Deep Learning

Lecture 2: Neural networks

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Today

Explain and motivate the basic constructs of neural networks.

- From linear discriminant analysis to logistic regression
- Stochastic gradient descent
- From logistic regression to the multi-layer perceptron
- Vanishing gradients and rectified networks
- Universal approximation theorem

Cooking recipe

- Get data (loads of them).
- Get good hardware.
- Define the neural network architecture as 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.

Neural networks

Threshold Logic Unit

The Threshold Logic Unit (McCulloch and Pitts, 1943) was the first mathematical model for a neuron. Assuming Boolean inputs and outputs, it is defined as:

$$f(\mathbf{x}) = 1_{\{\sum_i w_i x_i + b \geq 0\}}$$

This unit can implement:

- $\text{or}(a, b) = 1_{\{a+b-0.5 \geq 0\}}$
- $\text{and}(a, b) = 1_{\{a+b-1.5 \geq 0\}}$
- $\text{not}(a) = 1_{\{-a+0.5 \geq 0\}}$

Therefore, any Boolean function can be built with such units.

A Logical Calculus of Ideas Immanent in Nervous Activity

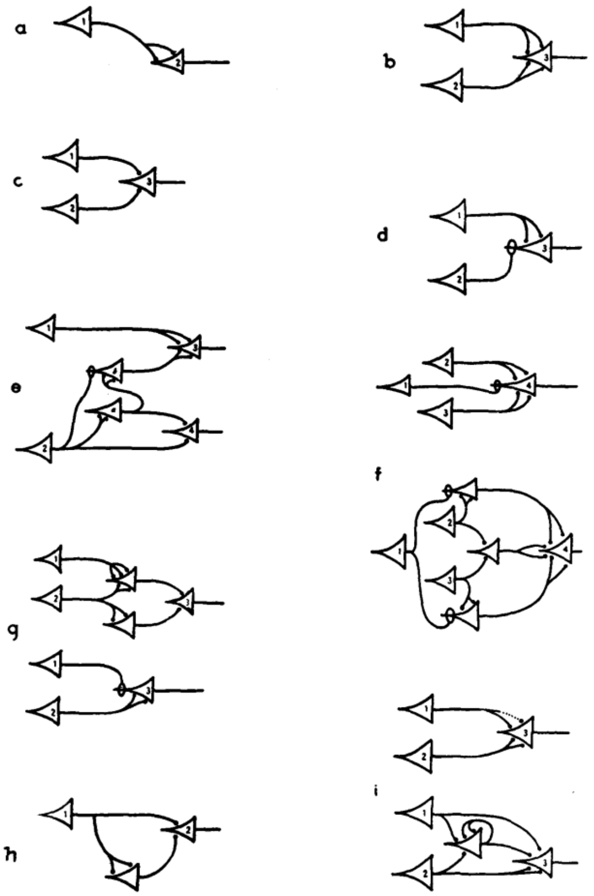


FIGURE 1

Credits: McCulloch and Pitts, A logical calculus of ideas immanent in nervous activity, 1943.

Perceptron

The perceptron (Rosenblatt, 1957) is very similar, except that the inputs are real:

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

This model was originally motivated by biology, with w_i being synaptic weights and x_i and f firing rates.

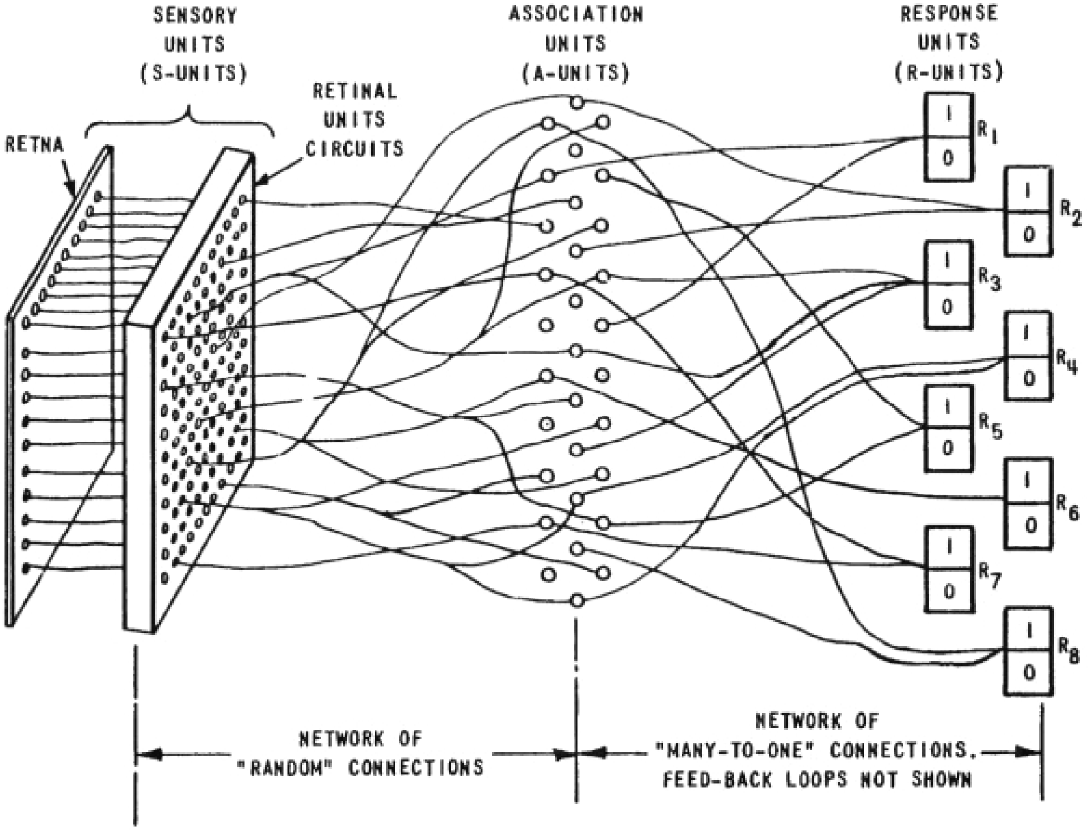
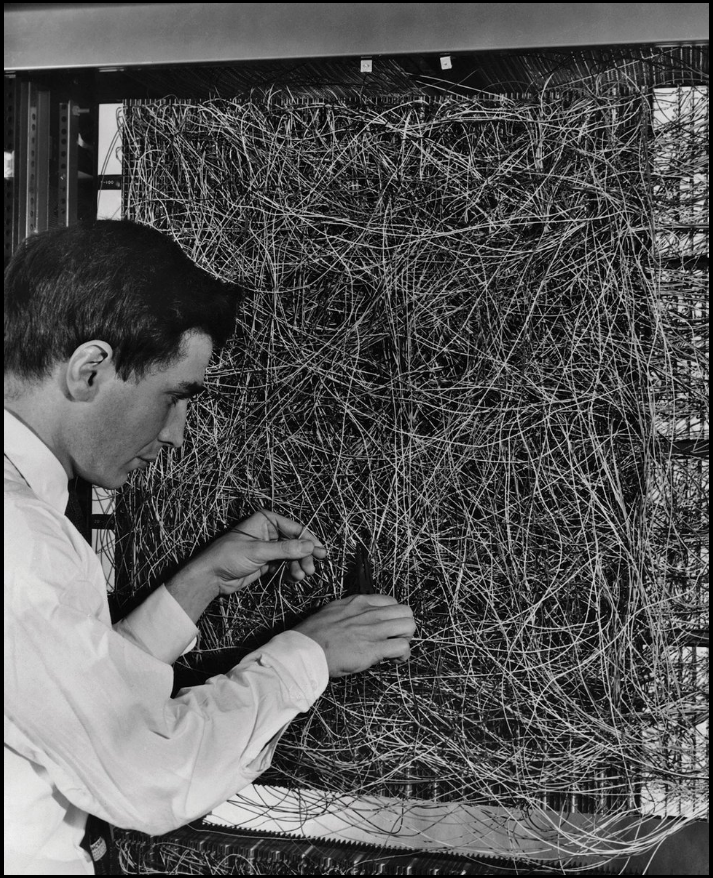
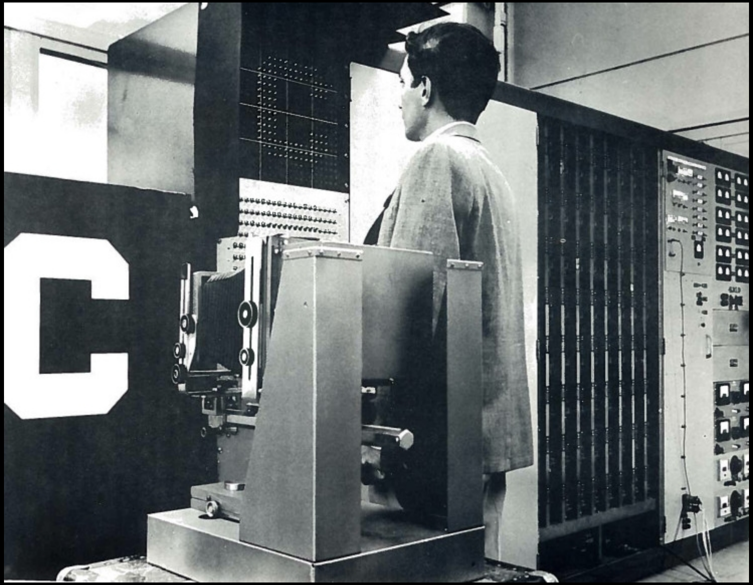

SENSORY UNITS (S-UNITS)
ASSOCIATION UNITS (A-UNITS)
RESPONSE UNITS (R-UNITS)
RETNA
RETINAL UNITS CIRCUITS
1
0
R_1
R_2
R_3
R_4
R_5
R_6
R_7
R_8
NETWORK OF "RANDOM" CONNECTIONS
NETWORK OF "MANY-TO-ONE" CONNECTIONS, FEED-BACK LOOPS NOT SHOWN

Figure 1 ORGANIZATION OF THE MARK I PERCEPTRON

Credits: Frank Rosenblatt, Mark I Perceptron operators' manual, 1960.





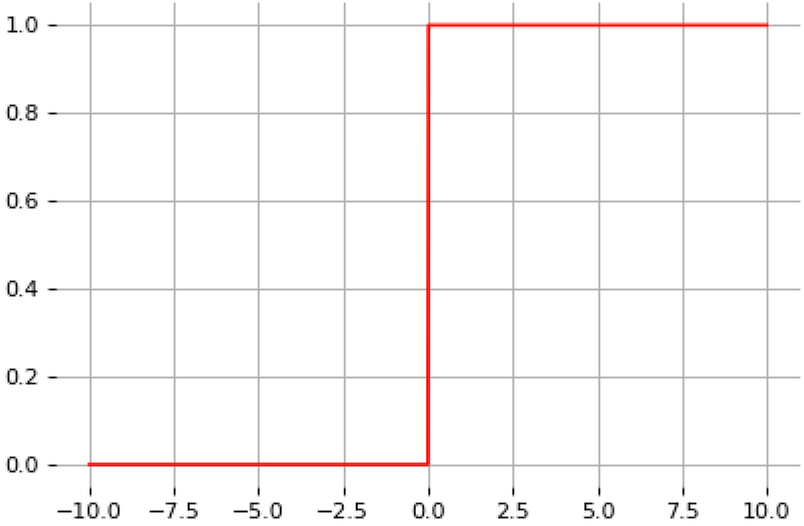
The Mark I Percetron (Frank Rosenblatt).

Perceptron Research from the 50's & 60's, clip

The Perceptron

Let us define the (non-linear) activation function:

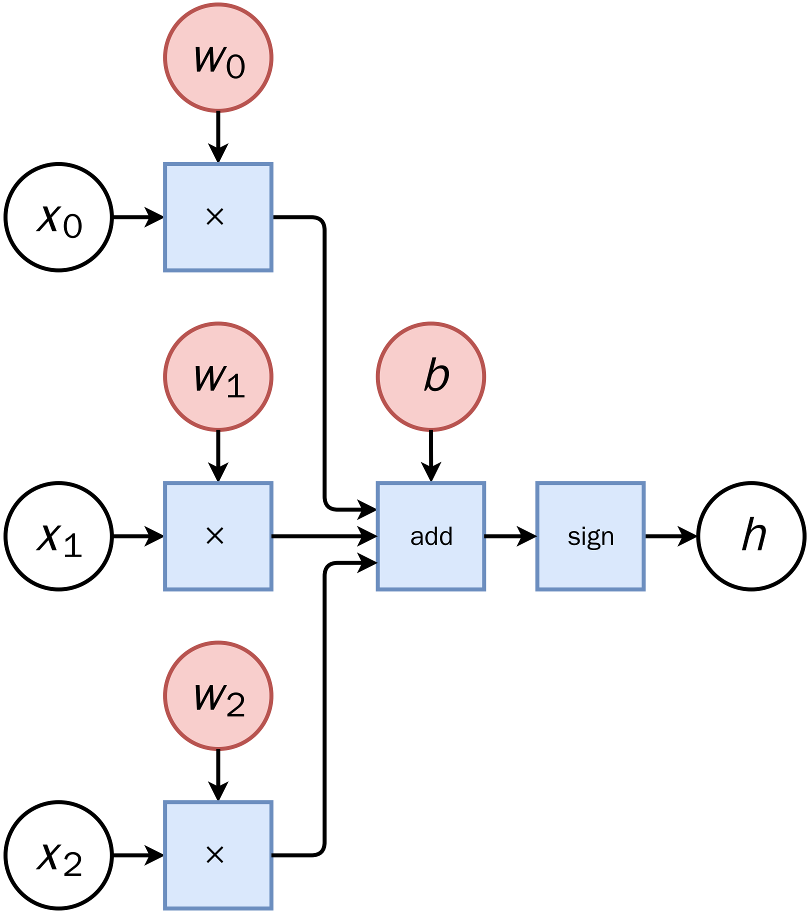
$$\text{sign}(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$



The perceptron classification rule can be rewritten as

$$f(\mathbf{x}) = \text{sign}(\sum_i w_i x_i + b).$$

Computational graphs



The computation of

$$f(\mathbf{x}) = \text{sign}(\sum_i w_i x_i + b)$$

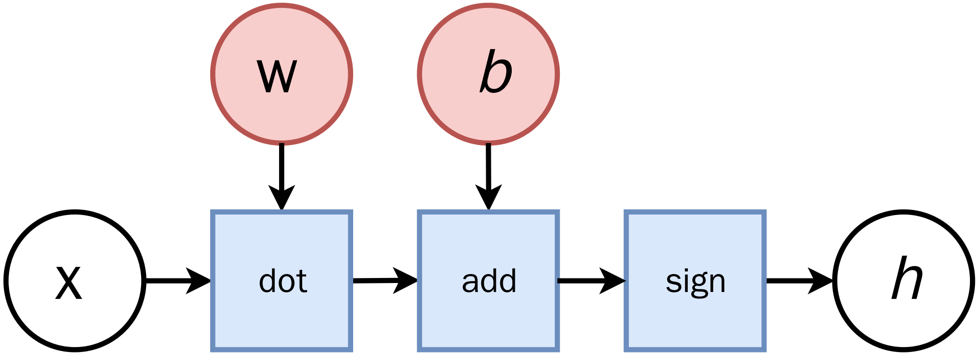
can be represented as a computational graph where

- white nodes correspond to inputs and outputs;
- red nodes correspond to model parameters;
- blue nodes correspond to intermediate operations.

