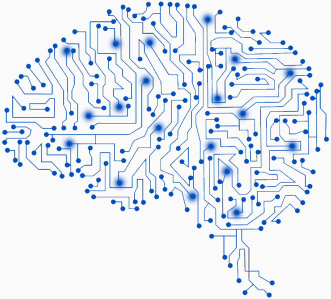
Master 2 Statistique & Data Science, Ingénierie Mathématique

Réseaux de neurones profonds pour l'apprentissage
Deep neural networks for machine learning

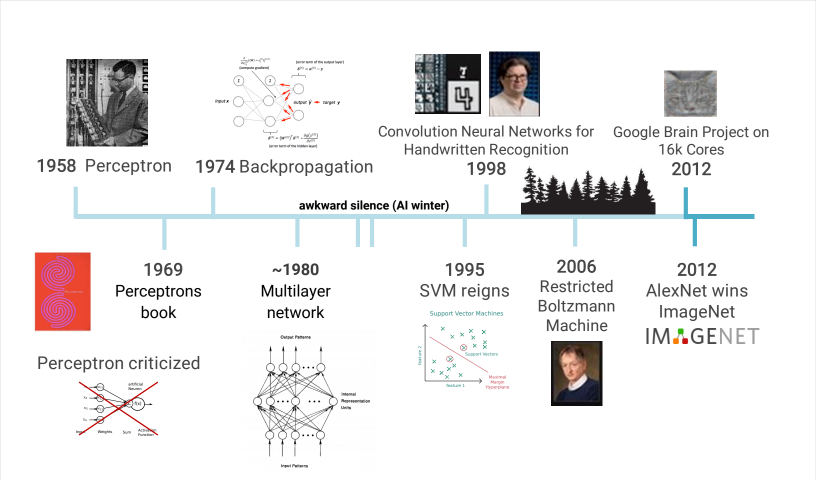
Course II – Introduction to Artificial Neural Networks: Backpropagation

Bruno Galerne

2024-2025

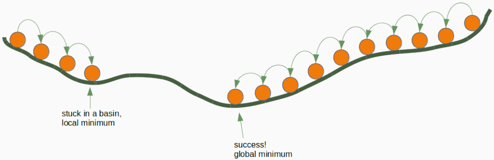


Timeline of (deep) learning

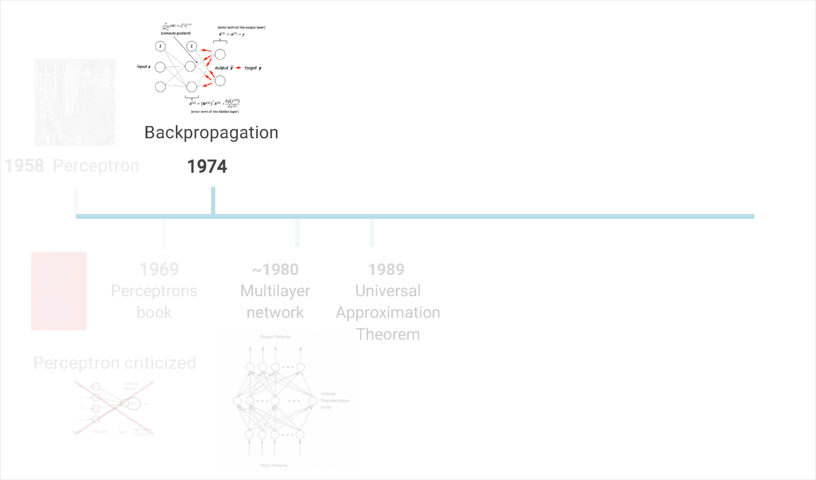


(Source: Lucas Masuch & Vincent Lepetit)

Backpropagation

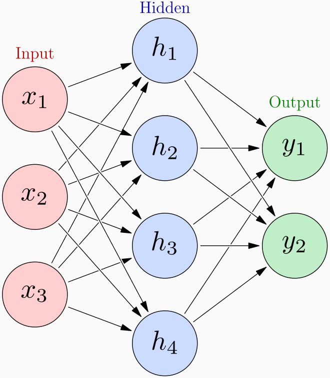


Learning with backpropagation



(Source: Lucas Masuch & Vincent Lepetit)

Artificial neural network / Multilayer perceptron / NeuralNet



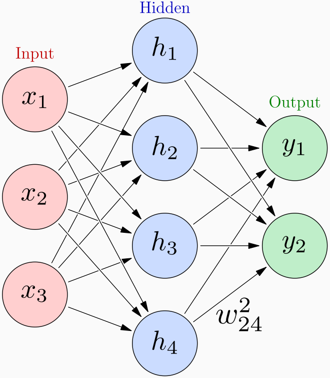
$$h_1 = g_1\left(w^1_{11}x_1 + w^1_{12}x_2 + w^1_{13}x_3 + b^1_1\right)$$
$$h_2 = g_1\left(w^1_{21}x_1 + w^1_{22}x_2 + w^1_{23}x_3 + b^1_2\right)$$
$$h_3 = g_1\left(w^1_{31}x_1 + w^1_{32}x_2 + w^1_{33}x_3 + b^1_3\right)$$
$$h_4 = g_1\left(w^1_{41}x_1 + w^1_{42}x_2 + w^1_{43}x_3 + b^1_4\right)$$

$$y_1 = g_2\left(w^2_{11}h_1 + w^2_{12}h_2 + w^2_{13}h_3 + w^2_{14}h_4 + b^2_1\right)$$
$$y_2 = g_2\left(w^2_{21}h_1 + w^2_{22}h_2 + w^2_{23}h_3 + w^2_{24}h_4 + b^2_2\right)$$

w^k_{ij} synaptic weight between previous node j and next node i at layer k.

g_k are any activation function applied to each coefficient of its input vector.

Artificial neural network / Multilayer perceptron / NeuralNet



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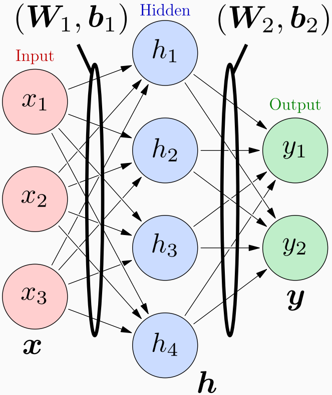
Artificial neural network / Multilayer perceptron / NeuralNet



$$h_1 = g_1\left(w_{11}^1 x_1 + w_{12}^1 x_2 + w_{13}^1 x_3 + b_1^1\right)$$
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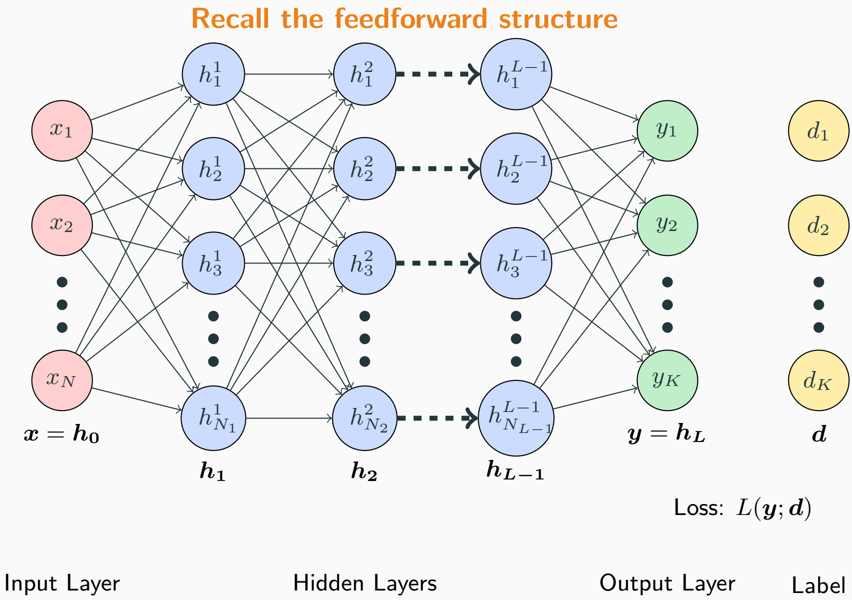
$$h_4 = g_1\left(w_{41}^1 x_1 + w_{42}^1 x_2 + w_{43}^1 x_3 + b_4^1\right)$$
$$\boldsymbol{h} = g_1\left(\boldsymbol{W}_1 \boldsymbol{x} + \boldsymbol{b}_1\right)$$

