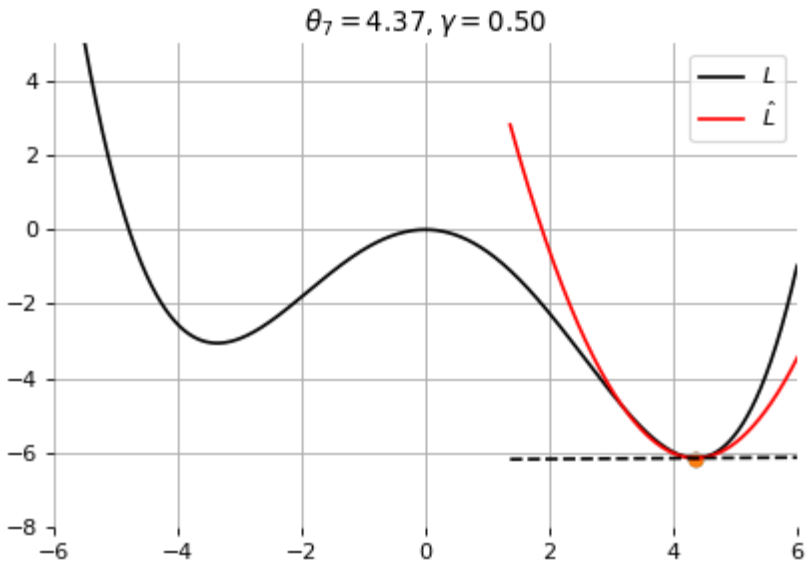

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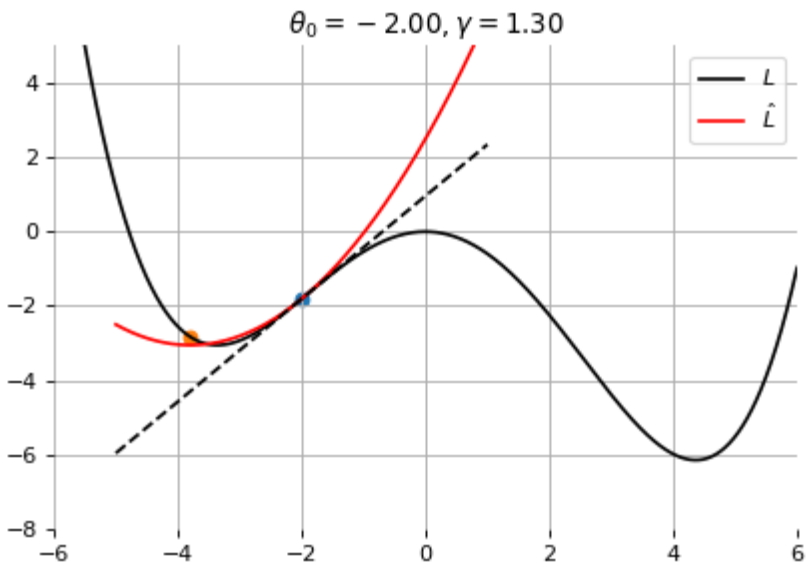
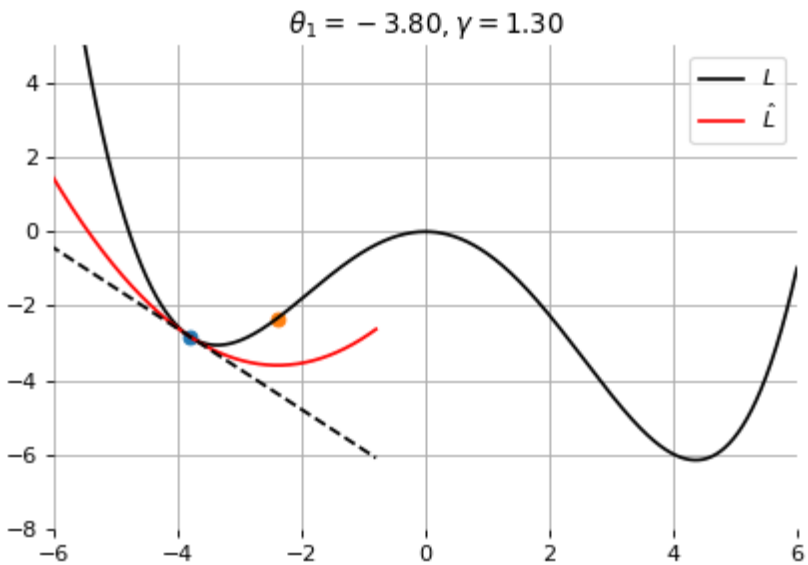


Example 3: Divergence due to a too large learning rate



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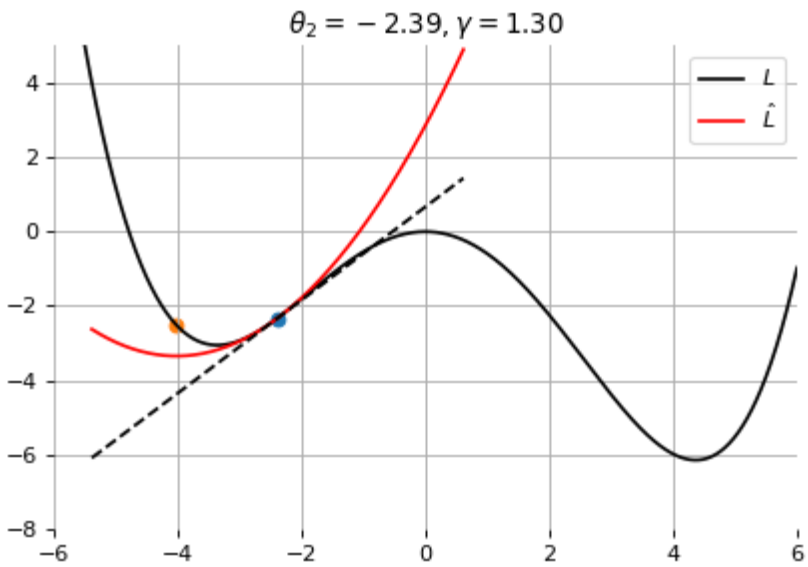

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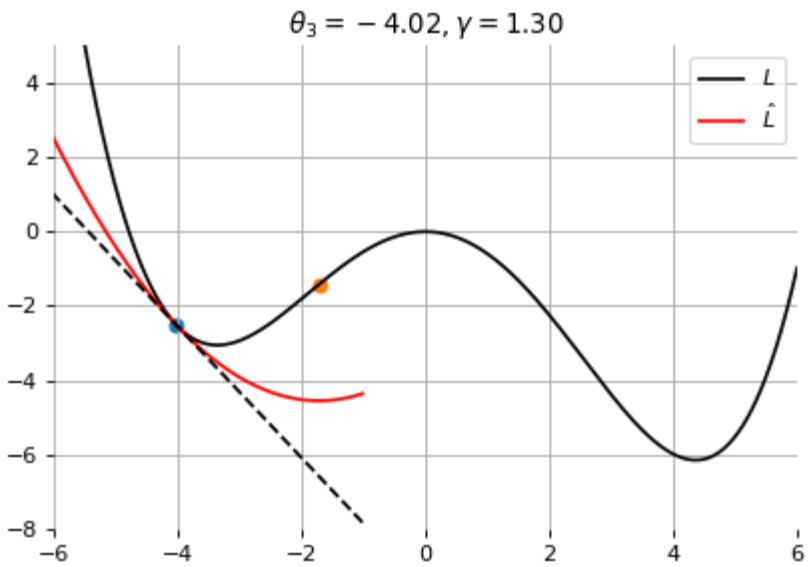

