Lecture 3:
A primer on fundamentals of deep learning

Advanced deep learning

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About this course

- Goal: In-depth understanding of important Deep Learning staples
  - Reinforce what you have already seen
  - Introduce state of the art models

- This is a hands-on course in pytorch
  - Minimal math
    - Enough to understand
  - Quite a bit of coding
  - Get comfortable with the standard pipeline

Course organization: 10 Lectures

- L1-2: Overview of Deep Learning (F. Precioso)
- L3-4: Fundamentals of Deep Learning (R. Sun)
- L5-6: Transformers (R. Sun)
- L7: Large models (LLMs, VLMs, Generators) (R. Sun)
- L8-9: Intro to generative models (P-A. Mattei)
- Tricks of the trade (R. Sun)

Today!

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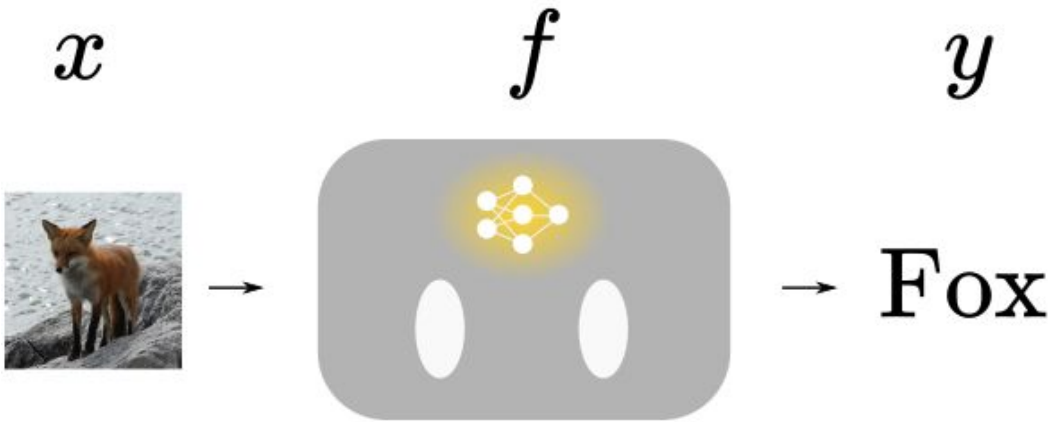
- Quick recap of deep learning fundamentals
  - Problem Statement and Empirical Risk Minimization
  - Neural Networks as classes of functions
  - Gradient Descent
  - Backpropagation

- Practical in pytorch: Training a MLP
  - Manual implementation
  - Progressive pytorch automation

1. Problem statement and risk

Problem statement: Ideal case



- Find (robot) f that classifies images well
  - Often based on neural networks

$$\forall (x, y) \in \mathcal{D}, f(x) = y$$

More formally

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- Definitions
  - X set of inputs
  - Y set of labels
  - $\Omega = X \times Y$
  - $\mathcal{D}$ Distribution over Ω with probability measure p

- Find function f: X -> Y such that

$$\forall (x, y) \in \mathcal{D}, f(x) = y$$

Assessing f with a criterion

- Finding exact correspondence functions is not always the thing to do
  - No exact matching
  - Other definitions of good solutions
  - Need to use restricted function space
    - Parametric function space

$$\mathcal{F} = \{f_\theta | \theta \in \mathbb{R}^d\}$$

- Introduce an assessment of how “good” f is with a loss l so that we try to have the lowest quantity $l(f(x), y)$

Minimizing Risk

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- Definitions
  - X set of inputs
  - Y set of labels
  - $\Omega = X \times Y$
  - $\mathcal{D}$ Distribution over Ω with probability measure p
  - l loss function assessing fit of f(x) to y
  - Find f in function space $\mathcal{F} = \{f_\theta | \theta \in \mathbb{R}^d\}$

- Minimize the ***Risk*** over the distribution

$$min_\theta \mathbb{E}_{x,y \sim \mathcal{D}}[l(f_\theta(x), y)]$$

Minimizing Risk

- Problem: we do not know $\mathcal{D}$!
  - Solved problem otherwise…
  - Evaluating the risk requires this distribution
- Solution: Use a dataset D of (x,y) sampled from $\mathcal{D}$
  - ***Empirical Risk Minimization***
  - If the (x,y) are i.i.d drawn from $\mathcal{D}$ can be expressed as a mean over the dataset

$$min_{\theta}\hat{\mathcal{R}}_{\theta} = \frac{1}{N}\sum_{i=0,\dots,N-1} l(f_{\theta}(x_i), y_i)$$

Takeaway

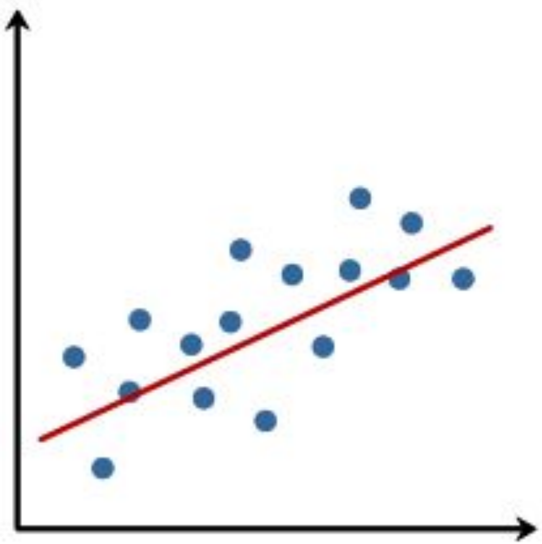
- Core problem: Find function matching inputs to outputs for any (x,y) of the target distribution

- Optimize over family of parametric functions
  - Assess functions with loss criterion

- Minimize the Risk function
  - Empirical Risk Minimization in practice

2. Example: linear regression

Linear problem

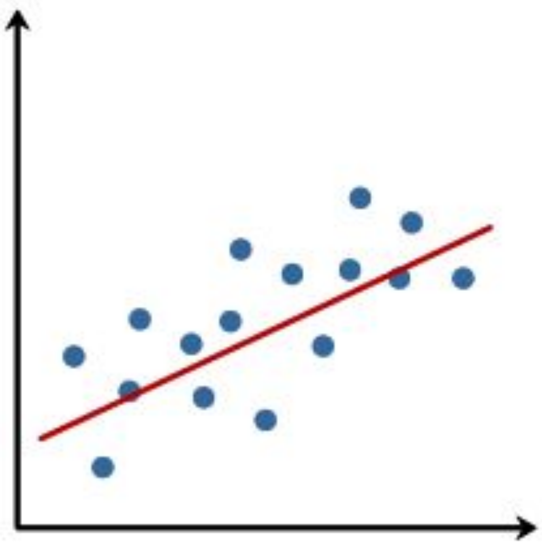


- Linearly correlated data
  - Input x (e.g. Voltage)
  - Output y (e.g. Intensity)

- Simple family of linear functions
  - Find linear coefficient

$$f_\theta(x) = \theta x$$

Minimization



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- Minimize the risk

Minimization

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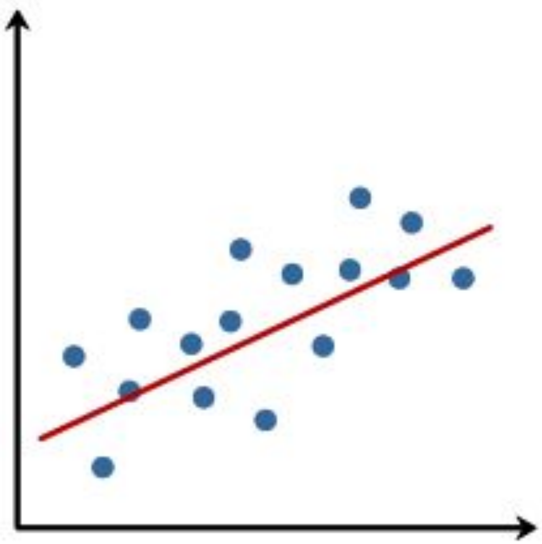
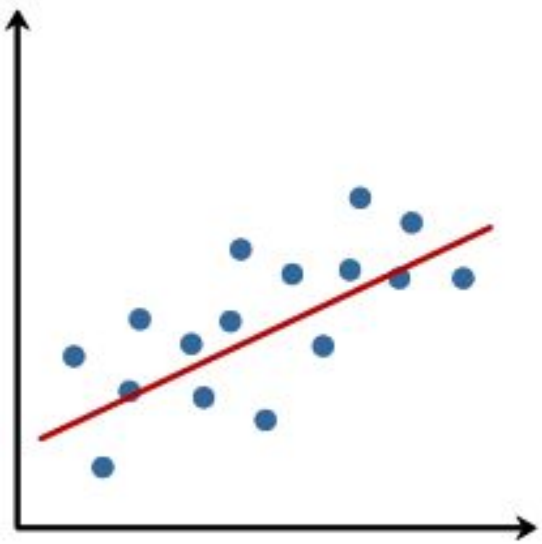


$$f_\theta(x) = \theta x$$

- Minimize the risk

$$min_\theta \hat{\mathcal{R}}_\theta = \frac{1}{N} \sum_{i=0,\ldots,N-1} (y_i - \theta x_i)$$