In terms of tensor operations, f can be rewritten as

$$f(\mathbf{x}) = \text{sign}(\mathbf{w}^T\mathbf{x} + b),$$

for which the corresponding computational graph of f is:



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

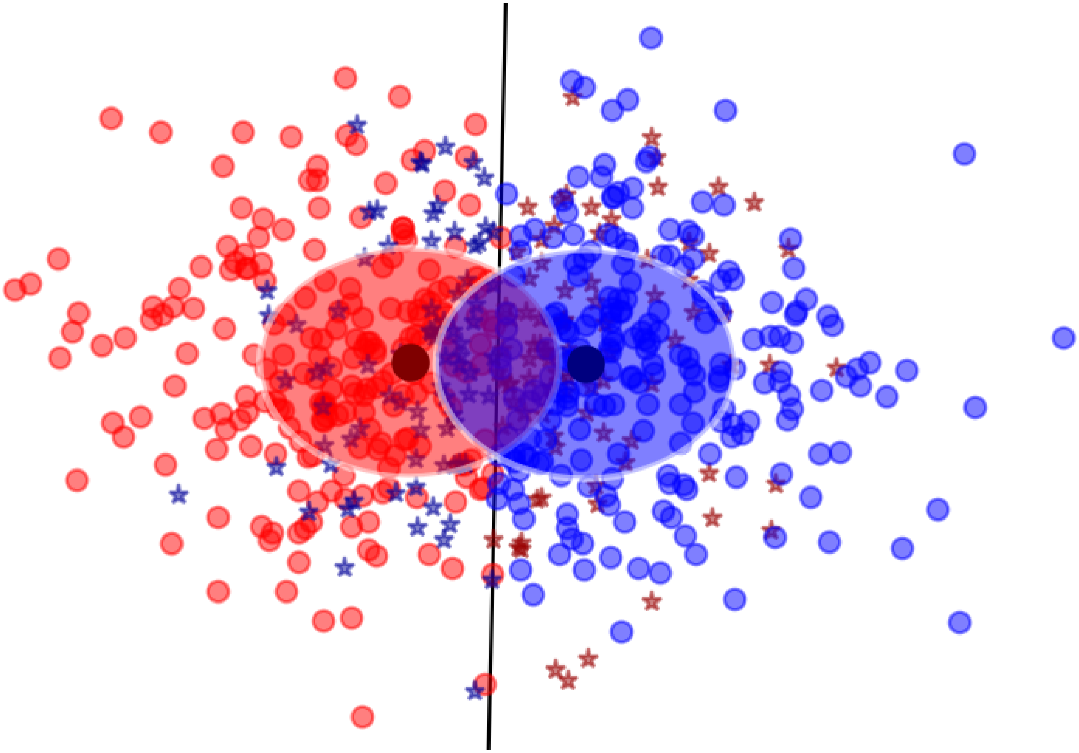
$$\sigma(x) = \frac{1}{1+\exp(-x)},$$

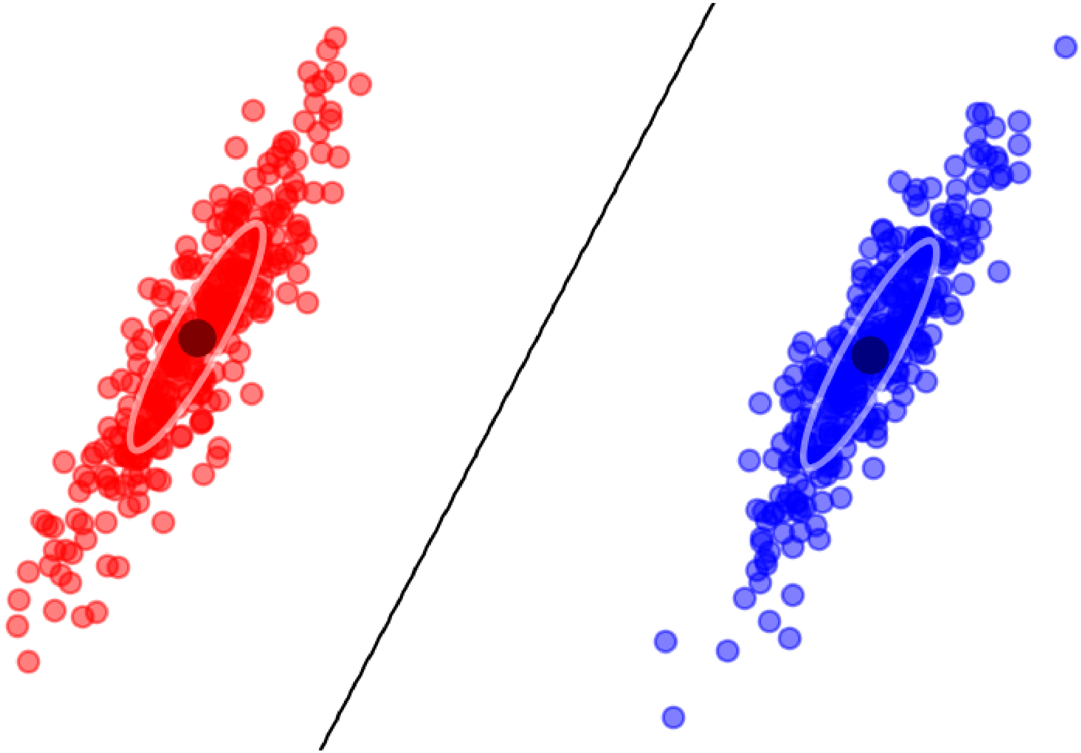
we get

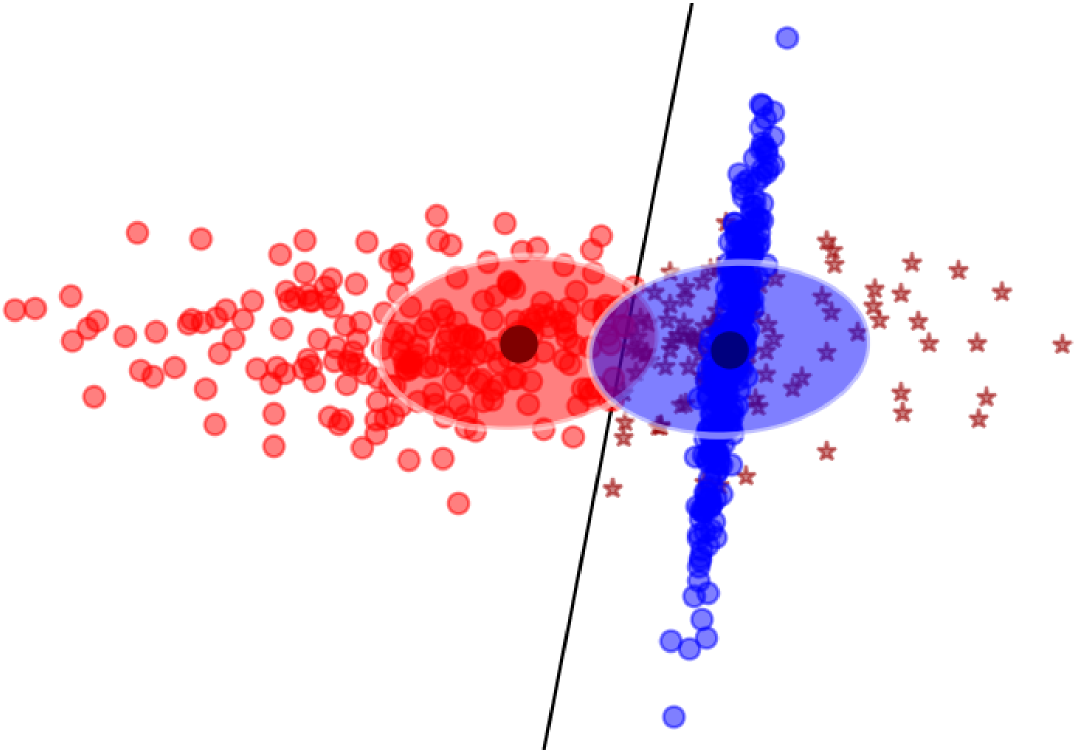
$$P(Y=1|\mathbf{x}) = \sigma\left(\log\frac{P(\mathbf{x}|Y=1)}{P(\mathbf{x}|Y=0)} + \log\frac{P(Y=1)}{P(Y=0)}\right).$$

Therefore,

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



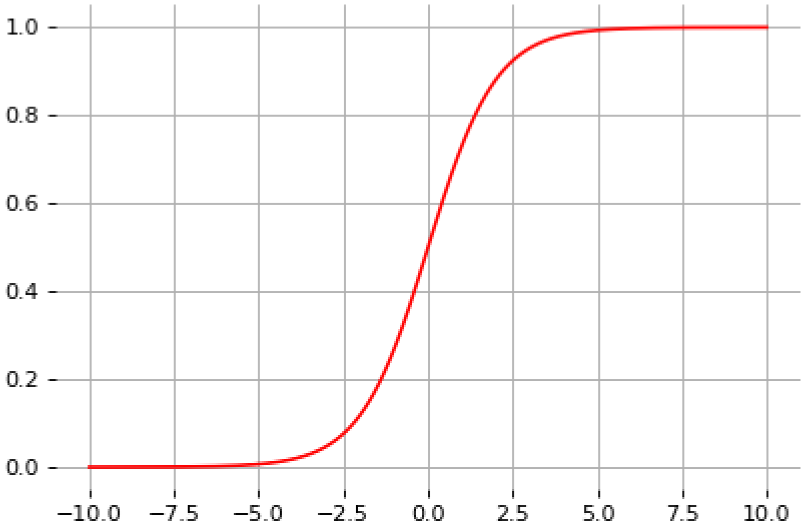




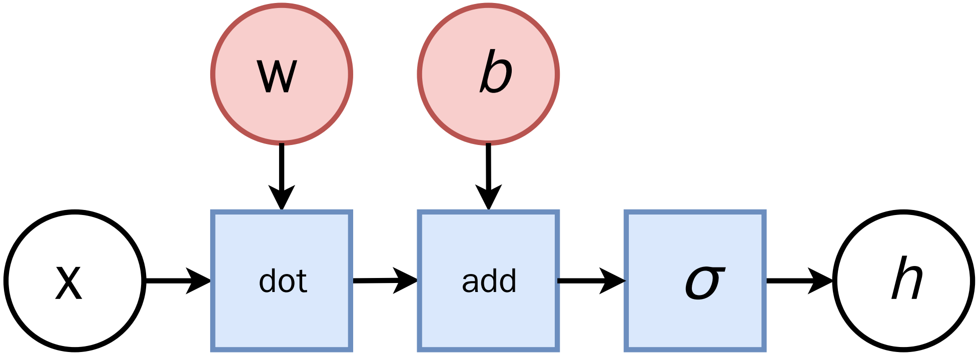
Note that the sigmoid function

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

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.



This unit is the lego brick of 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,

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

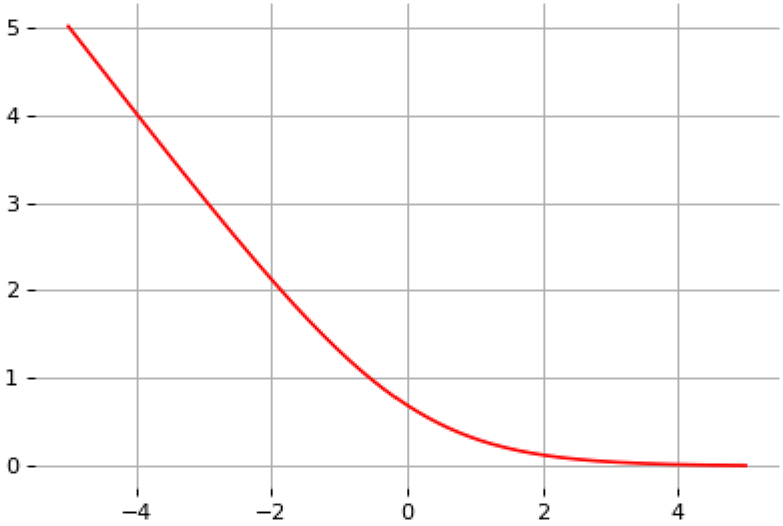
This loss is an instance of the cross-entropy

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

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.