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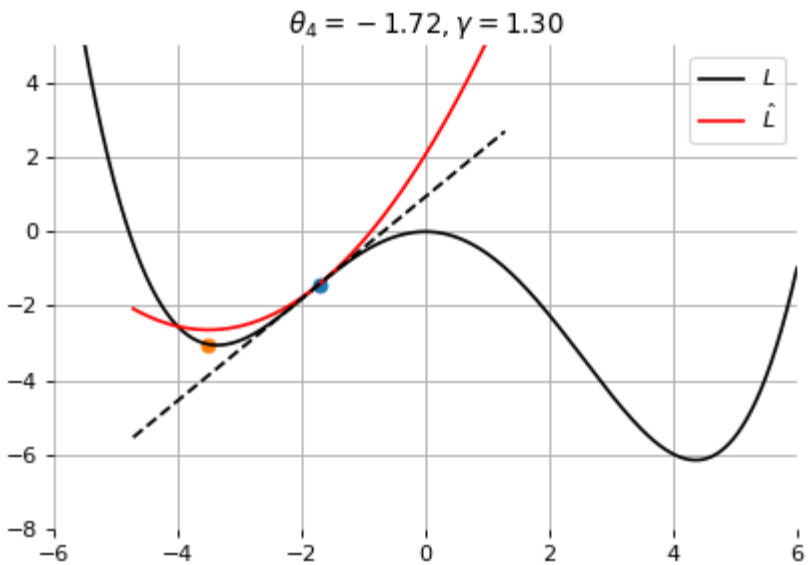

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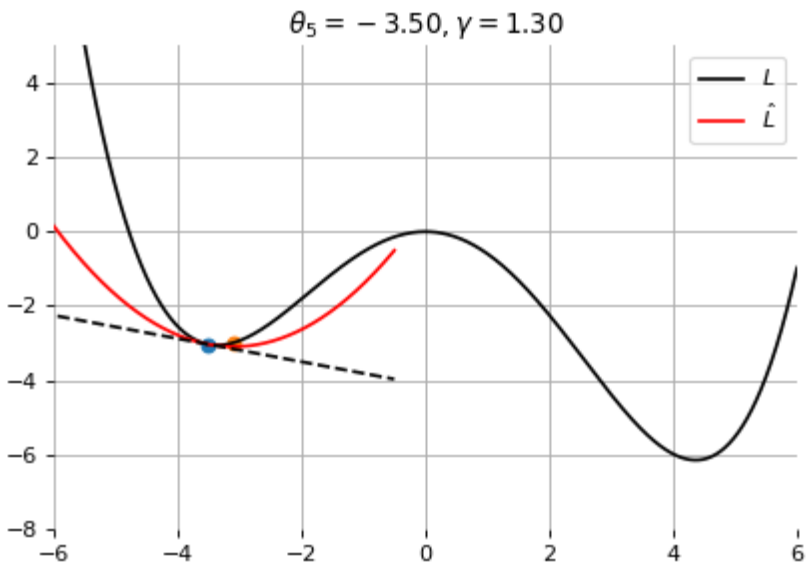

Example 3: Divergence due to a too large learning rate

Stochastic gradient descent

In the empirical risk minimization setup, $\mathcal{L}(\theta)$ and its gradient decompose as

$$\mathcal{L}(\theta) = \frac{1}{N} \sum_{\mathbf{x}_i, y_i \in \mathbf{d}} \ell(y_i, f(\mathbf{x}_i; \theta))$$

$$\nabla \mathcal{L}(\theta) = \frac{1}{N} \sum_{\mathbf{x}_i, y_i \in \mathbf{d}} \nabla \ell(y_i, f(\mathbf{x}_i; \theta)).$$

Therefore, in batch gradient descent the complexity of an update grows linearly with the size N of the dataset.

More importantly, since the empirical risk is already an approximation of the expected risk, it should not be necessary to carry out the minimization with great accuracy.

Instead, stochastic gradient descent uses as update rule:

$$\theta_{t+1} = \theta_t - \gamma \nabla \ell(y_{i(t+1)}, f(\mathbf{x}_{i(t+1)}; \theta_t))$$

- Iteration complexity is independent of N.
- The stochastic process $\{\theta_t | t = 1, ...\}$ depends on the examples $i(t)$ picked randomly at each iteration.

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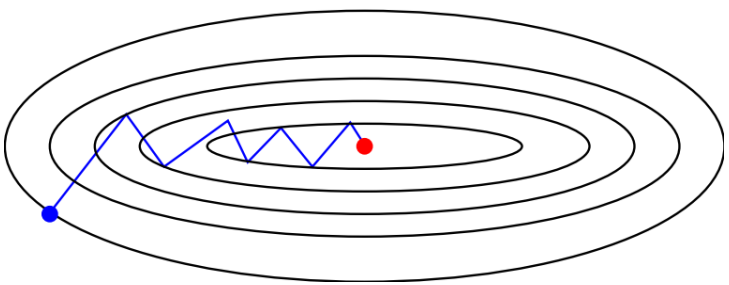
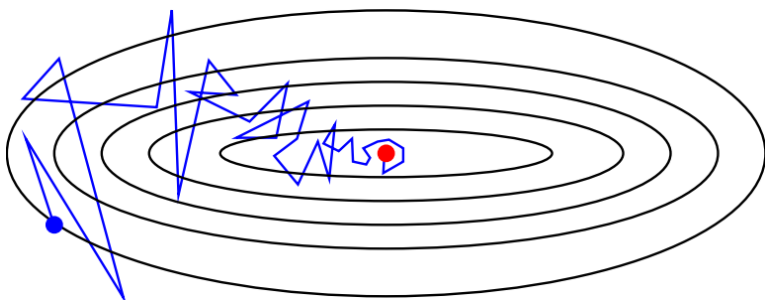


Batch gradient descent



Stochastic gradient descent

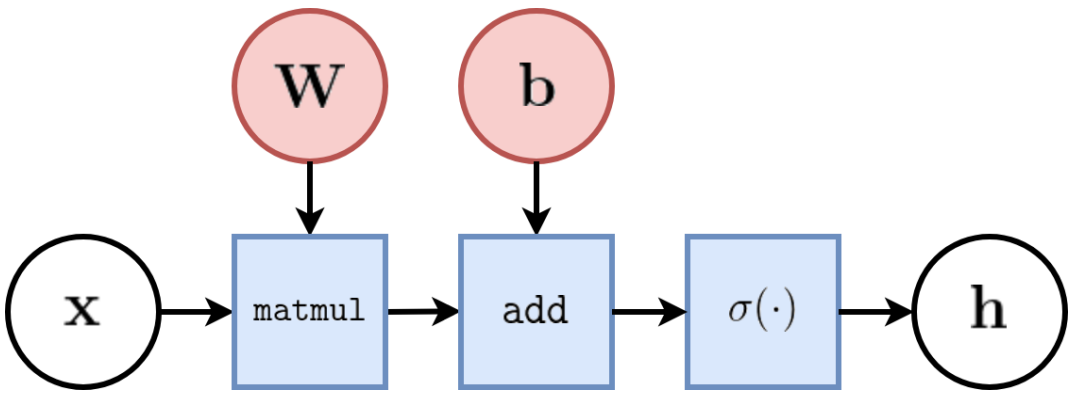
Layers

So far we considered the logistic unit $h = \sigma\left(\mathbf{w}^T\mathbf{x} + b\right)$, where $h \in \mathbb{R}, \mathbf{x} \in \mathbb{R}^p, \mathbf{w} \in \mathbb{R}^p$ and $b \in \mathbb{R}$.

