

14. Neural Networks

Network Data Analysis – NDA 2022–2023

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Sorbonne-LIP6



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Bibliography

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Linear Regression revisited

Stochastic Gradient Descent

The Simple Neuron

Deep Neural Network

Back-propagation

Linear regression

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Remember the problem of Linear Regression. Training data available
 $D_n = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$, with index $i = 1, \dots, n$

- ▶ Input data has d dimensions (features) $\mathbf{x}_i = (x_{i,1}, \dots, x_{i,d})$
- ▶ output data has 1 dimension y_i

Linear regression assumes that the output is an affine function of the input. Find (Θ, b) so that \hat{y} can approximate well y_i , $i = 1, \dots, n$ and can generalise to unknown inputs

$$\begin{aligned}\hat{y} &= w_1 x_1 + w_2 x_2 + \dots + w_d x_d + b \\ &= \Theta^T \mathbf{x} + b\end{aligned}$$

Least Squares

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The loss function is the *Residual Sum of Squares*

$$J_{RSS}(\Theta, b) = \frac{1}{2} \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \frac{1}{2} \sum_{i=1}^n (y_i - \Theta^T \mathbf{x}_i - b)^2$$

which we want to minimise w.r.t. the unknown model parameters

$$\min_{\Theta, b} J_{RSS}(\Theta, b)$$

Using the partial derivatives we get the gradient for each loss item i

$$\frac{\partial J_{RSS,i}}{\partial w_d} = -(y_i - \Theta^T \mathbf{x}_i - b)x_{i,d}$$

$$\frac{\partial J_{RSS,i}}{\partial b} = -(y_i - \Theta^T \mathbf{x}_i - b)$$

- ☞ In this linear model the solution has a closed form.
But can we solve for other more general models?

Gradient descent

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In general we have the **finite sum problem**

$$\min_{\Theta} J(\Theta) = \min_{\Theta} \frac{1}{n} \sum_{i=1}^n J_i(\Theta)$$

Basic gradient descent

$$\begin{aligned}\Theta_{t+1} &= \Theta_t - \eta_t \nabla J(\Theta_t) \\ &= \Theta_t - \eta_t \frac{1}{n} \sum_{i=1}^n \nabla J_i(\Theta_t)\end{aligned}$$

At every step t it moves monotonically towards the optimum.

In practice η_t is chosen either as constant, $\eta_t = \eta$, or as a square summable, but not summable function: $\sum_{t=1}^{\infty} \eta_t^2 < \infty$ and $\sum_{t=1}^{\infty} \eta_t = \infty$.

Question:

- ☞ What is the drawback of this iteration?

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Incremental gradient methods

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Stochastic Gradient Descent (SGD) At each iteration pick a random data-point $i(t) \in \{1, \dots, n\}$ and update

$$\Theta_{t+1} = \Theta_t - \eta_t \nabla J_{i(t)}(\Theta_t)$$

Sampling methods

- ▶ **Random Uniform:** Randomly pick an index i with replacement.
- ▶ **Permutation Based:** Pick index i in given order without replacement
(pre-shuffle dataset)

SGD characteristics

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- ▶ *n*-times faster to compute than the full $\nabla J(\Theta_t)$.
- ▶ But! it does not decrease monotonically.
- ▶ Very sensitive to the step size η_t .
- ▶ Converges fast to a region of confusion close to the optimum.
- ▶ Fluctuates around the optimum inside the region of confusion.
- ▶ The stochastic gradients are unbiased estimates of the true gradient!

Mini-batching

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Speed of convergence depends on how noisy the stochastic gradients are:

- ▶ The **variance** controls the convergence rate of the SGD.
- ▶ Smaller variance → faster convergence to the true gradient.

$$\Theta_{t+1} = \Theta_t - \eta_t \frac{1}{M} \sum_{i=1}^M \nabla J_i(\Theta_t)$$

Mini-batching

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Speed of convergence depends on how noisy the stochastic gradients are:

- ▶ The **variance** controls the convergence rate of the SGD.
- ▶ Smaller variance → faster convergence to the true gradient.

$$\Theta_{t+1} = \Theta_t - \eta_t \frac{1}{M} \sum_{i=1}^M \nabla J_i(\Theta_t)$$

- ▶ $M = 1$: vanilla SGD (cheap / high variance)
- ▶ $M = n$: full gradient descent (expensive / low variance)
- ▶ $1 < M < n$: in-between trade-off. Allows multi-core parallelism.

But if the batch is too large, we end up **over-fitting** the network.

Mini-batch convergence example

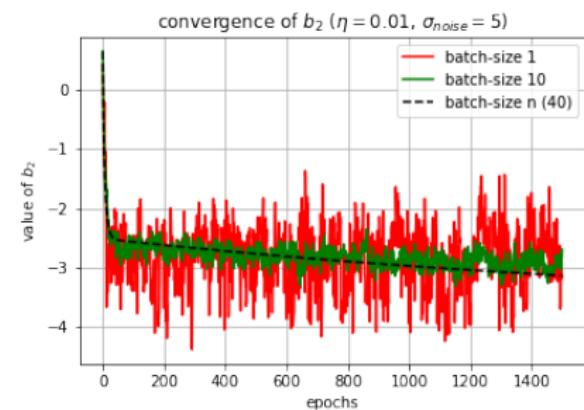
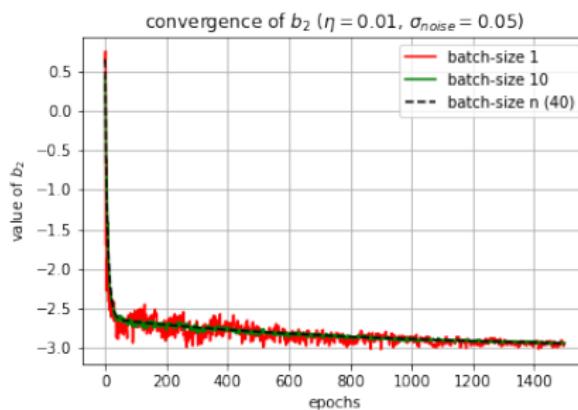
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Consider the data comes from the linear model

