



Lecture 3: A primer on fundamentals of deep learning

Advanced deep learning



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About this course

Advanced Deep Learning



- 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!

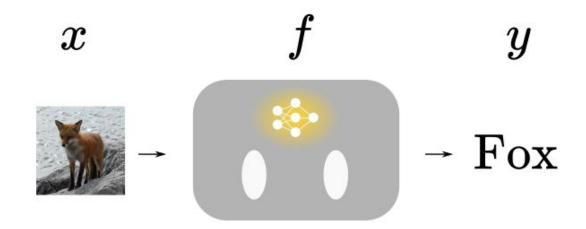


- Quick recap of deep learning fundamentals
 - Problem Statement and Empirical Risk Minimization
 - Neural Networks as classes of functions
 - Gradient Descent
 - Backpropagation
- Practical in pytorch: Training a MLP
 - Manual implementation
 - Progressive pytorch automation

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



- Definitions
 - X set of inputs
 - Y set of labels
 - \circ $\Omega = X \times Y$
 - \circ $\mathcal D$ 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 I so that we try to have the lowest quantity l(f(x), y)

Minimizing Risk



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

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

Minimizing Risk



- ullet 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}
 - <u>Empirical Risk Minimization</u>
 - 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

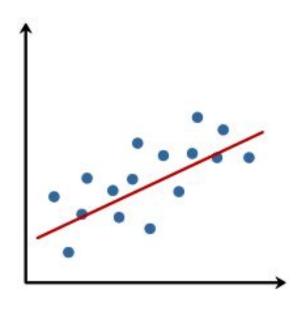
- Optimize over family of parametric functions
 - Assess functions with loss criterion

- Minimize the Risk function
 - Empirical Risk Minimization in practice

2. Example: linear regression

Linear problem

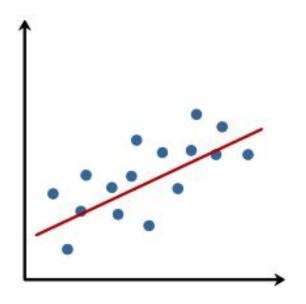




- Linearly correlated data
 - Input x (e.g. Voltage)
 - Output y (e.g. Intensity)
- Simple family of linear functions
 - Find linear coefficient

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

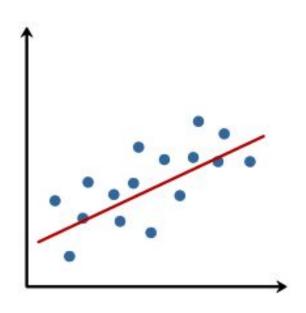




$$f_{\theta}(x) = \theta x$$

Minimize the risk



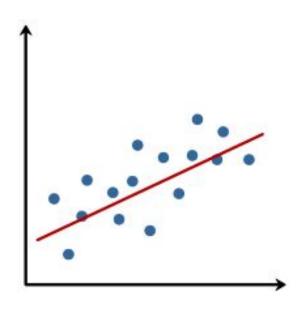


$$f_{\theta}(x) = \theta x$$

Minimize the risk

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





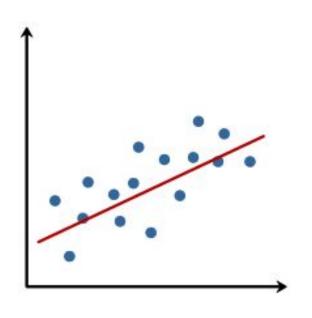
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Minimize the risk

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How?





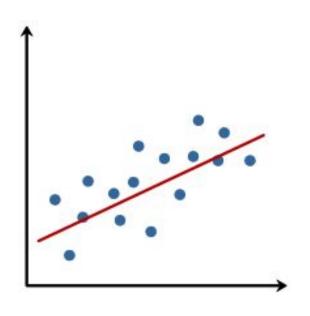
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Minimize the risk

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

- How?
 - Convex function!





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

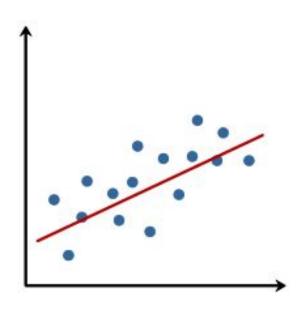
Minimize the risk

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

- How?

 - Convex function!Zero out the gradient!