These units can be composed in parallel to form a layer with q outputs:

$$\mathbf{h} = \sigma(\mathbf{W}^T\mathbf{x} + \mathbf{b})$$

where $\mathbf{h} \in \mathbb{R}^q, \mathbf{x} \in \mathbb{R}^p, \mathbf{W} \in \mathbb{R}^{p\times q}, b \in \mathbb{R}^q$ and where $\sigma(\cdot)$ is upgraded to the element-wise sigmoid function.



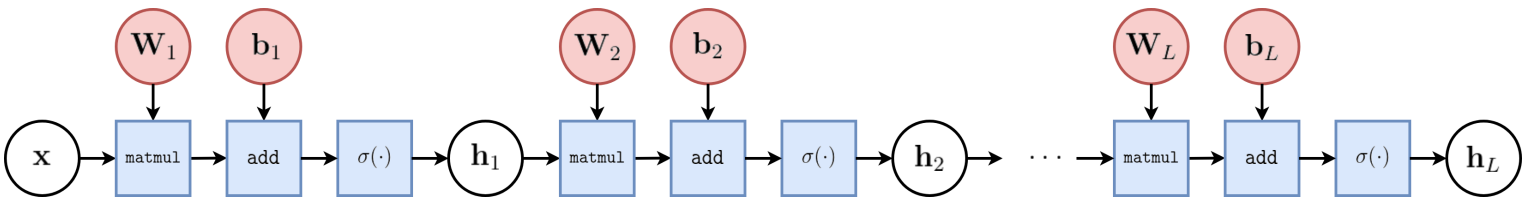
Multi-layer perceptron

Similarly, layers can be composed in series, such that:

$$\begin{aligned}
\mathbf{h}_0 &= \mathbf{x} \\
\mathbf{h}_1 &= \sigma(\mathbf{W}_1^T \mathbf{h}_0 + \mathbf{b}_1) \\
&\dots \\
\mathbf{h}_L &= \sigma(\mathbf{W}_L^T \mathbf{h}_{L-1} + \mathbf{b}_L) \\
f(\mathbf{x}; \theta) &= \mathbf{h}_L
\end{aligned}$$

where θ denotes the model parameters $\{\mathbf{W}_k, \mathbf{b}_k, ... | k = 1, ..., L\}$.

- This model is the multi-layer perceptron, also known as the fully connected feedforward network.
- Optionally, the last activation σ can be skipped to produce unbounded output values $\hat{y} \in \mathbb{R}$.


$\mathbf{W}_1$
$\mathbf{b}_1$
$\mathbf{W}_2$
$\mathbf{b}_2$
$\mathbf{W}_L$
$\mathbf{b}_L$
$\mathbf{x}$
matmul
add
$\sigma(\cdot)$
$\mathbf{h}_1$
matmul
add
$\sigma(\cdot)$
$\mathbf{h}_2$
$\cdots$
matmul
add
$\sigma(\cdot)$
$\mathbf{h}_L$

To minimize $\mathcal{L}(\theta)$ with stochastic gradient descent, we need the gradient $\nabla_\theta \ell(\theta_t)$.

Therefore, we require the evaluation of the (total) derivatives

$$\frac{\mathrm{d}\ell}{\mathrm{d}\mathbf{W}_k}, \frac{\mathrm{d}\ell}{\mathrm{d}\mathbf{b}_k}$$

of the loss ℓ with respect to all model parameters $\mathbf{W}_k, \mathbf{b}_k$, for $k = 1, ..., L$.

These derivatives can be evaluated automatically from the computational graph of ℓ using automatic differentiation.

Automatic differentiation

Consider a 1-dimensional output composition $f \circ g$, such that

$$y = f(\mathbf{u})$$
$$\mathbf{u} = g(x) = (g_1(x), ..., g_m(x)).$$

The chain rule of total derivatives states that

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \sum_{k=1}^{m} \frac{\partial y}{\partial u_k} \underbrace{\frac{\mathrm{d}u_k}{\mathrm{d}x}}_{\text{recursive case}}$$

- Since a neural network is a composition of differentiable functions, the total derivatives of the loss can be evaluated by applying the chain rule recursively over its computational graph.
- The implementation of this procedure is called (reverse) automatic differentiation (AD).
- AD is not numerical differentiation, nor symbolic differentiation.

As a guiding example, let us consider a simplified 2-layer MLP and the following loss function:

$$f(\mathbf{x}; \mathbf{W}_1, \mathbf{W}_2) = \sigma\left(\mathbf{W}_2^T \sigma\left(\mathbf{W}_1^T \mathbf{x}\right)\right)$$
$$\ell(y, \hat{y}; \mathbf{W}_1, \mathbf{W}_2) = \text{cross\_ent}(y, \hat{y}) + \lambda\left(||\mathbf{W}_1||_2 + ||\mathbf{W}_2||_2\right)$$

for $\mathbf{x} \in \mathbb{R}^p$, $y \in \mathbb{R}$, $\mathbf{W}_1 \in \mathbb{R}^{p \times q}$ and $\mathbf{W}_2 \in \mathbb{R}^q$.

