INF8225

Leçon 3

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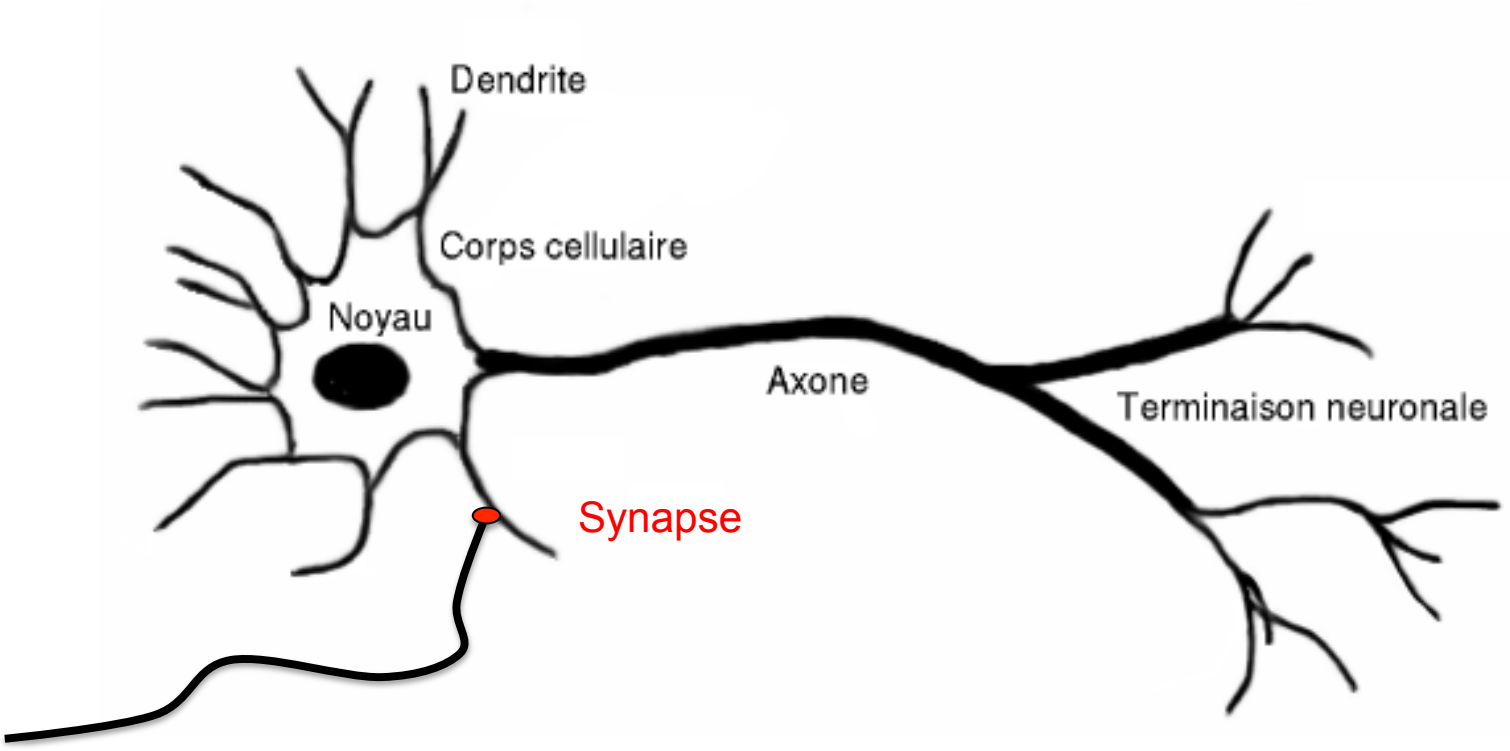
Plan du cours

- Réseaux de neurones
- Deep Learning
- Apprentissage avec rétropropagation
- Équations matricielles
- Apprentissage en pratique
  SGD, hyperparamètres, etc.

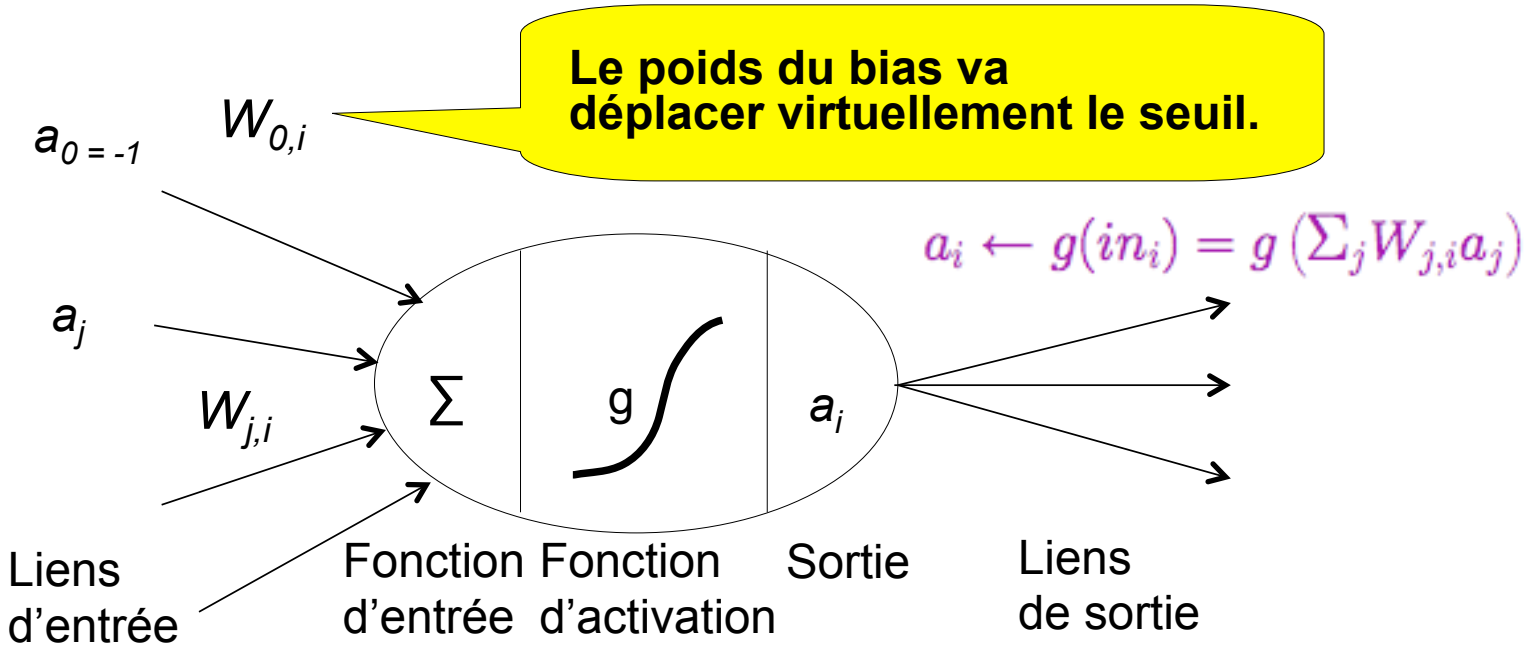
Réseaux de neurones

Réseaux de neurones

- 1ms-10ms temps pour des cycles
- 10^{11} neurones de plus de 20 types, 10^{14} synapses



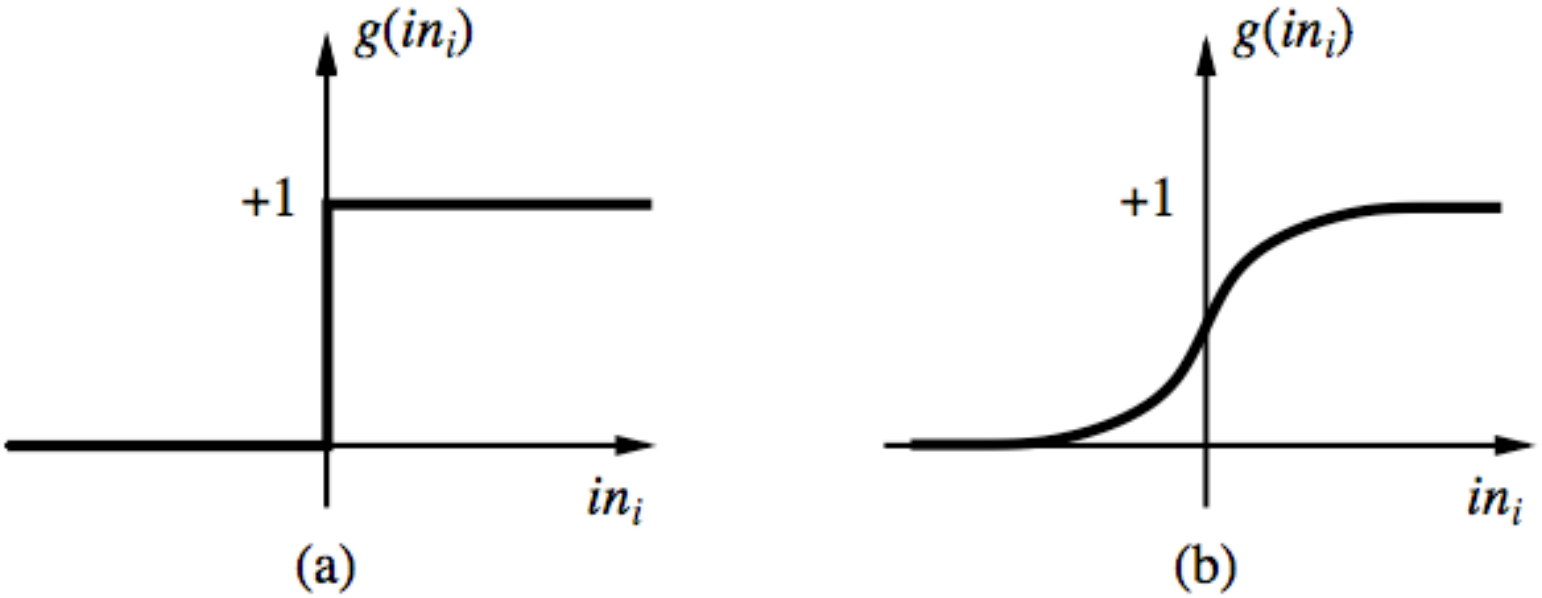
Modèle mathématique simple d'un neurone



- La fonction d'activation g est conçue pour répondre à des desiderata, on veut que l'unité soit :