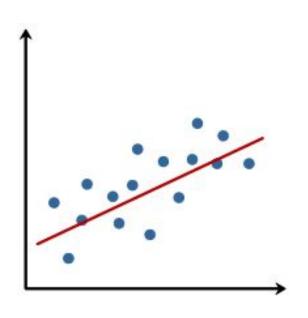




$$min_{\theta} \mathcal{R}_{\theta} = \frac{1}{N} \sum_{i=0,\dots,N-1} (y_i - \theta x_i)^2$$

Deriving gives condition:



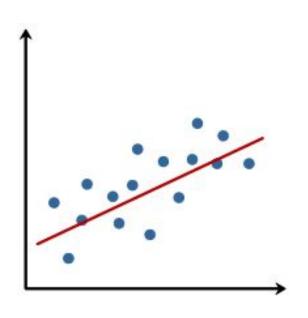


$$min_{\theta} \mathcal{R}_{\theta} = \frac{1}{N} \sum_{i=0,\dots,N-1} (y_i - \theta x_i)^2$$

Deriving gives condition:

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





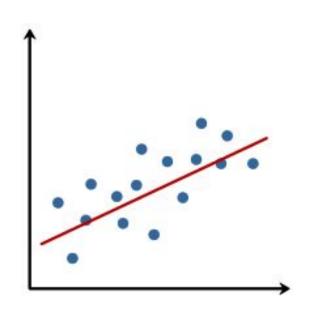
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• Solve for θ





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

• Deriving gives condition:

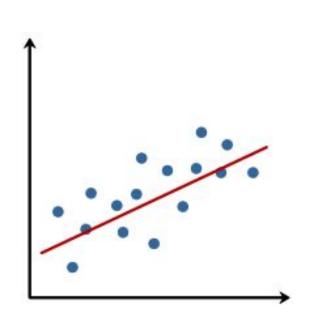
$$-\frac{2}{N} \sum_{i=0,...,N-1} (y_i - \theta x_i) x_i = 0$$

 \bullet / Solve for θ

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

Quickly analyzing the solution





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

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

If perfectly linear correlation

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

Takeaway



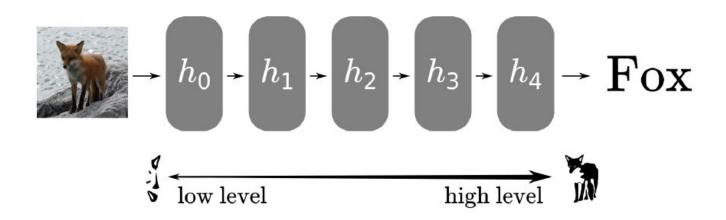
- Core problem: Find the right function in a family
 - Boils down to finding the right parameters
 - Depends on the data available

- 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



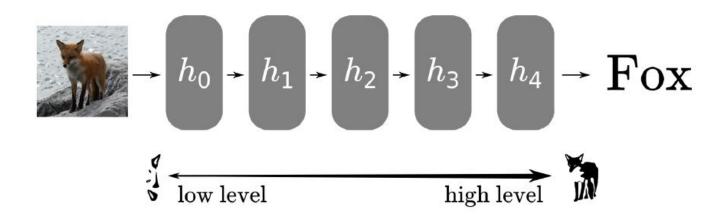


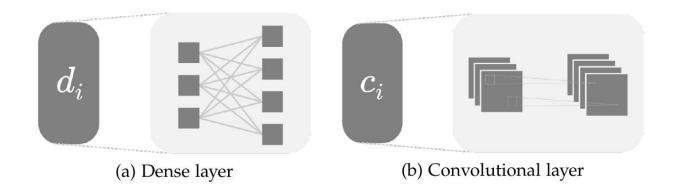
Neural networks are sequences of simple functions