$$y_1 = g_2\left(w_{11}^2 h_1 + w_{12}^2 h_2 + w_{13}^2 h_3 + w_{14}^2 h_4 + b_1^2\right)$$
$$y_2 = g_2\left(w_{21}^2 h_1 + w_{22}^2 h_2 + w_{23}^2 h_3 + w_{24}^2 h_4 + b_2^2\right)$$
$$\boldsymbol{y} = g_2\left(\boldsymbol{W}_2 \boldsymbol{h} + \boldsymbol{b}_2\right)$$

w_{ij}^k synaptic weight between previous node j and next node i at layer k.

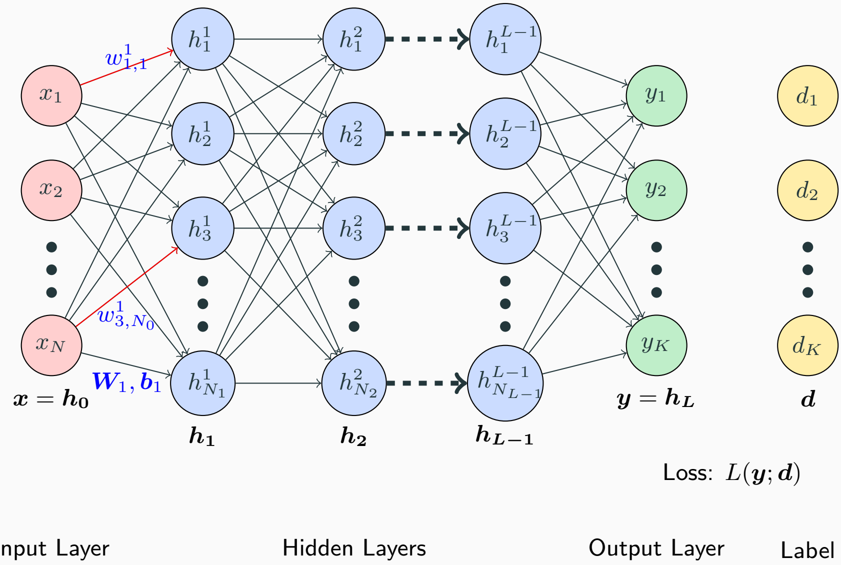
g_k are any activation function applied to each coefficient of its input vector.

The matrices $\boldsymbol{W_k}$ and biases $\boldsymbol{b}_k$ are learned from labeled training data.

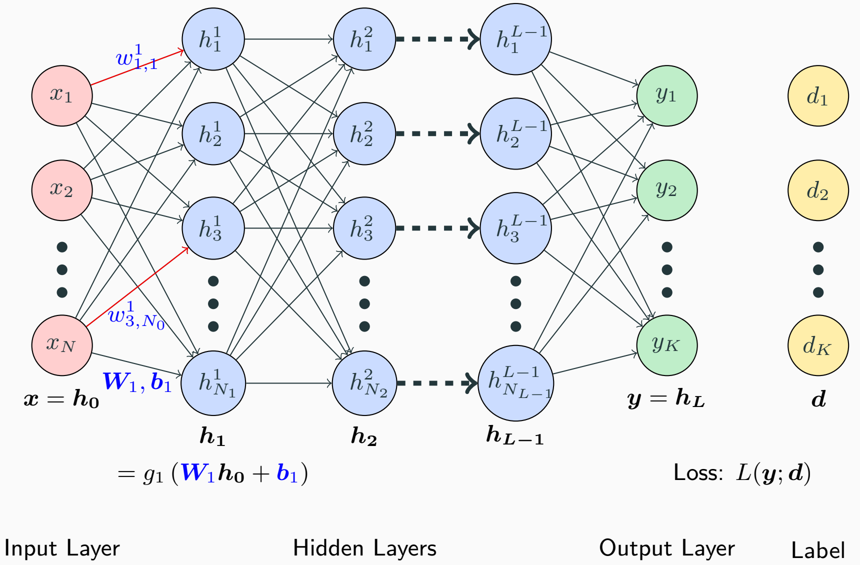

Recall the feedforward structure
x_1
x_2
x_N
$x = h_0$
h_1^1
h_2^1
h_3^1
$h_{N_1}^1$
h_1
h_1^2
h_2^2
h_3^2
$h_{N_2}^2$
h_2
h_1^{L-1}
h_2^{L-1}
h_3^{L-1}
$h_{N_{L-1}}^{L-1}$
h_{L-1}
y_1
y_2
y_K
$y = h_L$
d_1
d_2
d_K
d
Loss: $L(y; d)$
Input Layer
Hidden Layers
Output Layer
Label

Feedforward Artificial Neural Network

Recall the feedforward structure

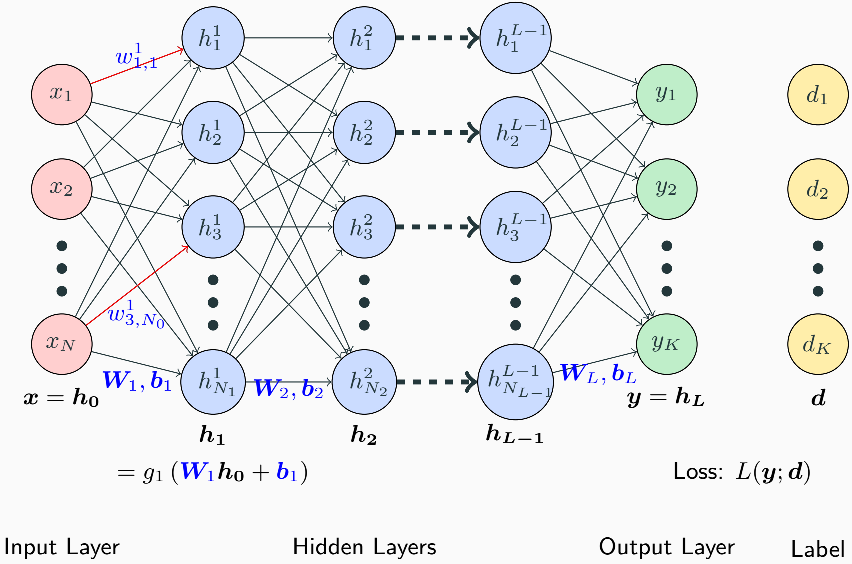


Recall the feedforward structure

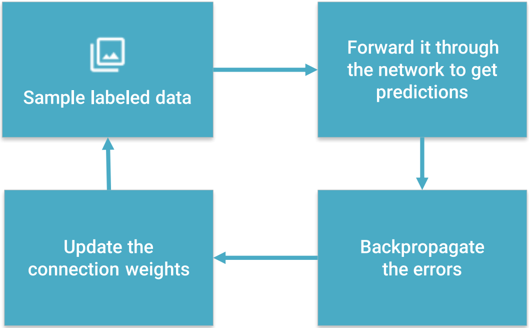


Feedforward Artificial Neural Network

Recall the feedforward structure



Training process



Learns by generating an error signal that measures the difference between the predictions of the network and the desired values and then using this error signal to change the weights (or parameters) so that predictions get more accurate.