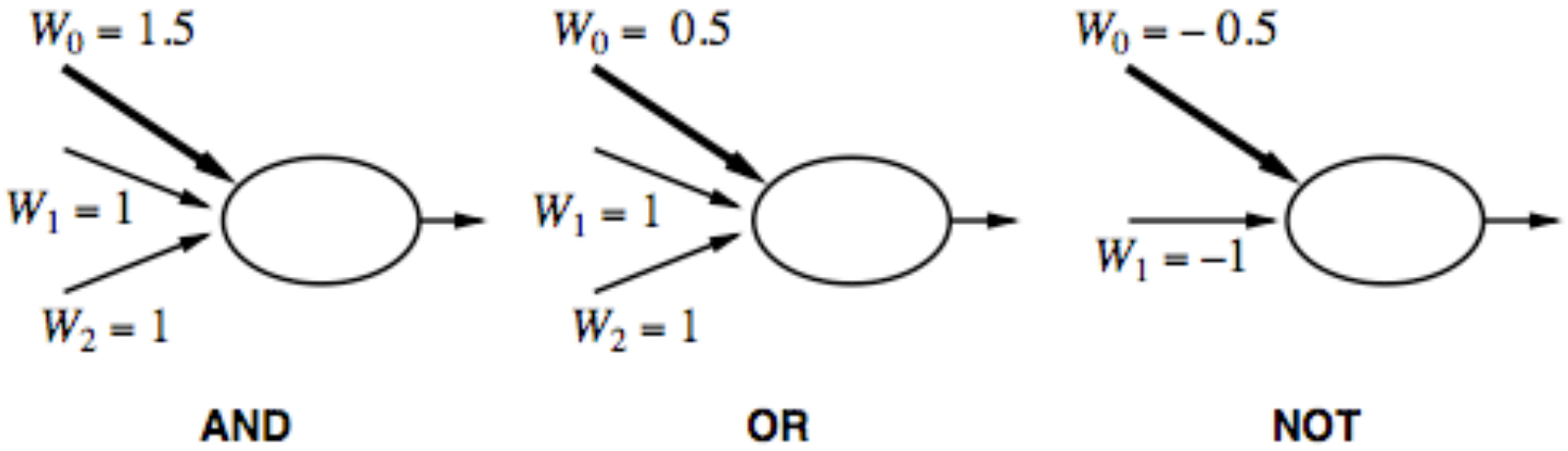
1. « active » (proche de +1) quand les « bonnes » entrées sont données
2. « inactive » (proche de 0) quand elles sont « mauvaises »
3. L'activation doit être non linéaire, sinon nous avons une simple fonction linéaire

La fonction d'activation



a) La fonction d'activation à seuil
b) La fonction sigmoïde (fonction logistique)

Les unités avec fonction d'activation peuvent représenter des portes logiques

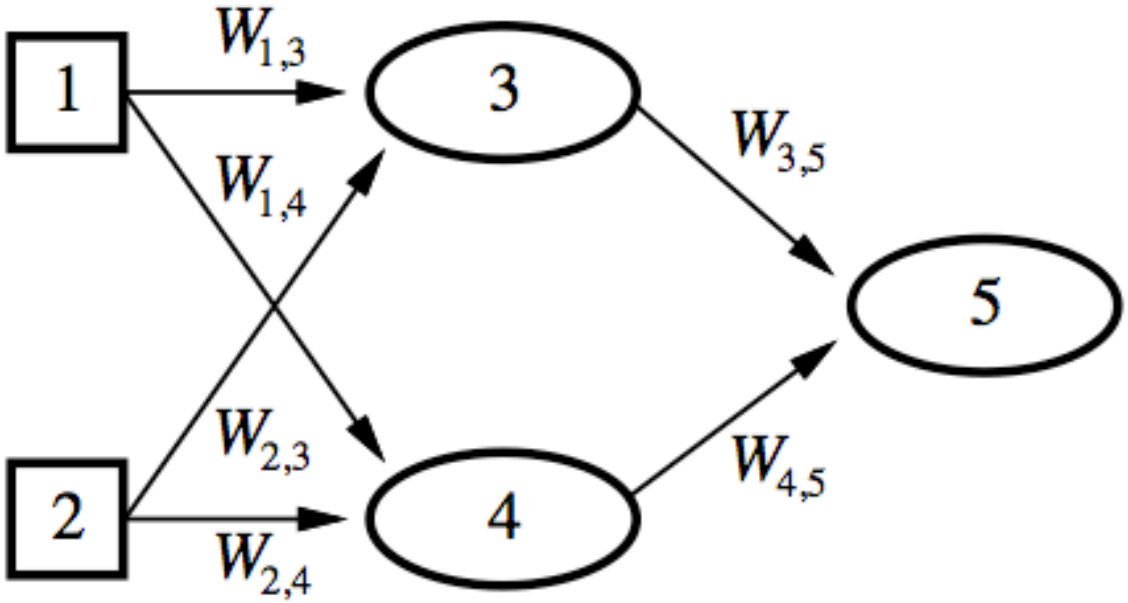


- Une motivation d'origine de la conception d'un modèle d'un neurone par McCulloch et Pitts, 1943.

Réseaux de neurones

- Plusieurs types de réseaux de neurones
  - réseaux « feed-forward » (perceptron multi-couches)
  - réseaux récurrents
- Principe d'apprentissage:
  - On fournit une entrée et la sortie désirée
  - On ajuste les poids en fonction de l'erreur
  - On fait la même chose avec les autres exemples
  - On répète jusqu'à ce qu'à un état où les poids varient très peu

Réseaux feed-forward

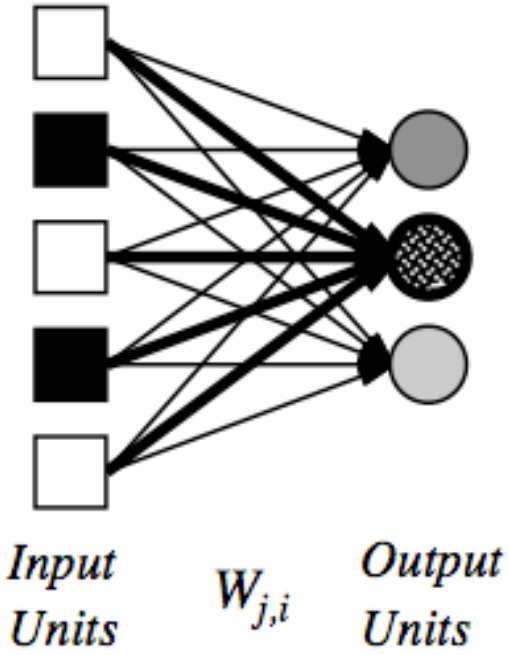


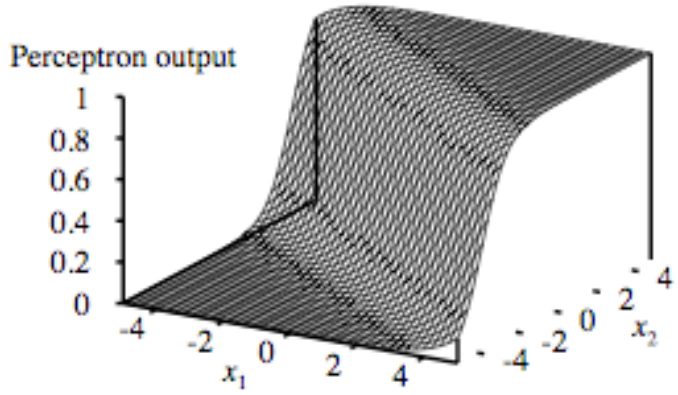
- Effectivement, c'est un paramétrage d'une famille de fonctions non linéaires

$$a_5 = g(W_{3,5} \cdot a_3 + W_{4,5} \cdot a_4)$$
$$= g(W_{3,5} \cdot g(W_{1,3} \cdot a_1 + W_{2,3} \cdot a_2) + W_{4,5} \cdot g(W_{1,4} \cdot a_1 + W_{2,4} \cdot a_2))$$

- Apprentissage = l'ajustement des poids

Un perceptron monocouche

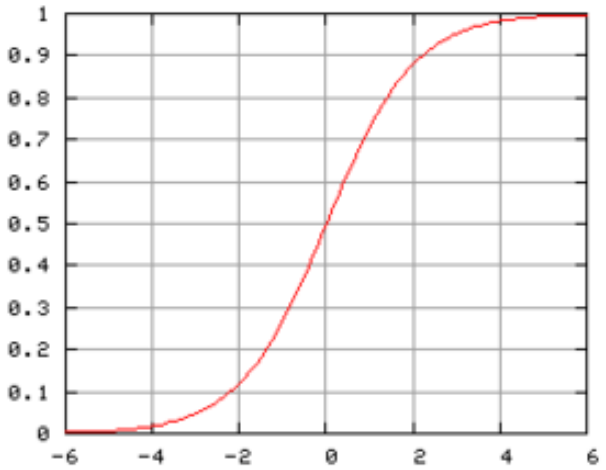




- Les ajustements des poids changent la position, l'orientation et la pente de la falaise

La fonction logistique

$$Logistique(z) = \frac{1}{1 + \exp(-z)}$$



- En utilisant un produit scalaire

$$h_{\mathbf{w}}(\mathbf{x}) = Logistique(\mathbf{w} \cdot \mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w} \cdot \mathbf{x})}$$

- Un avantage de cette fonction est que la dérivée satisfait g'(*z*)=g(*z*)(1-g(*z*))

Apprentissage perceptron classique

- Pour un seul exemple d'apprentissage avec une entrée x et une sortie vraie y, on écrit l'erreur quadratique

$$E = \frac{1}{2}Err^2 \equiv \frac{1}{2}(y - h_{\mathbf{W}}(\mathbf{x}))^2 \ ,$$

- En utilisant la descente de gradient

$$\begin{aligned}\frac{\partial E}{\partial W_j} &= Err \times \frac{\partial Err}{\partial W_j} = Err \times \frac{\partial}{\partial W_j}\left(y - g(\Sigma_{j=0}^{n} W_j x_j)\right) \\ &= -Err \times g'(in) \times x_j\end{aligned}$$