Minimization



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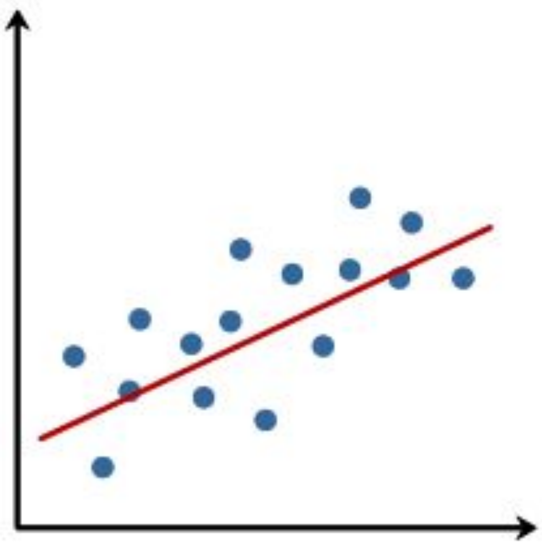
- Minimize the risk

$$min_\theta \hat{\mathcal{R}}_\theta = \frac{1}{N} \sum_{i=0,\ldots,N-1} (y_i - \theta x_i)$$

- How?

Minimization



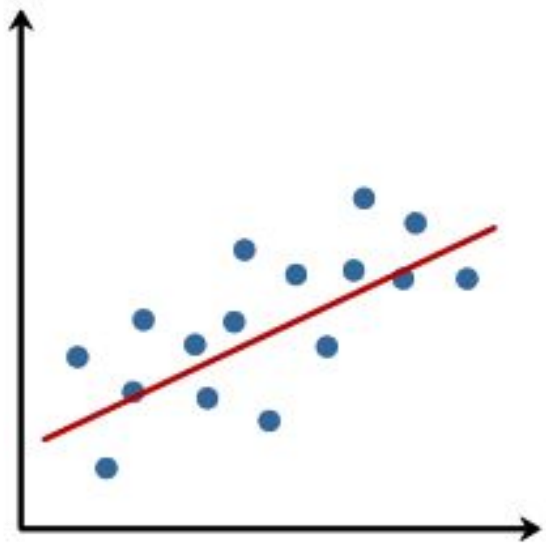
$$f_\theta(x) = \theta x$$

- Minimize the risk

$$min_\theta \hat{\mathcal{R}}_\theta = \frac{1}{N} \sum_{i=0,\ldots,N-1} (y_i - \theta x_i)^2$$

- How?
  - Convex function!

Minimization



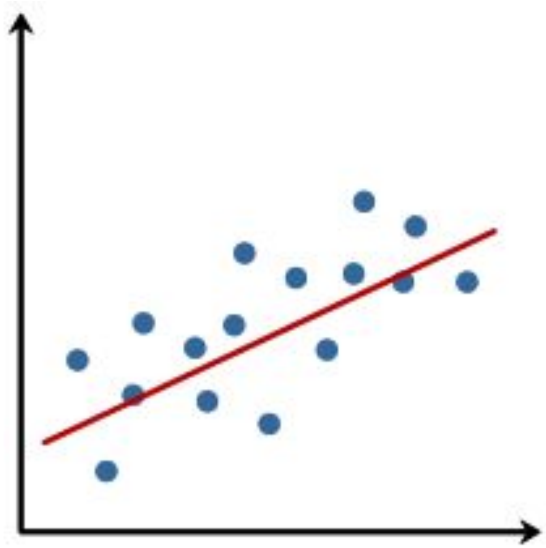
$$f_\theta(x) = \theta x$$

- Minimize the risk

$$min_\theta \hat{\mathcal{R}}_\theta = \frac{1}{N} \sum_{i=0,\dots,N-1} (y_i - \theta x_i)^2$$

- How?
  - Convex function!
  - Zero out the gradient!

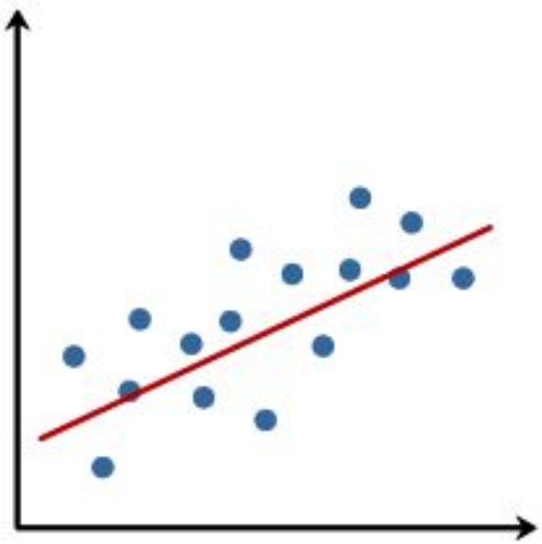
Solving the system



$$min_\theta \mathcal{R}_\theta = \frac{1}{N} \sum_{i=0,\ldots,N-1} (y_i - \theta x_i)^2$$

- Deriving gives condition:

Solving the system

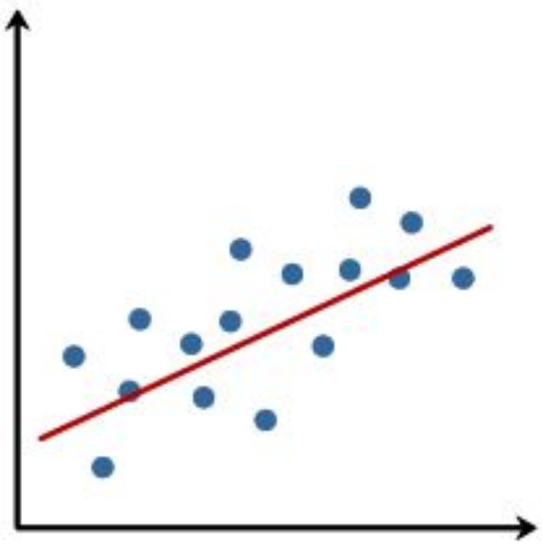


$$min_\theta \mathcal{R}_\theta = \frac{1}{N} \sum_{i=0,\dots,N-1} (y_i - \theta x_i)^2$$

- Deriving gives condition:

$$-\frac{2}{N} \sum_{i=0,\dots,N-1} (y_i - \theta x_i) x_i = 0$$

Solving the system



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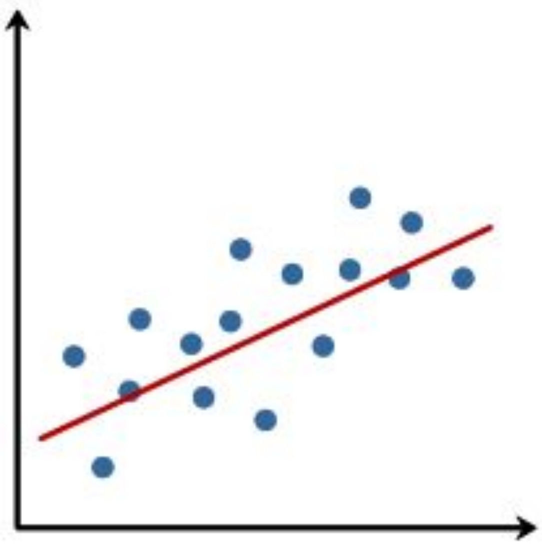
- Solve for θ

Solving the system



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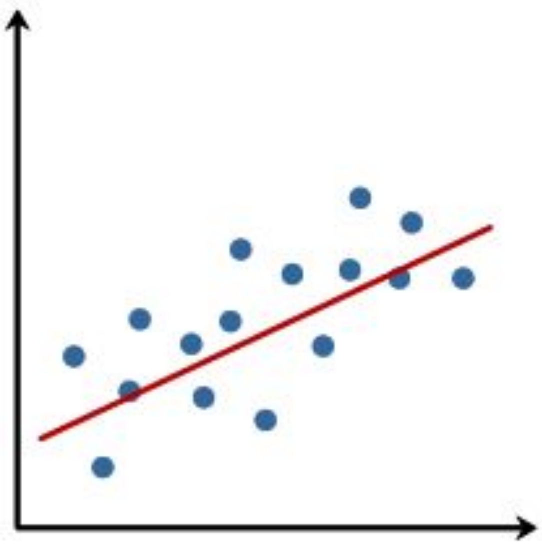
- Deriving gives condition:

$$-\frac{2}{N} \sum_{i=0,\ldots,N-1} (y_i - \theta x_i) x_i = 0$$

- Solve for θ

$$\theta = \frac{\sum_{i=0,\ldots,N-1} y_i x_i}{\sum_{i=0,\ldots,N-1} x_i^2}$$

Quickly analyzing the solution



$$f_\theta(x) = \theta x$$

$$\theta = \frac{\sum_{i=0,\ldots,N-1} y_i x_i}{\sum_{i=0,\ldots,N-1} x_i^2}$$

- If perfectly linear correlation

$$\theta = a\frac{\sum_{i=0,\ldots,N-1} x_i^2}{\sum_{i=0,\ldots,N-1} x_i^2} = a$$