(Source: Lucas Masuch)

- The parameters of the neural network are

$$\boldsymbol{W} = (\boldsymbol{W}_1, \boldsymbol{b}_1, \boldsymbol{W}_2, \boldsymbol{b}_2, \ldots, \boldsymbol{W}_L, \boldsymbol{b}_L)$$

- Training the network = minimizing the training loss $E(\boldsymbol{W})$

Objective: $\min_{\boldsymbol{W}} E(\boldsymbol{W})$ where $E(W) = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{T}} L(\boldsymbol{y}^i; \boldsymbol{d}^i)$

$$\Rightarrow \quad \nabla E(\boldsymbol{W}) = \begin{pmatrix} \frac{\partial E(\boldsymbol{W})}{\partial \boldsymbol{W}_1} & \frac{\partial E(\boldsymbol{W})}{\partial \boldsymbol{b}_1} & \ldots & \frac{\partial E(\boldsymbol{W})}{\partial \boldsymbol{W}_L} & \frac{\partial E(\boldsymbol{W})}{\partial \boldsymbol{b}_L} \end{pmatrix}^T = 0$$

- **Solution:** no closed-form solutions $\Rightarrow$ use (stochastic) gradient descent.
- $\frac{\partial E(\boldsymbol{W})}{\partial \boldsymbol{W}_k}$ not really rigorous, we will use the notation

$$\nabla_{\boldsymbol{W}_k} E(\boldsymbol{W}) \quad \text{and} \quad \nabla_{\boldsymbol{b}_k} E(\boldsymbol{W}).$$

Minimizing training loss

For multilayer neural networks $\boldsymbol{W} \mapsto E(\boldsymbol{W})$ is non-convex
$\Rightarrow$ No guarantee of convergence.
Even if convergence occurs, the solution depends on the initialization and the step size/learning rate γ.

Nevertheless, really good minima or saddle points are reached in practice by

$$\boldsymbol{W}^{t+1} \leftarrow \boldsymbol{W}^t - \gamma \nabla E(\boldsymbol{W}^t), \quad \gamma > 0$$

Gradient descent can be expressed coordinate by coordinate as:

$$w_{i,j}^{k,t+1} \leftarrow w_{i,j}^{k,t} - \gamma \frac{\partial E(\boldsymbol{W}^t)}{\partial w_{i,j}^k}$$

for all weights $w_{i,j}^k$ linking a node j to a node i in the next layer k.

$\Rightarrow$ The algorithm to compute $\dfrac{\partial E(\boldsymbol{W})}{\partial w_{i,j}^k}$ for ANNs is called **backpropagation**.

ANN – Optimization

- In practice we only use **stochastic** gradient descent with batch of training set.
- For some random small subset (e.g. batch) $\mathcal{S} \subset \mathcal{T}$, consider

$$E(\boldsymbol{W}; \mathcal{S}) = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{S}} L(\boldsymbol{y}^i; \boldsymbol{d}^i)$$

- Our **goal** is to compute the noisy gradient

$$\nabla_{\boldsymbol{W}_k} E(\boldsymbol{W}; \mathcal{S}) = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{S}} \nabla_{\boldsymbol{W}_k} L(\boldsymbol{y}^i; \boldsymbol{d}^i).$$

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- Why is this relevant to minimize $E(\boldsymbol{W}) = E(\boldsymbol{W};\mathcal{T})$?

ANN – Optimization

- **Stochastic** gradient descent: For some random small subset (e.g. batch) $\mathcal{S} \subset \mathcal{T}$, our **goal** is to compute the noisy gradient

$$\nabla_{\boldsymbol{W}_k} E(\boldsymbol{W}; \mathcal{S}) = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{S}} \nabla_{\boldsymbol{W}_k} L(\boldsymbol{y}^i; \boldsymbol{d}^i).$$

- **Unbiased approximation:** As soon as $\mathcal{S}$ spans uniformly the whole training set $\mathcal{T}$,

$$\begin{aligned}
\mathbb{E}_{\mathcal{S}}\left(\nabla_{\boldsymbol{W}_k} E(\boldsymbol{W}; \mathcal{S})\right) &= \mathbb{E}_{\mathcal{S}}\left(\sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{S}} \nabla_{\boldsymbol{W}_k} L(\boldsymbol{y}^i; \boldsymbol{d}^i)\right) \\
&= \mathbb{E}_{\mathcal{S}}\left(\sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{T}} \mathbf{1}_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{S}} \nabla_{\boldsymbol{W}_k} L(\boldsymbol{y}^i; \boldsymbol{d}^i)\right) \\
&= \frac{|\mathcal{S}|}{|\mathcal{T}|} \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{T}} \nabla_{\boldsymbol{W}_k} L(\boldsymbol{y}^i; \boldsymbol{d}^i) = \frac{|\mathcal{S}|}{|\mathcal{T}|} \nabla_{\boldsymbol{W}_k} E(\boldsymbol{W}).
\end{aligned}$$

- Conclusion: In expectation the noisy gradient is equal to the gradient using the whole training dataset (unbiased estimator).

ANN – Optimization

Loss functions: Classical loss functions are:

For regression: $\boldsymbol{d}^i \in \mathbb{R}^K$

- Square error

$$E(\boldsymbol{W}) = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{T}} \frac{1}{2} \|\boldsymbol{y}^i - \boldsymbol{d}^i\|_2^2 = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{T}} \frac{1}{2} \sum_k (y_k^i - d_k^i)^2$$

For multi-class classification: $d^i \in \{1, \ldots, K\}$, coded by $\boldsymbol{d}^i \in \{0, 1\}^K$,

- Cross-entropy with softmax as the last layer

$$E(\boldsymbol{W}) = -\sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i)} \sum_{k=1}^{K} d_k^i \log y_k^i \quad \text{with} \quad \boldsymbol{y}^i = f(\boldsymbol{x}^i; \boldsymbol{W}) = \text{softmax}(\boldsymbol{a}^i) \in (0, 1)^K.$$

- Cross-entropy with softmax included in loss (PyTorch convention): $\boldsymbol{y}^i = \boldsymbol{a}^i$ is the output of the last linear layer:

$$E(\boldsymbol{W}) = -\sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i)} \left[a_{d^i} - \log \left(\sum_{k=1}^{K} \exp(a_k) \right) \right] \quad \text{with } d^i \text{ the class of } \boldsymbol{x}^i.$$

ANN – Optimization

- The loss functions are of the form

$$E(\boldsymbol{W}) = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i)} L(\boldsymbol{y}^i; \boldsymbol{d}^i)$$

- By linearity,

$$\nabla E(\boldsymbol{W}) = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i)} \nabla L(\boldsymbol{y}^i; \boldsymbol{d}^i)$$