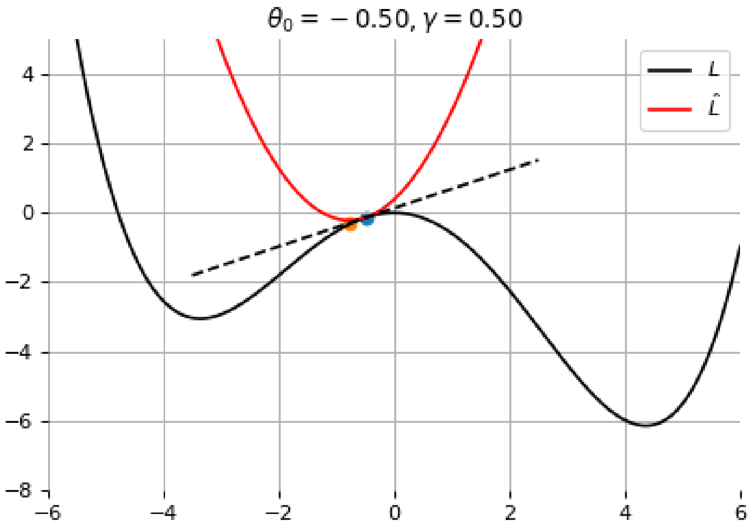
Gradient descent

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

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

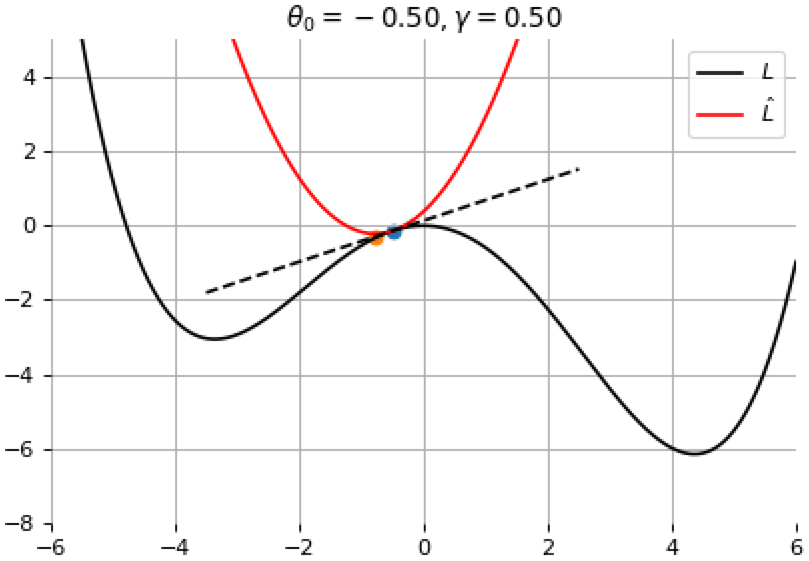
which results in the best improvement for the step $\epsilon = -\gamma \nabla_\theta \mathcal{L}(\theta_0)$.

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

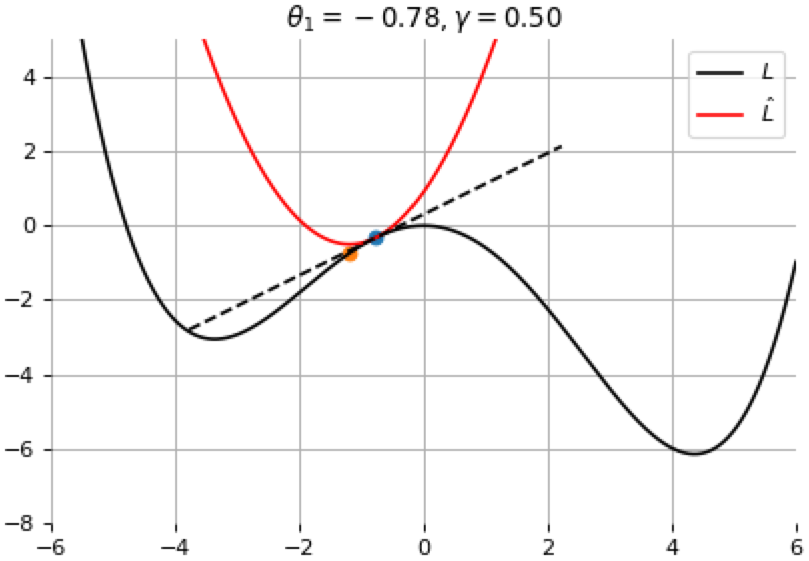
$$\theta_{t+1} = \theta_t - \gamma \nabla_\theta \mathcal{L}(\theta_t),$$

where

- 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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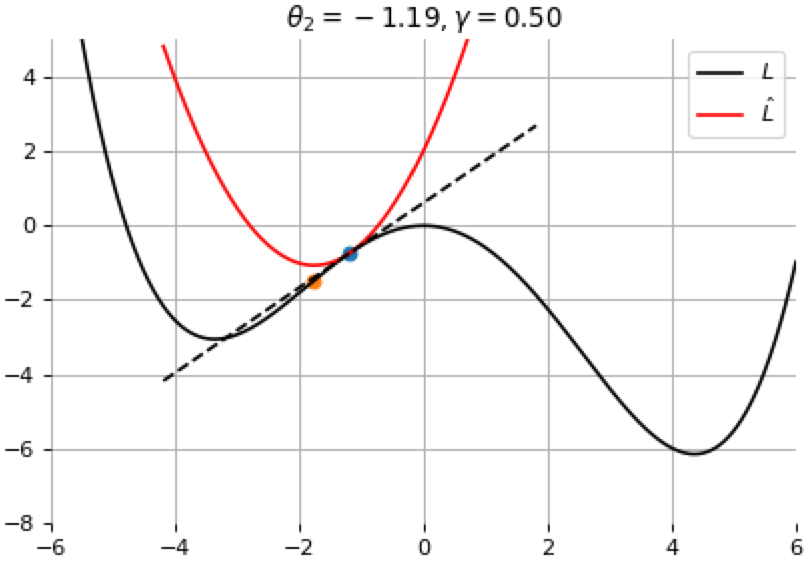

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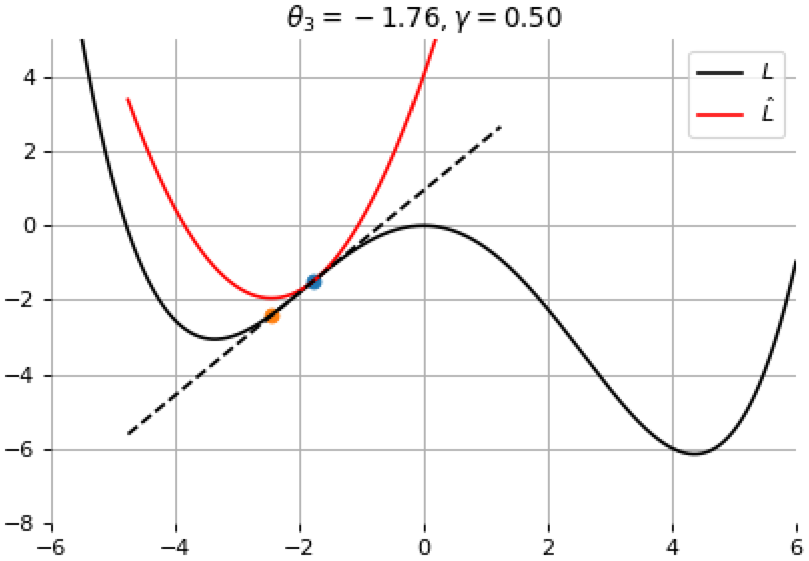

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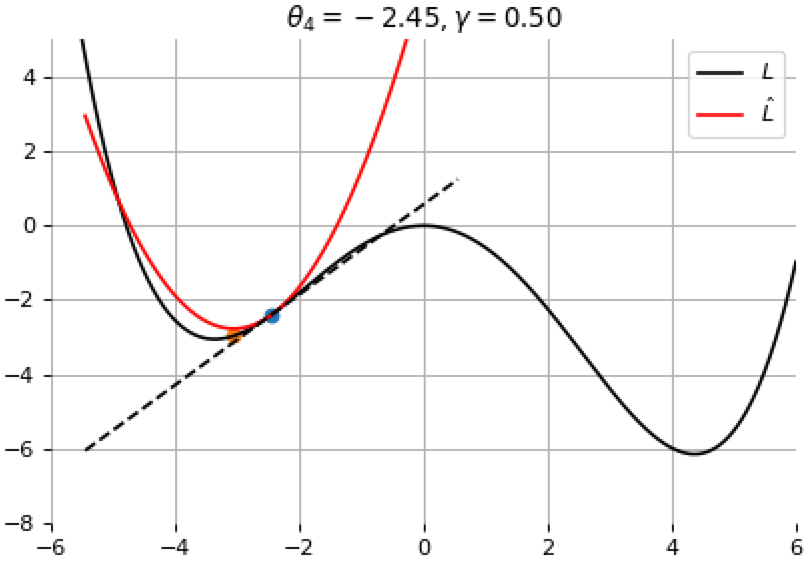

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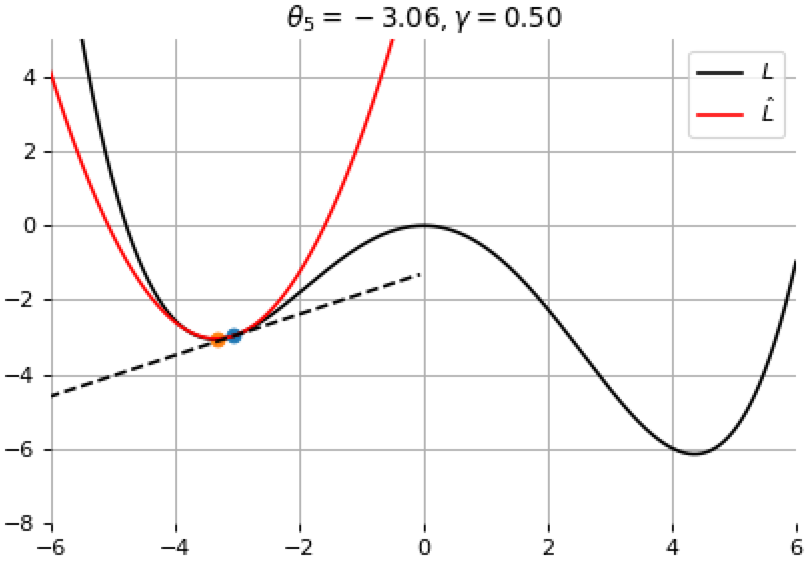

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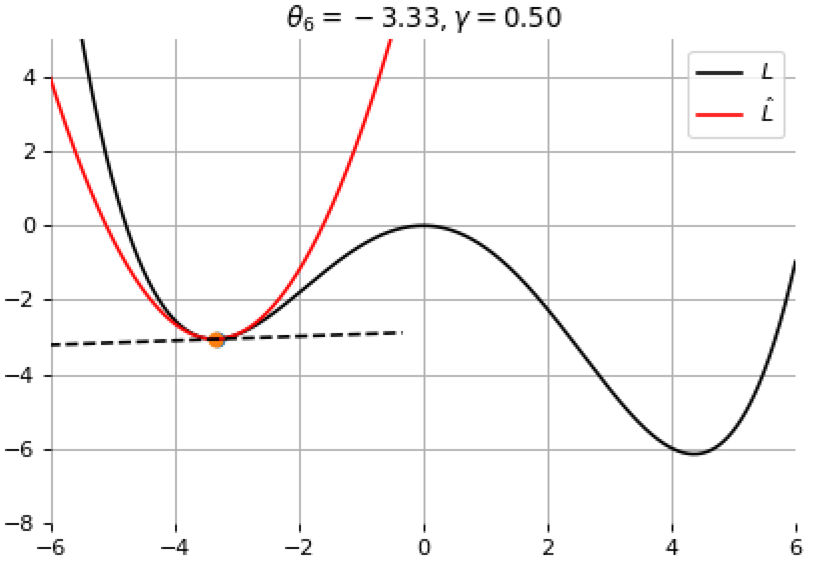

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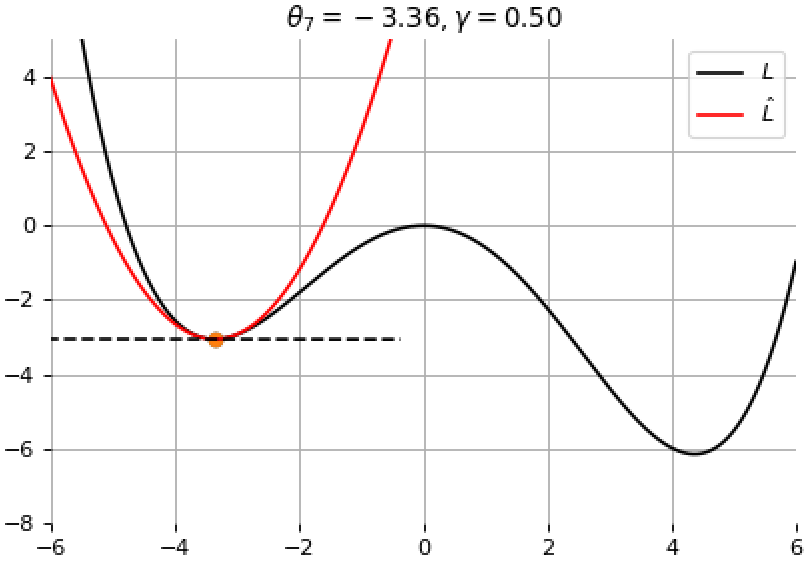