$$y = 5 + 2x_1 - 3x_2 + \epsilon$$

and we try to estimate with

$$\hat{y} = \hat{b}_0 + \hat{b}_1 x_1 + \hat{b}_2 x_2$$



Hyperparameters choice

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Hyperparameters:

- ▶ Learning rate η_t
- ▶ Mini-batch size M

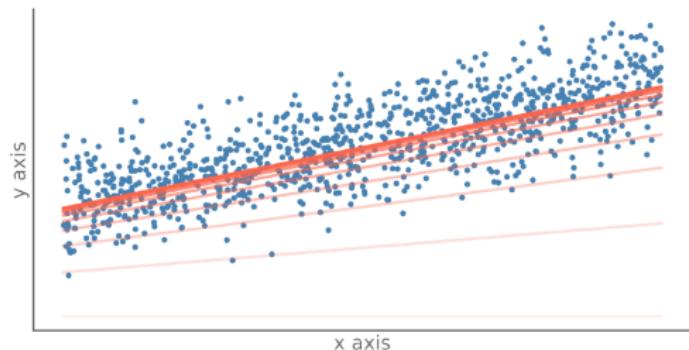
In general, the goal is **not** just to minimise the training loss.

☞ narrow minima of the training loss do not generalise well; wide minima are preferable.

☞ Run SGD with different hyperparameters and choose the pair that minimizes **validation loss**.

Regression Example

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#l	Loss	Gradient	Theta	
0	+12.481	-6.777	-1.732	-3.388 +0.000
20	+4.653	-4.066	-1.039	-2.033 +0.346
40	+1.835	-2.440	-0.624	-1.220 +0.554
60	+0.821	-1.464	-0.374	-0.732 +0.679
80	+0.455	-0.878	-0.224	-0.439 +0.754
100	+0.324	-0.527	-0.135	-0.263 +0.799
120	+0.277	-0.316	-0.081	-0.158 +0.826
140	+0.260	-0.190	-0.048	-0.095 +0.842
160	+0.253	-0.114	-0.029	-0.057 +0.851
180	+0.251	-0.068	-0.017	-0.034 +0.857
200	+0.250	-0.041	-0.010	-0.020 +0.861

Linear Regression revisited

Stochastic Gradient Descent

The Simple Neuron

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Back-propagation

From Linear Regression to Neural Networks

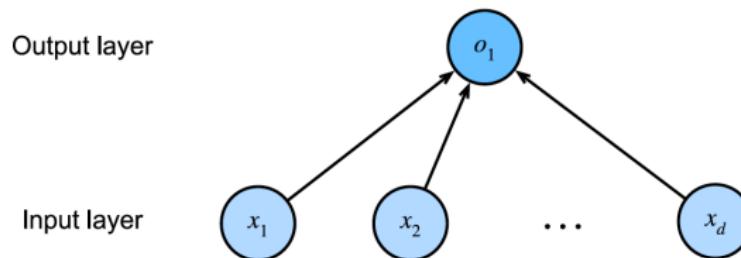
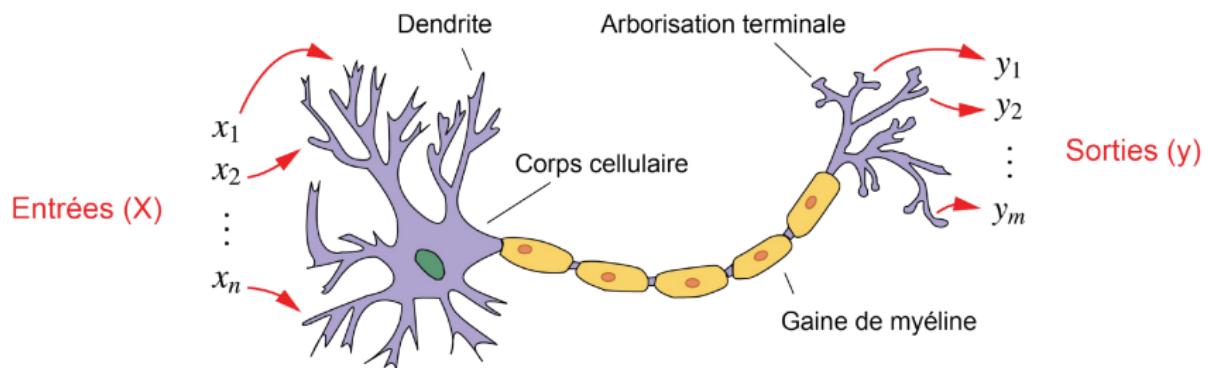


Fig. 3.1.2: Linear regression is a single-layer neural network.