- There the neural net output $\boldsymbol{y}^i = f(\boldsymbol{x}^i; \boldsymbol{W})$ is a function of the input data $\boldsymbol{x}^i$ and the neural weights $\boldsymbol{W}$.
- We know the gradient of $L(\boldsymbol{y}^i; \boldsymbol{d}^i)$ with respect to the variable $\boldsymbol{y}$
  - Regression/Square error:

$$L(\boldsymbol{y}; \boldsymbol{d}) = \frac{1}{2}\|\boldsymbol{y} - \boldsymbol{d}\|_2^2 \quad \Rightarrow \quad \nabla_{\boldsymbol{y}} L(\boldsymbol{y}; \boldsymbol{d}) = \boldsymbol{y} - \boldsymbol{d}$$

  - Multi-class classification/cross-entropy:

$$L(\boldsymbol{y}; \boldsymbol{d}) = -y_d + \log\left(\sum_{k=1}^{K} \exp(y_k)\right) \quad \Rightarrow \quad \nabla_{\boldsymbol{y}} L(\boldsymbol{y}; \boldsymbol{d}) = \text{softmax}(\boldsymbol{y}) - \boldsymbol{d}.$$

ANN – Optimization

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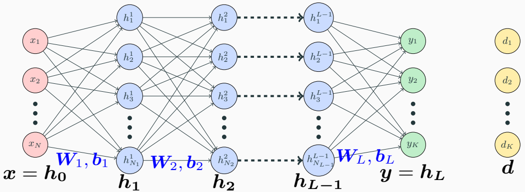
- We know the gradient of $L(\boldsymbol{y}^i; \boldsymbol{d}^i)$ with respect to the variable $\boldsymbol{y}$
- We still need to compute

$$\nabla_{\boldsymbol{W}_k} L(\boldsymbol{y}; \boldsymbol{d}) \quad \text{and} \quad \nabla_{\boldsymbol{b}_k} L(\boldsymbol{y}; \boldsymbol{d}) \quad \text{for } k = 0, \ldots, L.$$

- For simplicity above we will use the notation $E = L(\boldsymbol{y}; \boldsymbol{d})$, that is considering only one point.

ANN – Backpropagation



Loss: $E = L(\boldsymbol{y}; \boldsymbol{d})$

Forward pass

Initialization:

$\boldsymbol{h}_0 = \boldsymbol{x}$

for layer $k = 1$ **to** L **do**

- Linear unit:
- $\boldsymbol{a}_k = \boldsymbol{W}_k \boldsymbol{h}_{k-1} + \boldsymbol{b}_k$
- Componentwise non-linear activation:
- $\boldsymbol{h}_k = g_k(\boldsymbol{a}_k)$

end

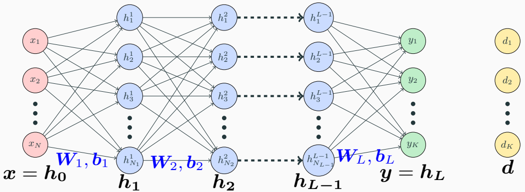
Output layer:

$\boldsymbol{y} = \boldsymbol{h}_L$

Compute loss:

$E = L(\boldsymbol{y}; \boldsymbol{d})$

ANN – Backpropagation



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Output layer:

$\boldsymbol{y} = \boldsymbol{h}_L$

Compute loss:

$E = L(\boldsymbol{y}; \boldsymbol{d})$

Backward pass

Goal: Compute the gradient with respect to all parameters

$$\frac{\partial E}{\partial w_{i,j}^k} = ? \qquad \frac{\partial E}{\partial b_i^k} = ?$$

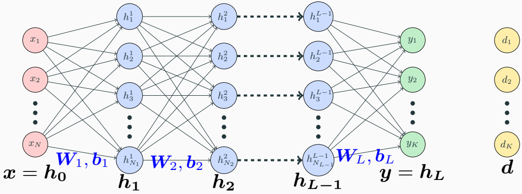
for all

$k \in \{1, \ldots, L\}$,

$i \in \{1, \ldots, N_k\}$,

$j \in \{1, \ldots, N_{k-1}\}$.

ANN – Backpropagation

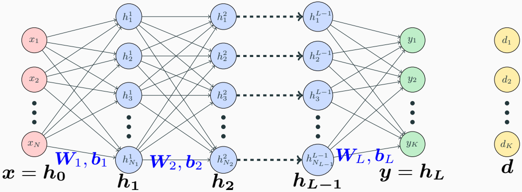


Loss: $E = L(\boldsymbol{y}; \boldsymbol{d})$

Going backward

- We know how to compute the loss function and its gradient:

$$\nabla_{\boldsymbol{h}_L} E = \nabla L(\boldsymbol{y}; \boldsymbol{d})$$



Loss: $E = L(\boldsymbol{y}; \boldsymbol{d})$

Gradient with respect to last linear unit output $\boldsymbol{a}_L$

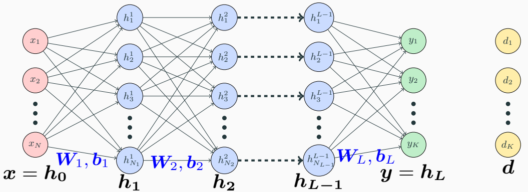
$$\boldsymbol{h}_L = g_L(\boldsymbol{a}_L)$$

That is for all $i \in \{1, \ldots, N_L\}$, $h_i^L = g_L(a_i^L)$. By the chain rule,

$$\frac{\partial E}{\partial a_i^L} = \frac{\partial E}{\partial h_i^L} \frac{\partial h_i^L}{\partial a_i^L} = [\nabla_{\boldsymbol{h}_L} E]_i \, g_L'(a_i^L)$$

Vector formula: $\nabla_{\boldsymbol{a}_L} E = \nabla_{\boldsymbol{h}_L} E \odot g_L'(\boldsymbol{a}_L)$

where $\odot$ is the componentwise product between vectors, ie Hadamard product.



Loss: $E = L(\boldsymbol{y}; \boldsymbol{d})$

Gradient with respect to bias of last linear unit b_L

$$\boldsymbol{a}_L = \boldsymbol{W}_L \boldsymbol{h}_{L-1} + \boldsymbol{b}_L$$

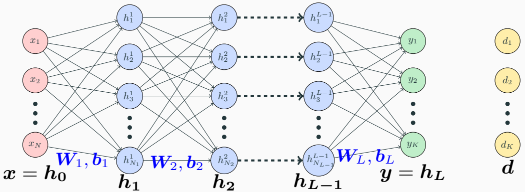
That is for all $i \in \{1, \ldots, N_L\}$, $a_i^L = \sum_{j=1}^{N_{L-1}} w_{i,j}^L h_j^{L-1} + b_i^L$.

By the chain rule, for all $i \in \{1, \ldots, N_L\}$,

$$\frac{\partial E}{\partial b_i^L} = \frac{\partial E}{\partial a_i^L} \underbrace{\frac{\partial a_i^L}{\partial b_i^L}}_{=1} = \frac{\partial E}{\partial a_i^L} = [\nabla_{\boldsymbol{a}_L} E]_i$$

Vector formula: $\nabla_{\boldsymbol{b}_L} E = \nabla_{\boldsymbol{a}_L} E$

ANN – Backpropagation



Loss: $E = L(\boldsymbol{y}; \boldsymbol{d})$

Gradient with respect to weights of last linear unit W_L

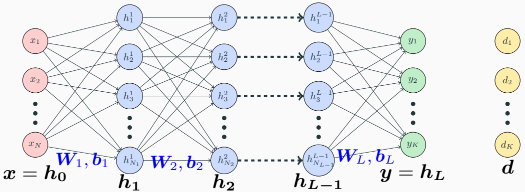
$$\boldsymbol{a}_L = \boldsymbol{W}_L \boldsymbol{h}_{L-1} + \boldsymbol{b}_L$$

That is for all $i \in \{1, \ldots, N_L\}$, $a_i^L = \sum_{j=1}^{N_{L-1}} w_{i,j}^L h_j^{L-1} + b_i^L$.