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

Neural network functions

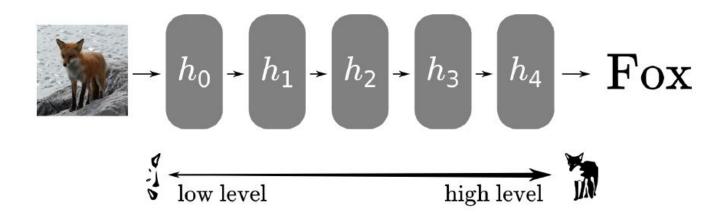


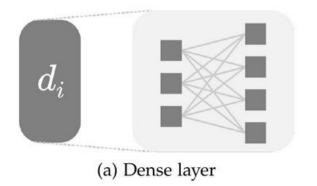




Interlude: Formalization of dense networks : UNIVERSITÉ CÔTE D'AZUR





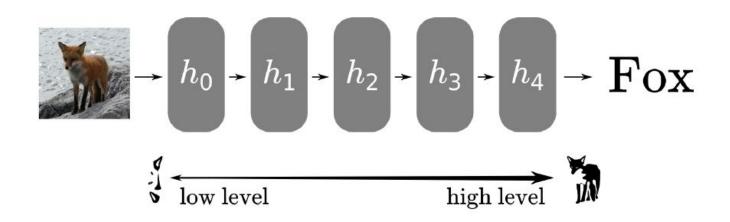


$$d_{\theta}(x) = \sigma(W_{\theta}x^{T} + b_{\theta})$$

$$\sigma(x) = ReLU(x) = max(0, x_{\parallel})$$

Interlude: Formalization of dense networks





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

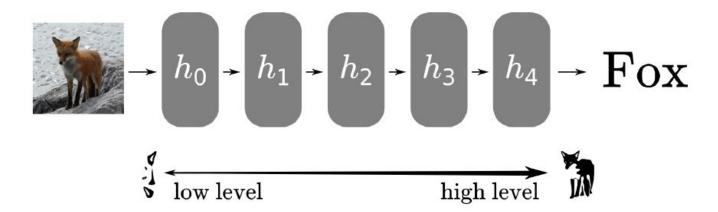
$$\sigma(x) = ReLU(x) = \max(0, x)$$

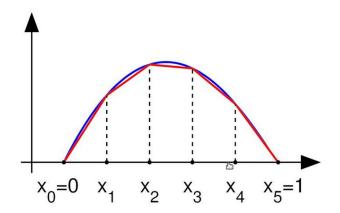
Piecewise linear!

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



- 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
 - \circ Piecewise polynomial with other σ
 - Similar reasoning on convolutional layers
- Universal approximation theorem [Cybenko '89]
 - Proof by contradiction

Takeaway



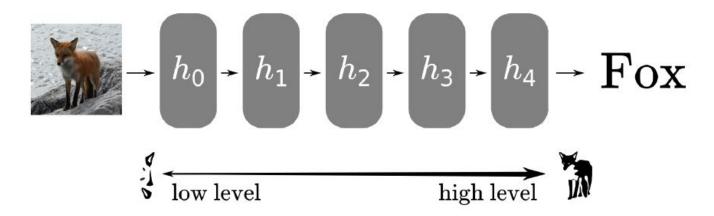
- Neural networks composed of simple functions
- Typical linear layer operations
- Non-linear activation functions

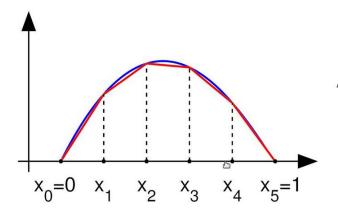
- High expressive power
 - Universal approximation with enough neurons
 - ReLU Feedforward networks are piecewise linear

4. Gradient descent

Let's find the best network then!



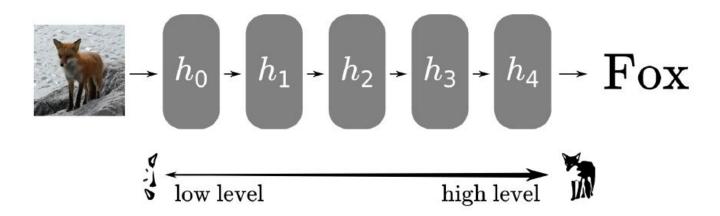


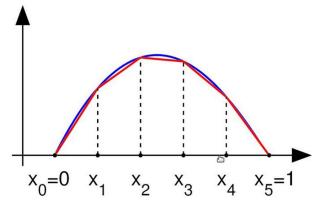


$$min_{\theta} \hat{\mathcal{R}}_{\theta} = \frac{1}{N} \sum_{i=0,\dots,N-1} l(f_{\theta}(x_i), y_i)$$

Let's find the best network then!



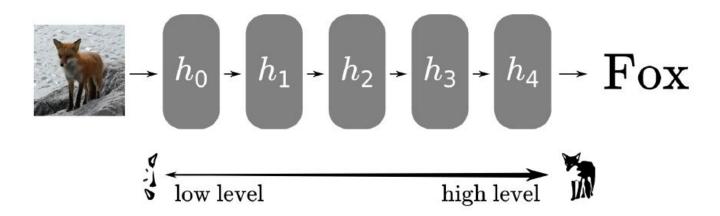


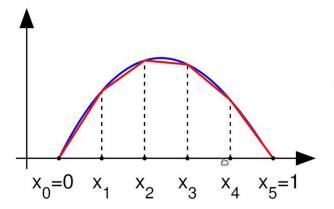


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Let's find the best network then!