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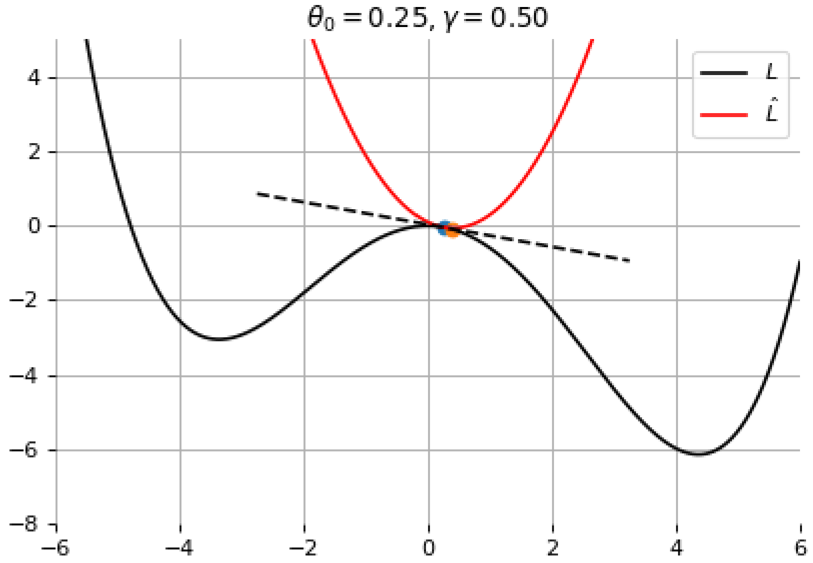
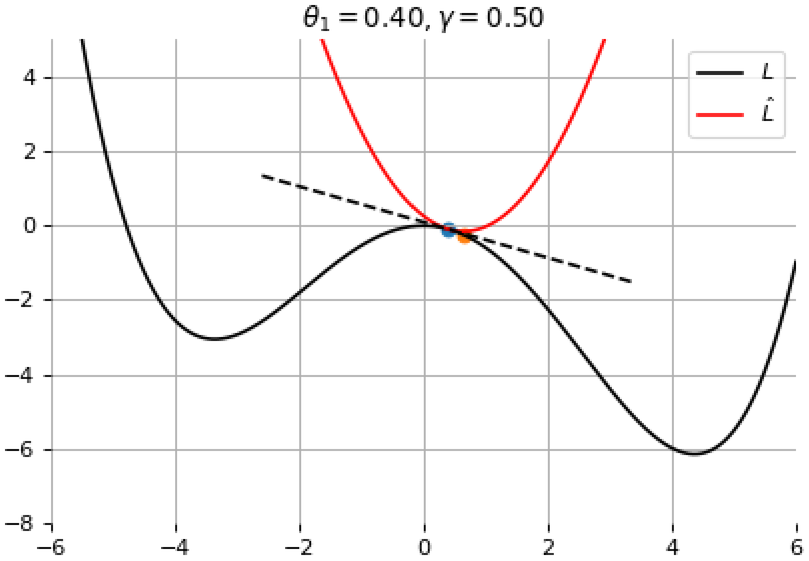


Example 2: Convergence to the global minima



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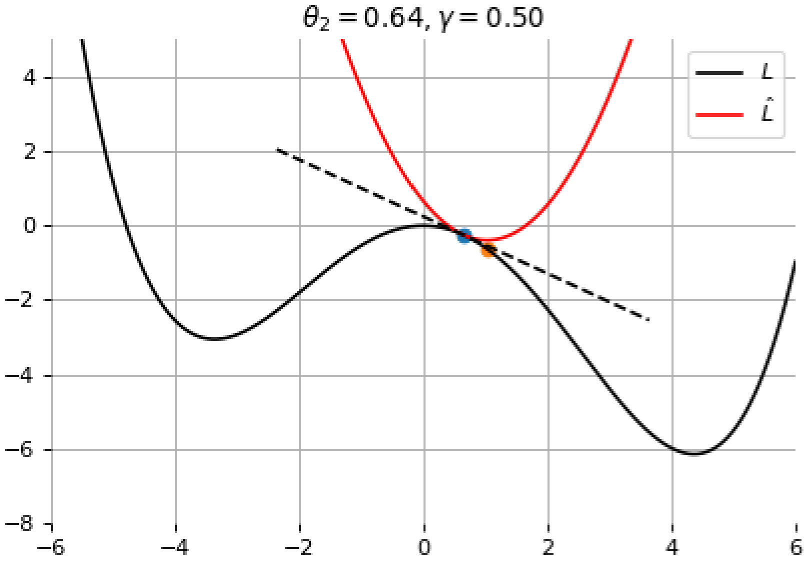

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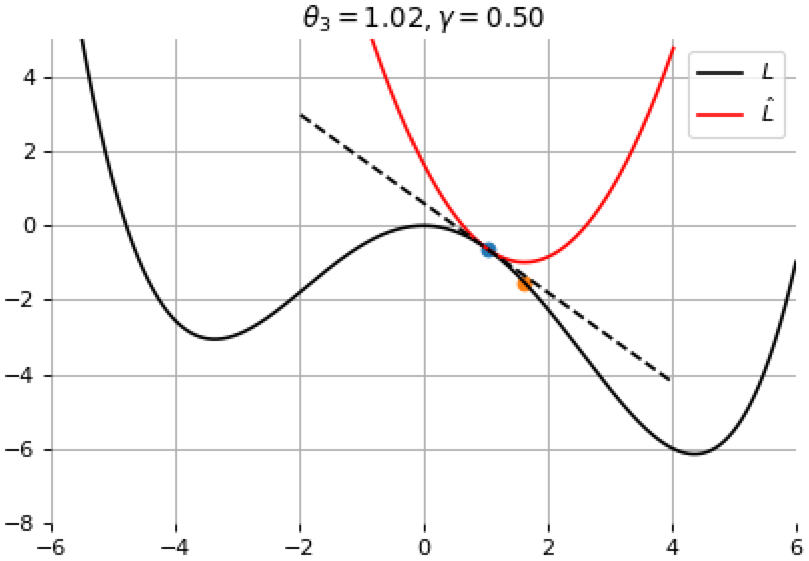

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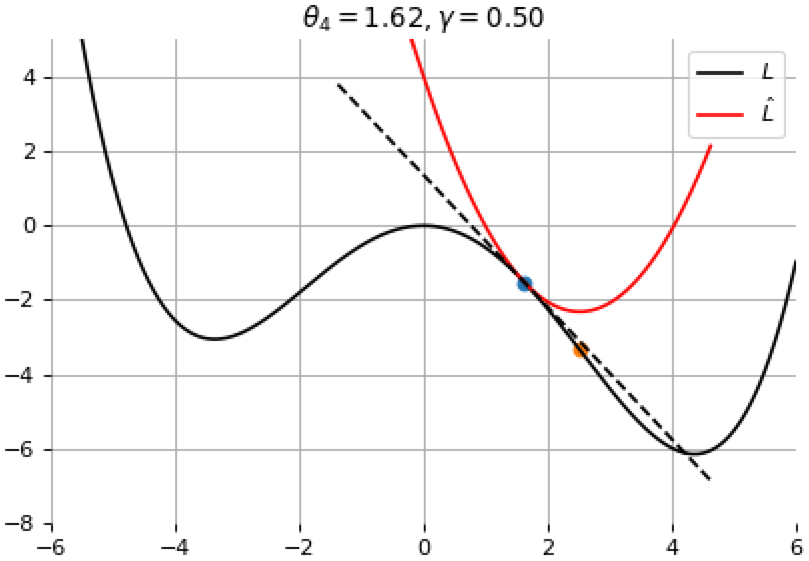

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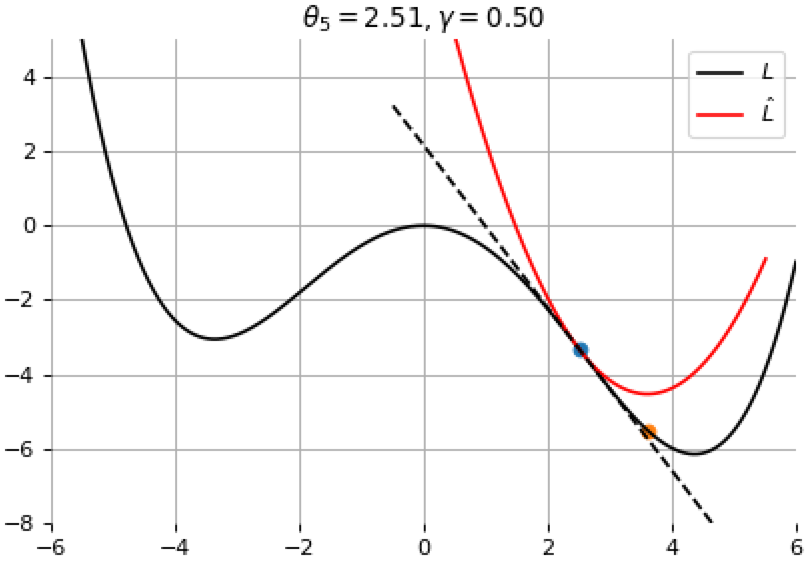

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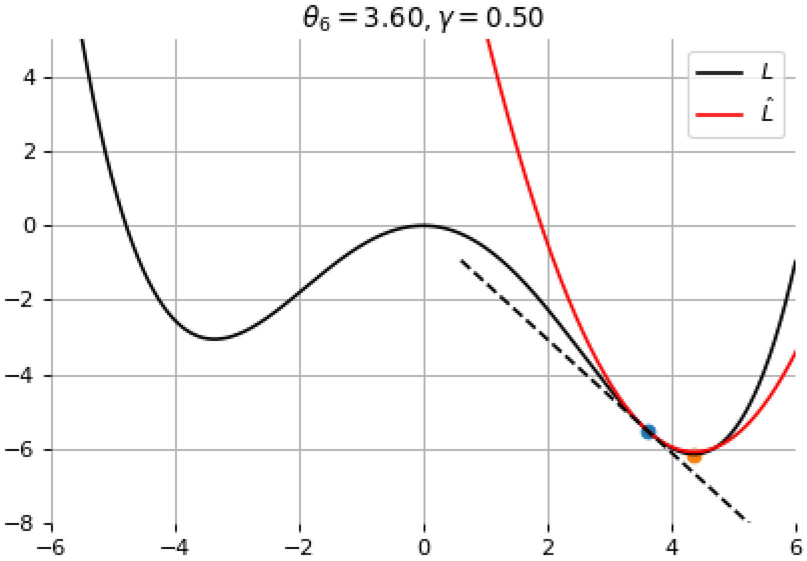

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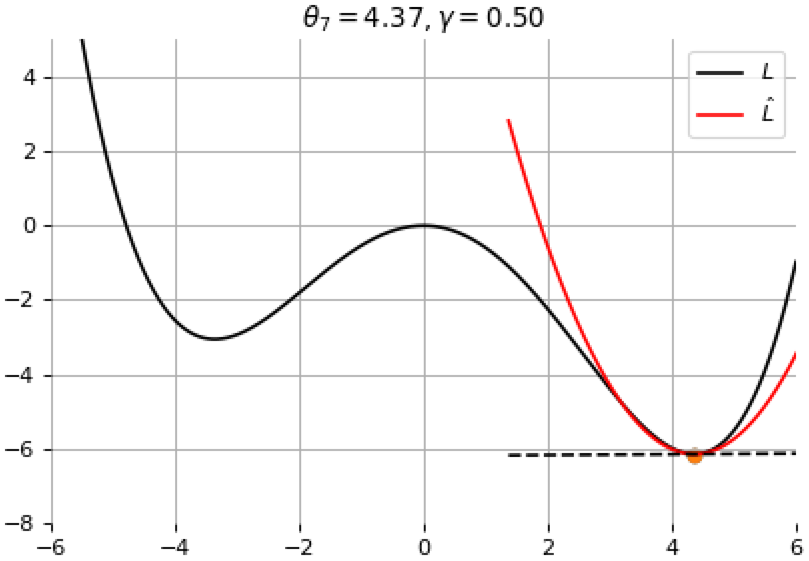

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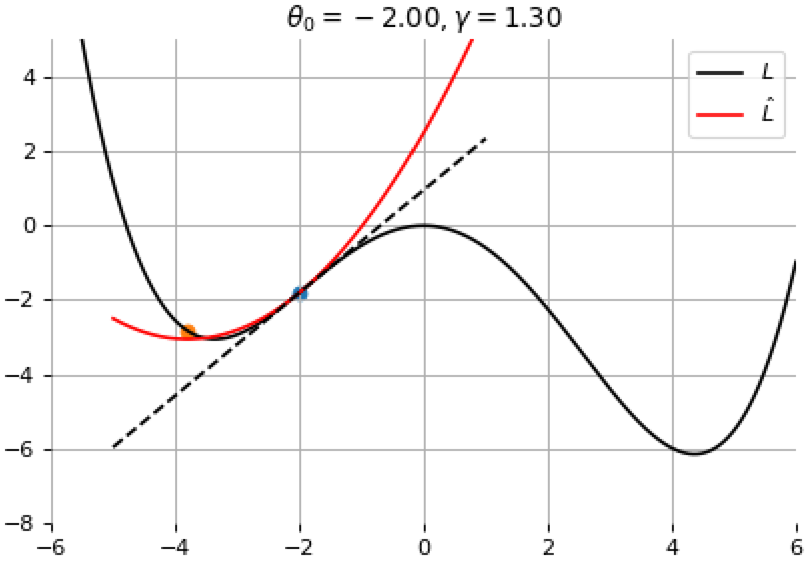
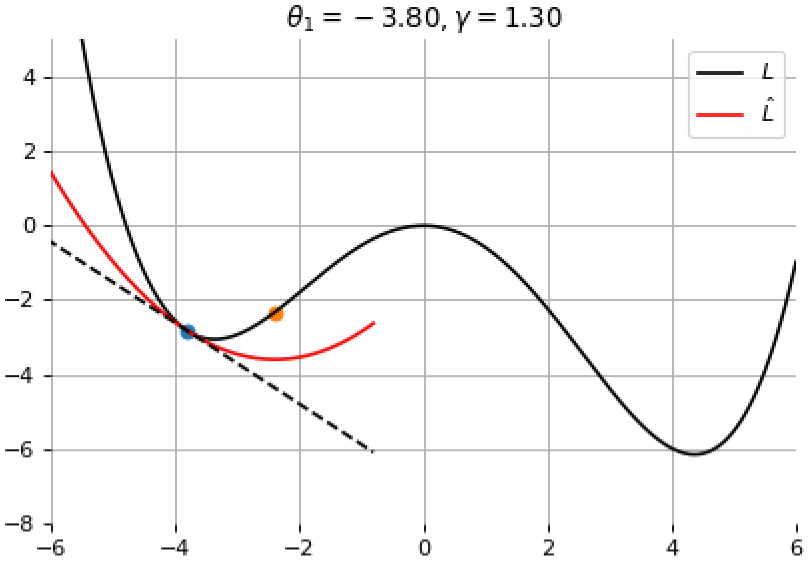