By the chain rule, for all $i \in \{1, \ldots, N_L\}$ and $j \in \{1, \ldots, N_{L-1}\}$

$$\frac{\partial E}{\partial w_{i,j}^L} = \frac{\partial E}{\partial a_i^L} \underbrace{\frac{\partial a_i^L}{\partial w_{i,j}^L}}_{=h_j^{L-1}} = \frac{\partial E}{\partial a_i^L} h_j^{L-1} = [\nabla_{\boldsymbol{a}_L} E]_i \, [\boldsymbol{h}_{L-1}]_j$$

Matrix formula: $\nabla_{\boldsymbol{W}_L} E = \nabla_{\boldsymbol{a}_L} E \, \boldsymbol{h}_{L-1}^T$



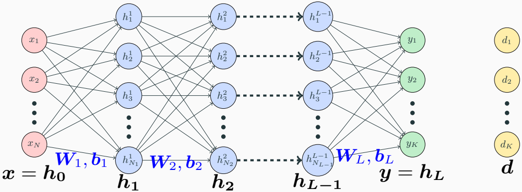
Loss: $E = L(\boldsymbol{y}; \boldsymbol{d})$

Gradients for last layer parameters

Given the gradient with respect to the output layer $\nabla_{\boldsymbol{h}_L} E$, so far we can compute:

- $\nabla_{\boldsymbol{a}_L} E = \nabla_{\boldsymbol{h}_L} E \odot g'_L(\boldsymbol{a}_L)$
- $\nabla_{\boldsymbol{b}_L} E = \nabla_{\boldsymbol{a}_L} E$
- $\nabla_{\boldsymbol{W}_L} E = \nabla_{\boldsymbol{a}_L} E \, \boldsymbol{h}_{L-1}^T$

ANN – Backpropagation



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Gradients for last layer parameters

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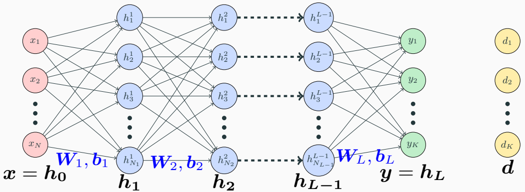
- $\nabla_{\boldsymbol{b}_L} E = \nabla_{\boldsymbol{a}_L} E$
- $\nabla_{\boldsymbol{W}_L} E = \nabla_{\boldsymbol{a}_L} E \, \boldsymbol{h}_{L-1}^T$

How can we compute the gradients for the parameters of layer $L - 1$?



Loss: $E = L(\boldsymbol{y}; \boldsymbol{d})$

Gradients for last layer parameters

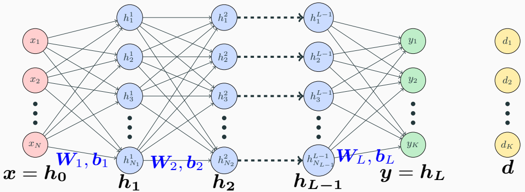
Given the gradient with respect to the output layer $\nabla_{\boldsymbol{h}_L} E$, so far we can compute:

- $\nabla_{\boldsymbol{a}_L} E = \nabla_{\boldsymbol{h}_L} E \odot g'_L(\boldsymbol{a}_L)$
- $\nabla_{\boldsymbol{b}_L} E = \nabla_{\boldsymbol{a}_L} E$
- $\nabla_{\boldsymbol{W}_L} E = \nabla_{\boldsymbol{a}_L} E \, \boldsymbol{h}_{L-1}^T$

How can we compute the gradients for the parameters of layer $L-1$?

We need the expression of the gradient with respect to the last but one hidden layer $\boldsymbol{h}_{L-1}$... and then the same formulas apply!

$$\nabla_{\boldsymbol{h}_{L-1}} E = ?$$

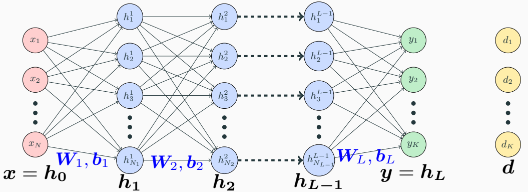


Loss: $E = L(\boldsymbol{y}; \boldsymbol{d})$

Gradient with respect to the last but one hidden layer $\boldsymbol{h}_{L-1}$

Here, even to compute the scalar partial derivative $\dfrac{\partial E}{\partial h_j^{L-1}}$, we need to use differential calculus for multivariate functions since h_j^{L-1} appears in each component of $\boldsymbol{a}_L$:

For all $i \in \{1, \ldots, N_L\}$, $a_i^L = \displaystyle\sum_{j=1}^{N_{L-1}} w_{i,j}^L h_j^{L-1} + b_i^L$.



Loss: $E = L(\boldsymbol{y}; \boldsymbol{d})$

Gradient with respect to the last but one hidden layer $\boldsymbol{h}_{L-1}$

Let us recall the derivative rule for composition with affine maps:

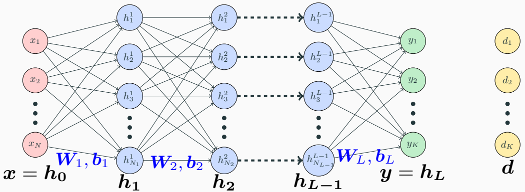
$$\text{For} \quad \varphi(\boldsymbol{x}) = f(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}) \quad \text{one has} \quad \nabla\varphi(\boldsymbol{x}) = \boldsymbol{A}^T \nabla f(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}).$$

Using the decomposition

$$\begin{array}{ccccc} \mathbb{R}^{N_{L-1}} & \to & \mathbb{R}^{N_L} & \to & \mathbb{R} \\ \boldsymbol{h}_{L-1} & \mapsto & \boldsymbol{a}_L = \boldsymbol{W}_L \boldsymbol{h}_{L-1} + \boldsymbol{b}_L & \mapsto & E \end{array}$$

Vector formula: $\nabla_{\boldsymbol{h}_{L-1}} E = {\boldsymbol{W}_L}^T \nabla_{\boldsymbol{a}_L} E$

ANN – Backpropagation



Loss: $E = L(\boldsymbol{y}; \boldsymbol{d})$

Forward pass

Initialization:

$\boldsymbol{h}_0 = \boldsymbol{x}$

for layer $k = 1$ **to** L **do**

  Linear unit:

  $\boldsymbol{a}_k = \boldsymbol{W}_k \boldsymbol{h}_{k-1} + \boldsymbol{b}_k$

  Componentwise non-linear activation:

  $\boldsymbol{h}_k = g_k(\boldsymbol{a}_k)$

end

Output layer:

$\boldsymbol{y} = \boldsymbol{h}_L$

Compute loss:

$E = L(\boldsymbol{y}; \boldsymbol{d})$

Backward pass

Initialization: Gradient of output layer:

$\nabla_{\boldsymbol{h}_L} E = \nabla L(\boldsymbol{y}; \boldsymbol{d})$

for layer $k = L$ **to** 1 **do**

  Componentwise gain of error:

  $\boldsymbol{\delta}_k = \nabla_{\boldsymbol{a}_k} E = \nabla_{\boldsymbol{h}_k} E \odot g_k'(\boldsymbol{a}_k)$