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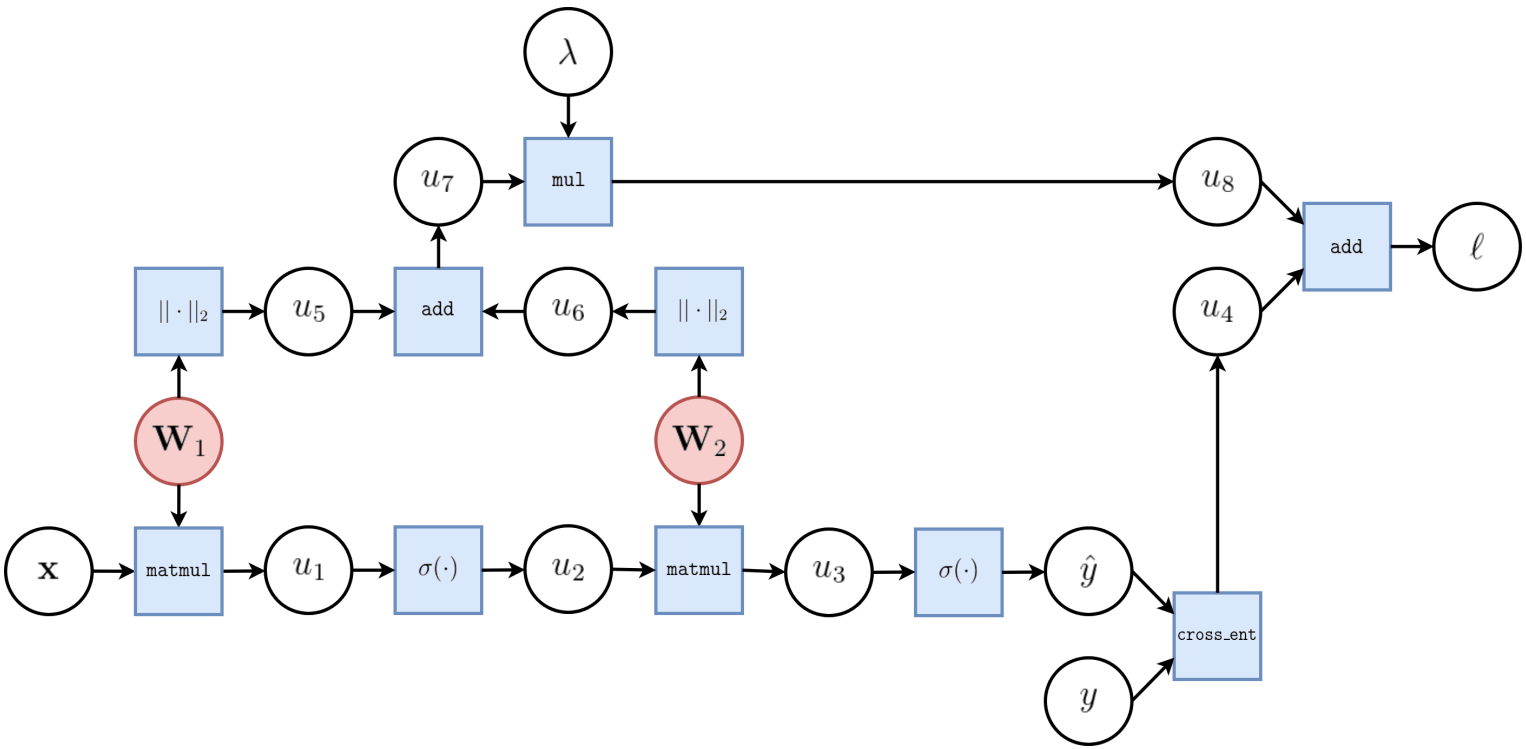
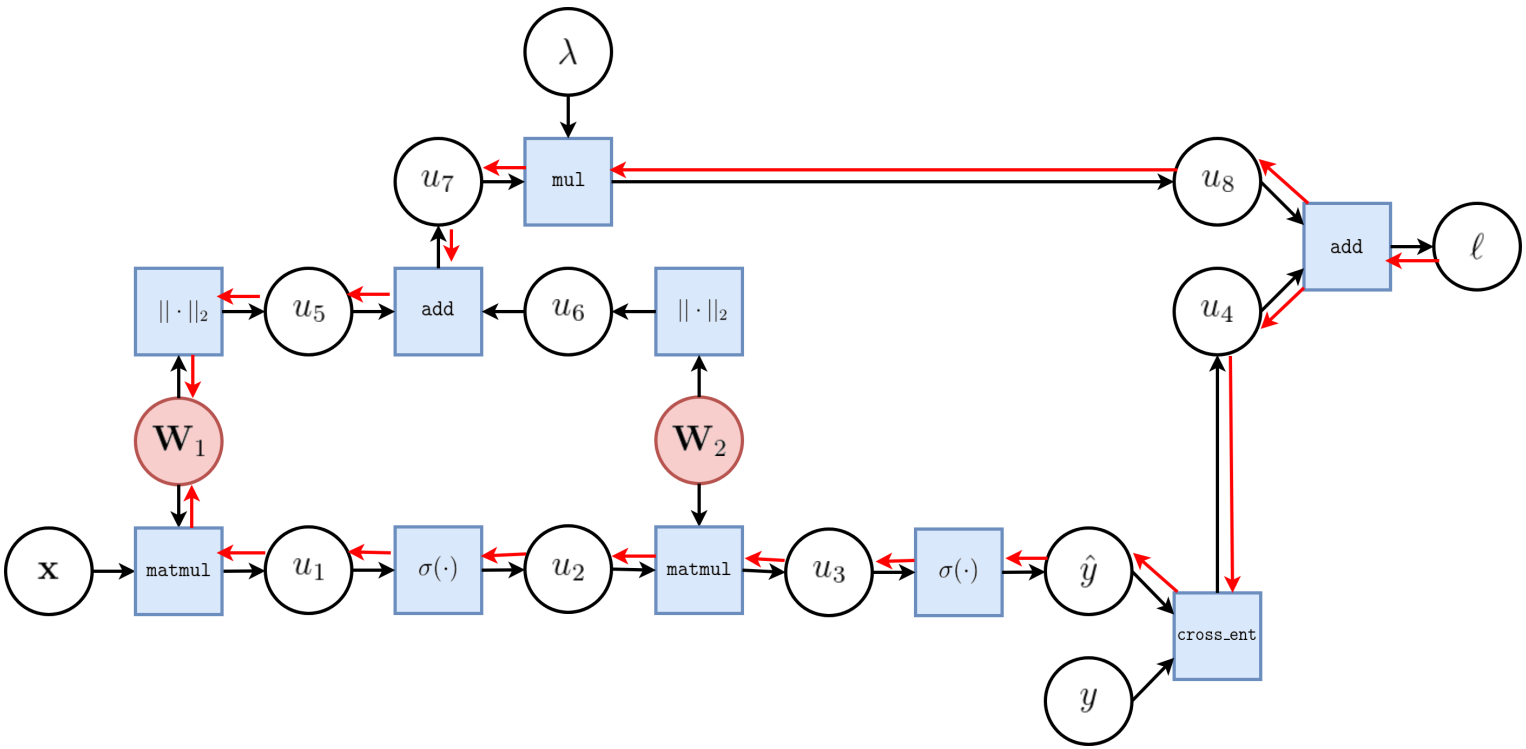


The total derivative $\frac{\mathrm{d}\ell}{\mathrm{d}\mathbf{W}_1}$ can be computed backward, by walking through all paths from ℓ to $\mathbf{W}_1$ in the computational graph and accumulating the terms:

$$\frac{\mathrm{d}\ell}{\mathrm{d}\mathbf{W}_1} = \frac{\partial \ell}{\partial u_8}\frac{\mathrm{d}u_8}{\mathrm{d}\mathbf{W}_1} + \frac{\partial \ell}{\partial u_4}\frac{\mathrm{d}u_4}{\mathrm{d}\mathbf{W}_1}$$