Example 3: Divergence due to a too large learning rate



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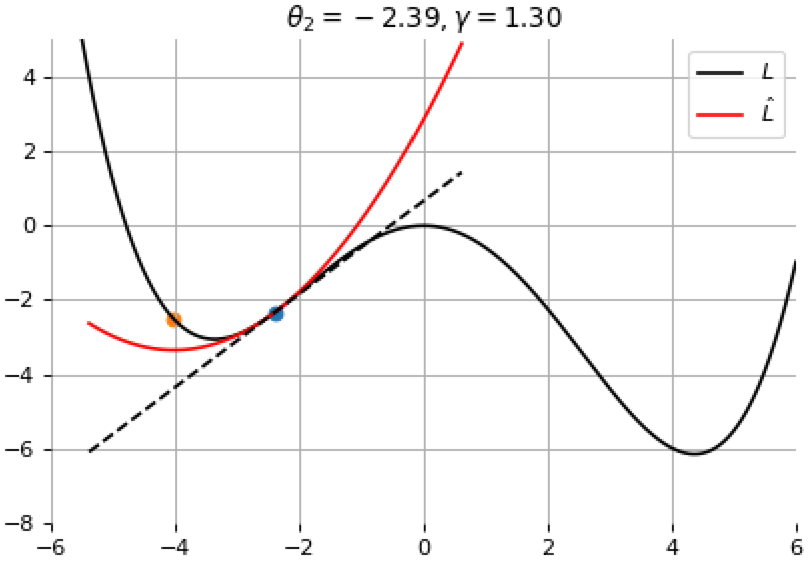

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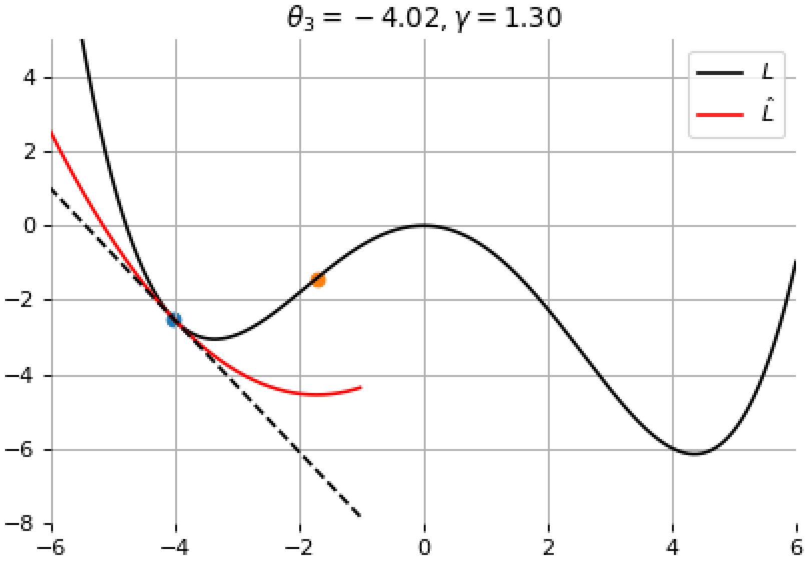

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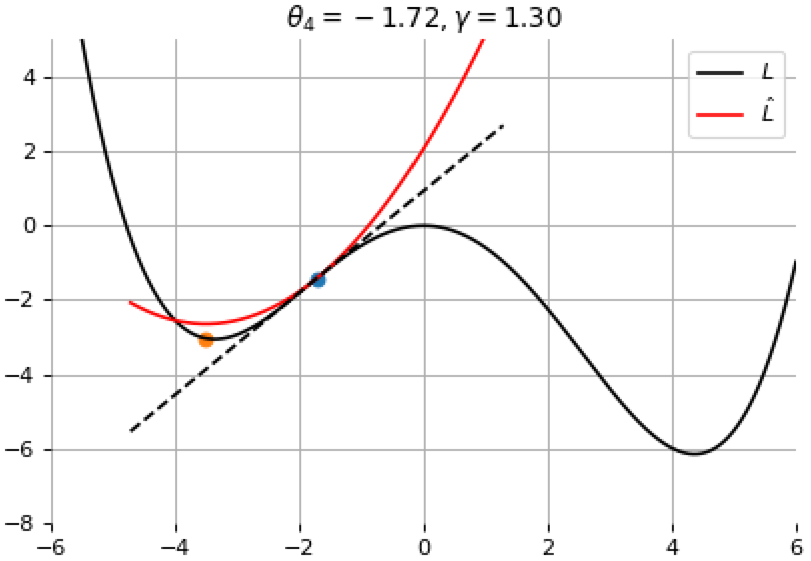

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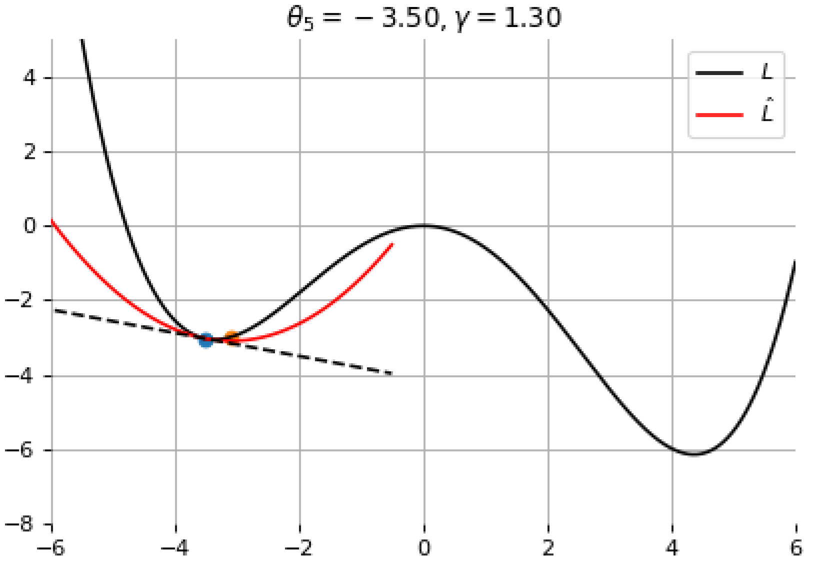

Example 3: Divergence due to a too large learning rate

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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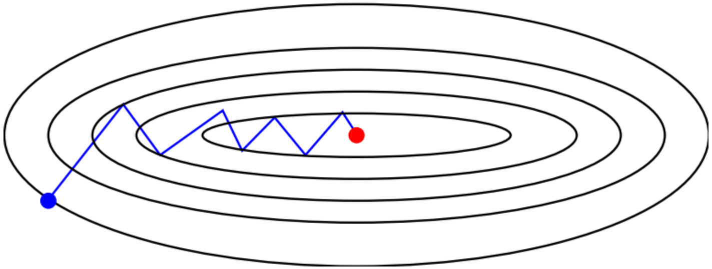
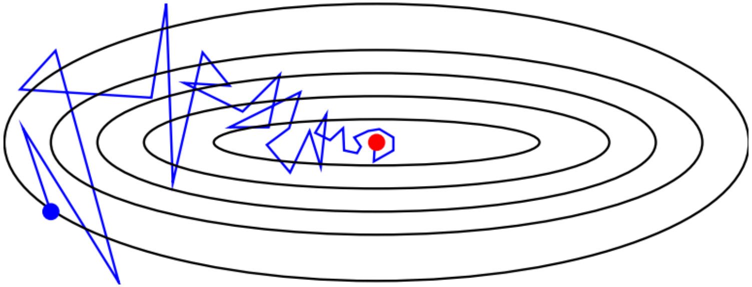


Batch gradient descent



Stochastic gradient descent

Why is stochastic gradient descent still a good idea?

- Informally, averaging the update

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

  over all choices $i(t+1)$ restores batch gradient descent.

- Formally, if the gradient estimate is unbiased, e.g., if

$$\begin{aligned} \mathbb{E}_{i(t+1)}[\nabla \ell(y_{i(t+1)}, f(\mathbf{x}_{i(t+1)}; \theta_t))] &= \frac{1}{N} \sum_{\mathbf{x}_i, y_i \in \mathbf{d}} \nabla \ell(y_i, f(\mathbf{x}_i; \theta_t)) \\ &= \nabla \mathcal{L}(\theta_t) \end{aligned}$$

  then the formal convergence of SGD can be proved, under appropriate assumptions (see references).

- Interestingly, if training examples $\mathbf{x}_i, y_i \sim P_{X,Y}$ are received and used in an online fashion, then SGD directly minimizes the expected risk.

When decomposing the excess error in terms of approximation, estimation and optimization errors, stochastic algorithms yield the best generalization performance (in terms of expected risk) despite being the worst optimization algorithms (in terms of empirical risk) (Bottou, 2011).

$$\begin{aligned}
&\mathbb{E}\left[R(\tilde{f}_*^{\mathbf{d}}) - R(f_B)\right] \\
&= \mathbb{E}\left[R(f_*) - R(f_B)\right] + \mathbb{E}\left[R(f_*^{\mathbf{d}}) - R(f_*)\right] + \mathbb{E}\left[R(\tilde{f}_*^{\mathbf{d}}) - R(f_*^{\mathbf{d}})\right] \\
&= \mathcal{E}_{\text{app}} + \mathcal{E}_{\text{est}} + \mathcal{E}_{\text{opt}}
\end{aligned}$$

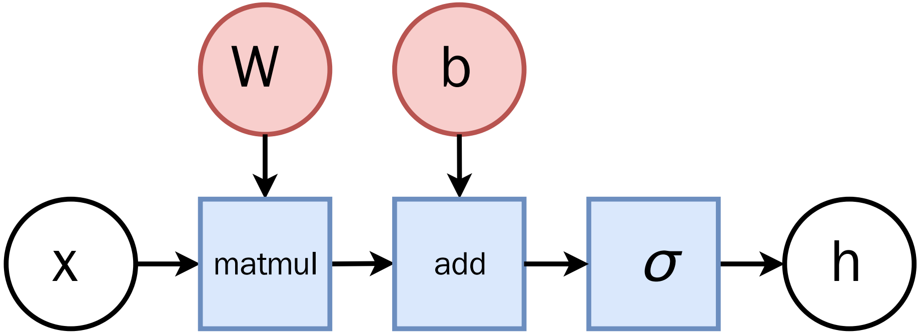
Layers

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.



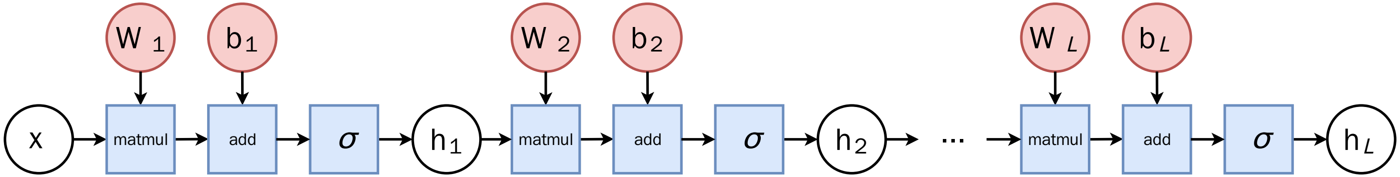
Multi-layer perceptron

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

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

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.


W 1
b1
W 2
b2
W L
bL
x
matmul
add
σ
h1
matmul
add
σ
h2
...
matmul
add
σ
hL

Classification

- For binary classification, the width q of the last layer L is set to 1, which results in a single output $h_L \in [0, 1]$ that models the probability $P(Y = 1|\mathbf{x})$.
- For multi-class classification, the sigmoid action σ in the last layer can be generalized to produce a (normalized) vector $\mathbf{h}_L \in [0, 1]^C$ of probability estimates $P(Y = i|\mathbf{x})$.

  This activation is the Softmax function, where its i-th output is defined as

$$\text{Softmax}(\mathbf{z})_i = \frac{\exp(z_i)}{\sum_{j=1}^{C} \exp(z_j)},$$

for $i = 1, ..., C$.

Regression

The last activation σ can be skipped to produce unbounded output values $h_L \in \mathbb{R}$.