  Gradient of layer bias:

  $\nabla_{\boldsymbol{b}_k} E = \boldsymbol{\delta}_k$

  Gradient of weights:

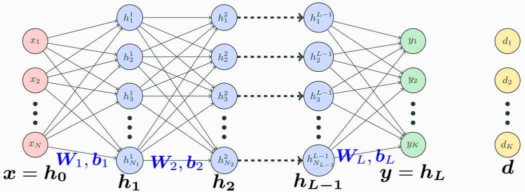
  $\nabla_{\boldsymbol{W}_k} E = \boldsymbol{\delta}_k \boldsymbol{h}_{k-1}^T$

  Gradient of previous hidden layer:

  $\nabla_{\boldsymbol{h}_{k-1}} E = \boldsymbol{W}_k^T \boldsymbol{\delta}_k$

end

ANN – Backpropagation



Loss: $E = L(\boldsymbol{y}; \boldsymbol{d})$

Forward pass

Initialization:

$\boldsymbol{h}_0 = \boldsymbol{x}$

for layer $k = 1$ **to** L **do**

Linear unit:

$\boldsymbol{a}_k = \boldsymbol{W}_k \boldsymbol{h}_{k-1} + \boldsymbol{b}_k$ **(stored)**

Componentwise non-linear activation:

$\boldsymbol{h}_k = g_k(\boldsymbol{a}_k)$ **(stored)**

end

Output layer:

$\boldsymbol{y} = \boldsymbol{h}_L$

Compute loss:

$E = L(\boldsymbol{y}; \boldsymbol{d})$

Backward pass

Initialization: Gradient of output layer:

$\nabla_{\boldsymbol{h}_L} E = \nabla L(\boldsymbol{y}; \boldsymbol{d})$

for layer $k = L$ **to** 1 **do**

Componentwise gain of error:

$\boldsymbol{\delta}_k = \nabla_{\boldsymbol{a}_k} E = \nabla_{\boldsymbol{h}_k} E \odot g_k'(\boldsymbol{a}_k)$

Gradient of layer bias:

$\nabla_{\boldsymbol{b}_k} E = \boldsymbol{\delta}_k$

Gradient of weights:

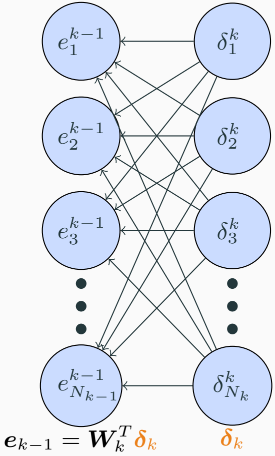
$\nabla_{\boldsymbol{W}_k} E = \boldsymbol{\delta}_k \boldsymbol{h}_{k-1}^T$

Gradient of previous hidden layer:

$\nabla_{\boldsymbol{h}_{k-1}} E = \boldsymbol{W}_k^T \boldsymbol{\delta}_k$

end

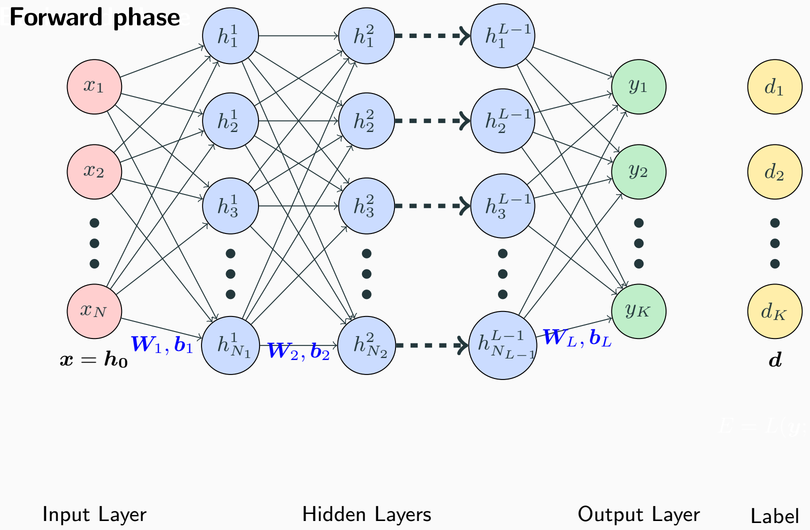
Error backpropagation



- Gradient of previous hidden layer: $\boldsymbol{e}_{k-1} = \nabla_{\boldsymbol{h}_{k-1}} E = \boldsymbol{W}_k^T \boldsymbol{\delta}_k$
- Multiplying by $\boldsymbol{W}_k^T$ corresponds to passing to the linear layer in reverse order.
- The error is backpropagated layer by layer to compute the gradient with respect to each layer parameters.