Takeaway

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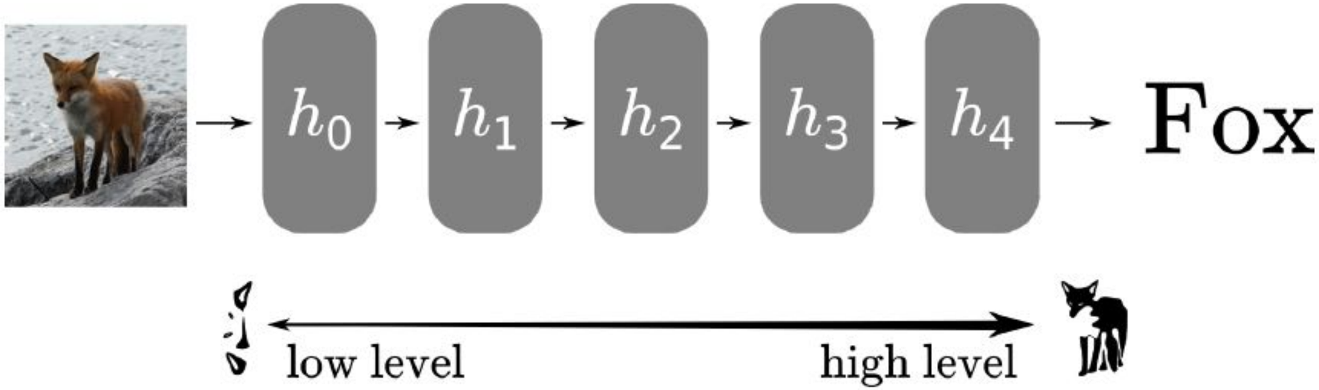
- Core problem: Find the right function in a family
  - Boils down to finding the right parameters
  - Depends on the data available

- Minimizing the risk is finding the best fit solution
  - Shown on univariate linear regression
  - Generalizes to multiple dimensions
  - ***Pointless if the data does not fit!***

3. Neural network functions

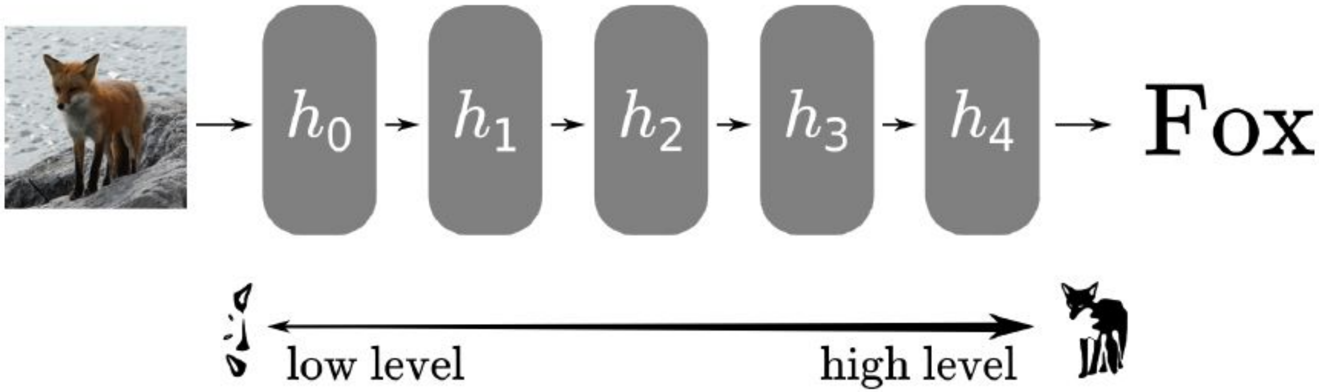
Neural network functions

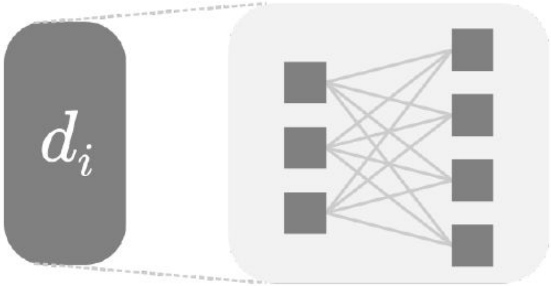


- Neural networks are sequences of simple functions

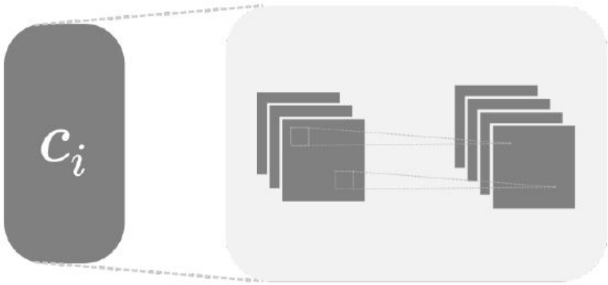
$$f_\theta = h_\theta^0 \circ h_\theta^1 \circ \cdots \circ h_\theta^{L-1}$$