$$\frac{\mathrm{d}u_8}{\mathrm{d}\mathbf{W}_1} = \dots$$

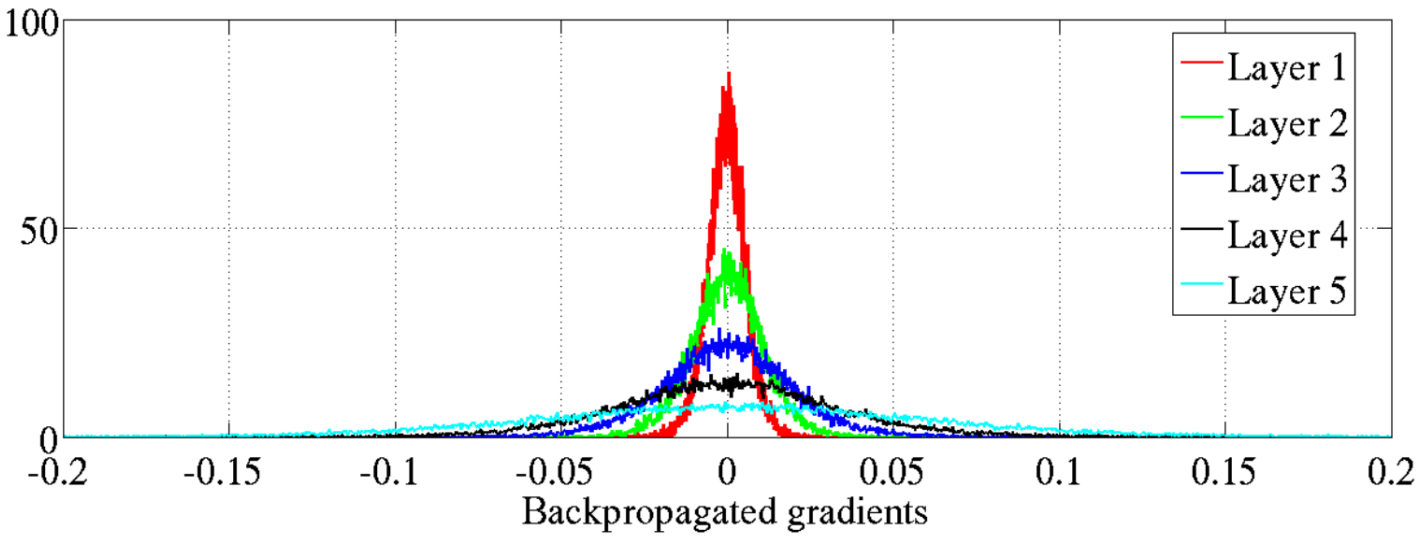


- This algorithm is known as reverse-mode automatic differentiation, also called backpropagation.
- An equivalent procedure can be defined to evaluate the derivatives in forward mode, from inputs to outputs.

Vanishing gradients

Training deep MLPs with many layers has for long (pre-2011) been very difficult due to the vanishing gradient problem.

- Small gradients slow down, and eventually block, stochastic gradient descent.
- This results in a limited capacity of learning.



Backpropagated gradients normalized histograms (Glorot and Bengio, 2010).
Gradients for layers far from the output vanish to zero.

Consider a simplified 3-layer MLP, with $x, w_1, w_2, w_3 \in \mathbb{R}$, such that

$$f(x; w_1, w_2, w_3) = \sigma\left(w_3 \sigma\left(w_2 \sigma\left(w_1 x\right)\right)\right).$$

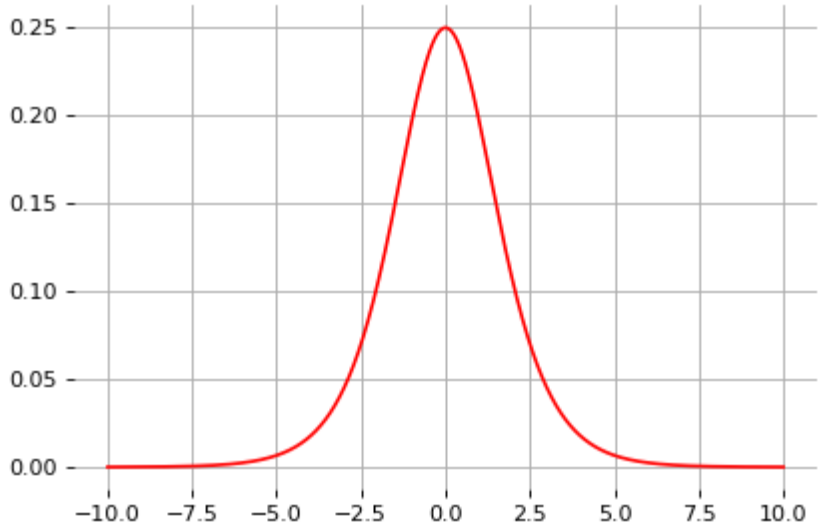
Under the hood, this would be evaluated as

$$\begin{aligned} u_1 &= w_1 x \\ u_2 &= \sigma(u_1) \\ u_3 &= w_2 u_2 \\ u_4 &= \sigma(u_3) \\ u_5 &= w_3 u_4 \\ \hat{y} &= \sigma(u_5) \end{aligned}$$

and its derivative $\frac{\mathrm{d}\hat{y}}{\mathrm{d}w_1}$ as

$$\begin{aligned} \frac{\mathrm{d}\hat{y}}{\mathrm{d}w_1} &= \frac{\partial \hat{y}}{\partial u_5}\frac{\partial u_5}{\partial u_4}\frac{\partial u_4}{\partial u_3}\frac{\partial u_3}{\partial u_2}\frac{\partial u_2}{\partial u_1}\frac{\partial u_1}{\partial w_1} \\ &= \frac{\partial \sigma(u_5)}{\partial u_5} w_3 \frac{\partial \sigma(u_3)}{\partial u_3} w_2 \frac{\partial \sigma(u_1)}{\partial u_1} x \end{aligned}$$

The derivative of the sigmoid activation function σ is:



$$\frac{\mathrm{d}\sigma}{\mathrm{d}x}(x) = \sigma(x)(1 - \sigma(x))$$

Notice that $0 \leq \frac{\mathrm{d}\sigma}{\mathrm{d}x}(x) \leq \frac{1}{4}$ for all x.

Assume that weights w_1, w_2, w_3 are initialized randomly from a Gaussian with zero-mean and small variance, such that with high probability $-1 \leq w_i \leq 1$.

Then,

$$\frac{\mathrm{d}\hat{y}}{\mathrm{d}w_1} = \underbrace{\frac{\partial \sigma(u_5)}{\partial u_5}}_{\leq \frac{1}{4}} \underbrace{w_3}_{\leq 1} \underbrace{\frac{\partial \sigma(u_3)}{\partial u_3}}_{\leq \frac{1}{4}} \underbrace{w_2}_{\leq 1} \underbrace{\frac{\sigma(u_1)}{\partial u_1}}_{\leq \frac{1}{4}} x$$

This implies that the gradient $\frac{\mathrm{d}\hat{y}}{\mathrm{d}w_1}$ exponentially shrinks to zero as the number of layers in the network increases.

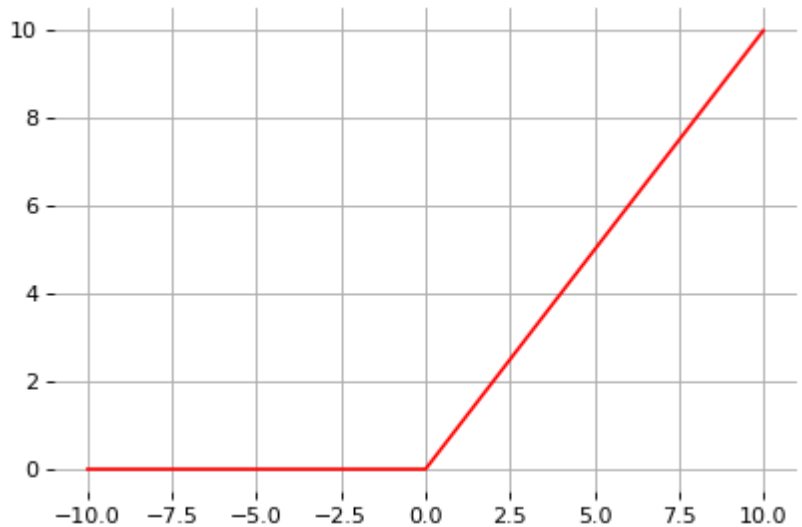
Hence the vanishing gradient problem.

- In general, bounded activation functions (sigmoid, tanh, etc) are prone to the vanishing gradient problem.
- Note the importance of a proper initialization scheme.