Biology inspired neuron

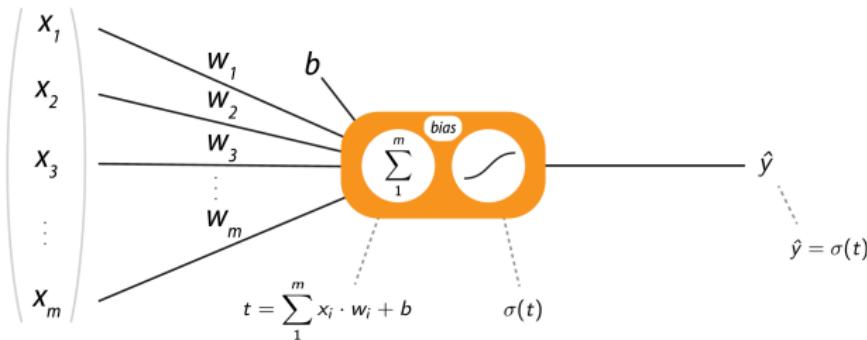
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Simple artificial neuron

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$$\hat{y} = \sigma(\Theta^T \cdot X + b)$$



Input	Bias / Weight	Activation function	Output
X	Θ, b	$\sigma(t)$	\hat{y}

Reminder: Logistic Regression

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Find the probability for y to be in class 1 based on the features \mathbf{x}

$$p(\mathbf{x}) = \mathbf{P}[y = 1 \mid \mathbf{x}] = \frac{e^{\Theta^T \cdot \mathbf{x} + b}}{1 + e^{\Theta^T \cdot \mathbf{x} + b}} = \frac{1}{e^{-\Theta^T \cdot \mathbf{x} - b} + 1}$$

The weights (Θ, b) should minimize the negative log-likelihood cost

$$J(\Theta, b) = - \sum_{i=1}^n \{y_i \log p(\mathbf{x}_i) + (1 - y_i) \log(1 - p(\mathbf{x}_i))\}$$

The minimization is achieved by (Stochastic) Gradient Descent

$$\Theta_{t+1} = \Theta_t - \eta_t \frac{1}{M} \sum_{i \in \text{minibatch}} \nabla_{\Theta} J(\Theta, b)$$

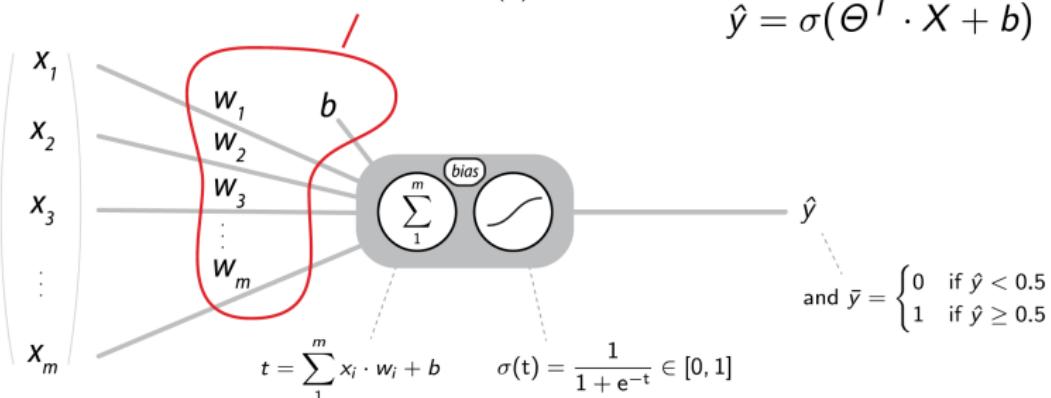
$$b_{t+1} = b_t - \eta_t \frac{1}{M} \sum_{i \in \text{minibatch}} \nabla_b J(\Theta, b)$$

Logistic Regression

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Determined by the minimisation
of a cost function $J(\Theta)$

$$\hat{y} = \sigma(\Theta^T \cdot X + b)$$

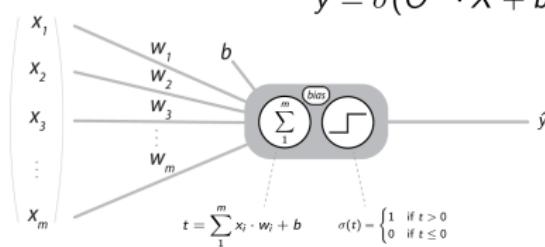


Input	Bias / Weight	Activation function	Output
X	Θ	$\sigma(t)$	\hat{y}

From [B.5] 01-history-and-basic-concepts

The Perceptron

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THE PERCEPTRON

sets of which are tend to sets of

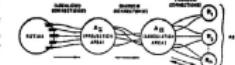


Fig. 1. Organization of a perceptron.
The cells in the projection area ea
receives a number of connections. f

Perceptron
Frank Rosenblatt
1958

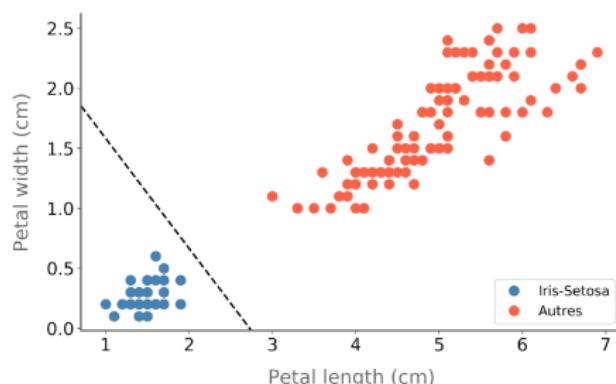
Linear and binary classifier

Perceptron Example

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Iris plants dataset

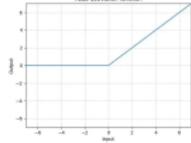
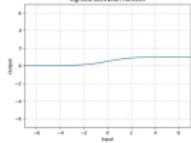
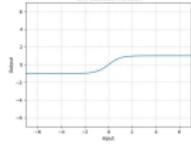
Dataset from : Fisher, R.A. "The use of multiple measurements in taxonomic problems" Annual Eugenics, 7, Part II, 179-188 (1936)