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

No closed form!

Approximation: Gradient Descent

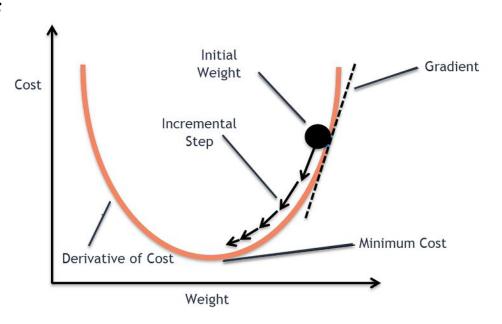


Iteratively make steps of size η to minimize risk

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

Elementwise form:

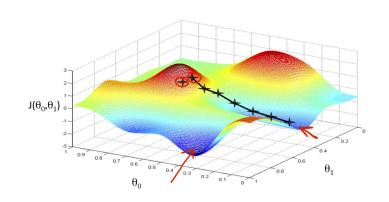
$$\theta_i^{t+1} := \theta_i^t - \eta \frac{\partial \hat{\mathcal{R}}_{\theta}}{\partial \theta_i}$$



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



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

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

Noisier process

Takeaway



- No closed form Risk Minimization solution
 - Networks are too complex
 - Much worse behaved than linear regression
- Solution: Gradient Descent
 - \circ Find direction of θ that minimizes the risk
 - Make a step in the direction
 - Repeat

5. Backprop

We need the gradient...



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

Requires finding the risk gradient wrt parameters

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

Boils down to computing gradients for one sample

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

Backpropagation (Informal)



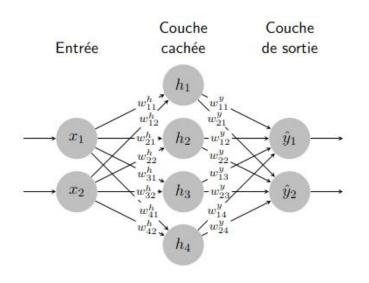
$$l := l(f_{\theta}(x), y)$$

- Networks are complex but made of simple parts!
 - Simple gradients of component functions
 - $\begin{array}{ccc} \circ & \text{Chain-rule allows} \\ & \text{decomposition into} & \frac{\partial l}{\partial w} = \\ & \text{simple gradients} & \end{array}$



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





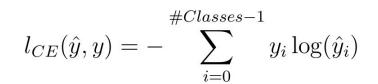
- Simple 1 hidden layer MLP
 - 2 inputs
 - 2 outputs
 - 4 hidden activations

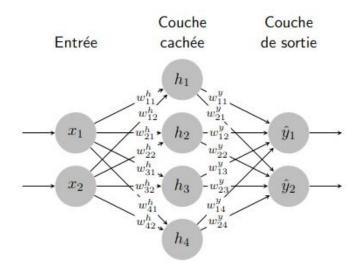
Classification problem

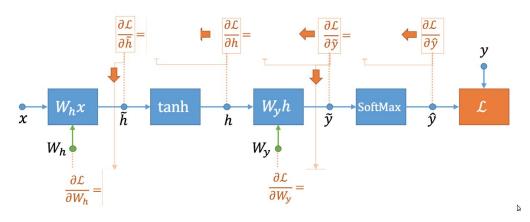
- Outputs probabilities
- ✓ Cross-entropy loss

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



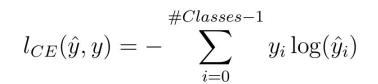


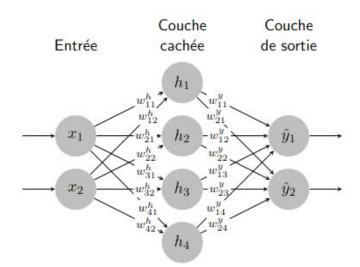


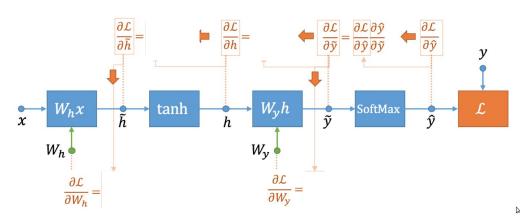


$$\begin{cases} \tilde{h}_i = \sum_{j=1}^{n_x} W_{i,j}^h \ x_j + b_i^h \\ h_i = \tanh(\tilde{h}_i) \\ \tilde{y}_i = \sum_{j=1}^{n_h} W_{i,j}^y \ h_j + b_i^y \\ \hat{y}_i = \operatorname{SoftMax}(\tilde{y}_i) = \frac{e^{\tilde{y}_i}}{\sum\limits_{j=1}^{n_y} e^{\tilde{y}_j}} \end{cases}$$