- Nous avons une règle simple pour une mise à jour

$$W_j \leftarrow W_j + \alpha \times Err \times g'(in) \times x_j$$

Apprentissage perceptron

répéter:

pour chaque exemple **faire**

pour chaque noeud j de la couche d'entrée du réseau **faire**

$a_j \leftarrow$ item j dans le vecteur d'entrée de l'exemple

$in \leftarrow \sum_j W_j \times a_j$

$a_{out} \leftarrow g(in)$

// soit y la sortie désirée pour cet exemple

$\Delta \leftarrow g'(in) \times (y - a_{out})$

$W_j \leftarrow W_j + \alpha \times a_j \times \Delta_i$

jusqu'à ce que le critère d'arrêt soit satisfait

Perceptron - exemple

répéter:
  pour chaque exemple **faire**
    pour chaque noeud j de la couche d'entrée du réseau **faire**
      $a_j \leftarrow$ item j dans le vecteur d'entrée de l'exemple
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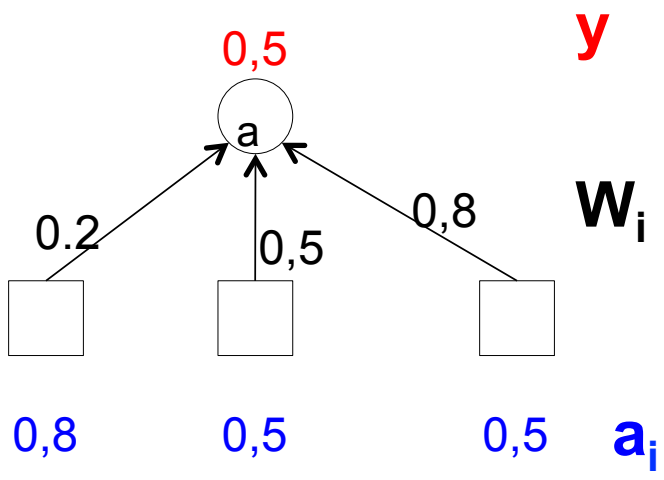

α = 0,9

- in = .2*.8 + .5*.5 + .8*.5 = .81

Perceptron - exemple

répéter:
  pour chaque exemple **faire**
    pour chaque noeud j de la couche d'entrée du réseau **faire**
      $a_j \leftarrow$ item j dans le vecteur d'entrée de l'exemple
    $in \leftarrow \sum_j W_j \times a_j$
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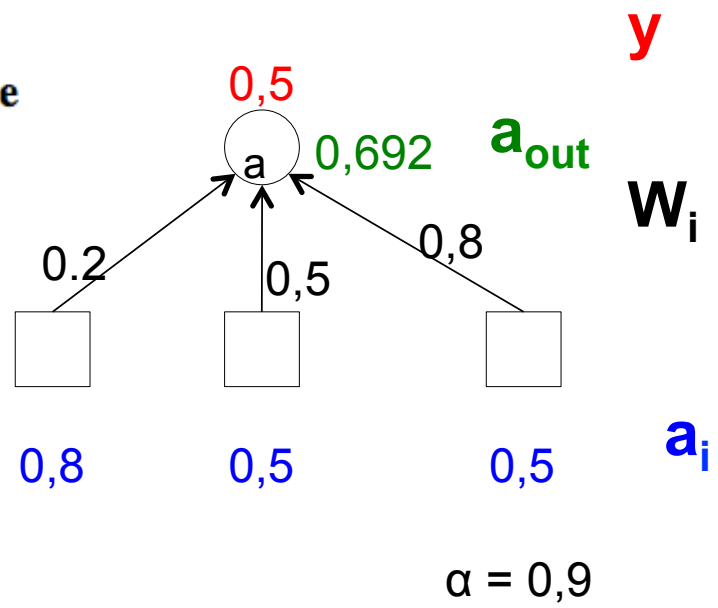

$$a_{out} = g(.81) = \frac{1}{1 + \exp(-.81)} = .692$$

Perceptron - exemple

répéter:
  pour chaque exemple **faire**
    pour chaque noeud j de la couche d'entrée du réseau **faire**
      $a_j \leftarrow$ item j dans le vecteur d'entrée de l'exemple
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    // soit y la sortie désirée pour cet exemple
    $\Delta \leftarrow g'(in) \times (y - a_{out})$
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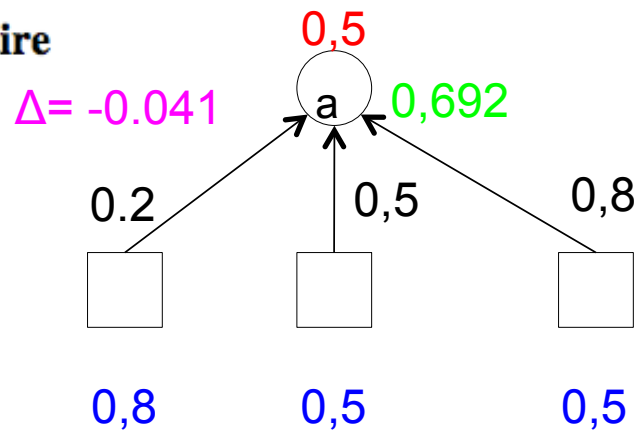

α = 0,9

$$\Delta = g'(in) \times (y - a_{out})$$
$$= g(z)(1 - g(z)) \times (y - g(z))$$
$$= .692(1 - .692) \times (.5 - .692) = -0.041$$

Perceptron - exemple

répéter:
  pour chaque exemple **faire**
    pour chaque noeud j de la couche d'entrée du réseau **faire**
      $a_j \leftarrow$ item j dans le vecteur d'entrée de l'exemple
    $in \leftarrow \sum_j W_j \times a_j$
    $a_{out} \leftarrow g(in)$
    // soit y la sortie désirée pour cet exemple
    $\Delta \leftarrow g'(in) \times (y - a_{out})$
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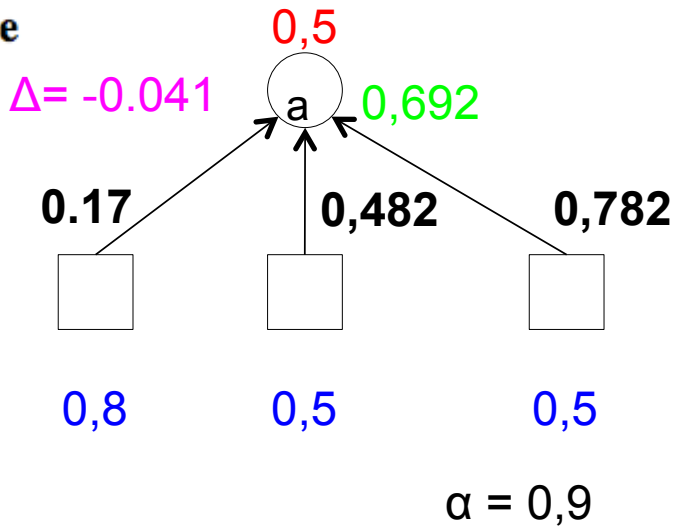
jusqu'à ce que le critère d'arrêt soit satisfait



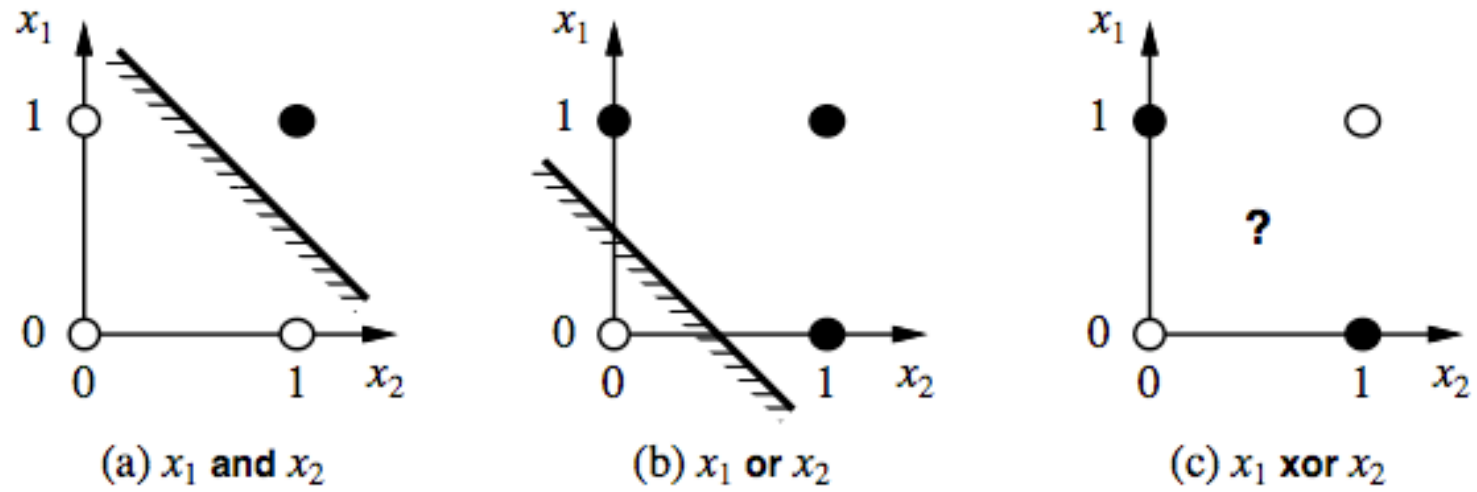
$W_1 = .2 + .9 \times .8 \times -.041 = \mathbf{.17}$