Length x_1	Width x_2	Iris Setosa (0/1) y
1.4	1.4	1
1.6	1.6	1
1.4	1.4	1
1.5	1.5	1
1.4	1.4	1
4.7	4.7	0
4.5	4.5	0
4.9	4.9	0
4.0	4.0	0
4.6	4.6	0
(...)		

Activation functions

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Function	Description	Plot	Characteristics
ReLU	$\max(0, z)$		positive values only
Sigmoid	$\frac{1}{1+e^{-z}}$		[0, +1] binary class
Softmax	$\frac{e^{z_i}}{\sum_j e^{z_j}}$		[0, +1] multi-class
Tanh	$\tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$		[-1, +1] values

Loss functions

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- ▶ Regression:

- ▶ Mean Squared Error Loss

$$\text{MSELoss}(i) = (y_{i,\text{true}} - y_{i,\text{pred}})^2$$

- ▶ Classification

- ▶ (2 classes): Binary Cross Entropy Loss

$$\text{BCELoss}(i) = -[y_i \log(p(\mathbf{x}_i)) + (1 - y_i) \log(1 - p(\mathbf{x}_i))]$$

- ▶ (c classes): Negative Log-Likelihood Loss

$$\text{NLLLoss}(i) = \log \text{softmax}_{(y_i)} (\Theta_1^T \mathbf{x}_i, \dots, \Theta_c^T \mathbf{x}_i)$$

where,

$$\text{softmax}_{(y_i=k)} (\Theta_1^T \mathbf{x}_i, \dots, \Theta_c^T \mathbf{x}_i) = \frac{e^{\Theta_k^T \mathbf{x}_i}}{\sum_{\ell=1}^c e^{\Theta_\ell^T \mathbf{x}_i}}$$

- ☞ The last layer of your network should be `LogSoftmax()`.