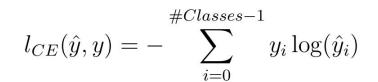


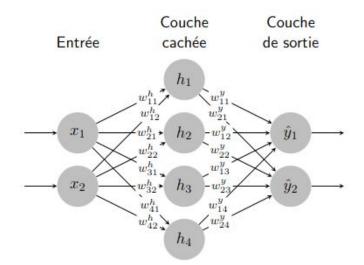


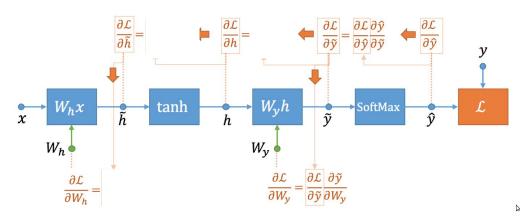


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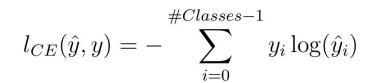


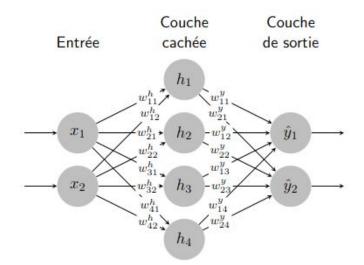


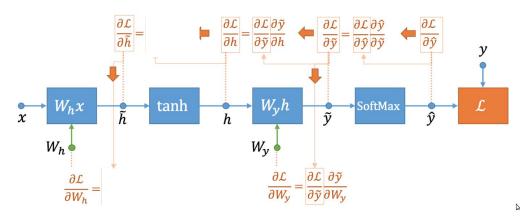


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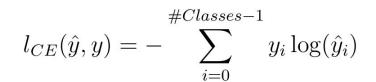


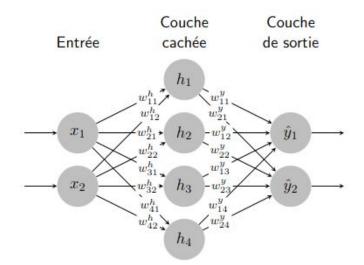


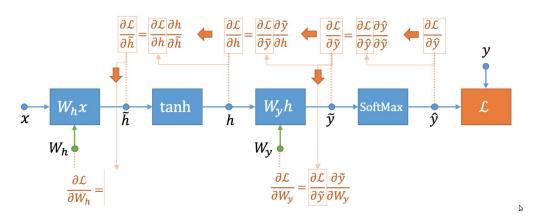


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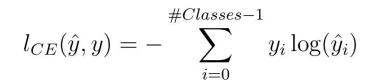


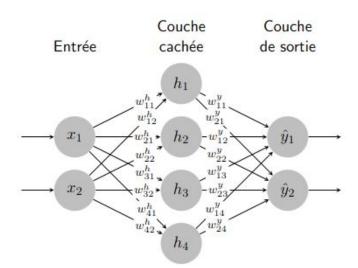


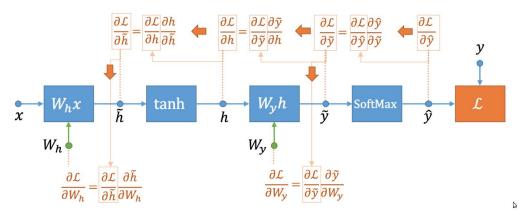


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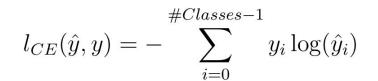