Neural network functions



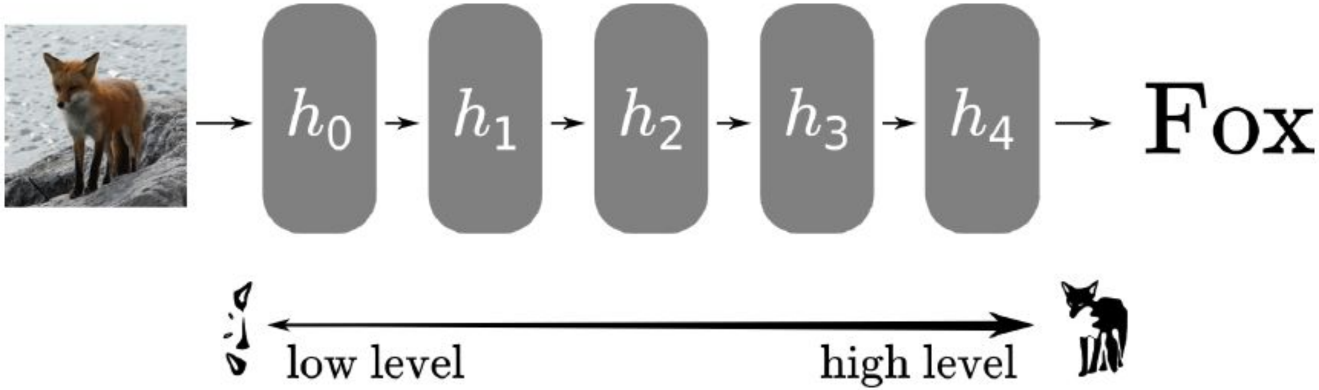


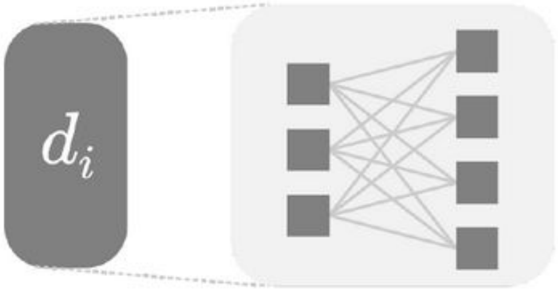
(a) Dense layer



(b) Convolutional layer

Interlude: Formalization of dense networks



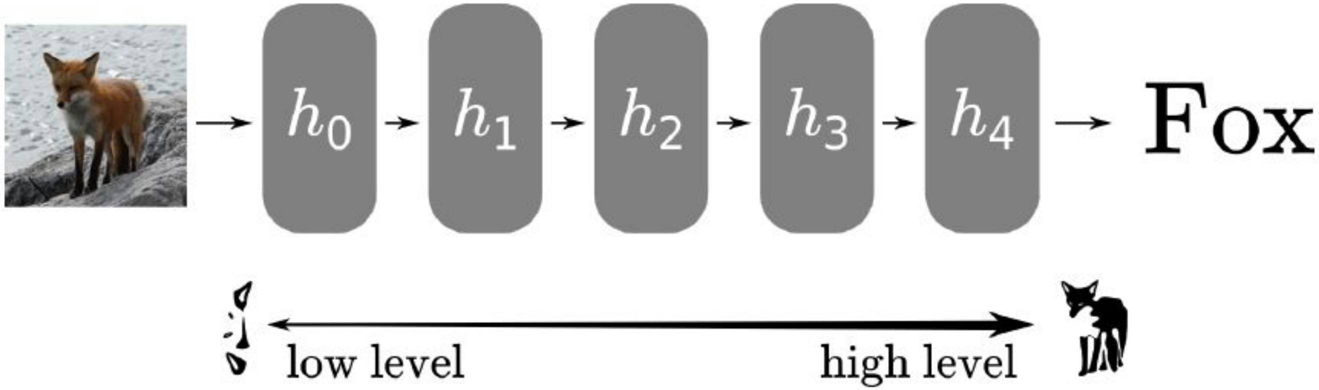


(a) Dense layer

$$d_\theta(x) = \sigma(W_\theta x^T + b_\theta)$$

$$\sigma(x) = ReLU(x) = max(0, x)$$

Interlude: Formalization of dense networks



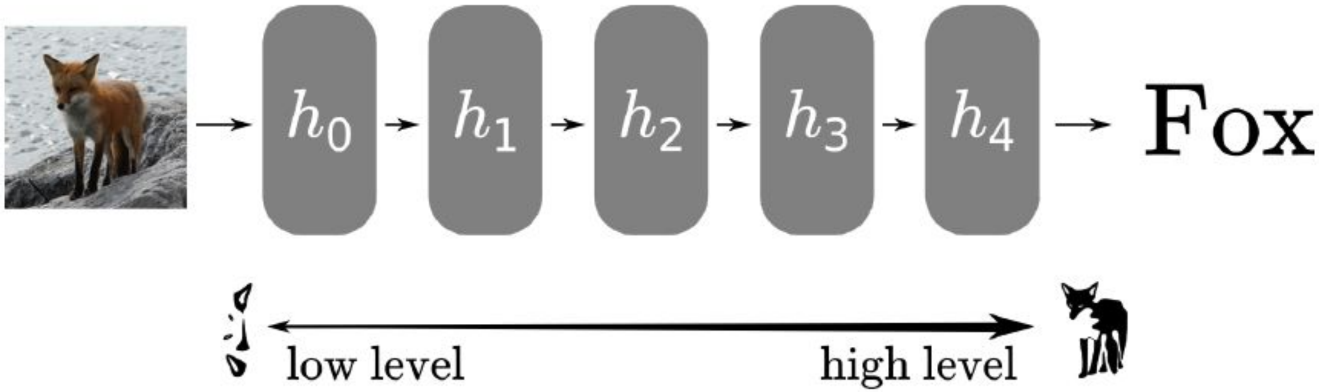
$$d_\theta(x) = \sigma(W_\theta x^T + b_\theta)$$

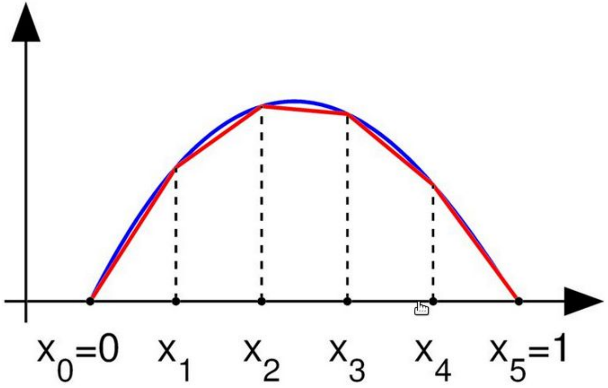
$$\sigma(x) = ReLU(x) = max(0, x)$$

Piecewise linear!

Individual layers are piecewise linear, composition preserves piecewise linearity

Interlude: Formalization of dense networks





- Highly expressive
  - Can fit many types of distributions

Some more properties

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- Upper bound on number of linear pieces wrt number of layers and units per layer
    - Exercise: Proof by recurrence

- Similar properties with other deep networks
    - Piecewise polynomial with other σ
    - Similar reasoning on convolutional layers

- Universal approximation theorem [Cybenko '89]
    - Proof by contradiction

Takeaway

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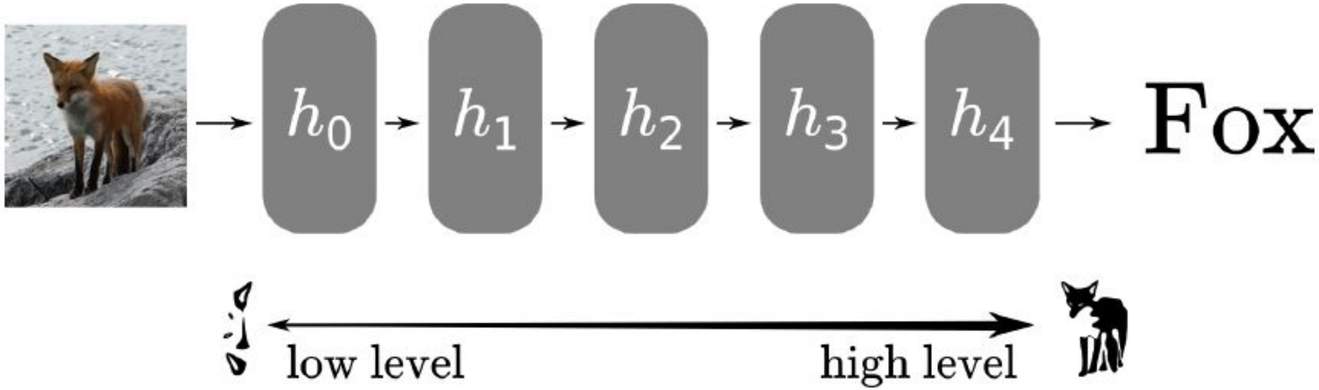
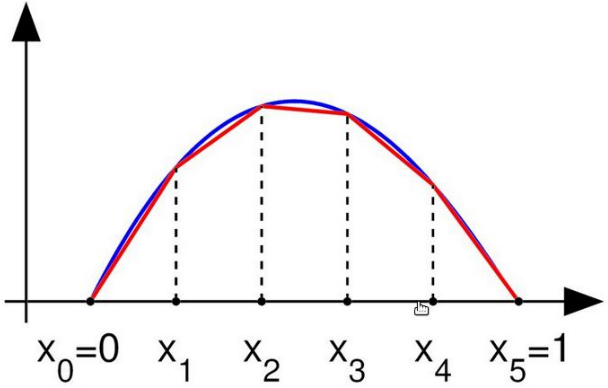
- Neural networks composed of simple functions
  - Typical linear layer operations
  - Non-linear activation functions

- High expressive power
  - Universal approximation with enough neurons
  - ReLU Feedforward networks are piecewise linear

4. Gradient descent

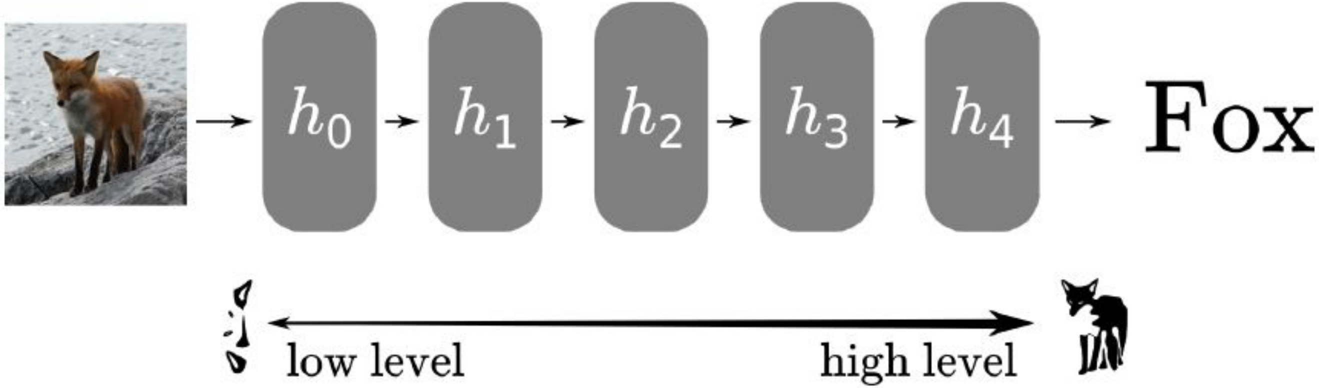
Let’s find the best network then!

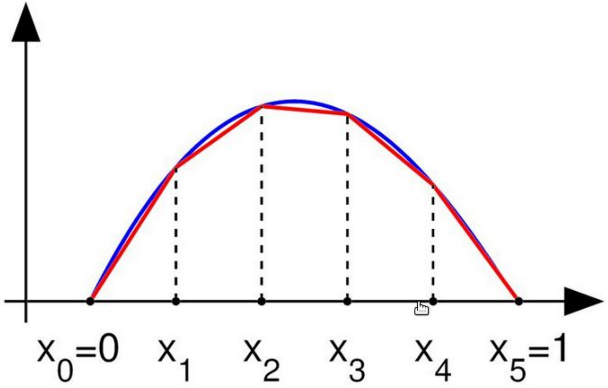




$$min_\theta \hat{\mathcal{R}}_\theta = \frac{1}{N} \sum_{i=0,\ldots,N-1} l(f_\theta(x_i), y_i)$$

Let's find the best network then!