Linear Regression revisited

Stochastic Gradient Descent

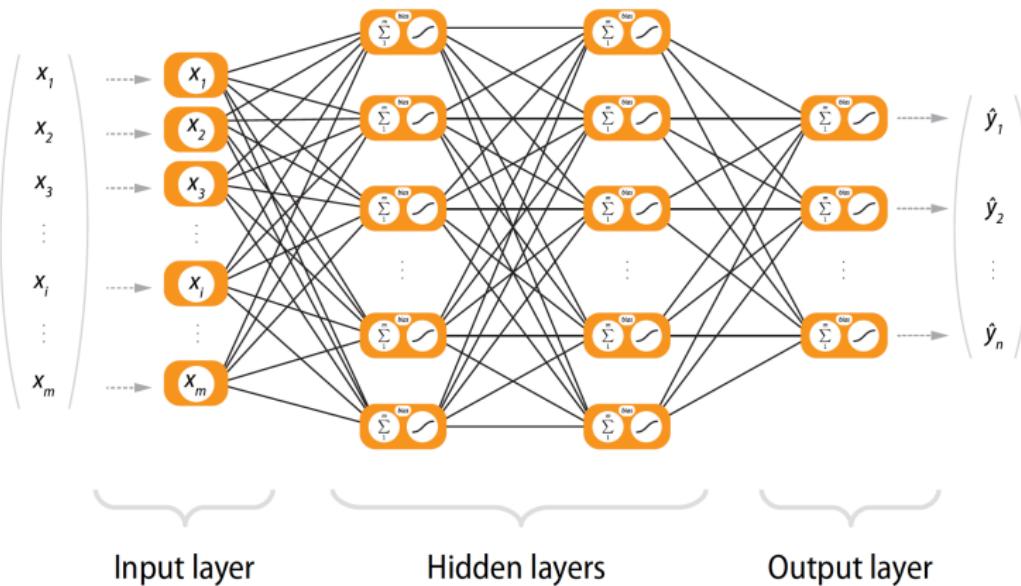
The Simple Neuron

Deep Neural Network

Back-propagation

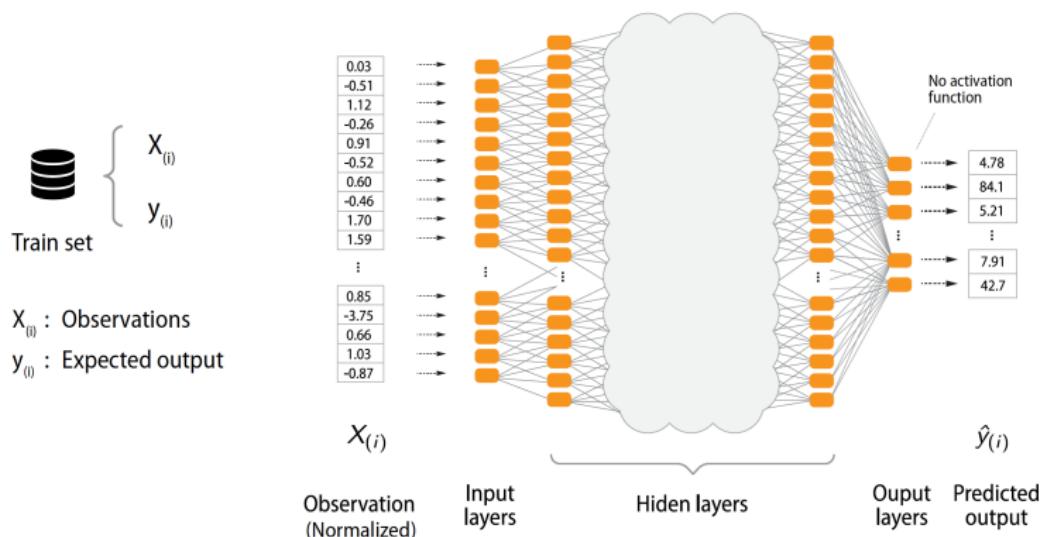
Multi-Layer Perceptron

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Hidden Layers (Regression)

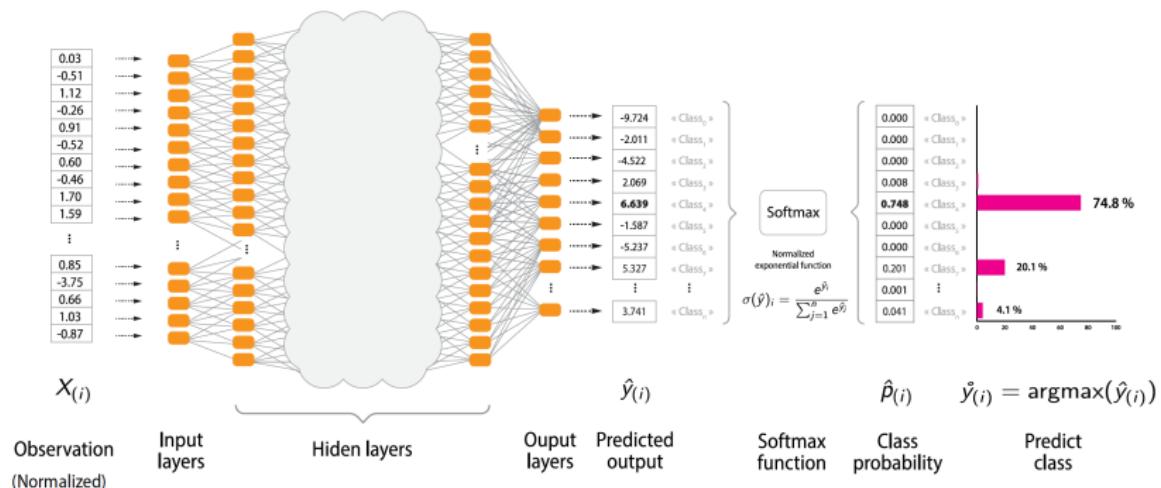
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From [B.5] 01-history-and-basic-concepts

Hidden Layers (Classification)

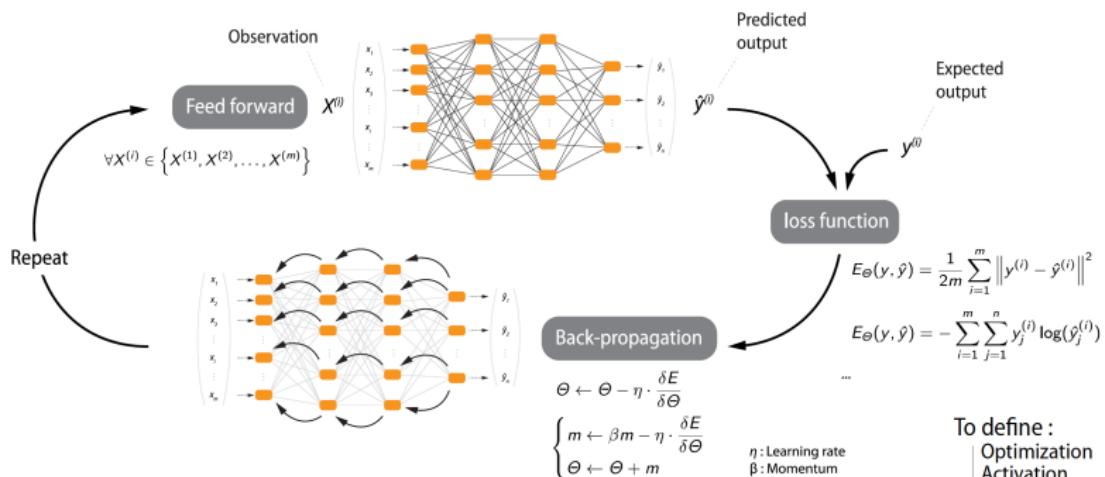
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From [B.5] 01-history-and-basic-concepts

Deep Learning Iteration Cycle

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Back-propagation

Learning process

From [B.5] 01-history-and-basic-concepts

Linear Regression revisited

Stochastic Gradient Descent

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Back-propagation

Automatic Differentiation

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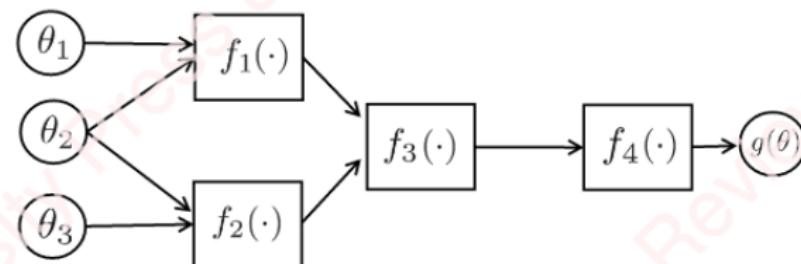
Automatic differentiation is based on the differentiation **chain rule**.