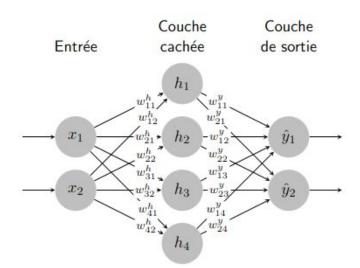


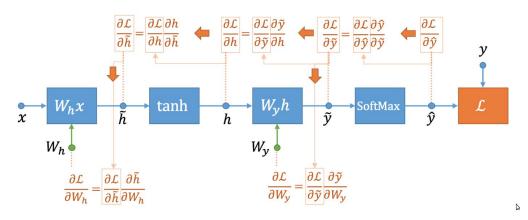


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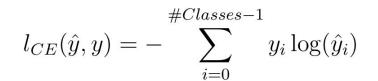


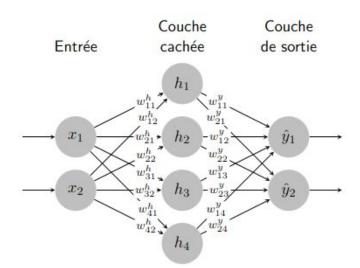


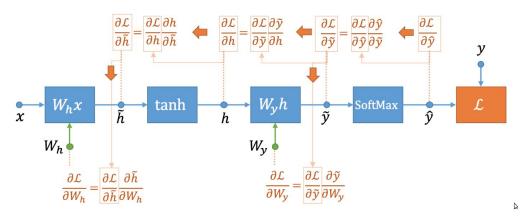
$$\begin{cases} \tilde{h}_i = \sum_{j=1}^{n_x} W_{i,j}^h \ x_j + b_i^h \\ h_i = \tanh(\tilde{h}_i) \\ \tilde{y}_i = \sum_{j=1}^{n_h} W_{i,j}^y \ h_j + b_i^y \\ \hat{y}_i = \operatorname{SoftMax}(\tilde{y}_i) = \frac{e^{\tilde{y}_i}}{\sum\limits_{j=1}^{n_y} e^{\tilde{y}_j}} \end{cases}$$

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



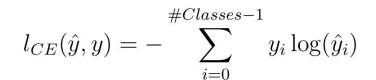


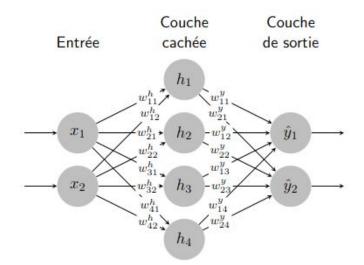


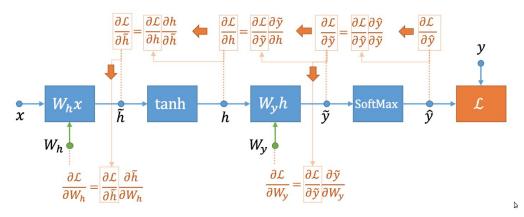


$$\begin{cases} \tilde{h}_{i} = \sum_{j=1}^{n_{x}} W_{i,j}^{h} \ x_{j} + b_{i}^{h} \\ h_{i} = \tanh(\tilde{h}_{i}) \\ \tilde{y}_{i} = \sum_{j=1}^{n_{h}} W_{i,j}^{y} \ h_{j} + b_{i}^{y} \\ \hat{y}_{i} = \operatorname{SoftMax}(\tilde{y}_{i}) = \frac{e^{\tilde{y}_{i}}}{\sum_{j=1}^{n_{y}} e^{\tilde{y}_{j}}} \end{cases} \begin{cases} \delta_{i}^{y} = \frac{\partial \ell}{\partial \tilde{y}_{i}} = \hat{y}_{i} - y_{i} \\ \frac{\partial \ell}{\partial W_{i,j}^{y}} = \delta_{i}^{y} \ h_{j} \\ \frac{\partial \ell}{\partial b_{i}^{y}} = \delta_{i}^{y} \end{cases}$$









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

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

$$\delta_i^h = \frac{\partial \ell}{\partial \tilde{h}_i} = (1 - h_i^2) \sum_{j=1}^{n_y} \delta_j^y W_{j,i}^y \\ \frac{\partial \ell}{\partial W_{i,j}^h} = \delta_i^h x_j \\ \frac{\partial \ell}{\partial b_i^h} = \delta_i^h \end{cases}$$

Takeaway

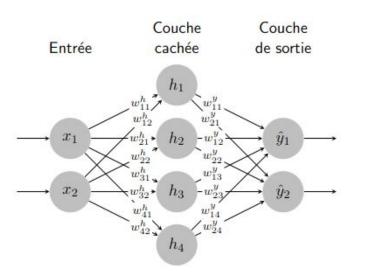


Core problem: Find gradient updates

- 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





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

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

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