Automatic differentiation

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

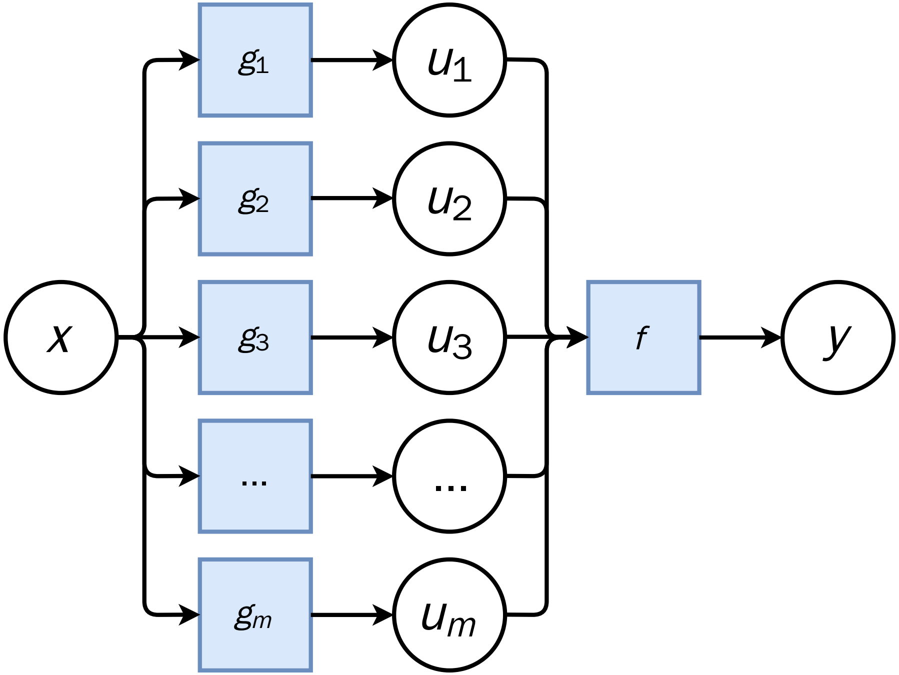
Therefore, we require the evaluation of the (total) derivatives

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

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.

Chain rule



Let us consider a 1-dimensional output composition $f \circ g$, such that

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

The chain rule states that $(f \circ g)' = (f' \circ g)g'$.

For the total derivative, the chain rule generalizes to

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

Reverse automatic differentiation

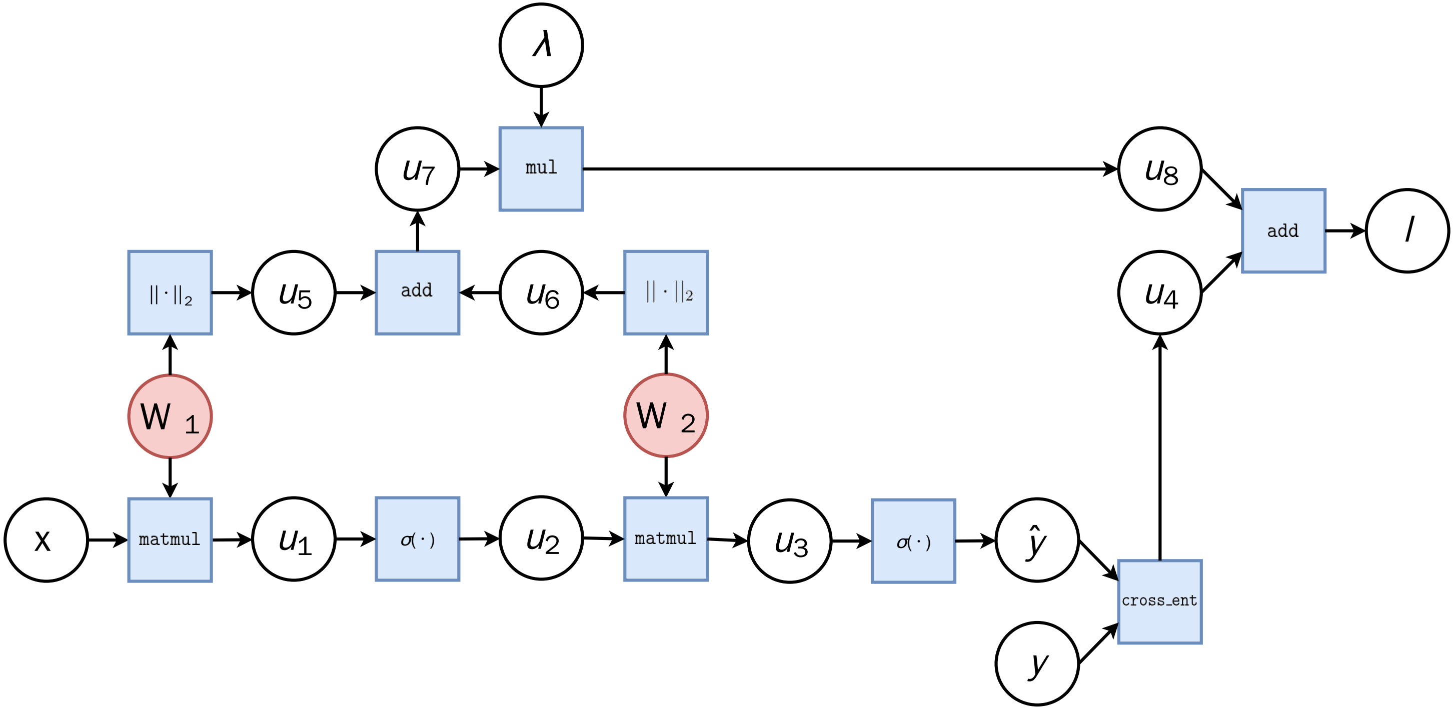
- Since a neural network is a composition of differentiable functions, the total derivatives of the loss can be evaluated backward, by applying the chain rule recursively over its computational graph.
- The implementation of this procedure is called reverse automatic differentiation.

Let us consider a simplified 2-layer MLP and the following loss function:

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

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

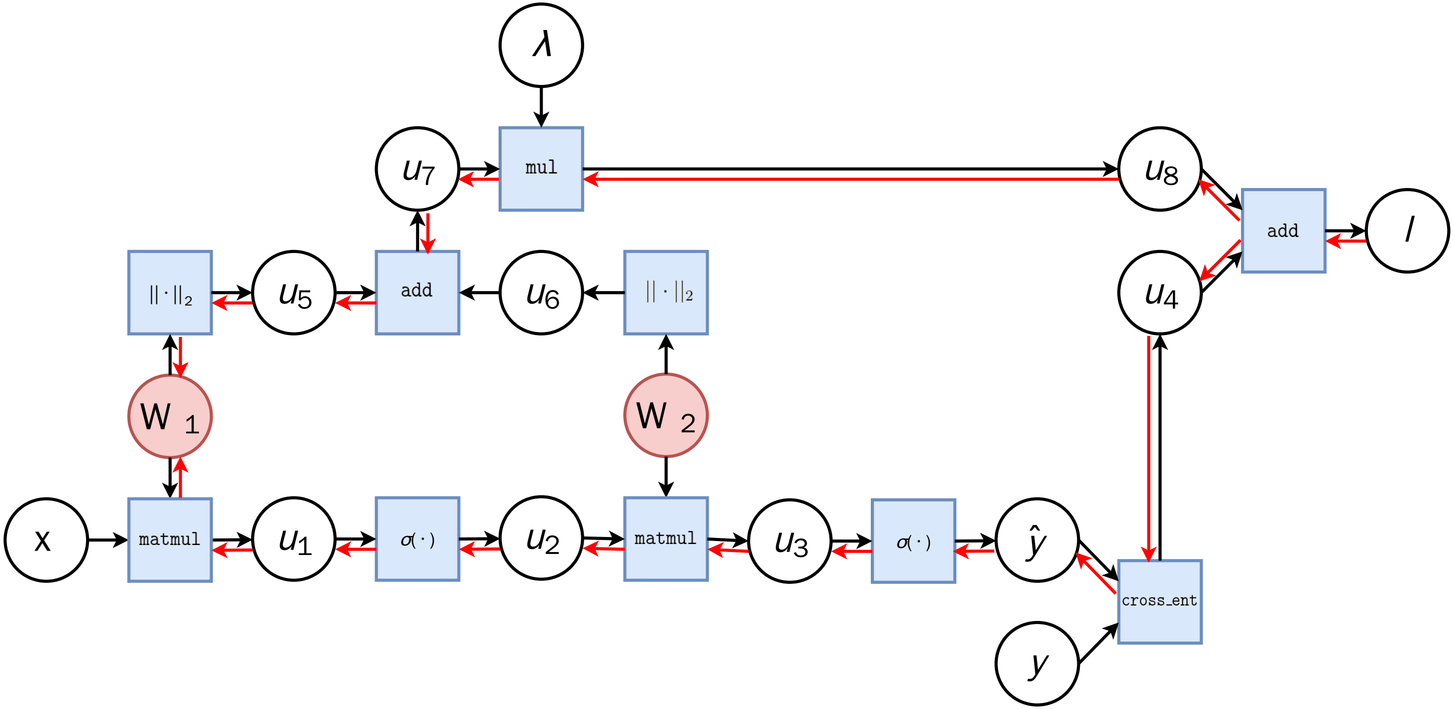
In the forward pass, intermediate values are all computed from inputs to outputs, which results in the annotated computational graph below:

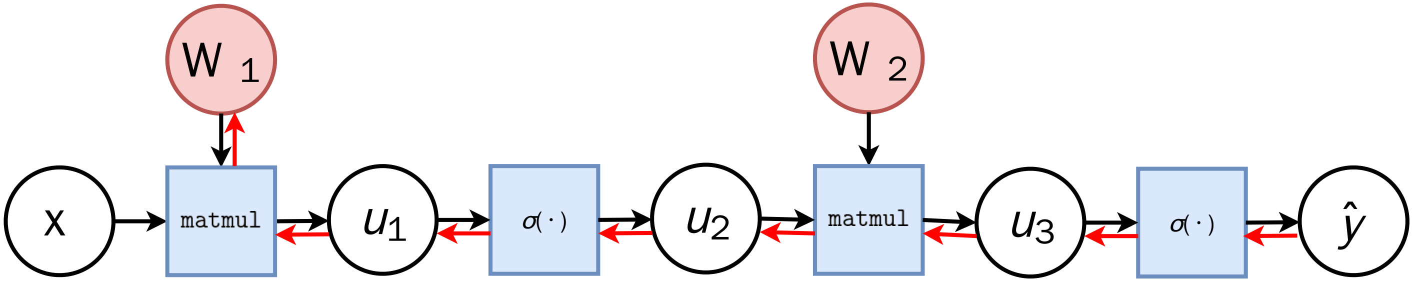


The total derivative can be computed through a backward pass, by walking through all paths from outputs to parameters in the computational graph and accumulating the terms. For example, for $\frac{\mathrm{d}\ell}{\mathrm{d}\mathbf{W}_1}$ we have:

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

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





Let us zoom in on the computation of the network output $\hat{y}$ and of its derivative with respect to $\mathbf{W}_1$.

- Forward pass: values u_1, u_2, u_3 and $\hat{y}$ are computed by traversing the graph from inputs to outputs given $\mathbf{x}$, $\mathbf{W}_1$ and $\mathbf{W}_2$.
- Backward pass: by the chain rule we have

$$\begin{aligned}\frac{\mathrm{d}\hat{y}}{\mathrm{d}\mathbf{W}_1} &= \frac{\partial \hat{y}}{\partial u_3}\frac{\partial u_3}{\partial u_2}\frac{\partial u_2}{\partial u_1}\frac{\partial u_1}{\partial \mathbf{W}_1} \\ &= \frac{\partial \sigma(u_3)}{\partial u_3}\frac{\partial \mathbf{W}_2^T u_2}{\partial u_2}\frac{\partial \sigma(u_1)}{\partial u_1}\frac{\partial \mathbf{W}_1^T u_1}{\partial \mathbf{W}_1}\end{aligned}$$

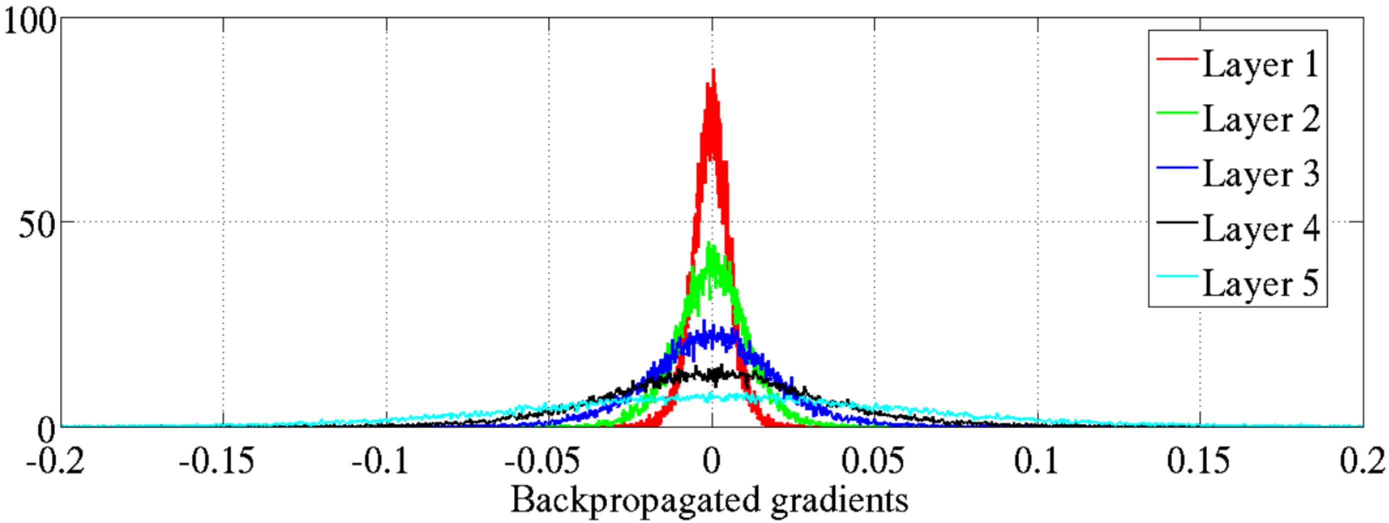
Note how evaluating the partial derivatives requires the intermediate values computed forward.

- This algorithm is also known as backpropagation.
- An equivalent procedure can be defined to evaluate the derivatives in forward mode, from inputs to outputs.
- Since differentiation is a linear operator, automatic differentiation can be implemented efficiently in terms of tensor operations.