Backpropagation (or backprop) is key for training neural networks.

- ▶ For a given vector θ it computes the numerical value $\nabla g(\theta)$.
- ▶ The function $g(\theta)$ is seen as a composition of **elementary functions** $\{f_i\}$, whose **local derivatives** are easy to compute.
- ▶ All elementary functions output a **single scalar**.

Computational graph

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$$g(\theta) = f_4(f_3(f_1(\theta_1, \theta_2), f_2(\theta_2, \theta_3)))$$

☞ **Directed acyclic graph**: input nodes $\{\theta_i\}_{i=1}^d$, computational blocks $f_i(\cdot)$, and output node $g(\theta)$.

Source [B.4], Chapter 5

Chain rule of differentiation

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Consider the function for $\theta \in \mathbb{R}^d$

$$g(\theta) = f_{K+1}(f_1(\theta), f_2(\theta), \dots, f_K(\theta))$$

Chain Rule

$$\frac{\partial g(\theta)}{\partial \theta_i} = \sum_{k=1}^K \frac{\partial f_{K+1}(f_1, \dots, f_K)}{\partial f_k} \cdot \frac{\partial f_k(\theta)}{\partial \theta_i}$$

- ☞ The derivatives multiply along each influence path and the contributions of all paths sum.

Forward mode of automatic differentiation

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1. Each block $f_k(\cdot)$ computes the local partial derivative $\frac{\partial f_k(\theta)}{\partial \theta_i}$.
 2. The message is passed to computational block $f_{K+1}(\cdot)$, which multiplies it by the local partial derivative $\partial f_{K+1}(f_1, \dots, f_K) / \partial f_k$.
 3. The block $f_{K+1}(\cdot)$ sums up all product terms $\partial f_{K+1} / \partial f_k \cdot \partial f_k(\theta) / \partial \theta_i$ to obtain the final result $\partial g(\theta) / \partial \theta_i$.
- ☞ To compute the full gradient $\nabla g(\theta)$ this procedure should be repeated for every entry $\theta_i \rightarrow$ inefficient for large dimensions d .

Backpropagation

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- ☞ The forward pass is for the calculation of $g(\theta)$ through the computational graph, and the backward pass to compute all partial derivatives $\partial g(\theta)/\partial\theta_i$, simultaneously.

Algorithm 5.3: Backprop to compute all partial derivatives (5.82) for the computational graph in Fig. 5.16

Forward pass:

- Given an input vector θ , by following the direction of the edges in the computational graph, each k th computational block $f_k(\cdot)$ evaluates its output f_k for $k = 1, \dots, K + 1$.
- Each computational block $f_k(\cdot)$ also evaluates the local derivatives $\partial f_k(\theta)/\partial\theta_i$ with respect to its inputs $\theta_1, \dots, \theta_D$ with $k = 1, \dots, K$.
- Computational block $f_{K+1}(\cdot)$ evaluates all the local partial derivatives $\partial f_{K+1}(f_1, \dots, f_K)/\partial f_k$ with respect to all its inputs f_k , with $k = 1, 2, \dots, K$.

Backward pass:

- Block $f_{K+1}(\cdot)$ passes each message $\partial f_{K+1}(f_1, \dots, f_K)/\partial f_k$ back to the respective block $f_k(\cdot)$.
 - Each block $f_k(\cdot)$ multiplies the message $\partial f_{K+1}(f_1, \dots, f_K)/\partial f_k$ by the corresponding local derivative $\partial f_k(\theta)/\partial\theta_i$.
 - Each block $f_k(\cdot)$ sends the computed message $\partial f_{K+1}(f_1, \dots, f_K)/\partial f_k \cdot \partial f_k(\theta)/\partial\theta_i$ for $i = 1, \dots, D$ back to variable node θ_i .
 - Finally, each variable node θ_i sums up all its received upstream messages to obtain (5.82).
-

Example 1

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Figure 5.19 Forward pass to compute the gradient $\nabla g(\theta)$ at $\theta = [1, -1, 1]^T$ for function $g(\theta) = \theta_1^2 + 2\theta_2^2 - \theta_3^2$.

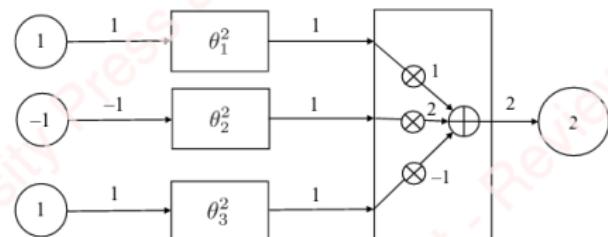
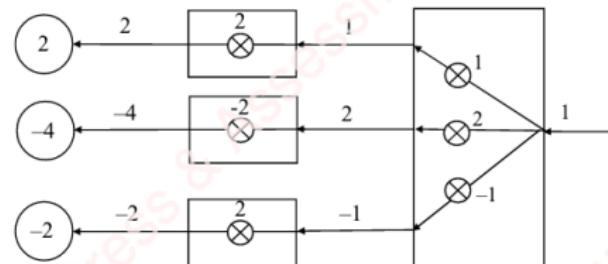


Figure 5.20 Backward pass to compute the gradient $\nabla g(\theta)$ at $\theta = [1, -1, 1]^T$ for function $g(\theta) = \theta_1^2 + 2\theta_2^2 - \theta_3^2$.