$W_2 = .5 + .9 \times .5 \times -.041 = \mathbf{.482}$

$W_3 = .8 + .9 \times .5 \times -.041 = \mathbf{.782}$

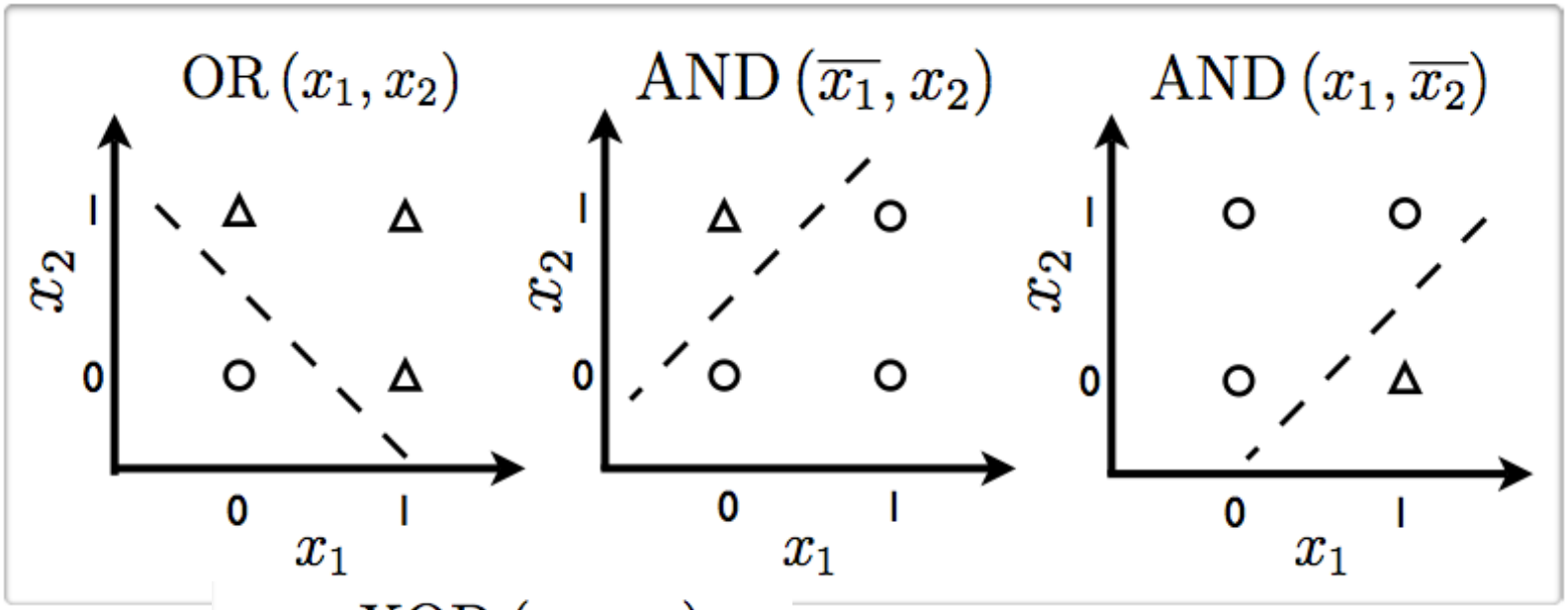
Problèmes avec un séparateur linéaire

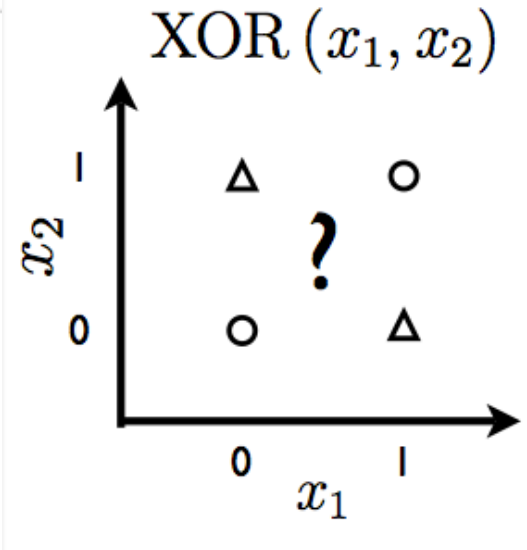
$\Sigma_j W_j x_j > 0$ or $\mathbf{W} \cdot \mathbf{x} > 0$



- Il peut représenter AND, OR et NOT mais pas XOR
- … sauf si vous pouvez trouver une meilleure représentation. Q: La définition d'XOR est ?

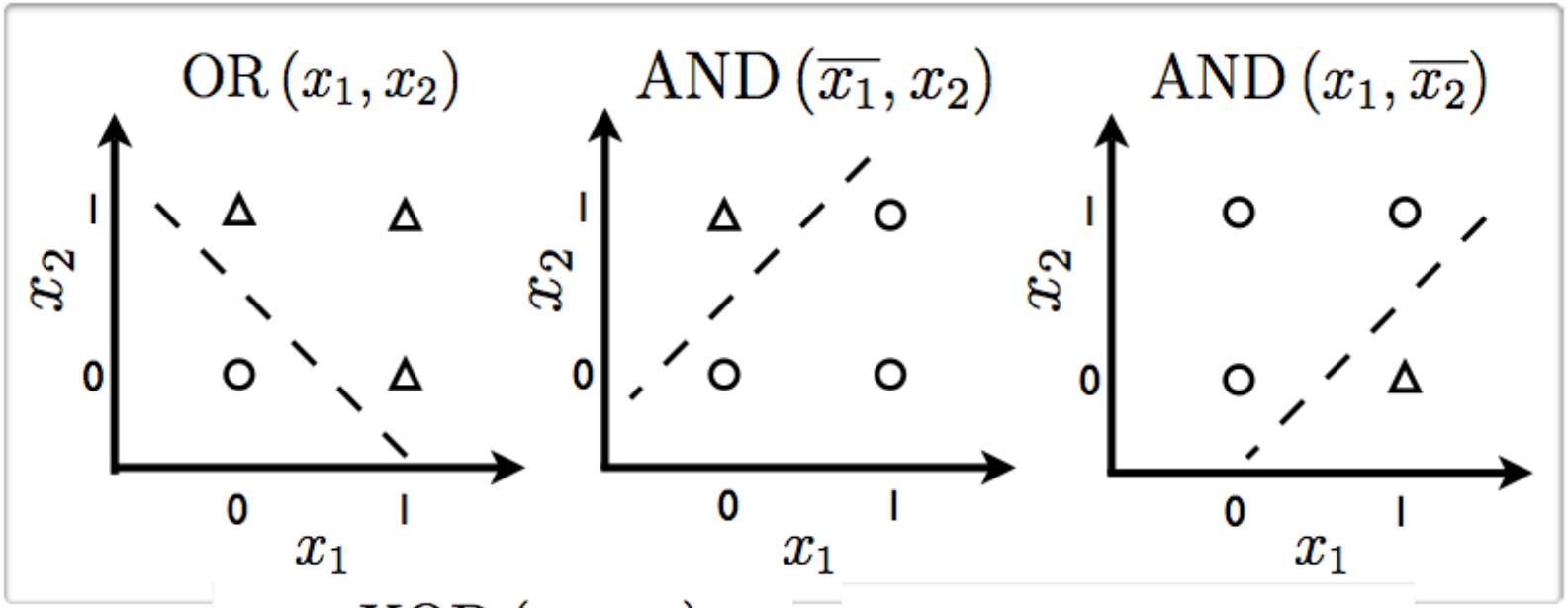
Exercice: utilisez la definition d'XOR pour transformer les donnees