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.

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

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

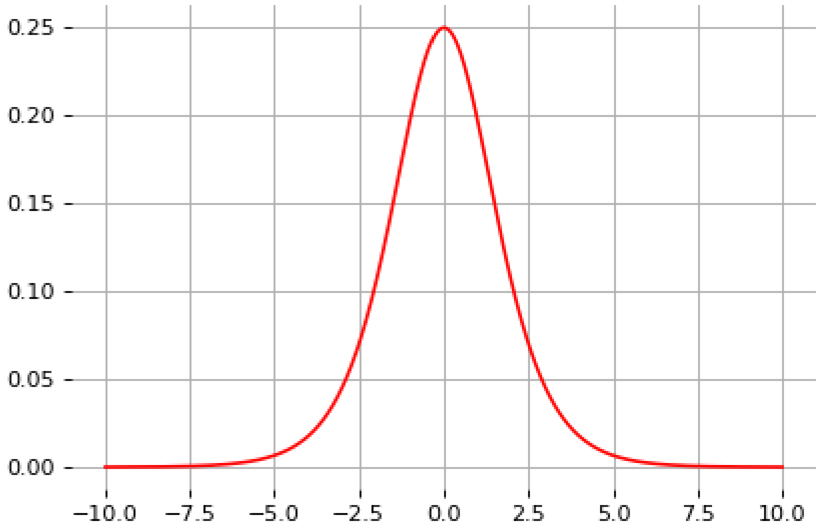
Under the hood, this would be evaluated as

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

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.

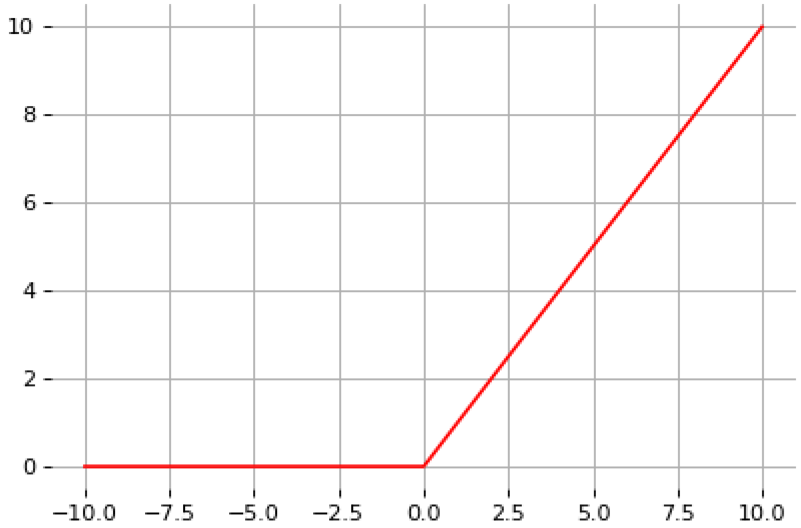
Hence the vanishing gradient problem.

- 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

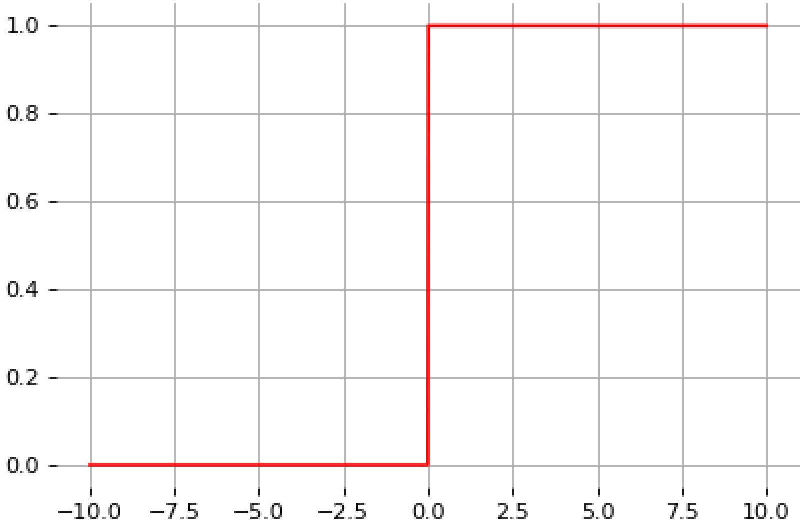
Instead of the sigmoid activation function, modern neural networks are for most based on rectified linear units (ReLU) (Glorot et al, 2011):

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



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

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

  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 $v_i, w_i, b_i, i = 1, ..., q$ 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).

Theorem (Barron, 1992) The mean integrated square error between the estimated network $\hat{F}$ and the target function f is bounded by

$$O\left(\frac{C_f^2}{q} + \frac{qp}{N}\log N\right)$$

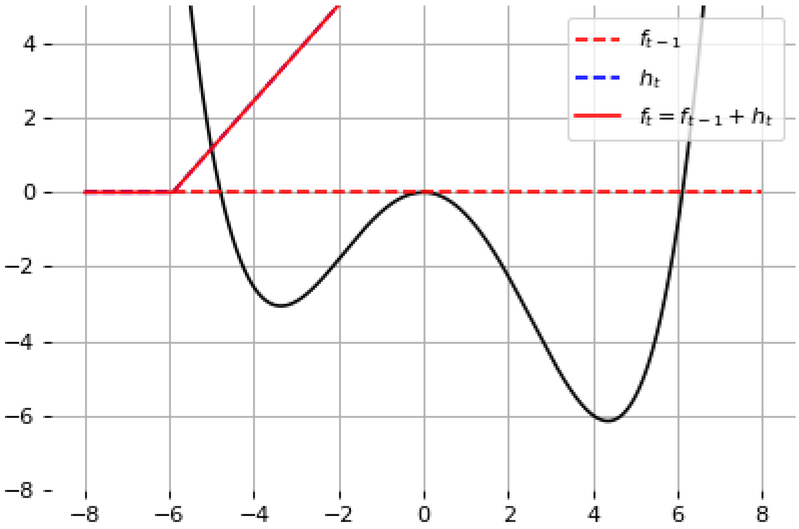
where N is the number of training points, q is the number of neurons, p is the input dimension, and C_f measures the global smoothness of f.

- Combines approximation and estimation errors.
- Provided enough data, it guarantees that adding more neurons will result in a better approximation.

Let us consider the 1-layer MLP

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

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



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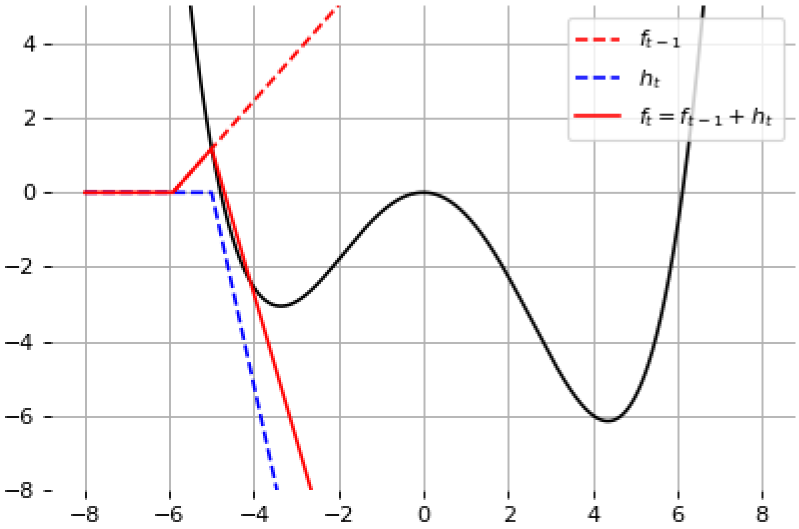

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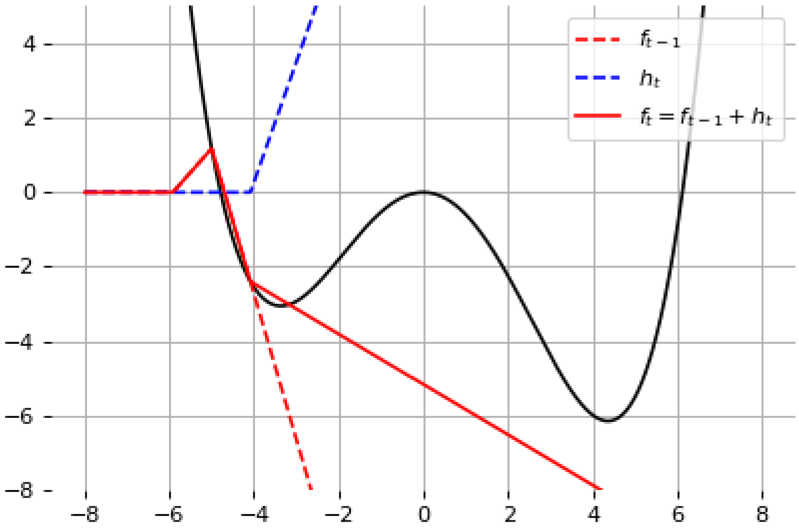

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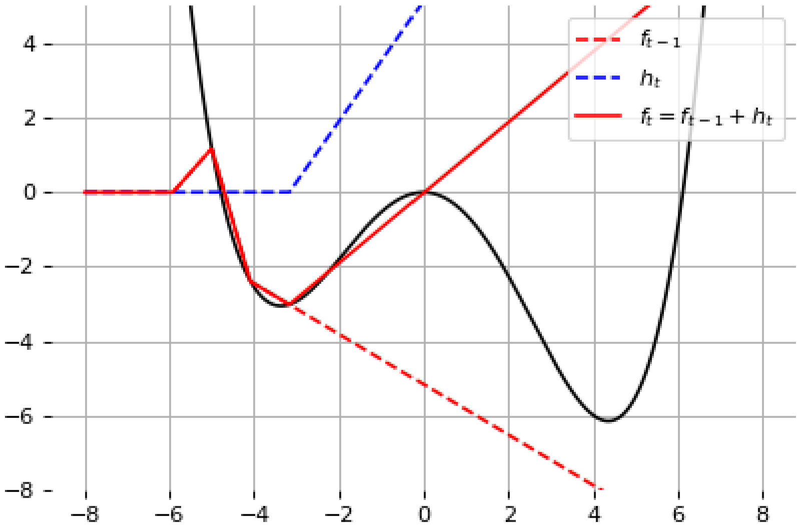

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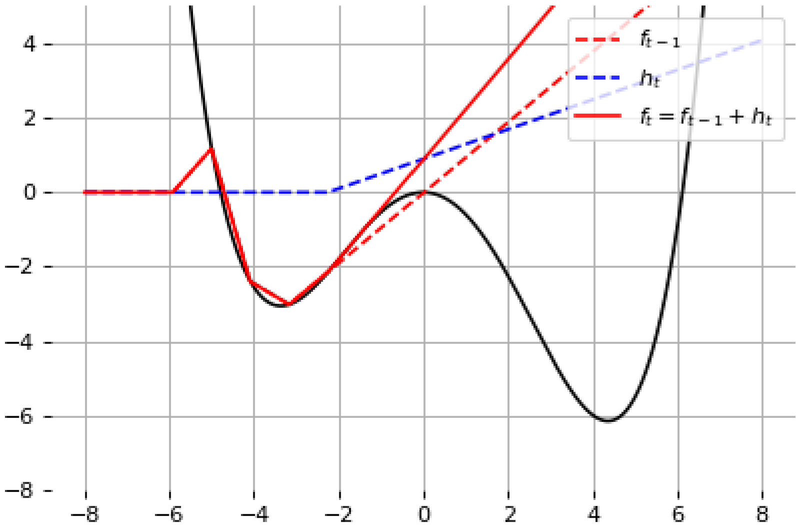

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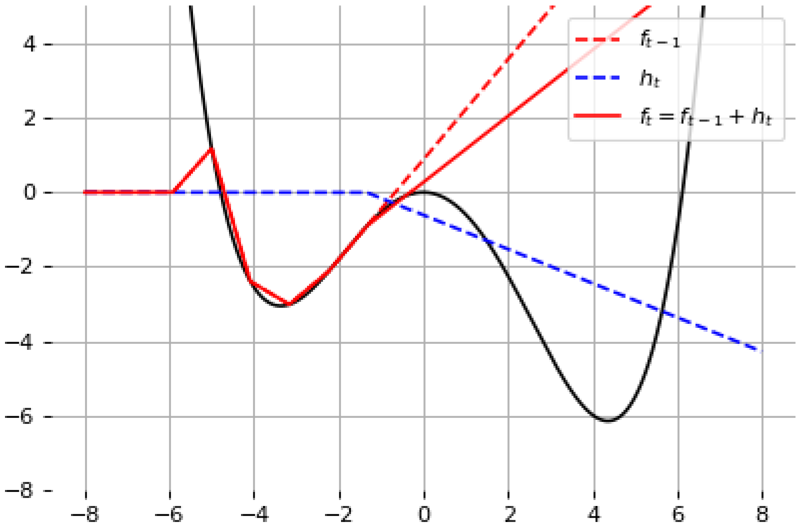

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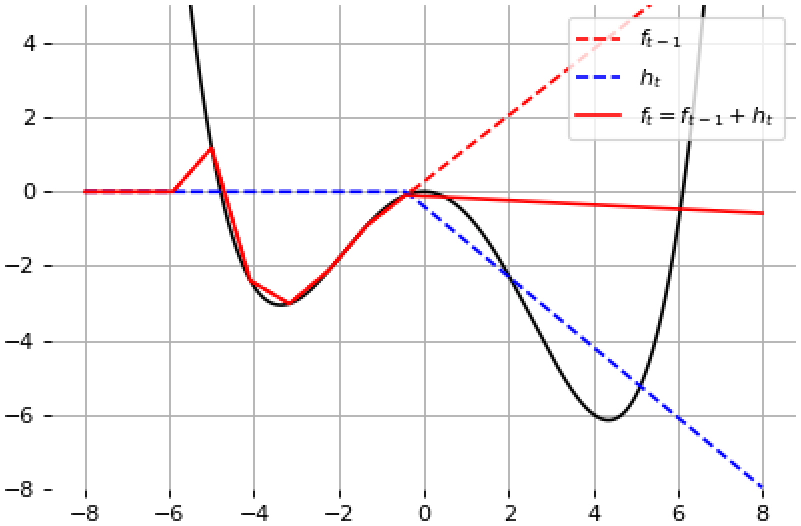