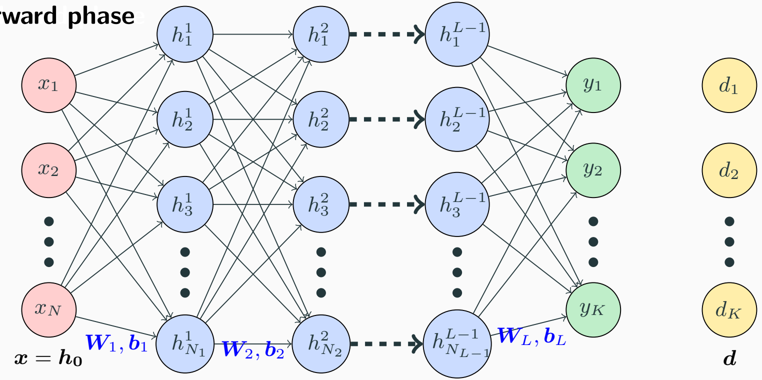
ANN – Backpropagation

Error backpropagation



Error backpropagation

Forward phase

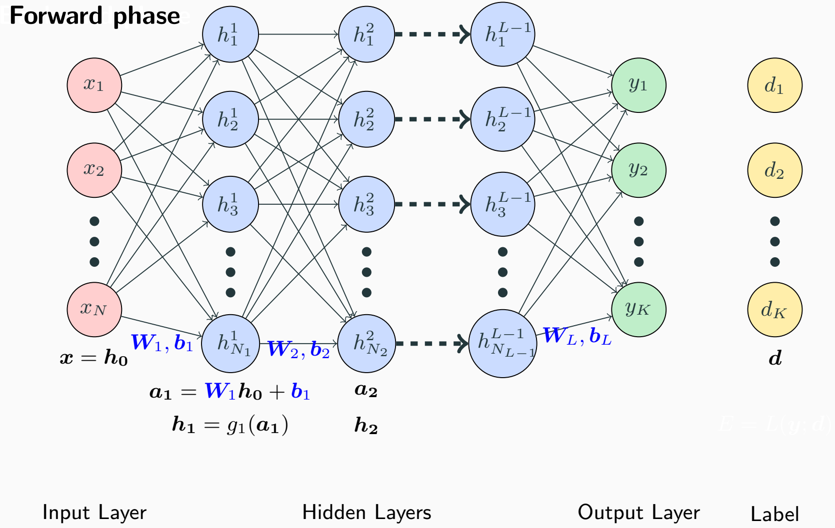


$$\boldsymbol{a_1} = \boldsymbol{W}_1 \boldsymbol{h_0} + \boldsymbol{b}_1$$

$$\boldsymbol{h_1} = g_1(\boldsymbol{a_1})$$

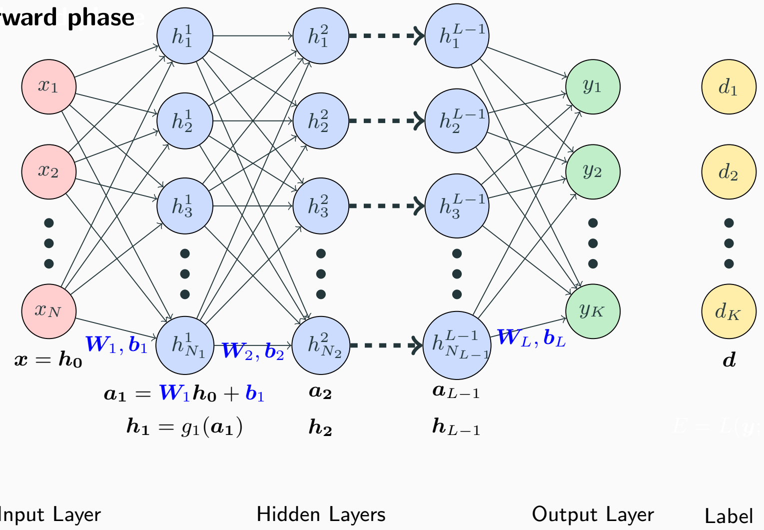
Input Layer | Hidden Layers | Output Layer | Label