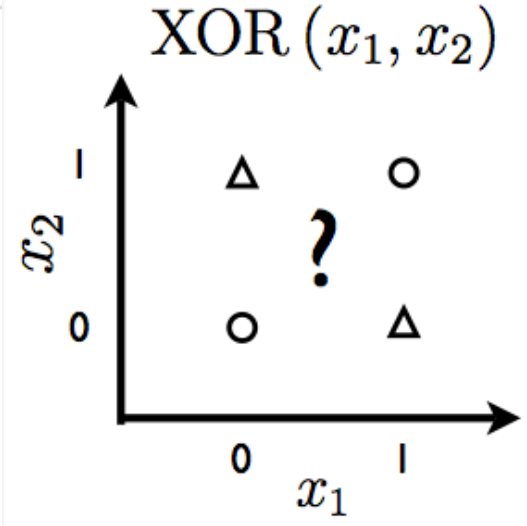


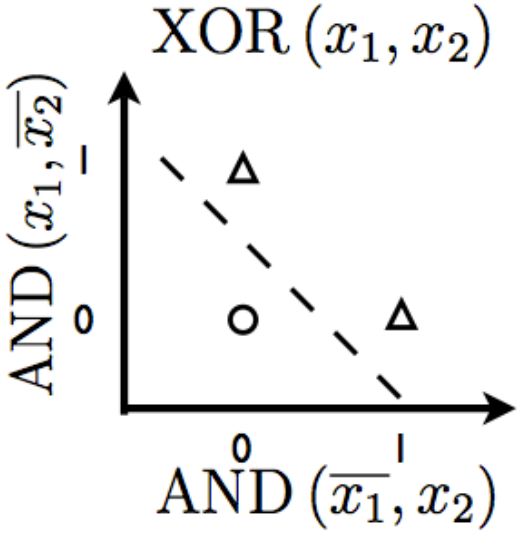


De Hugo Larochelle

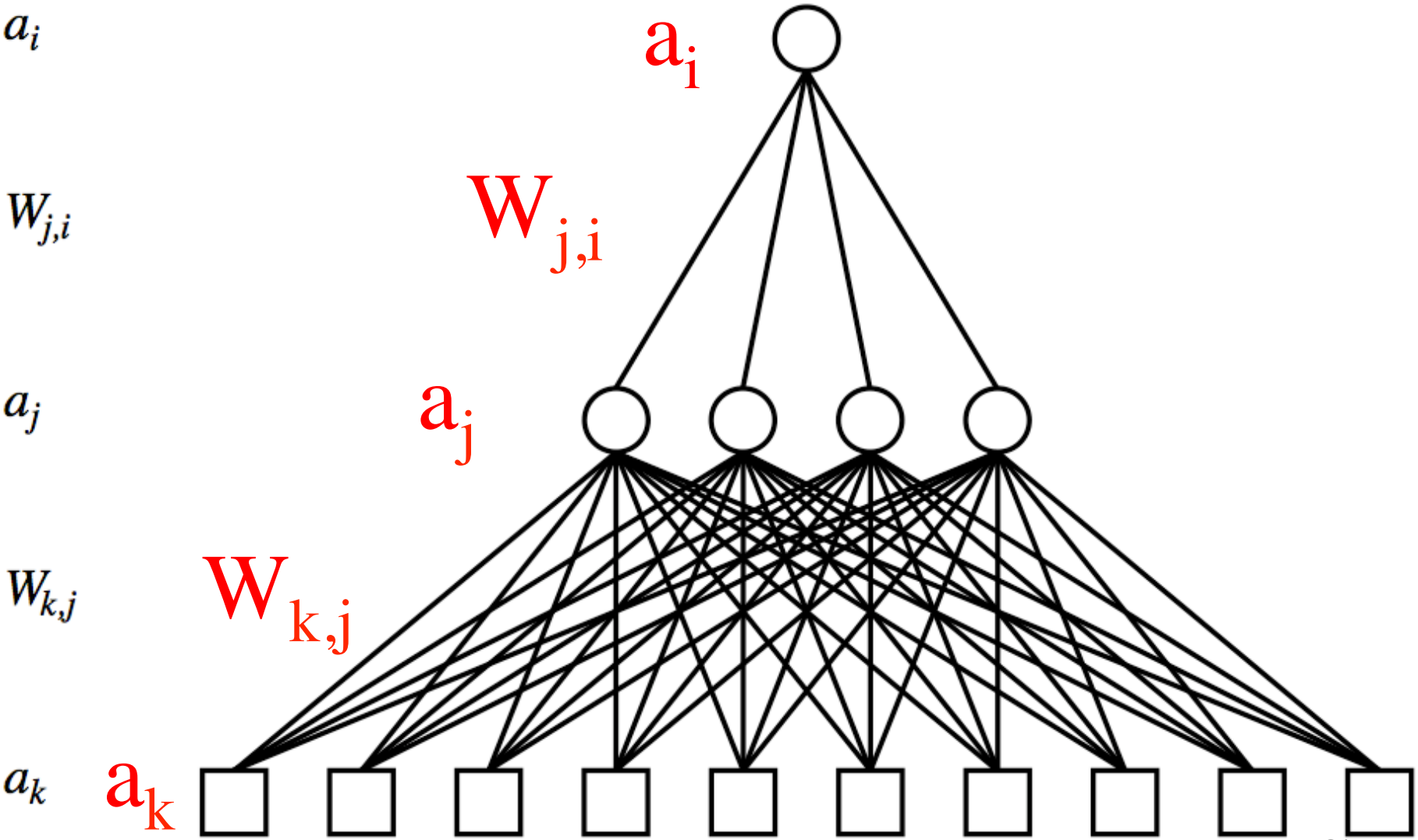
Exercice: utilisez la definition d'XOR pour transformer les donnees





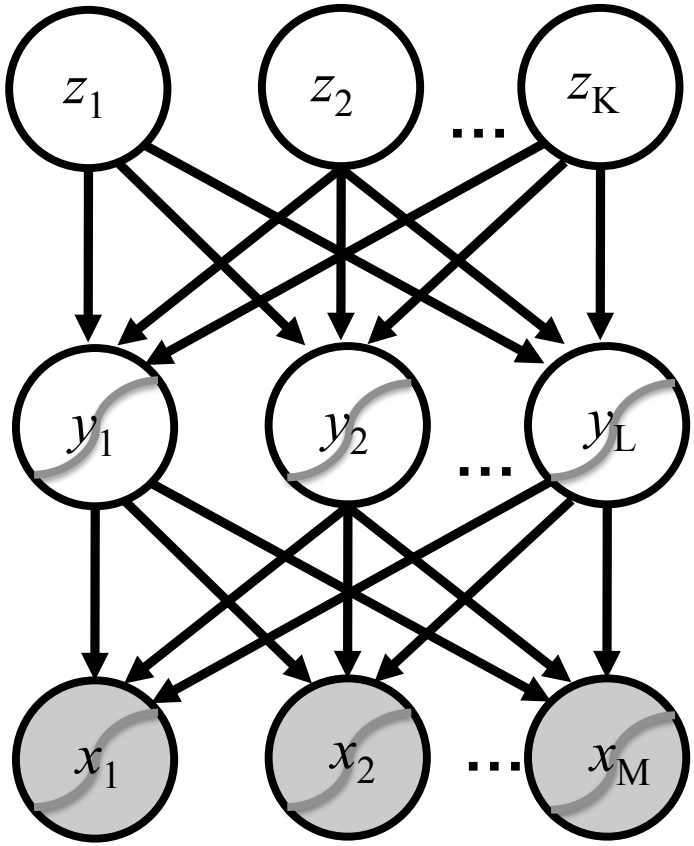


Réseau de neurones multicouche

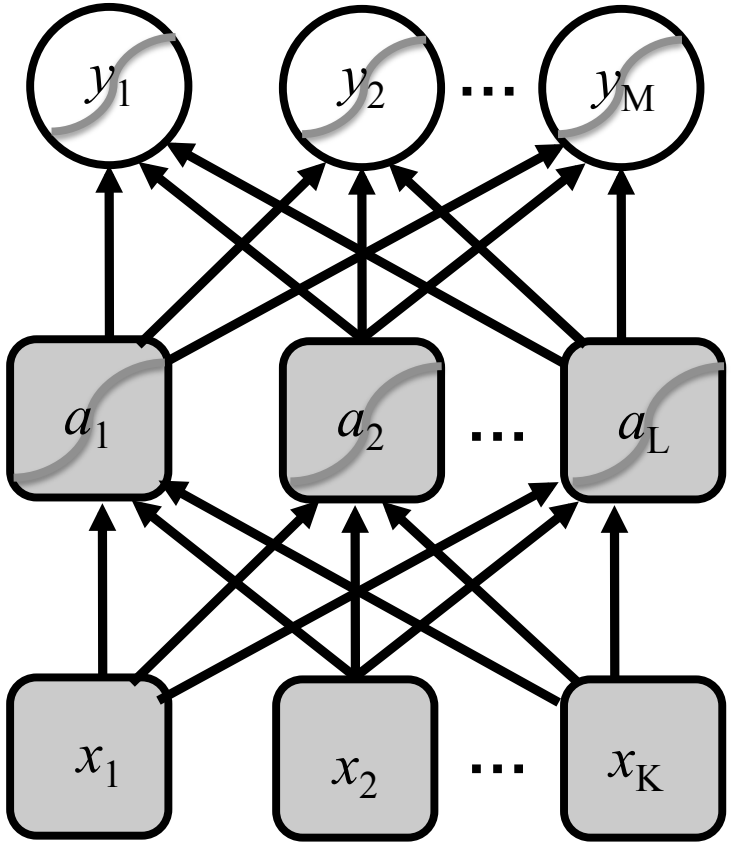


Important : BNs vs NNs

Réseau de Bayes



Réseau de neurones



Variables stochastique

Observé

non-observé

Variables déterministe

Observé

Rétropropagation

Pour notre couche de sortie, on fait la mise à jour de même façon que d'une réseau avec un seule couche

$$W_{j,i} \leftarrow W_{j,i} + \alpha \times a_j \times \Delta_i \quad \text{où} \quad \Delta_i = Err_i \times g'(in_i)$$

Comparez avec notre mise à jour pour un seule couche

$$W_j \leftarrow W_j + \alpha \times Err \times g'(in) \times x_j$$

Couche caché: rétropropager l'erreur de la couche de sortie

$$\Delta_j = g'(in_j) \sum_i W_{j,i} \Delta_i \ .$$

Règle de mise à jour pour les poids de la couche caché:

$$W_{k,j} \leftarrow W_{k,j} + \alpha \times a_k \times \Delta_j \ .$$

Dérivation des équations de rétropropagation

En commençant avec l'erreur quadratique

$$E = \frac{1}{2}\sum_i (y_i - a_i)^2 \ ,$$

Où la somme est effectuée sur les nœuds de la couche de sortie

$$\begin{aligned}
\frac{\partial E}{\partial W_{j,i}} &= -(y_i - a_i)\frac{\partial a_i}{\partial W_{j,i}} = -(y_i - a_i)\frac{\partial g(in_i)}{\partial W_{j,i}} \\
&= -(y_i - a_i)g'(in_i)\frac{\partial in_i}{\partial W_{j,i}} = -(y_i - a_i)g'(in_i)\frac{\partial}{\partial W_{j,i}}\left(\sum_j W_{j,i}a_j\right) \\
&= -(y_i - a_i)g'(in_i)a_j = -a_j\Delta_i
\end{aligned}$$