Example 2

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Figure 5.25 Forward pass for the calculation of the gradient $\nabla g(\theta)$ at $\theta = [1, -2, 1]^T$ for the computational graph in Fig. 5.15 with the elementary functions detailed in Example 5.25. Within each computational block, we have also indicated the local partial derivatives to be used in the backward phase by the corresponding input.

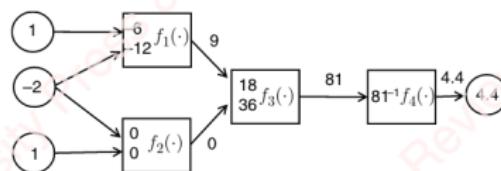
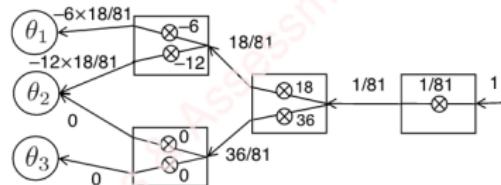


Figure 5.26 Backward pass for the calculation of the gradient $\nabla g(\theta)$ at $\theta = [1, -2, 1]^T$ for the computational graph in Fig. 5.15 with the elementary functions detailed in Example 5.25.



$$f_1(x_1, x_2) = f_2(x_1, x_2) = f_3(x_1, x_2) = (x_1 + 2x_2)^2, \quad f_4(x_1) = \log(x_1)$$

Source [B.4], Chapter 5

Example 2

A. Giovanidis 2022

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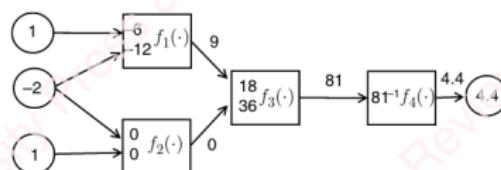
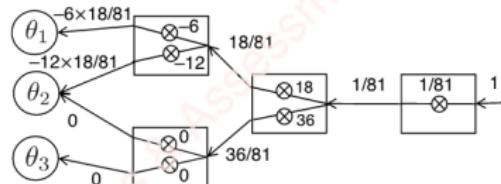


Figure 5.26 Backward pass for the calculation of the gradient $\nabla g(\theta)$ at $\theta = [1, -2, 1]^T$ for the computational graph in Fig. 5.15 with the elementary functions detailed in Example 5.25.

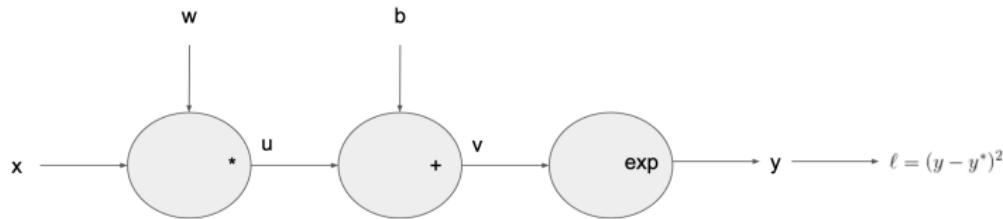


$$f_1(x_1, x_2) = f_2(x_1, x_2) = f_3(x_1, x_2) = (x_1 + 2x_2)^2, \quad f_4(x_1) = \log(x_1)$$

Example 3

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FORWARD PASS



$$u = wx$$

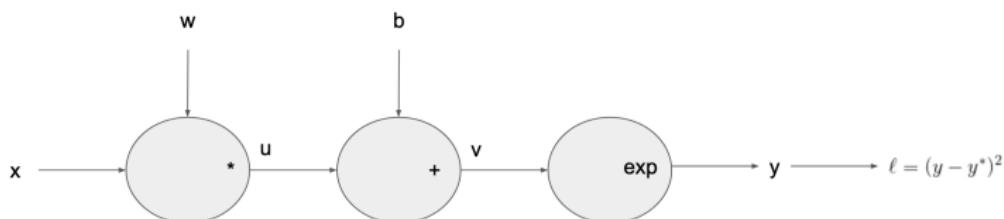
$$v = u + b$$

$$y = e^v$$

$$\ell = (y - y^*)^2$$

Example 3

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$$u = wx$$

$$v = u + b$$

$$y = e^v$$

$$\ell = (y - y^*)^2$$

$$\frac{\partial u}{\partial w} = x$$

$$\frac{\partial v}{\partial b} = 1, \quad \frac{\partial v}{\partial u} = 1$$

$$\frac{\partial y}{\partial v} = e^v = y.$$

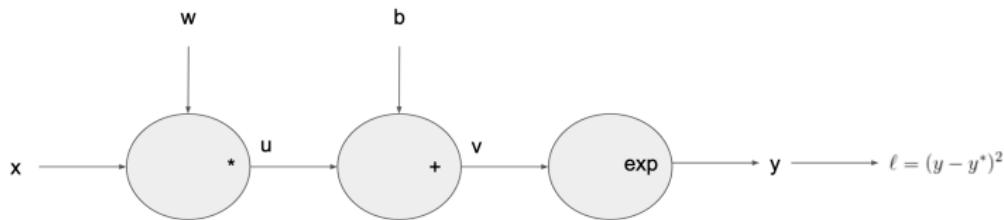
$$\frac{\partial \ell}{\partial w} = \frac{\partial \ell}{\partial y} \frac{\partial y}{\partial w}$$

$$\frac{\partial \ell}{\partial b} = \frac{\partial \ell}{\partial y} \frac{\partial y}{\partial b}$$