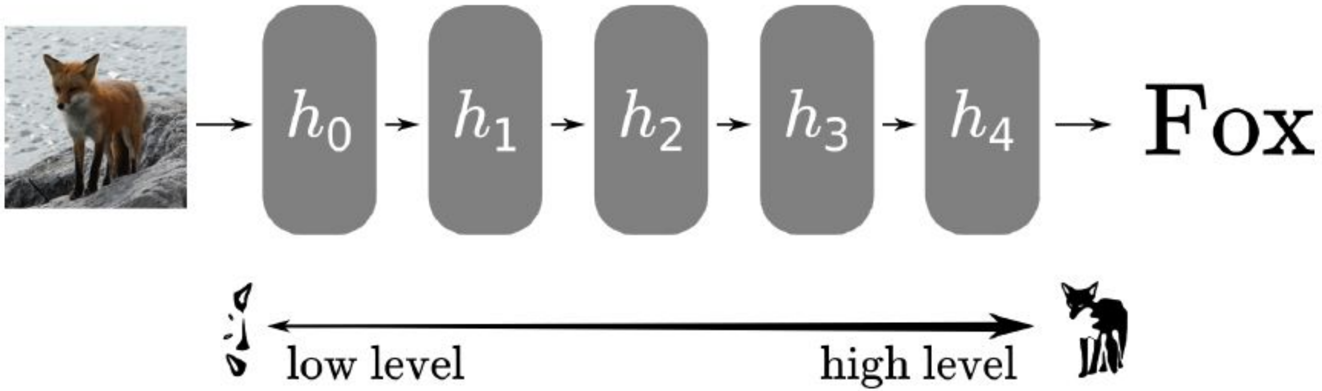


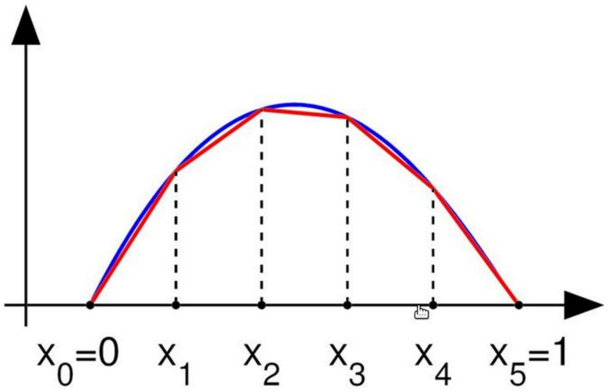


$$min_\theta \hat{\mathcal{R}_\theta} = \frac{1}{N} \sum_{i=0,\dots,N-1} l(f_\theta(x_i), y_i)$$

?????????????

Let’s find the best network then!





$$min_\theta \hat{\mathcal{R}}_\theta = \frac{1}{N} \sum_{i=0,\ldots,N-1} l(f_\theta(x_i), y_i)$$

No closed form!

Approximation: Gradient Descent

- Iteratively make steps of size η to minimize risk

$$\theta^{t+1} := \theta^t - \eta \nabla_\theta \hat{\mathcal{R}}_\theta$$

- Elementwise form:

$$\theta_i^{t+1} := \theta_i^t - \eta \frac{\partial \hat{\mathcal{R}}_\theta}{\partial \theta_i}$$

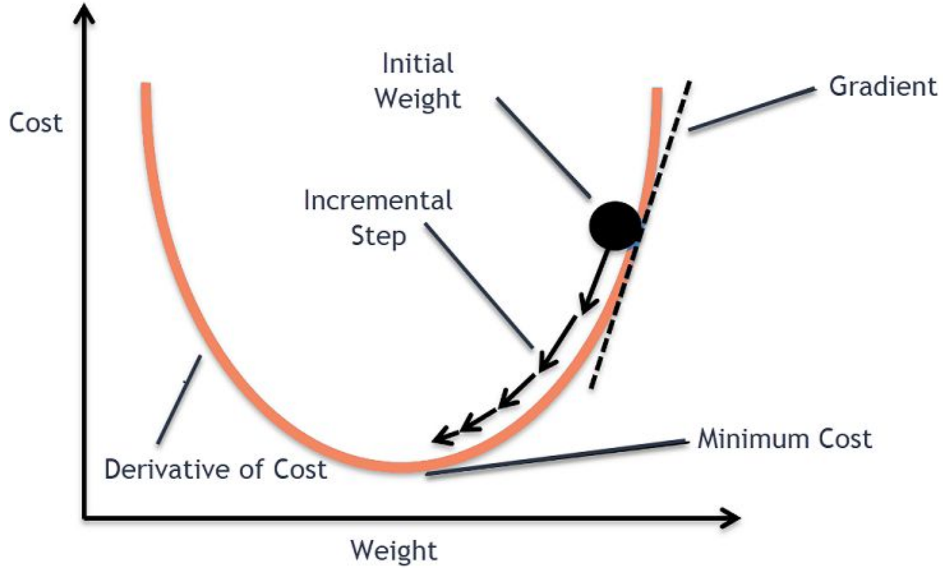


Image from Analytics Vidhya

Interlude: A few nice things to know

- Guarantees on convergence under conditions
  - Lipschitz gradient gives nice upper bounds
  - Adaptive gradient steps can offer guarantees
    - Steps traditionally fixed

- No guarantee to find a global optimum
  - Quite unlikely
  - Gravitates towards Local optimum

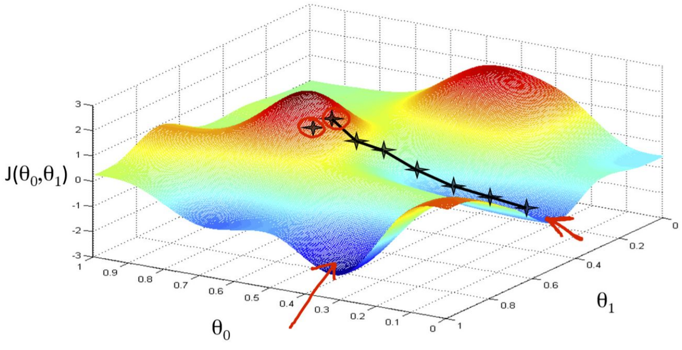


Image from Towards Data Science

In practice: Stochastic Gradient Descent

- Deep learning deals in large-scale
  - Big datasets
  - Big models
  - GD can get expensive!

- Stochastic Gradient Descent
  - Work on small batches of data B instead of D

$$\theta^{t+1} := \theta^t - \eta \nabla_\theta \hat{\mathcal{R}_\theta}(B)$$

  - Noisier process

Takeaway

- No closed form Risk Minimization solution
  - Networks are too complex
  - Much worse behaved than linear regression

- Solution: Gradient Descent
  - Find direction of θ that minimizes the risk
  - Make a step in the direction
  - Repeat

5. Backprop

We need the gradient…

$$\theta^{t+1} := \theta^t - \eta \nabla_\theta \mathcal{R}_\theta\hat{(}B)$$

- Requires finding the risk gradient wrt parameters

$$\nabla_\theta \mathcal{R}_\theta\hat{(}B) = \frac{1}{\#B} \sum_{k=0,\ldots,B-1} \nabla_\theta l(f_\theta(x_k), y_k)$$

- Boils down to computing gradients for one sample

$$\nabla_\theta l(f_\theta(x), y)$$

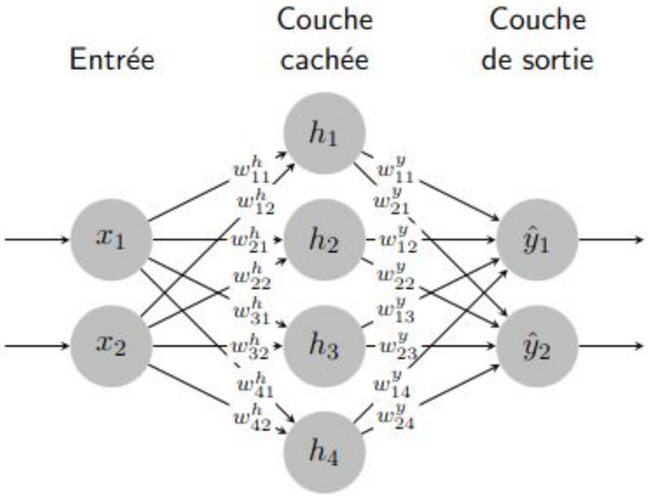
Backpropagation (Informal)

$$l := l(f_\theta(x), y)$$

- Networks are complex but made of simple parts!
  - Simple gradients of component functions
  - Chain-rule allows decomposition into simple gradients $$\frac{\partial l}{\partial w} = \frac{\partial l}{\partial a}\frac{\partial a}{\partial w}$$

- Need to store intermediate activations "a" to evaluate partial derivatives $$\frac{\partial a}{\partial w}$$