avec

$$\Delta_i = Err_i \times g'(in_i)$$

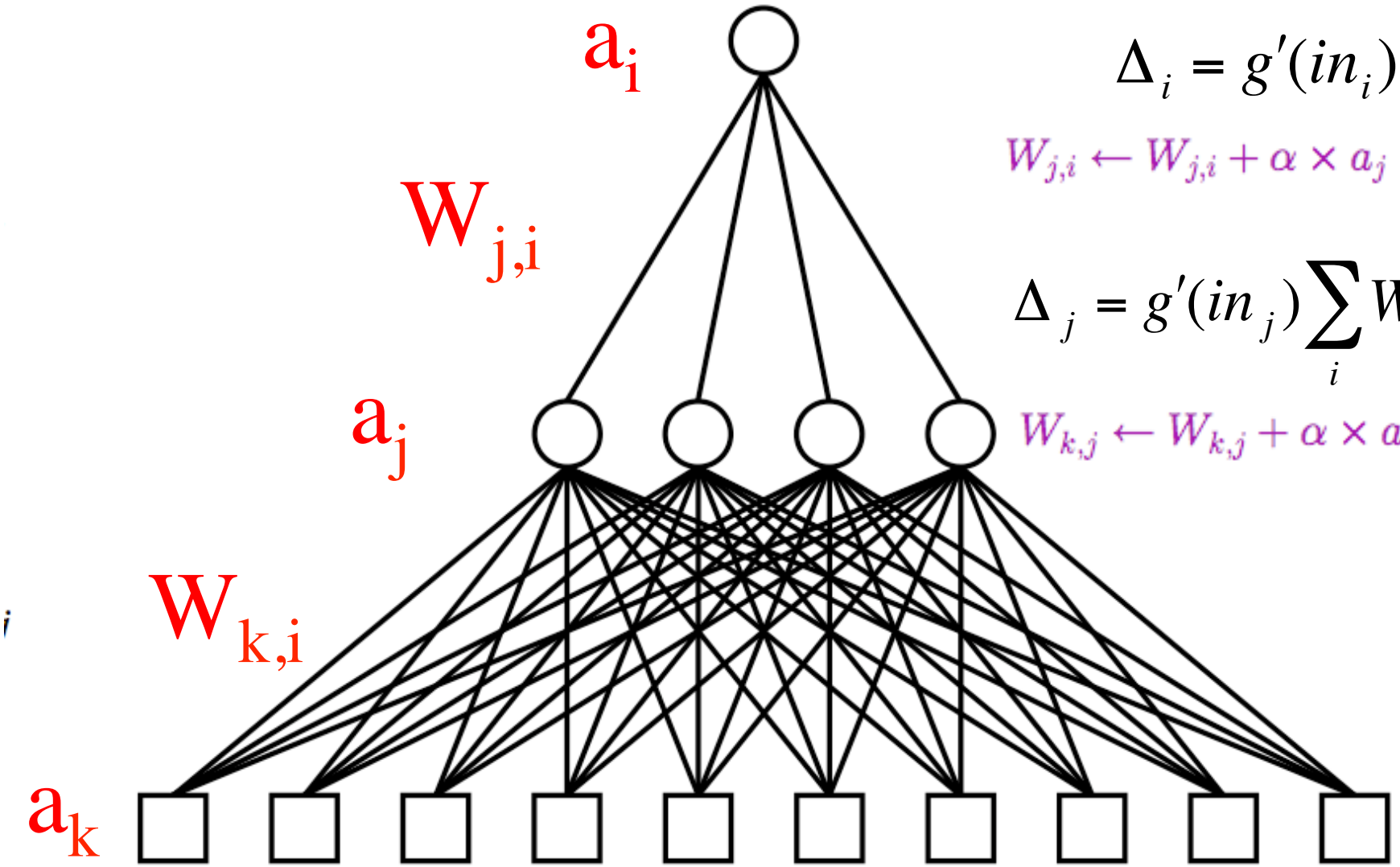
L'algorithme de rétropropagation

- Le processus de rétropropagation peut se résumer comme suit :
- Calculer les valeurs Δ pour les unités de sortie en utilisant l'erreur observée
- En commençant par la couche de sortie, répéter les étapes suivantes pour chaque couche du réseau, jusqu'à ce que la dernière couche cachée ait été atteinte
  - Rétropropager les valeurs Δ à la couche précédente
  - Mettre à jour les poids entre les deux couches

Dérivation de rétropropagation

$$
\begin{aligned}
\frac{\partial E}{\partial W_{k,j}} &= -\sum_i (y_i - a_i)\frac{\partial a_i}{\partial W_{k,j}} = -\sum_i (y_i - a_i)\frac{\partial g(in_i)}{\partial W_{k,j}} \\
&= -\sum_i (y_i - a_i) g'(in_i)\frac{\partial in_i}{\partial W_{k,j}} = -\sum_i \Delta_i \frac{\partial}{\partial W_{k,j}}\left(\sum_j W_{j,i} a_j\right) \\
&= -\sum_i \Delta_i W_{j,i}\frac{\partial a_j}{\partial W_{k,j}} = -\sum_i \Delta_i W_{j,i}\frac{\partial g(in_j)}{\partial W_{k,j}} \\
&= -\sum_i \Delta_i W_{j,i} g'(in_j)\frac{\partial in_j}{\partial W_{k,j}} \\
&= -\sum_i \Delta_i W_{j,i} g'(in_j)\frac{\partial}{\partial W_{k,j}}\left(\sum_k W_{k,j} a_k\right) \\
&= -\sum_i \Delta_i W_{j,i} g'(in_j) a_k = -a_k \Delta_j
\end{aligned}
$$

Réseau de neurones multicouche



$$\Delta_i = g'(in_i)Err_i$$

$$W_{j,i} \leftarrow W_{j,i} + \alpha \times a_j \times \Delta_i$$

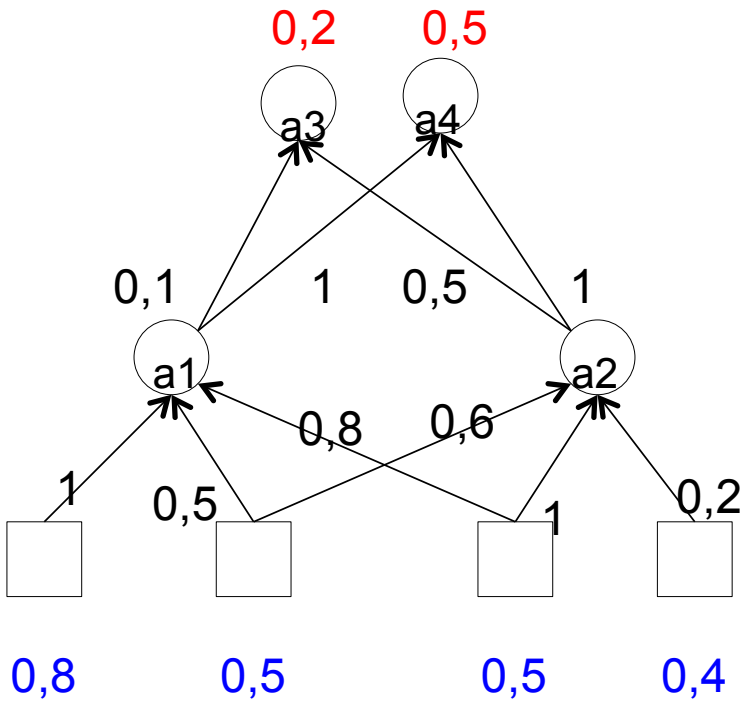
$$\Delta_j = g'(in_j)\sum_i W_{j,i}\Delta_i$$

$$W_{k,j} \leftarrow W_{k,j} + \alpha \times a_k \times \Delta_j$$

Apprentissage avec rétropropagation

// Soit un réseau qui contient M couches
répéter:
  pour chaque exemple **faire**
    pour chaque noeud j de la couche d'entrée du réseau **faire**
      $a_j \leftarrow$ item j dans le vecteur d'entrée de l'exemple
    pour $l = 2$ à M **faire**
      $in_i \leftarrow \sum_j W_{j,i} \times a_j$
      $a_i \leftarrow g(in_i)$
    pour chaque noeud i de la couche de sortie **faire**
      // soit y_i la sortie désirée pour le noeud i et a_i la sortie obtenue
      $\Delta_i \leftarrow g'(in_i) \times (y_i - a_i)$
    pour $l = M$-1 à 1 **faire**
      pour chaque noeud j de la couche l faire
        $\Delta_j \leftarrow g'(in_j) \times \sum_i W_{j,i} \Delta_i$
        pour chaque noeud i de la couche l+1 faire
          $W_{j,i} \leftarrow W_{j,i} + \alpha \times a_j \times \Delta_i$
jusqu'à ce que le critère d'arrêt soit satisfait

Réseau de neurones - exemple



Réseau de neurones - exemple

pour chaque noeud *j* de la couche d'entrée du réseau **faire**

$a_j = x_j$ ou item *j* dans le vecteur d'entrée de l'exemple

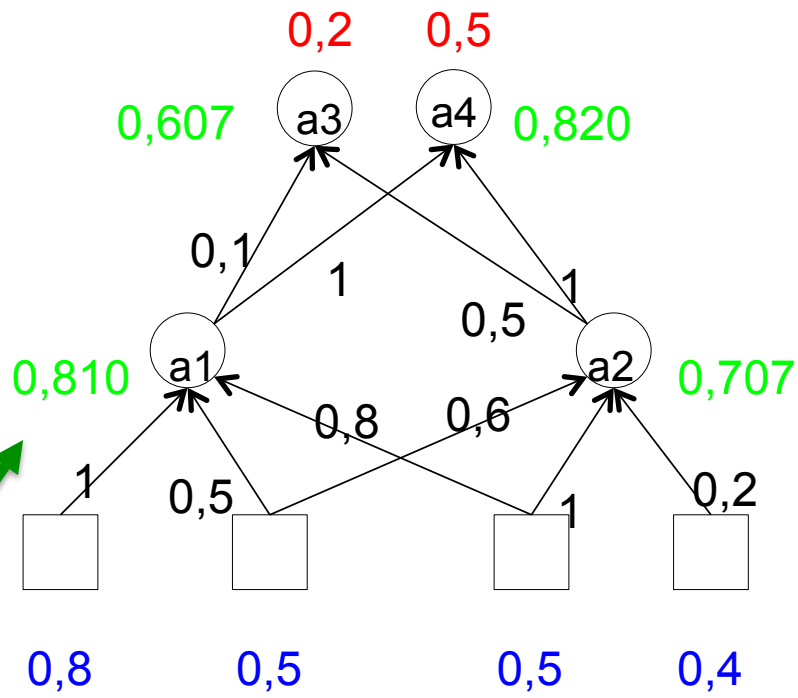
pour *I* = 2 à *M* **faire**

$in_i = \sum_j W_{j,i} \times a_j$

$a_i = g(in_i)$

Exemple:

$$a_1 = g(w \cdot a)$$
$$= g([1 \quad .5 \quad .8] \cdot [.8 \quad .5 \quad .5])$$
$$= g(1.45)$$
$$= \frac{1}{1+\exp(-1.45)} = .810$$



Réseau de neurones - exemple

pour chaque noeud *j* de la couche d'entrée du réseau **faire**

$a_j = x_j$ ou item *j* dans le vecteur d'entrée de l'exemple

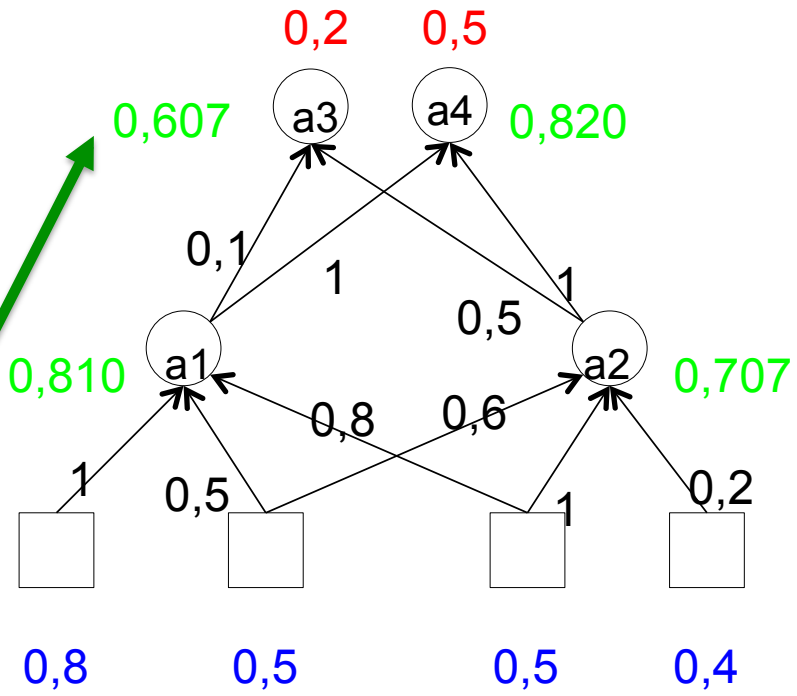
pour *l* = 2 à *M* **faire**

$in_i = \sum_j W_{j,i} \times a_j$

$a_i = g(in_i)$

Exemple:

$$a_1 = g(w \cdot a)$$
$$= g([.1 \quad .5] \cdot [.810 \quad .707])$$
$$= g(.4345)$$
$$= \frac{1}{1+\exp(-.4345)} = .607$$