Example 3

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CHAIN RULE



$$u = wx$$

$$v = u + b$$

$$y = e^v$$

$$\ell = (y - y^*)^2$$

$$\frac{\partial u}{\partial w} = x$$

$$\frac{\partial v}{\partial b} = 1, \quad \frac{\partial v}{\partial u} = 1$$

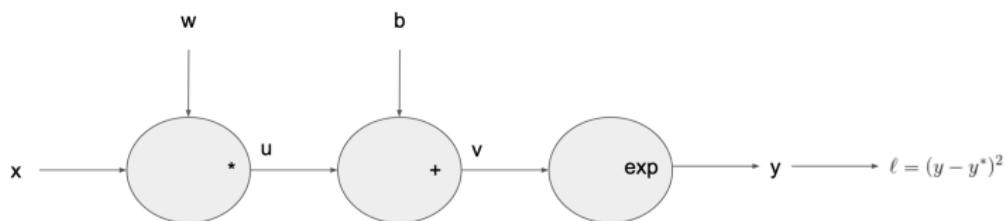
$$\frac{\partial y}{\partial v} = e^v = y.$$

$$\frac{\partial y}{\partial w} = \frac{\partial y}{\partial v} \frac{\partial v}{\partial u} \frac{\partial u}{\partial w} \quad \frac{\partial \ell}{\partial w} = \frac{\partial \ell}{\partial y} \frac{\partial y}{\partial w}$$

$$\frac{\partial y}{\partial b} = \frac{\partial y}{\partial v} \frac{\partial v}{\partial b} \quad \frac{\partial \ell}{\partial b} = \frac{\partial \ell}{\partial y} \frac{\partial y}{\partial b}$$

Example 3

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$$u = wx$$

$$v = u + b$$

$$y = e^v$$

$$\ell = (y - y^*)^2$$

$$\begin{aligned}\frac{\partial u}{\partial w} &= x \\ \frac{\partial v}{\partial b} &= 1, \quad \frac{\partial v}{\partial u} = 1 \\ \frac{\partial y}{\partial v} &= e^v = y.\end{aligned}$$

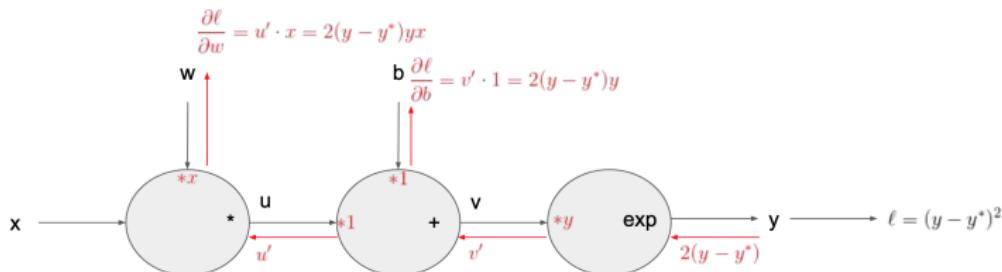
$$\begin{aligned}\frac{\partial \ell}{\partial w} &= 2(y - y^*) \cdot y \cdot 1 \cdot x \\ \frac{\partial \ell}{\partial b} &= 2(y - y^*) \cdot y \cdot 1\end{aligned}$$

$$\begin{aligned}\frac{\partial y}{\partial w} &= \frac{\partial y}{\partial v} \frac{\partial v}{\partial u} \frac{\partial u}{\partial w} \\ \frac{\partial y}{\partial b} &= \frac{\partial y}{\partial v} \frac{\partial v}{\partial b} \\ \frac{\partial \ell}{\partial b} &= \frac{\partial \ell}{\partial y} \frac{\partial y}{\partial b}\end{aligned}$$

Example 3

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BACKWARD PASS



$$\begin{aligned} u &= wx \\ v &= u + b \\ y &= e^v \\ \ell &= (y - y^*)^2 \end{aligned}$$

$$\begin{aligned} \frac{\partial u}{\partial w} &= x \\ \frac{\partial v}{\partial b} &= 1, \quad \frac{\partial v}{\partial u} = 1 \\ \frac{\partial y}{\partial v} &= e^v = y. \end{aligned} \quad \begin{aligned} \frac{\partial \ell}{\partial w} &= 2(y - y^*) \cdot y \cdot 1 \cdot x \\ \frac{\partial \ell}{\partial b} &= 2(y - y^*) \cdot y \cdot 1 \end{aligned}$$

$$\begin{aligned} v' &= 2(y - y^*) \cdot y \\ u' &= v' \cdot 1 \end{aligned}$$

Practical implementation

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« Deep learning for humans »



Keras

By François Chollet (Google)
High level API
Part of TensorFlow since 2017
MIT licence



Most used DL framework
Supported by Google
Low level API – an hard way
Apache licence

Widely used in the implementation of practical solutions

Widely used in the field of AI research



From Torch library
Supported by Facebook
BSD licence



python™



NumPy



jupyter

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END