Example: Tanh MLP



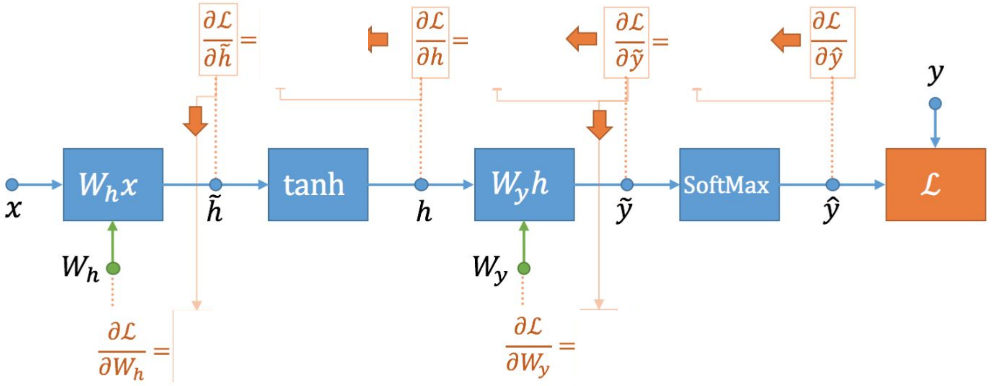
- Simple 1 hidden layer MLP
  - 2 inputs
  - 2 outputs
  - 4 hidden activations

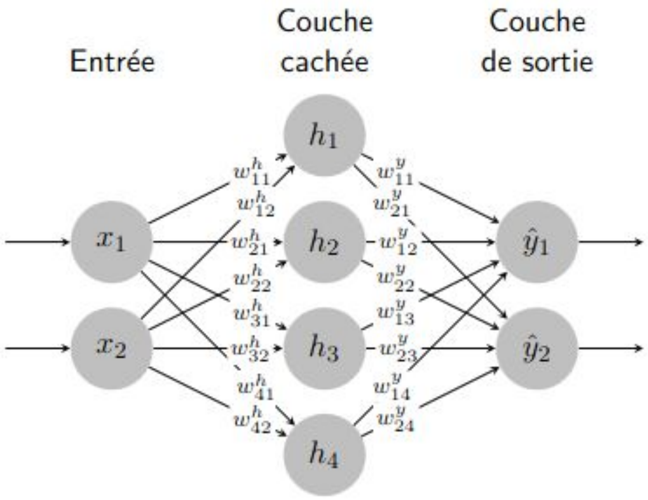
- Classification problem
  - Outputs probabilities
  - Cross-entropy loss

$$l_{CE}(\hat{y}, y) = - \sum_{i=0}^{\#Classes-1} y_i \log(\hat{y}_i)$$

Example: Tanh MLP

$$l_{CE}(\hat{y}, y) = -\sum_{i=0}^{\#Classes-1} y_i \log(\hat{y}_i)$$





$$\begin{cases} \tilde{h}_i = \sum_{j=1}^{n_x} W^h_{i,j} \; x_j + b^h_i \\ h_i = \tanh(\tilde{h}_i) \\ \tilde{y}_i = \sum_{j=1}^{n_h} W^y_{i,j} \; h_j + b^y_i \\ \hat{y}_i = \mathrm{SoftMax}(\tilde{y}_i) = \dfrac{e^{\tilde{y}_i}}{\sum_{j=1}^{n_y} e^{\tilde{y}_j}} \end{cases}$$

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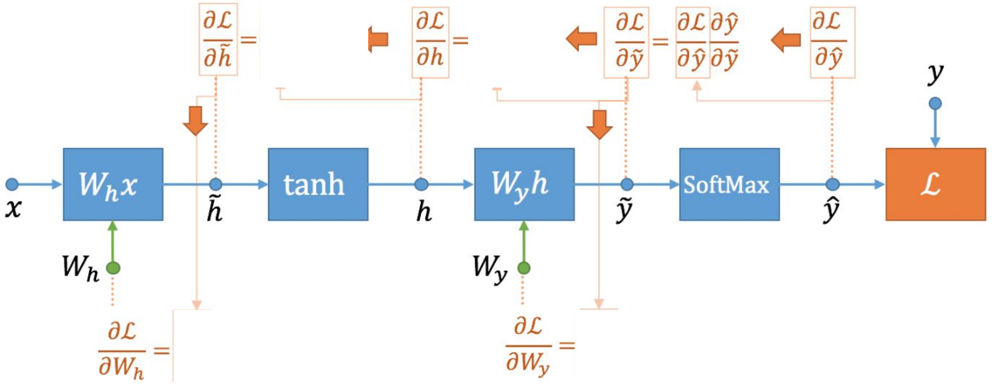
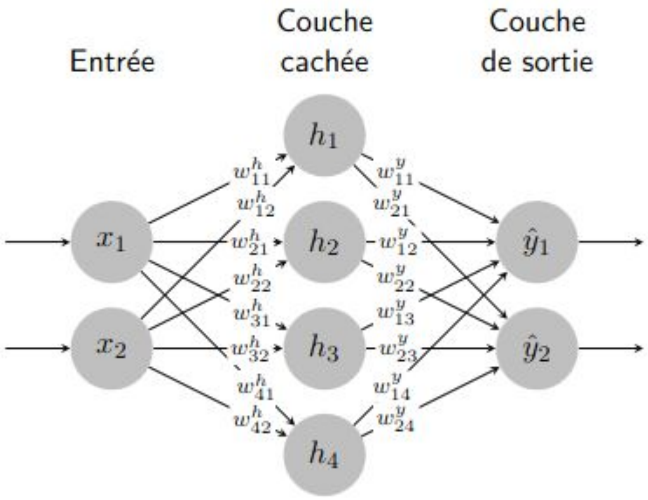
$$l_{CE}(\hat{y}, y) = -\sum_{i=0}^{\#Classes-1} y_i \log(\hat{y}_i)$$





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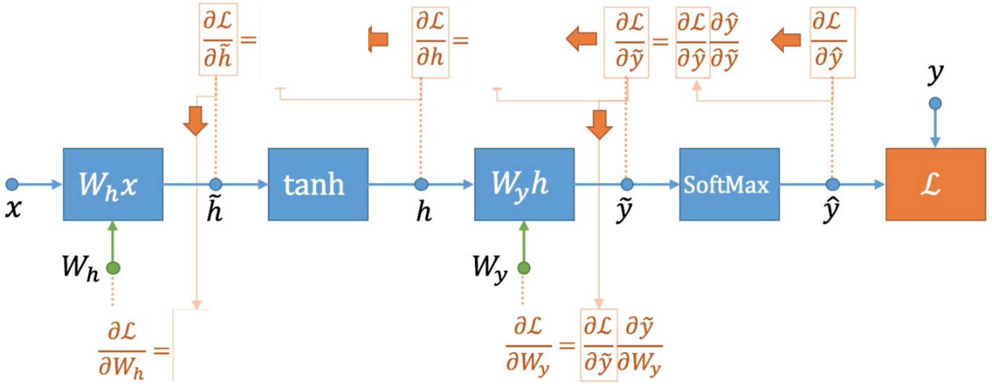

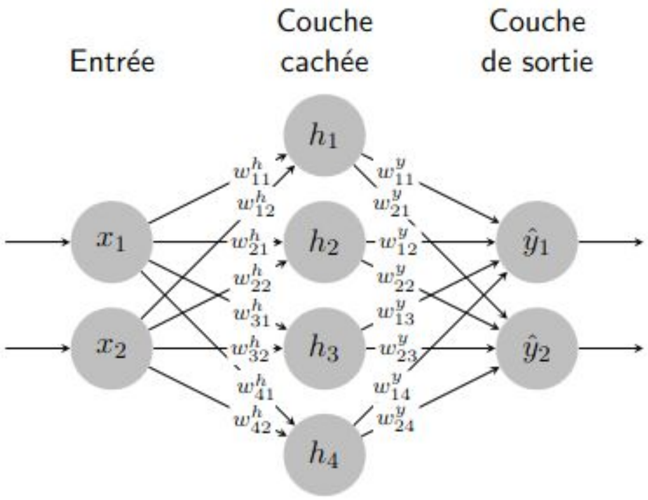

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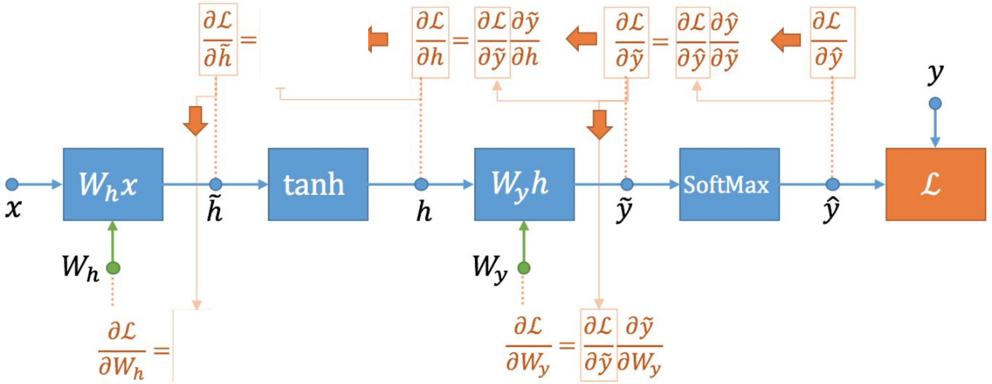