Réseau de neurones - exemple

// soit y_i la sortie désirée pour le noeud i et a_i la sortie obtenue

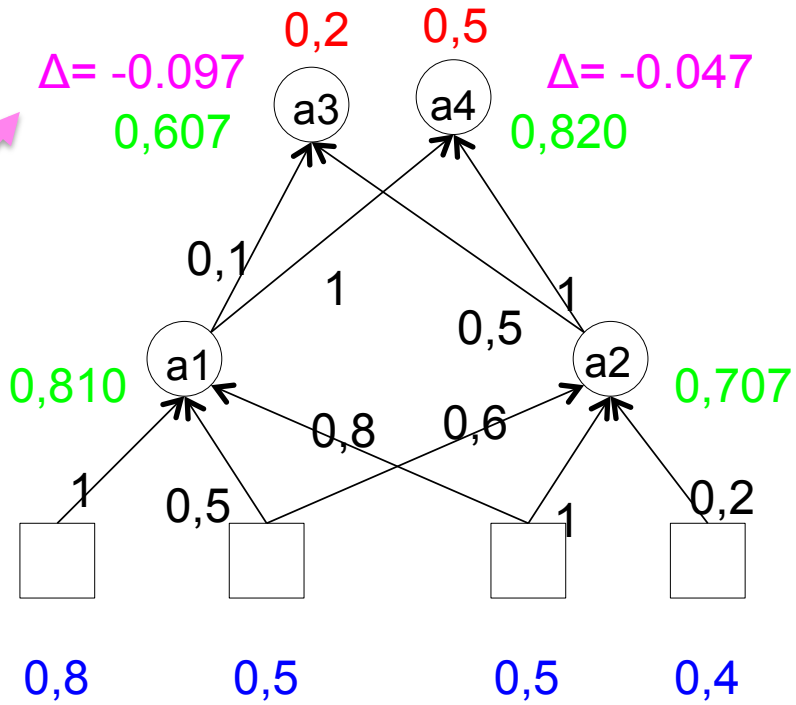
$\Delta_i = g'(in_i) \times (y_i - a_i)$

pour $l = M$-1 à 1 **faire**

  pour chaque noeud j

    de la couche l faire

      $\Delta_j = g'(in_j) \times \sum_i W_{j,i} \Delta_i$

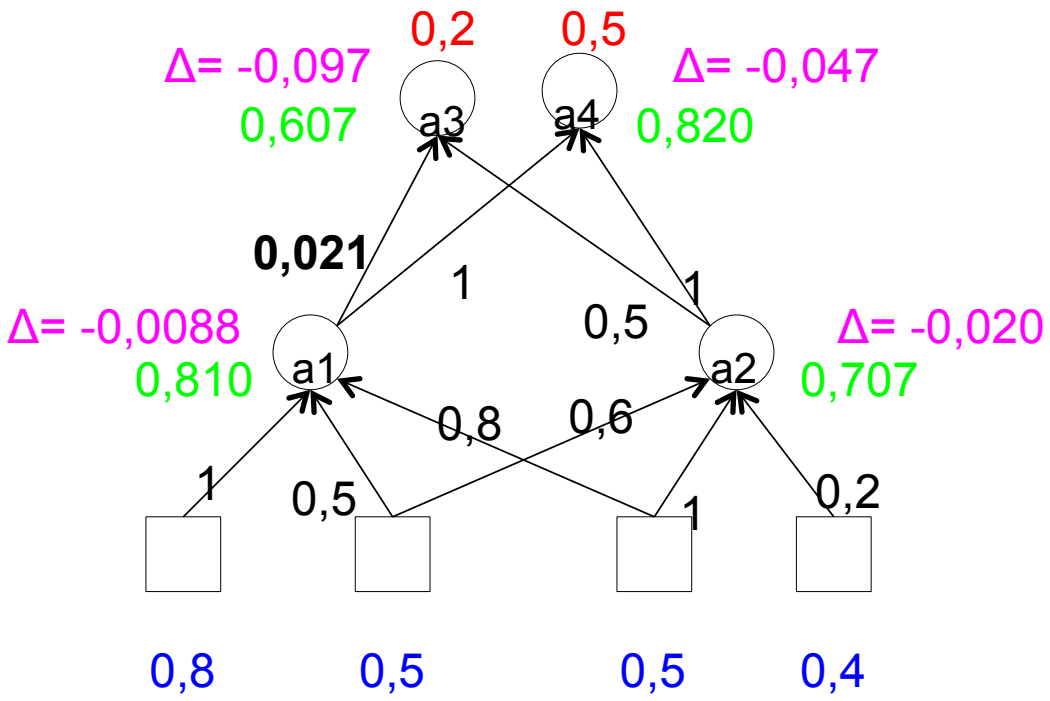


$$\Delta_i = g'(in_i) \times (y_i - a_i)$$
$$= g(z)(1 - g(z)) \times (y - g(z))$$
$$= .607(1 - .607) \times (.2 - .607) = -0.097$$

Réseau de neurones - exemple

pour chaque noeud *i* de la couche *l*+1 faire

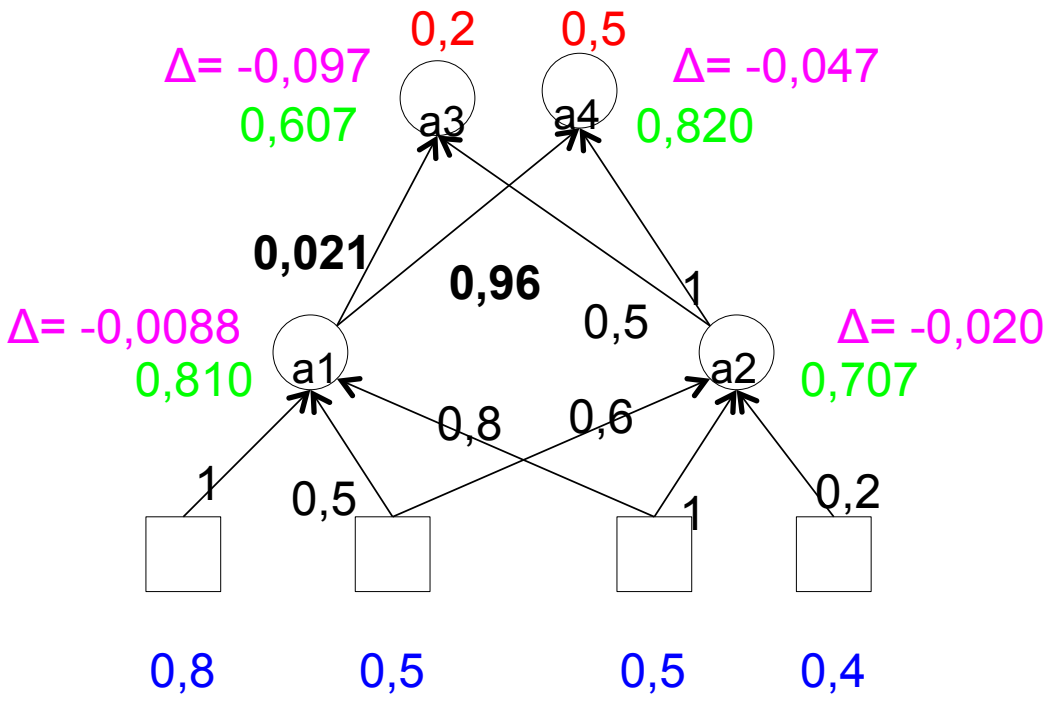
$W_{j,i} = W_{j,i} + \alpha \times a_j \times \Delta_i$



Réseau de neurones - exemple

pour chaque noeud *i* de la couche *l*+1 faire

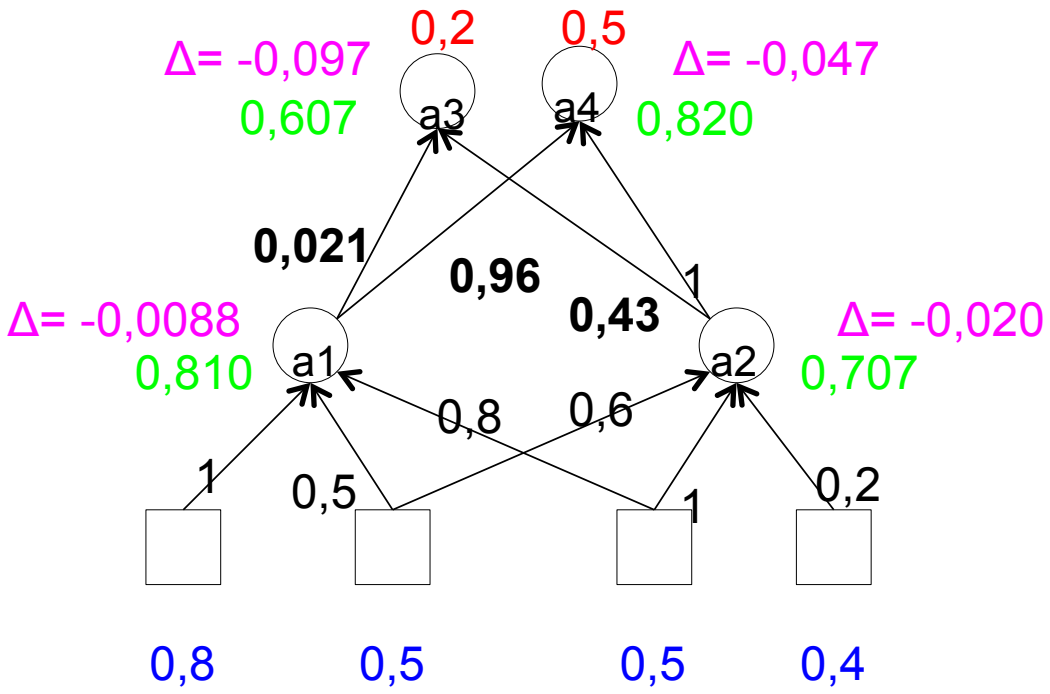
$W_{j,i} = W_{j,i} + \alpha \times a_j \times \Delta_i$