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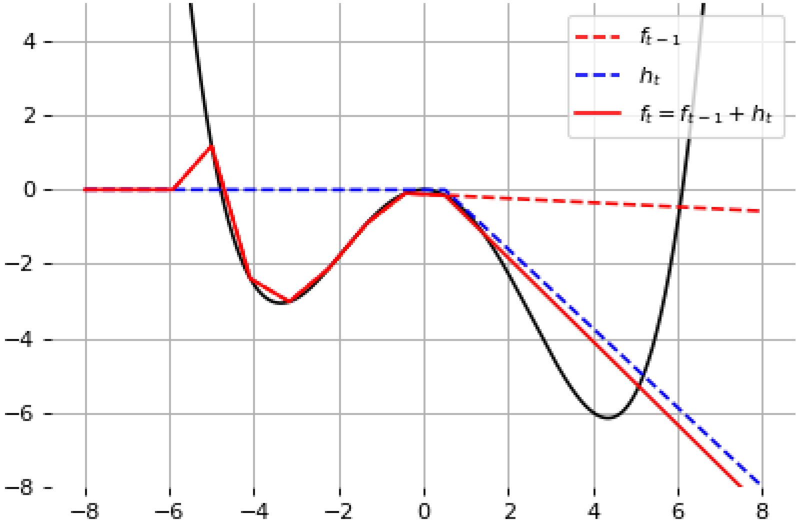

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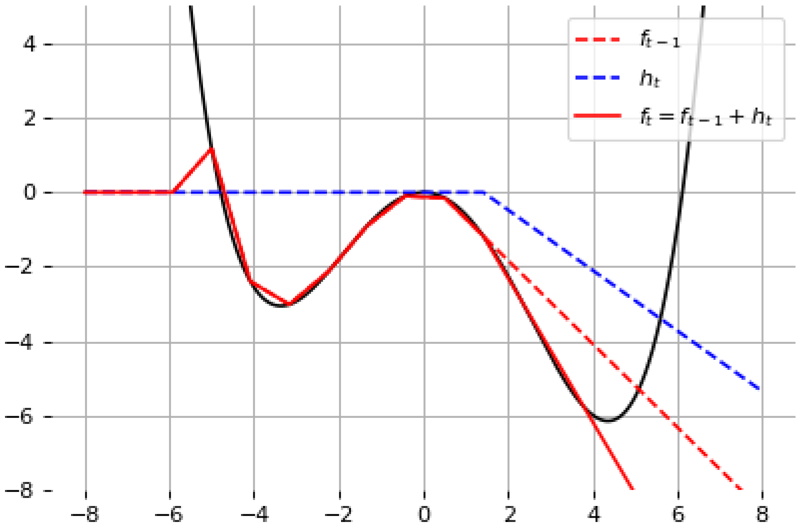

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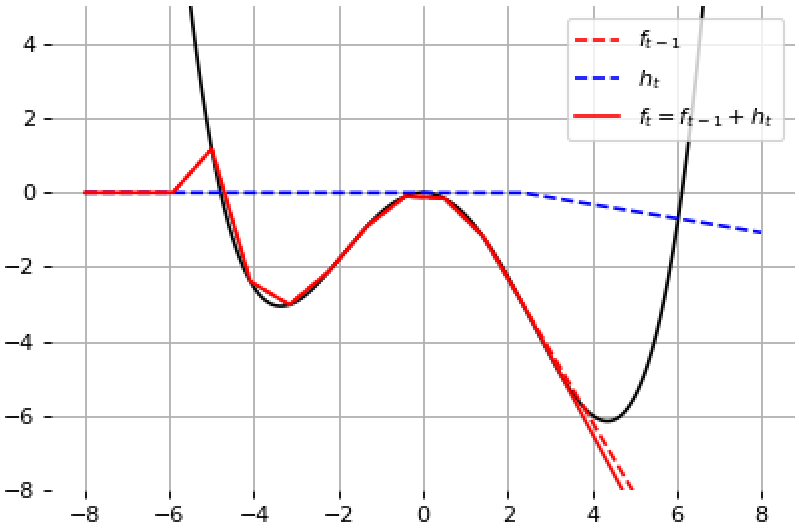

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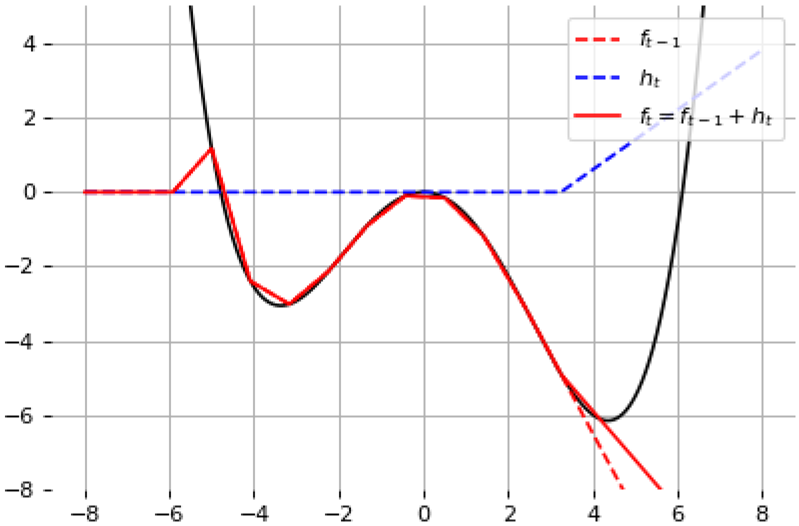

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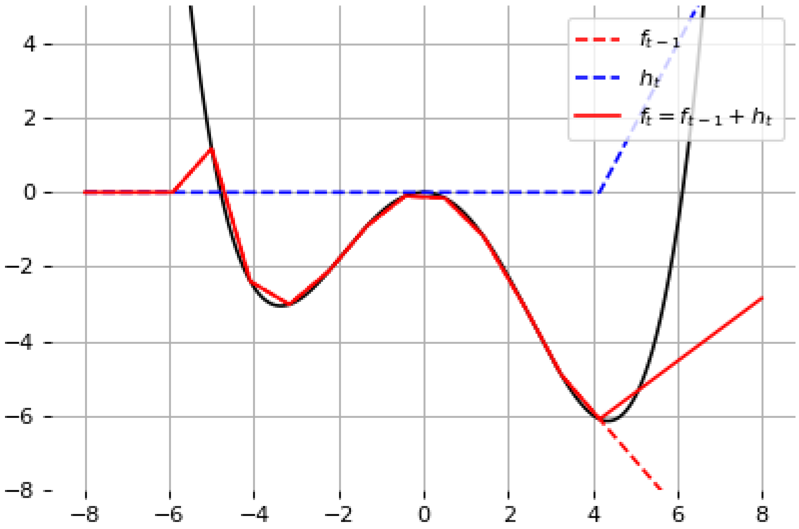

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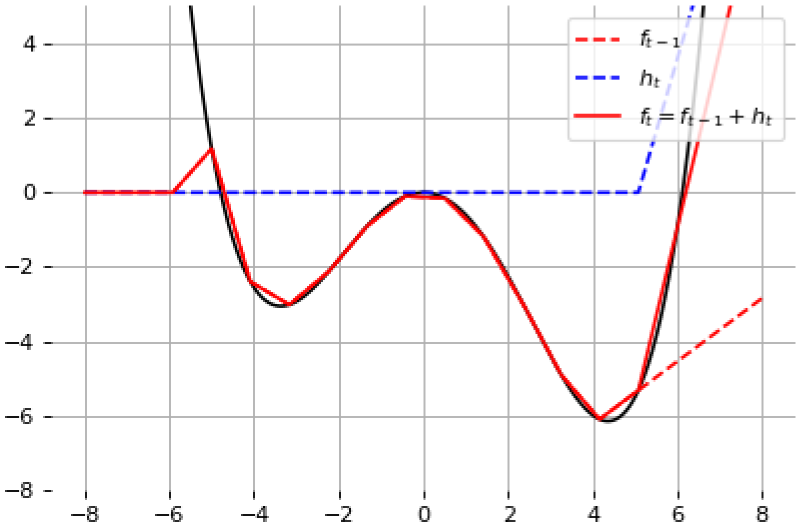
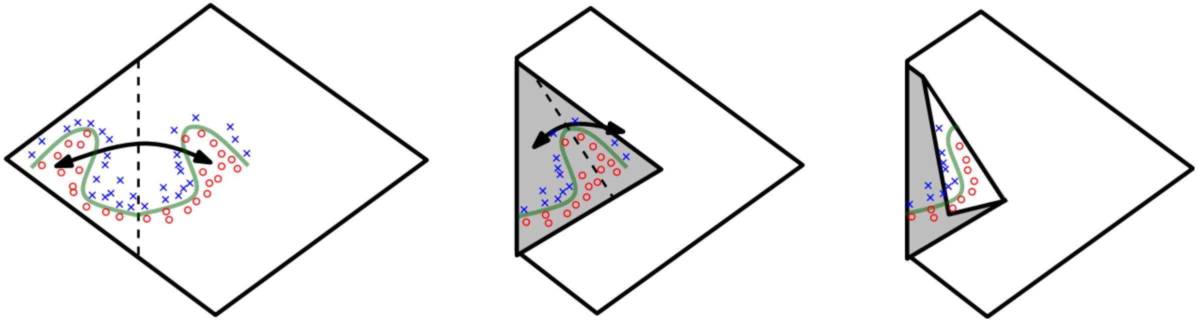


Effect of depth



Theorem (Montúfar et al, 2014) A rectifier neural network with p input units and L hidden layers of width $q \geq p$ can compute functions that have $\Omega((\frac{q}{p})^{(L-1)p} q^p)$ linear regions.

- That is, the number of linear regions of deep models grows exponentially in L and polynomially in q.
- Even for small values of L and q, deep rectifier models are able to produce substantially more linear regions than shallow rectifier models.

Deep learning

Recent advances and model architectures in deep learning are built on a natural generalization of a neural network: a graph of tensor operators, taking advantage of

- the chain rule
- stochastic gradient descent
- convolutions
- parallel operations on GPUs.

This does not differ much from networks from the 90s, as covered in Today's lecture.

Credits: Francois Fleuret, EE559 Deep Learning, EPFL.

This generalization allows to compose and design complex networks of operators, possibly dynamically, dealing with images, sound, text, sequences, etc. and to train them end-to-end.

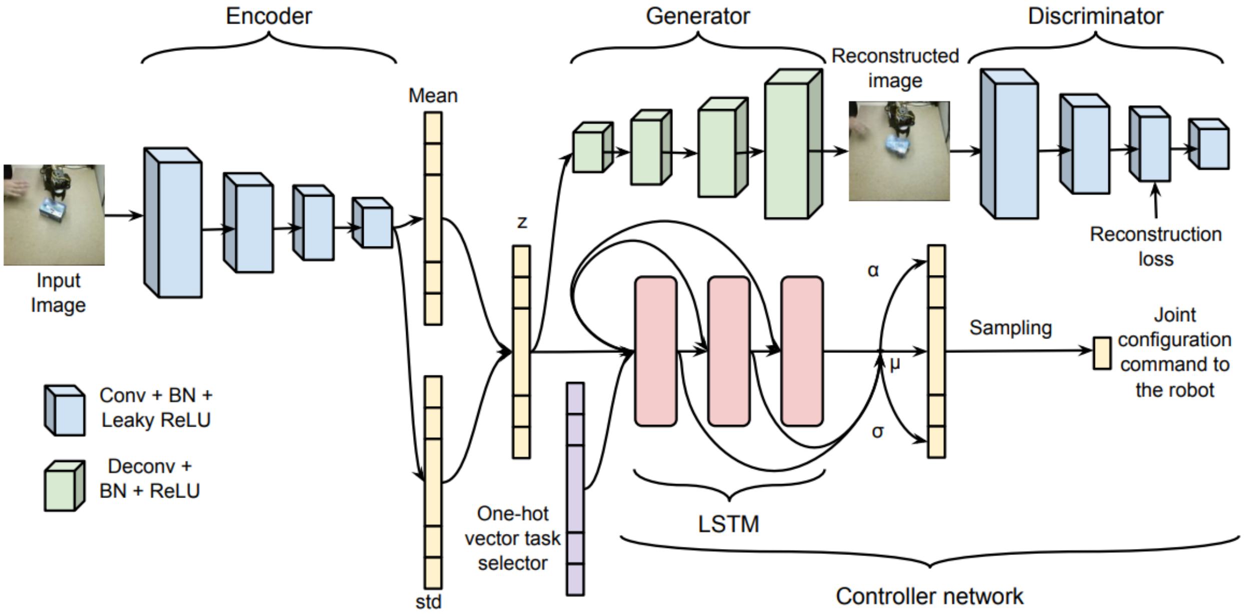


Fig. 2: Our proposed architecture for multi-task robot manipulation learning. The neural network consists of a controller network that outputs joint commands based on a multi-modal autoregressive estimator and a VAE-GAN autoencoder that reconstructs the input image. The encoder is shared between the VAE-GAN autoencoder and the controller network and extracts some shared features that will be used for two tasks (reconstruction and controlling the robot).

Credits: Francois Fleuret, EE559 Deep Learning, EPFL; Rahmatizadeh et al, 2017, arXiv:1707.02920.

The end.

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