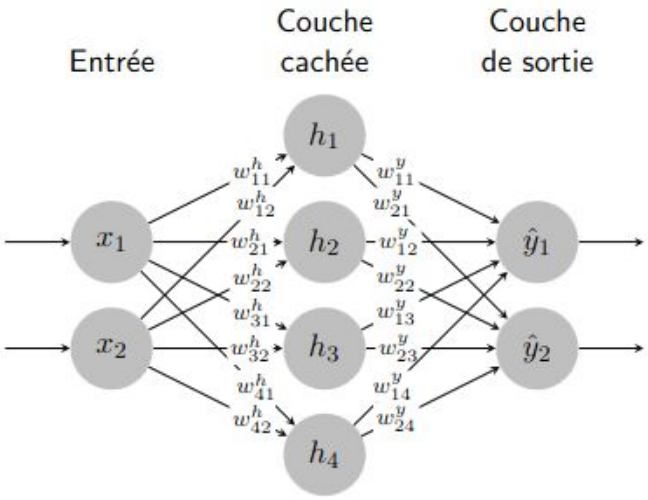

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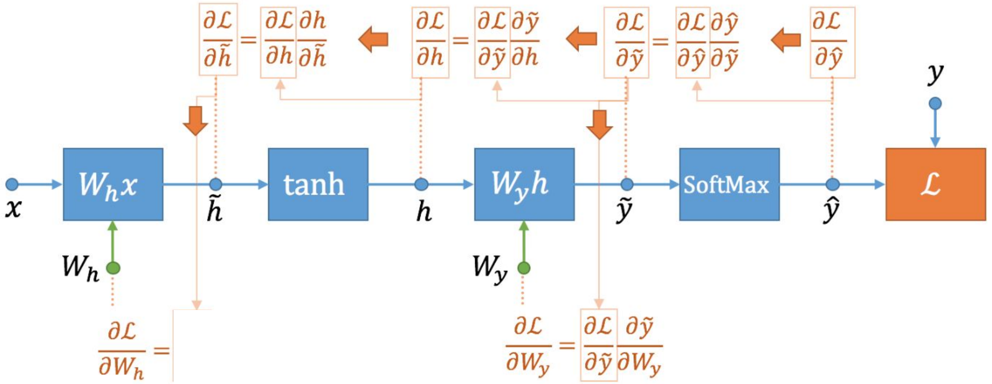
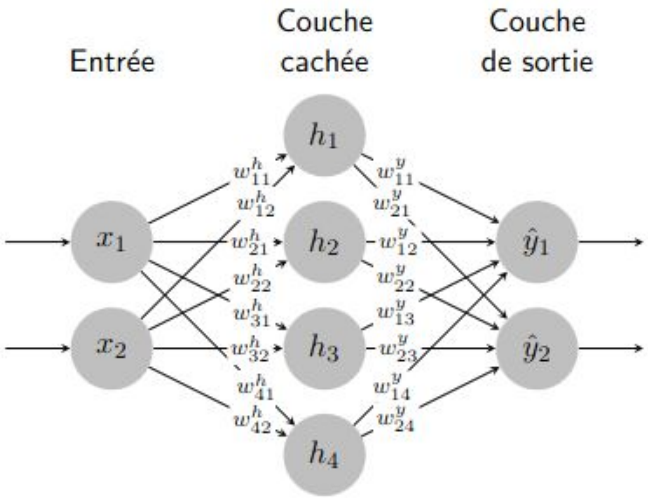
Example: Tanh MLP

$$l_{CE}(\hat{y}, y) = -\sum_{i=0}^{\#Classes-1} y_i \log(\hat{y}_i)$$





$$\begin{cases} \tilde{h}_i = \sum_{j=1}^{n_x} W^h_{i,j}\, x_j + b^h_i \\ h_i = \tanh(\tilde{h}_i) \\ \tilde{y}_i = \sum_{j=1}^{n_h} W^y_{i,j}\, h_j + b^y_i \\ \hat{y}_i = \mathrm{SoftMax}(\tilde{y}_i) = \dfrac{e^{\tilde{y}_i}}{\sum_{j=1}^{n_y} e^{\tilde{y}_j}} \end{cases}$$

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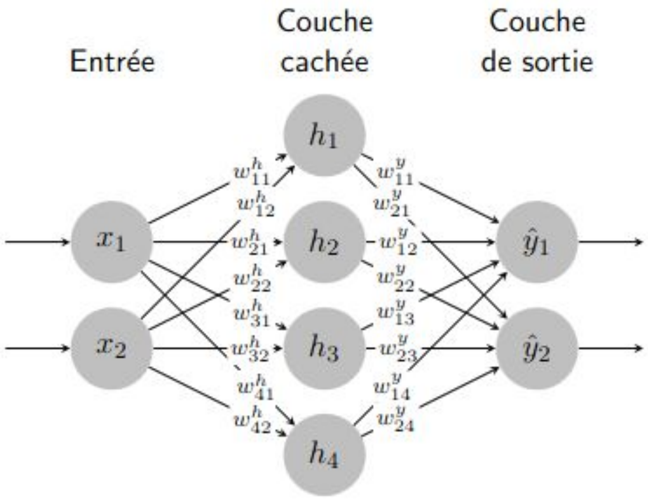

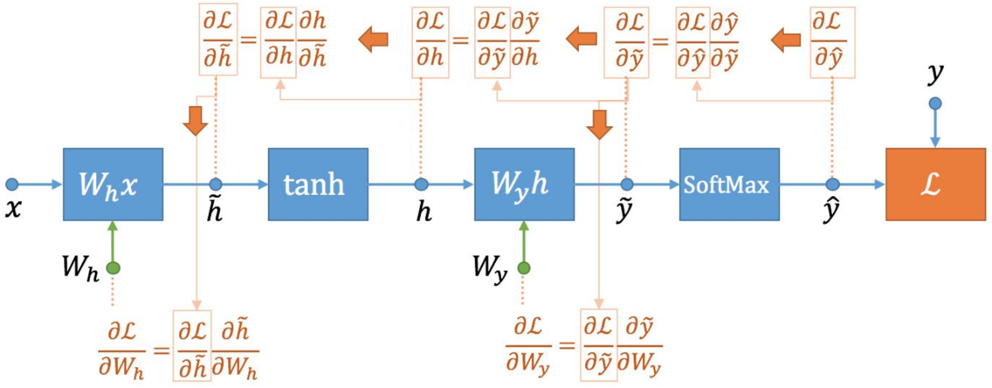

$$\begin{cases} \tilde{h}_i = \sum_{j=1}^{n_x} W_{i,j}^h \; x_j + b_i^h \\ h_i = \tanh(\tilde{h}_i) \\ \tilde{y}_i = \sum_{j=1}^{n_h} W_{i,j}^y \; h_j + b_i^y \\ \hat{y}_i = \mathrm{SoftMax}(\tilde{y}_i) = \dfrac{e^{\tilde{y}_i}}{\sum_{j=1}^{n_y} e^{\tilde{y}_j}} \end{cases}$$

$$\begin{cases} \delta_i^y = \dfrac{\partial \ell}{\partial \tilde{y}_i} = \\ \dfrac{\partial \ell}{\partial W_{i,j}^y} = \\ \dfrac{\partial \ell}{\partial b_i^y} = \end{cases}$$

Example: Tanh MLP

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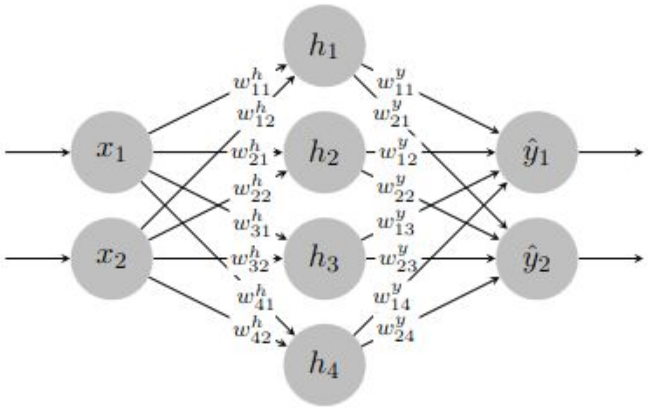
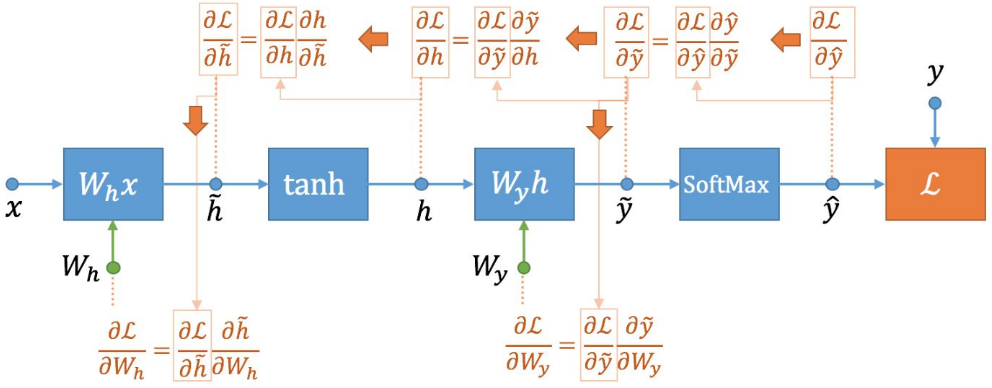
$$l_{CE}(\hat{y}, y) = -\sum_{i=0}^{\#Classes-1} y_i \log(\hat{y}_i)$$