Rectified linear units

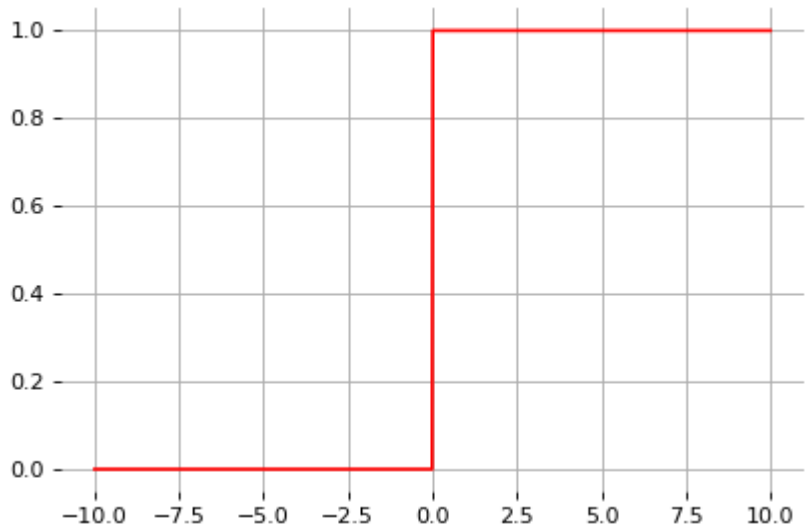
Instead of the sigmoid activation function, modern neural networks are for most based on rectified linear units (ReLU) (Glorot et al, 2011):

$$\mathrm{ReLU}(x) = \max(0, x)$$



Note that the derivative of the ReLU function is

$$\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{ReLU}(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ 1 & \text{otherwise} \end{cases}$$



For $x = 0$, the derivative is undefined. In practice, it is set to zero.

Therefore,

$$\frac{\mathrm{d}\hat{y}}{\mathrm{d}w_1} = \underbrace{\frac{\partial\sigma(u_5)}{\partial u_5}}_{=1} w_3 \underbrace{\frac{\partial\sigma(u_3)}{\partial u_3}}_{=1} w_2 \underbrace{\frac{\partial\sigma(u_1)}{\partial u_1}}_{=1} x$$

This solves the vanishing gradient problem, even for deep networks! (provided proper initialization)

Note that:

- The ReLU unit dies when its input is negative, which might block gradient descent.
- This is actually a useful property to induce sparsity.
- This issue can also be solved using leaky ReLUs, defined as

$$\mathrm{LeakyReLU}(x) = \max(\alpha x, x)$$

for a small $\alpha \in \mathbb{R}^+$ (e.g., $\alpha = 0.1$).

Universal approximation

Theorem. (Cybenko 1989; Hornik et al, 1991) Let $\sigma(\cdot)$ be a bounded, non-constant continuous function. Let I_p denote the p-dimensional hypercube, and $C(I_p)$ denote the space of continuous functions on I_p. Given any $f \in C(I_p)$ and $\epsilon > 0$, there exists $q > 0$ and $v_i, w_i, b_i, i = 1, \ldots, q$ such that

$$F(x) = \sum_{i \leq q} v_i \sigma(w_i^T x + b_i)$$

satisfies

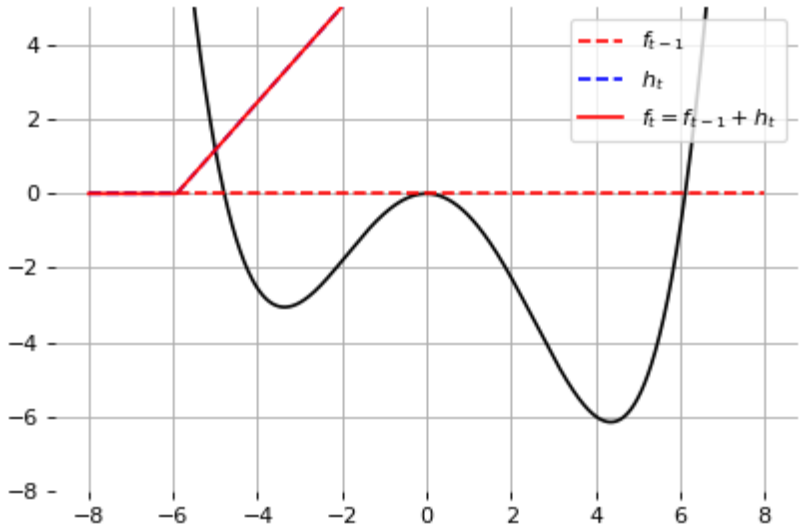
$$\sup_{x \in I_p} |f(x) - F(x)| < \epsilon.$$

- It guarantees that even a single hidden-layer network can represent any classification problem in which the boundary is locally linear (smooth);
- It does not inform about good/bad architectures, nor how they relate to the optimization procedure.
- The universal approximation theorem generalizes to any non-polynomial (possibly unbounded) activation function, including the ReLU (Leshno, 1993).

Consider the 1-layer MLP

$$f(x) = \sum w_i \mathrm{ReLU}(x + b_i).$$

This model can approximate any smooth 1D function, provided enough hidden units.



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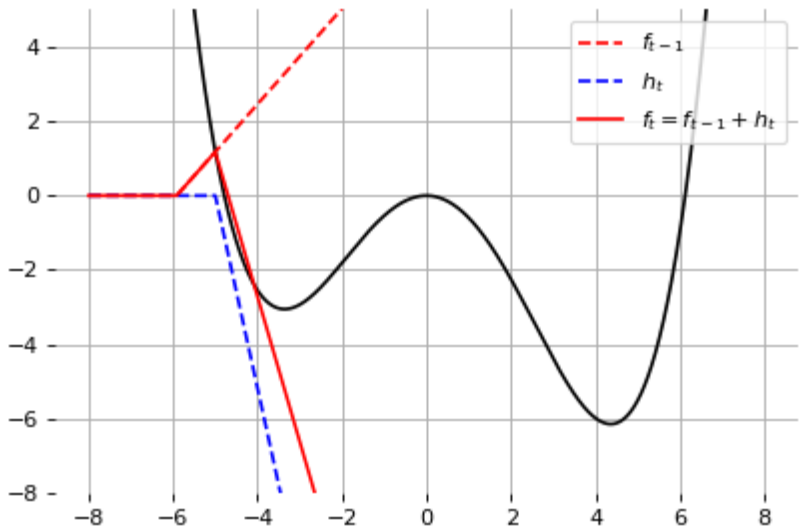

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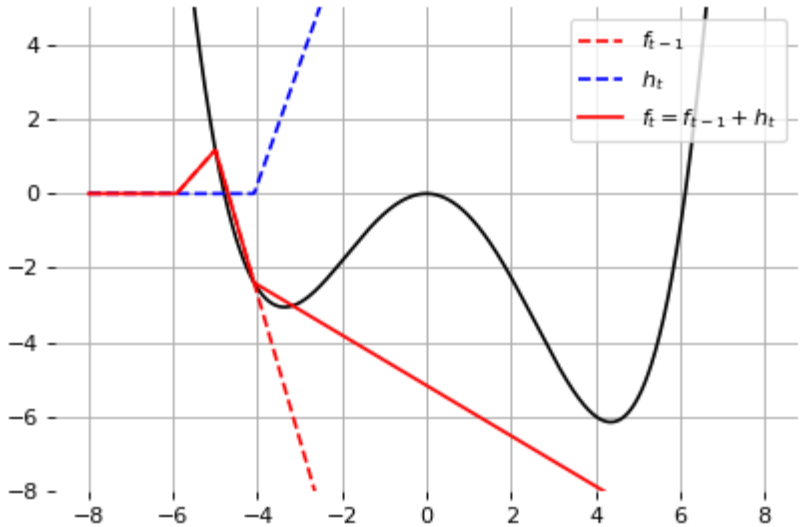