Error backpropagation

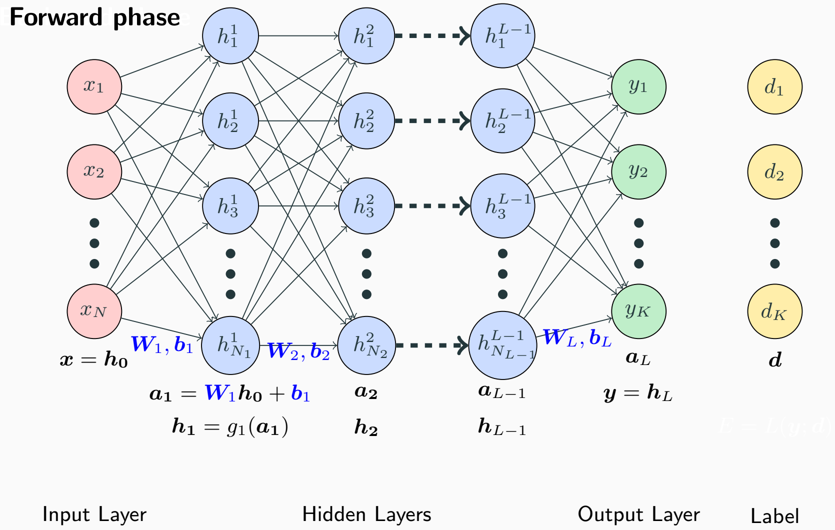


Error backpropagation

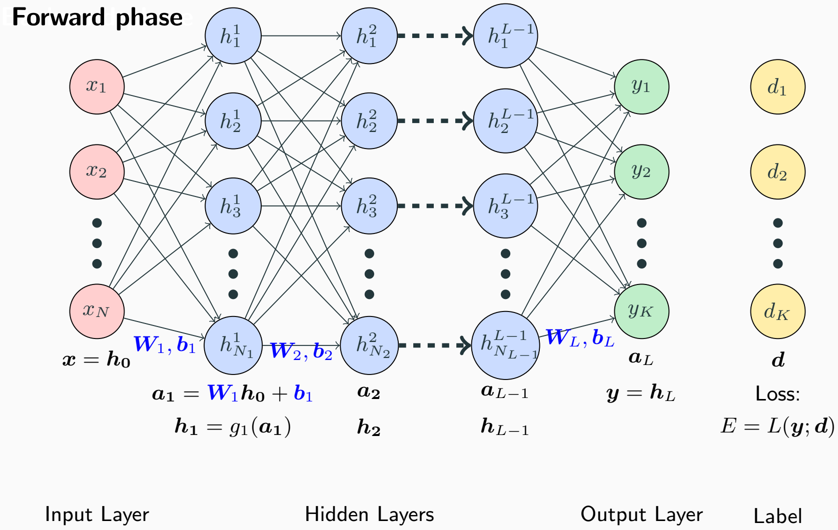
Forward phase



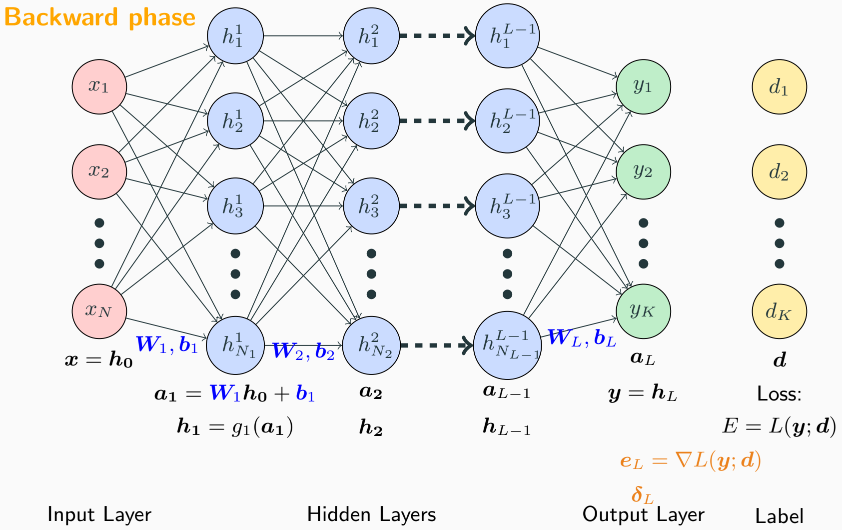
Error backpropagation



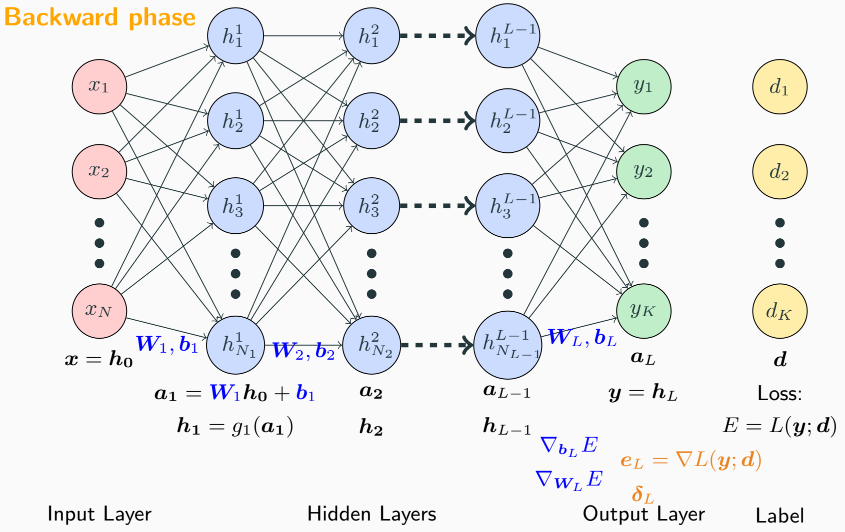
Error backpropagation



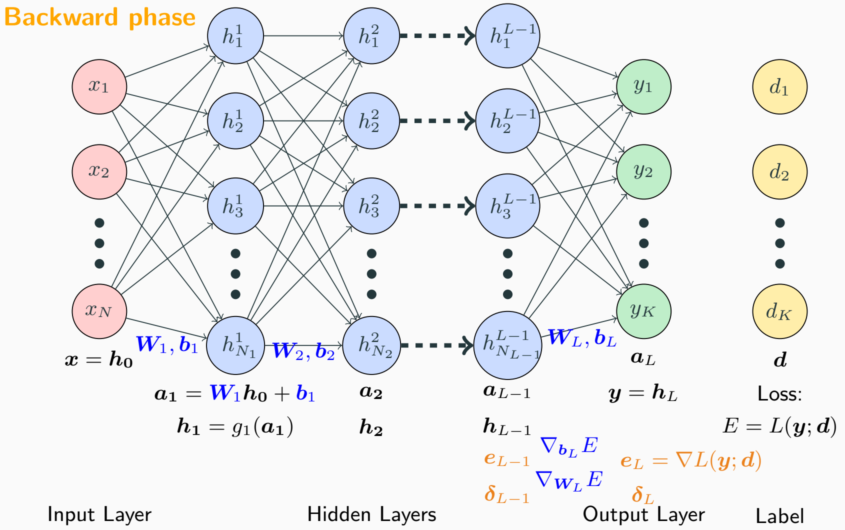
Error backpropagation



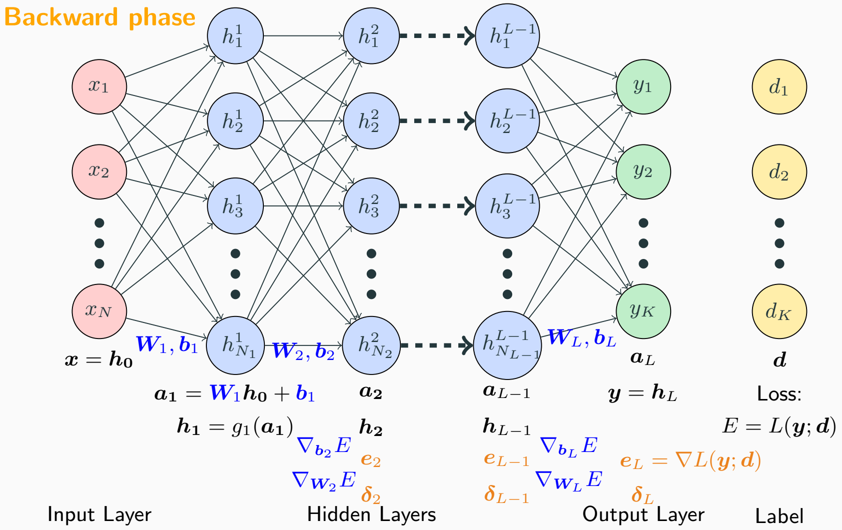
Error backpropagation



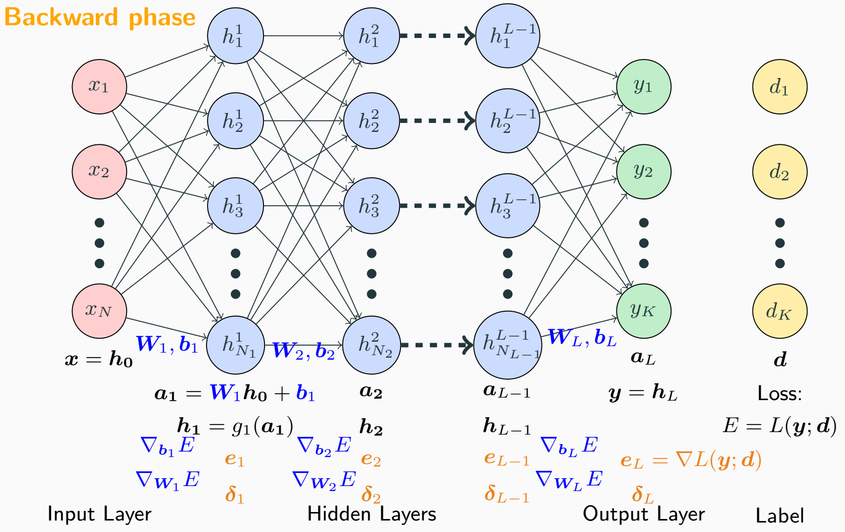
Error backpropagation



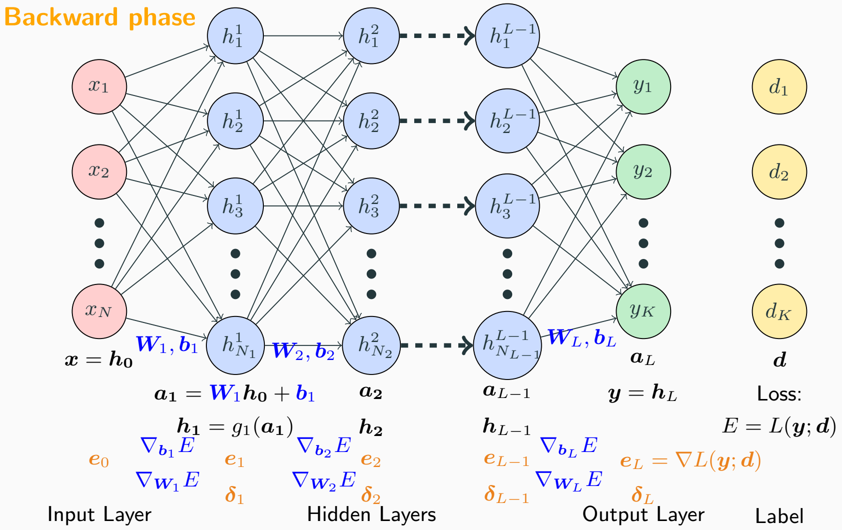
Error backpropagation



Error backpropagation



Error backpropagation



Error backpropagation in practice

Training loss:

$$E(\boldsymbol{W}) = \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{T}} L(\boldsymbol{y}^i; \boldsymbol{d}^i)$$

- The backpropagation procedure computes $\nabla_{\boldsymbol{W}} L(\boldsymbol{y}^i; \boldsymbol{d}^i) = \nabla_{\boldsymbol{W}} L(f(\boldsymbol{x}^i; \boldsymbol{W}); \boldsymbol{d}^i)$.
- This has to be done for each data point $\boldsymbol{x}^i \in \mathcal{T}$.
- By linearity, the final gradient $\nabla E(\boldsymbol{W})$ is the sum of all individual gradients $\nabla_{\boldsymbol{W}} L(\boldsymbol{y}^i; \boldsymbol{d}^i)$.
- These gradients are summed sequentially (no need to store each individual gradients).
- In general we do not compute the exact gradient...

Error backpropagation in practice

Batch loss:

$$E(\boldsymbol{W}) \approx \sum_{(\boldsymbol{x}^i, \boldsymbol{d}^i) \in \mathcal{S}} L(\boldsymbol{y}^i; \boldsymbol{d}^i), \quad \text{with} \quad \mathcal{S} \subset \mathcal{T}$$

- The backpropagation has to be done for each visited data point $\boldsymbol{x}^i \in \mathcal{S}$ of the batch.
- The gradient for each point $\boldsymbol{x}^i$ is added to the running gradient = current gradient estimation.
- Once the noisy estimated gradient is used as a gradient step, one needs to set the gradients to zero: See PyTorch `torch.zero_grad()` procedure.

Questions?

Sources, images courtesy and acknowledgment

Charles Deledalle **V. Lepetit** **L. Masuch**