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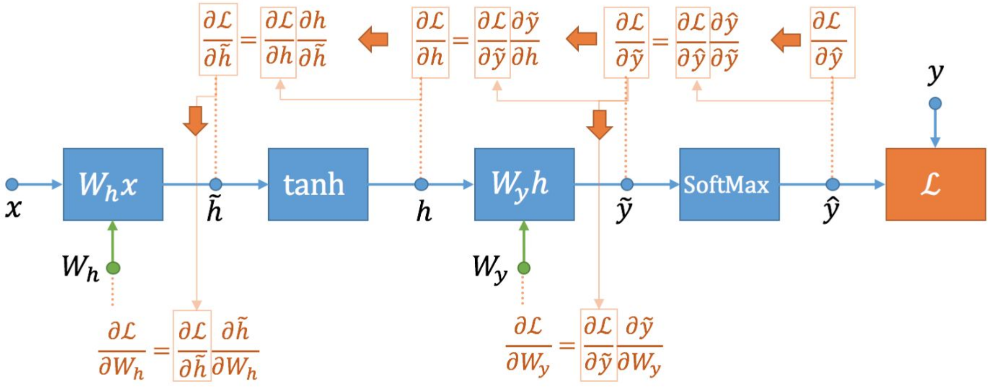
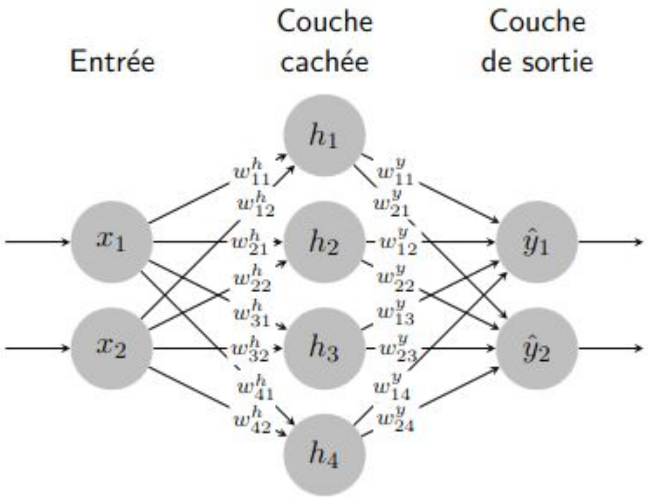
$$\begin{cases} \delta_i^y = \dfrac{\partial \ell}{\partial \tilde{y}_i} = \hat{y}_i - y_i \\ \dfrac{\partial \ell}{\partial W_{i,j}^y} = \delta_i^y \; h_j \\ \dfrac{\partial \ell}{\partial b_i^y} = \delta_i^y \end{cases}$$

Example: Tanh MLP

$$l_{CE}(\hat{y}, y) = -\sum_{i=0}^{\#Classes-1} y_i \log(\hat{y}_i)$$





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Example: Tanh MLP

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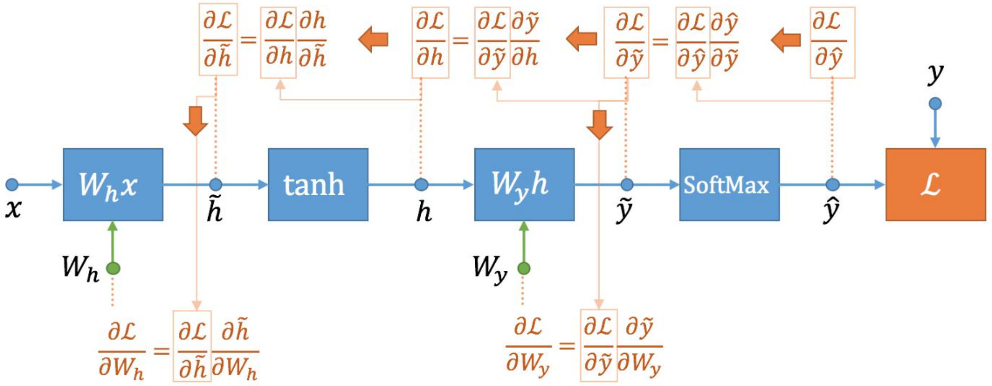

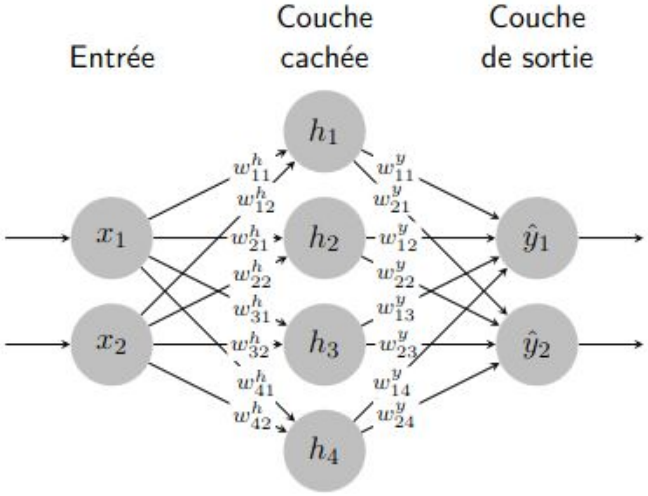

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$$\begin{cases} \delta^y_i = \dfrac{\partial\ell}{\partial\tilde{y}_i} = \hat{y}_i - y_i \\ \dfrac{\partial\ell}{\partial W^y_{i,j}} = \delta^y_i\; h_j \\ \dfrac{\partial\ell}{\partial b^y_i} = \delta^y_i \\ \delta^h_i = \dfrac{\partial\ell}{\partial\tilde{h}_i} = (1-h_i^2)\sum_{j=1}^{n_y}\delta^y_j W^y_{j,i} \\ \dfrac{\partial\ell}{\partial W^h_{i,j}} = \delta^h_i\; x_j \\ \dfrac{\partial\ell}{\partial b^h_i} = \delta^h_i \end{cases}$$

Takeaway

- Core problem: Find gradient updates

- Gradient can be computed efficiently with backpropagation
  - Chain rule starting from the "end" of the network
  - Keep network activation to evaluate gradients
  - Simple layers mean simple gradient blocks

Your turn! Go as far as you can

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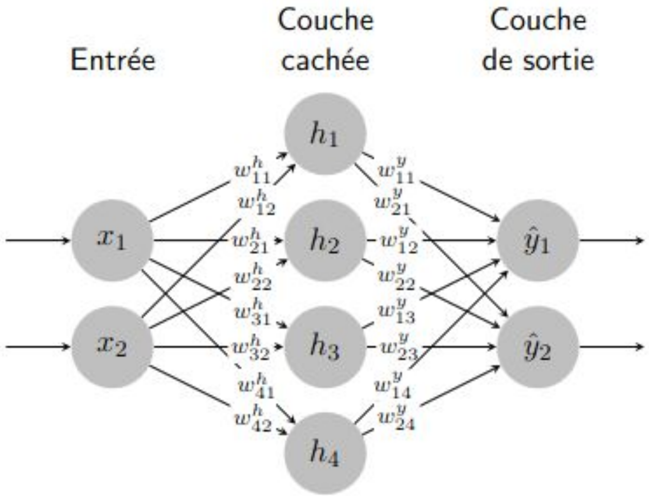

$$\begin{cases} \tilde{\mathbf{h}} = \mathbf{x}{\mathbf{W}^h}^\top + \mathbf{b}^h \\ \mathbf{h} = \tanh(\tilde{\mathbf{h}}) \\ \tilde{\mathbf{y}} = \mathbf{h}{\mathbf{W}^y}^\top + \mathbf{b}^y \\ \hat{\mathbf{y}} = \mathrm{SoftMax}(\tilde{\mathbf{y}}) \end{cases}$$

$$\begin{cases} \nabla_{\tilde{\mathbf{y}}} = \hat{\mathbf{y}} - \mathbf{y} \\ \nabla_{\mathbf{W}^y} = {\nabla_{\tilde{\mathbf{y}}}}^\top \mathbf{h} \\ \nabla_{\mathbf{b}^y} = \nabla_{\tilde{\mathbf{y}}}^\top \\ \nabla_{\tilde{\mathbf{h}}} = (\nabla_{\tilde{\mathbf{y}}} \mathbf{W}^y) \odot (1 - \mathbf{h}^2) \\ \nabla_{\mathbf{W}^h} = {\nabla_{\tilde{\mathbf{h}}}}^\top \mathbf{x} \\ \nabla_{\mathbf{b}^h} = \nabla_{\tilde{\mathbf{h}}}^\top \end{cases}$$

- Lab 3 practical notebook on Moodle
  - Implement this by hand with basic torch!
  - Careful with batch dimension!