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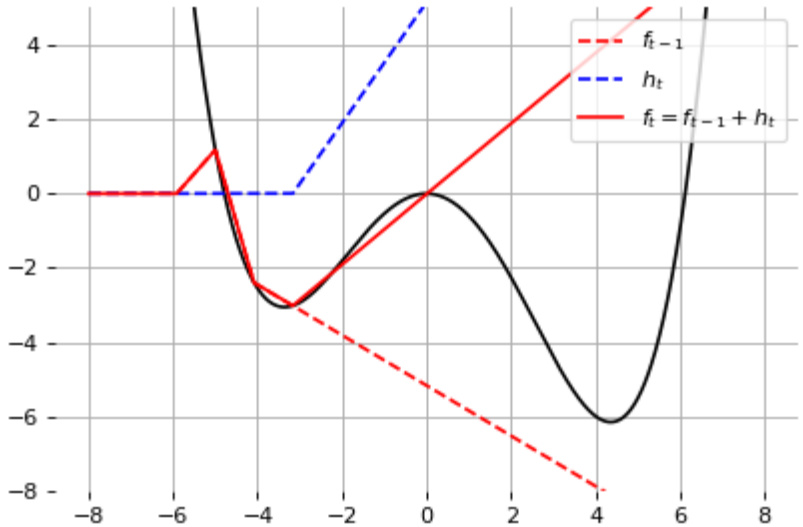

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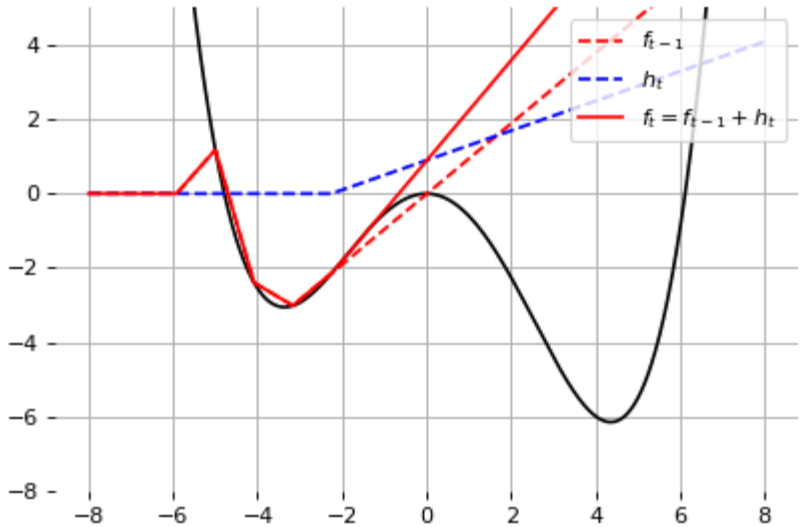

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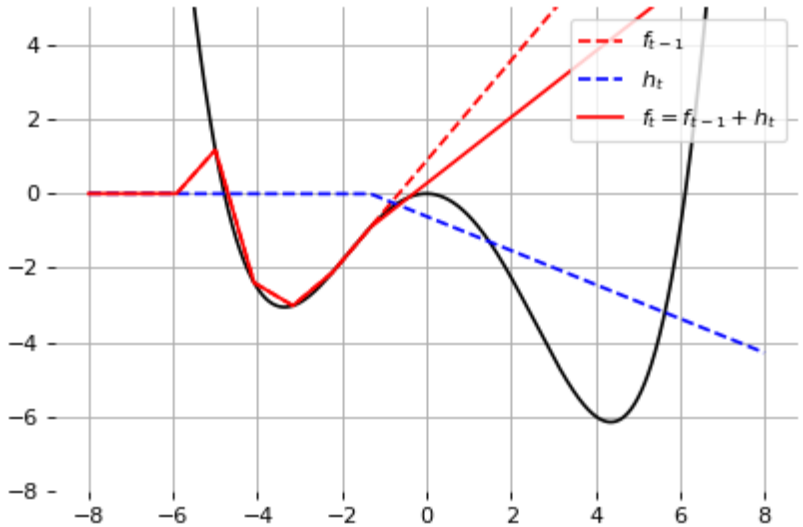

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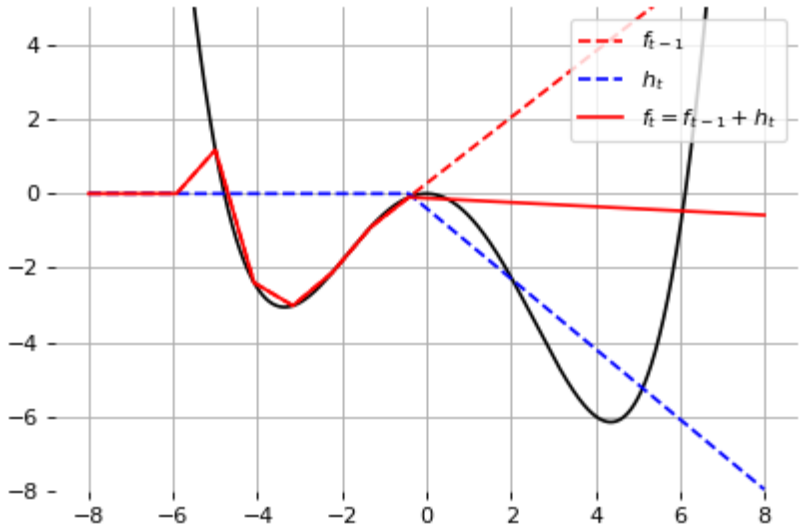

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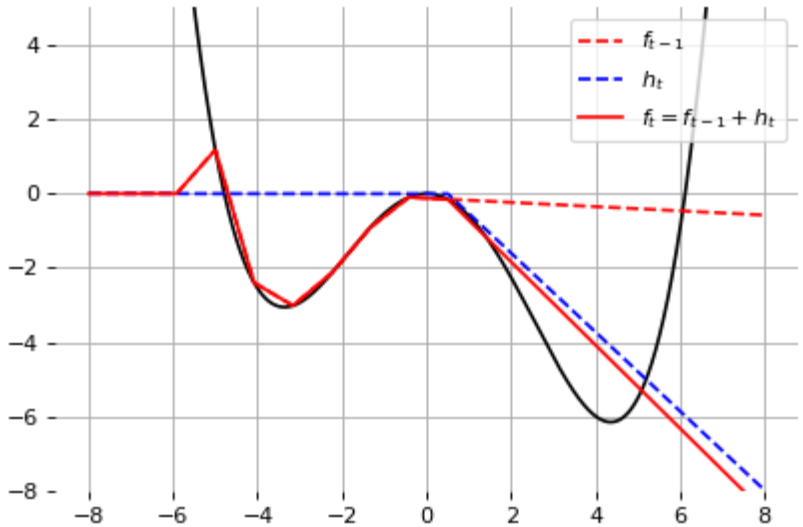

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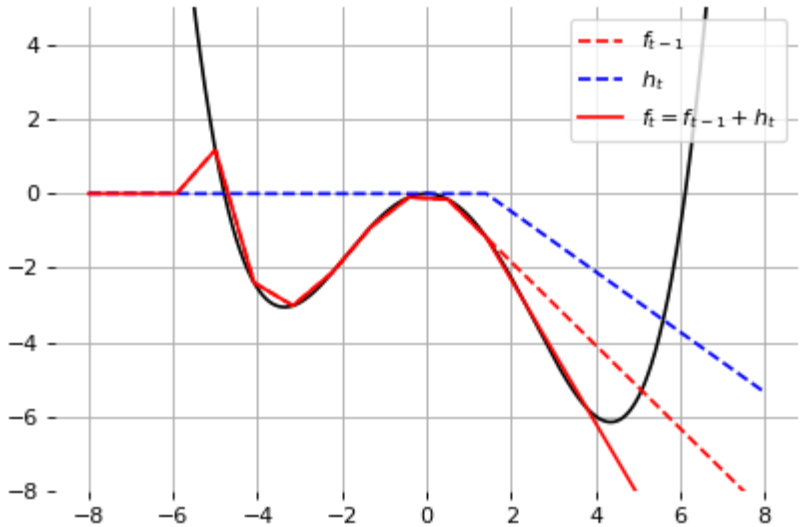

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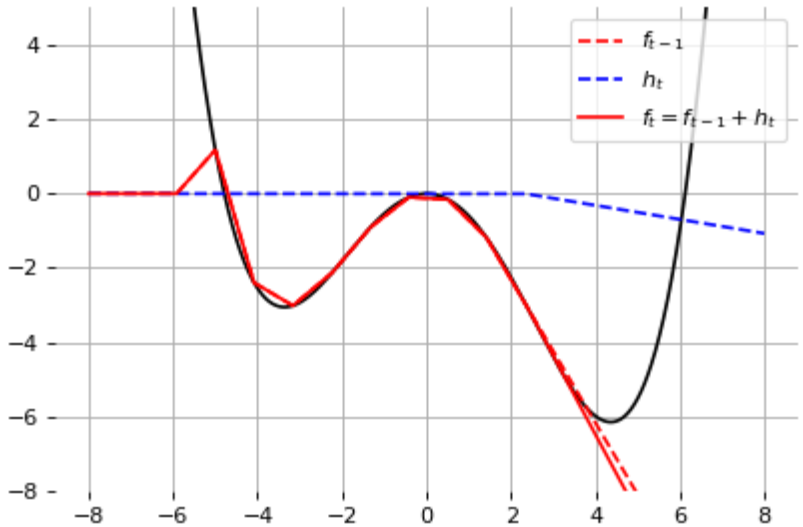

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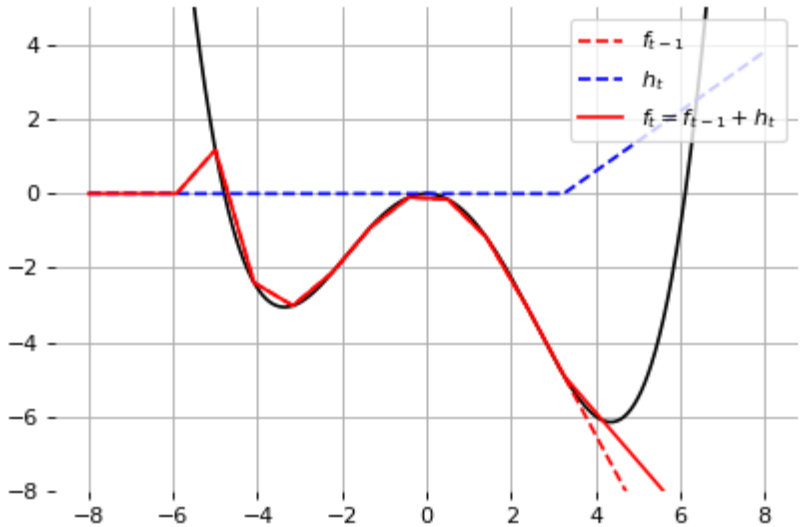

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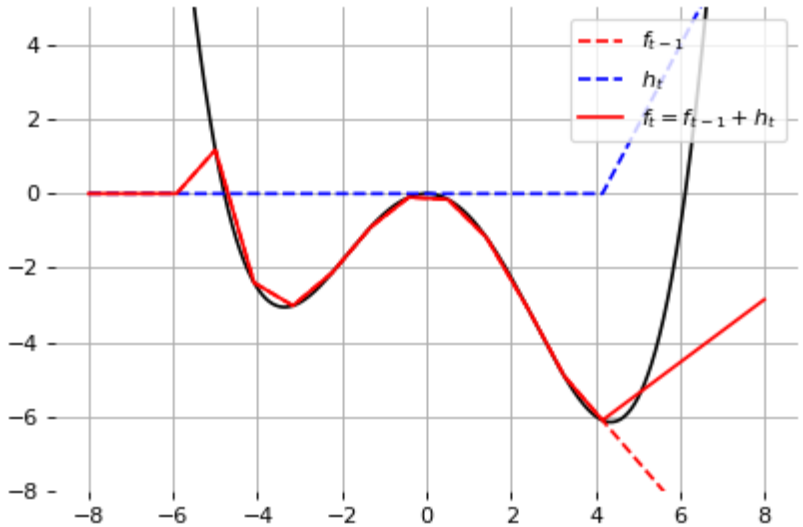

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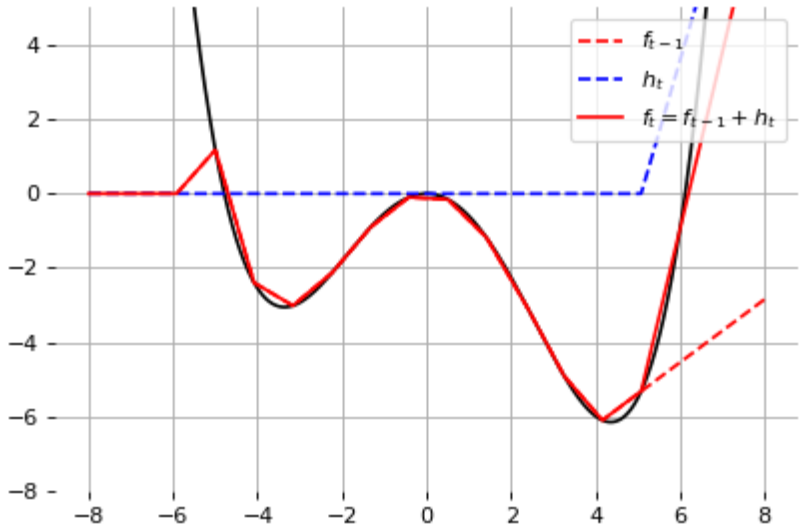

Cooking recipe

- Get data (loads of them).
- Get good hardware.
- Define the neural network architecture.
  - A neural network is a composition of differentiable functions.
  - Stick to non-saturating activation function to avoid vanishing gradients.
  - Prefer deep over shallow architectures.
- Optimize with (variants of) stochastic gradient descent.
  - Evaluate gradients with automatic differentiation.

The end.

References

Materials from the first part of the lecture are inspired from the excellent Deep Learning Course by Francois Fleuret (EPFL, 2018).

- Lecture 3a: Linear classifiers, perceptron
- Lecture 3b: Multi-layer perceptron

Further references:

- Introduction to ML and Stochastic optimization (Gower, 2017)
- Why are deep neural networks hard to train? (Nielsen, 2017)
- Automatic differentiation in machine learning: a survey (Baydin, 2015)