Réseau de neurones - exemple

pour chaque noeud *i* de la couche *l*+1 faire

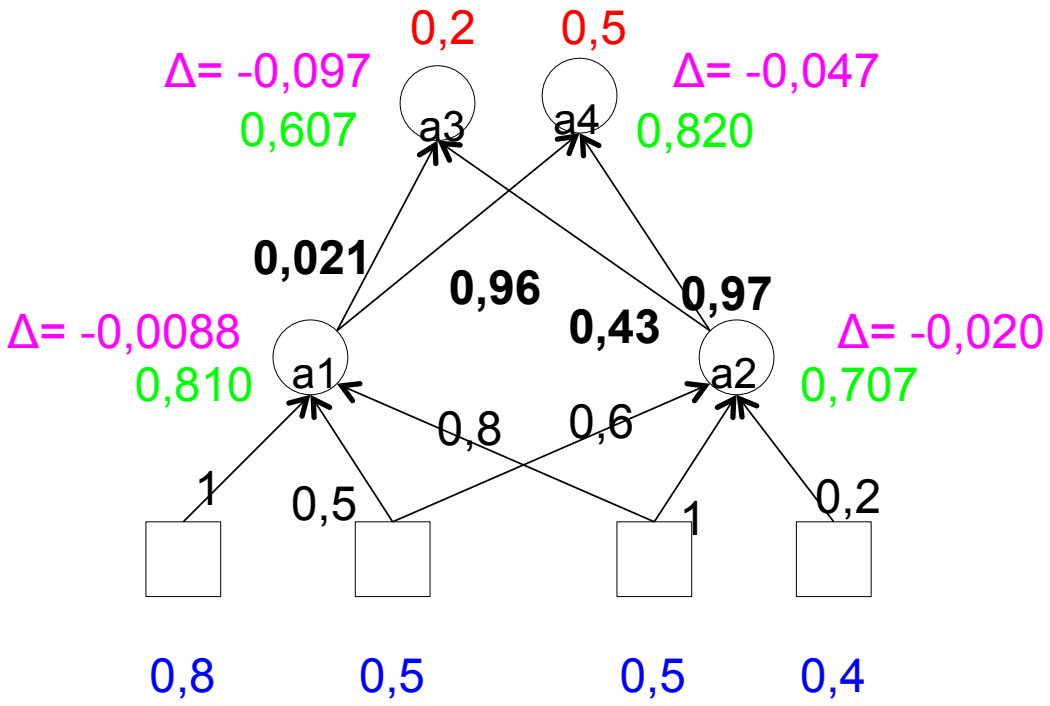
$W_{j,i} = W_{j,i} + \alpha \times a_j \times \Delta_i$



Réseau de neurones - exemple

pour chaque noeud *i* de la couche *l*+1 faire

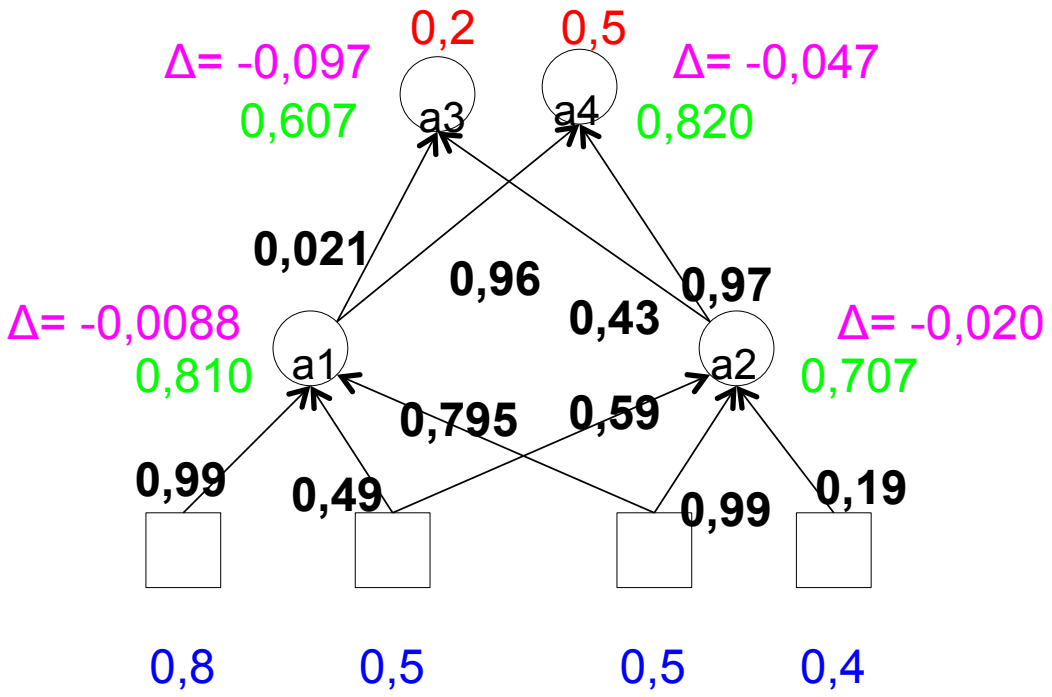
$W_{j,i} = W_{j,i} + \alpha \times a_j \times \Delta_i$



Réseau de neurones - exemple

pour chaque noeud *i* de la couche *l*+1 faire

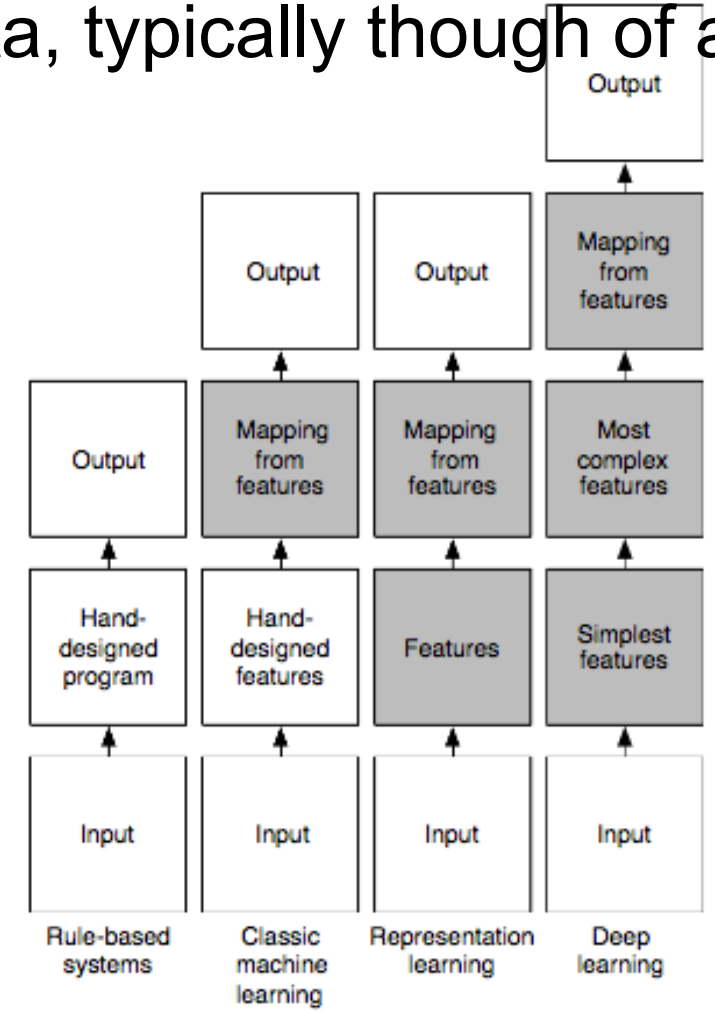
$W_{j,i} = W_{j,i} + \alpha \times a_j \times \Delta_i$



Deep Learning

Deep Learning

- Deep Learning methods seek to learn representations through a sequence of transformations of the data, typically though of as layers in a network
- Flow charts from Bengio et al. (2014) “showing how the different parts of an AI system relate to each other within different AI disciplines.
- Shaded boxes indicate components that are able to learn from data”



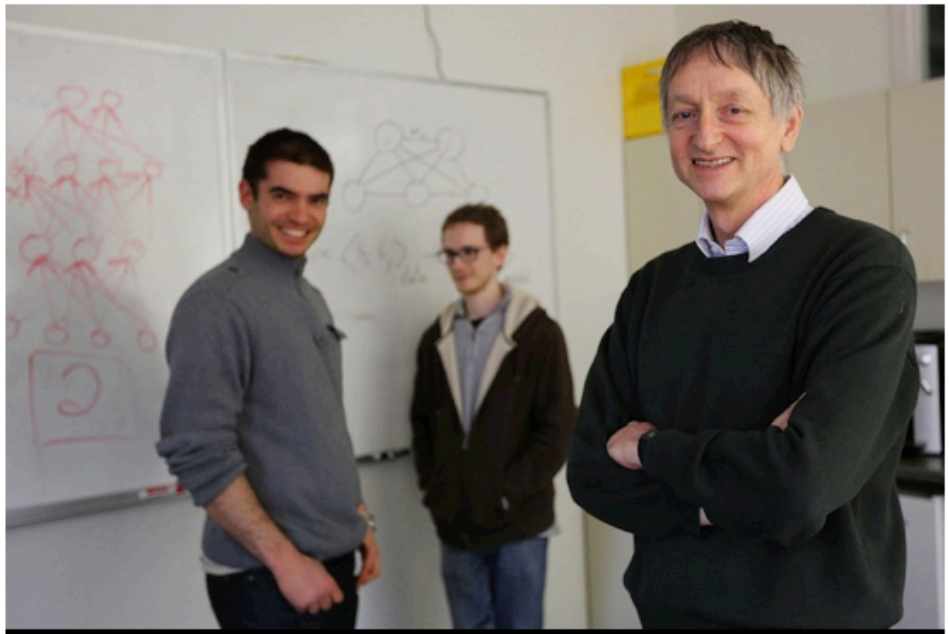
Why are Deep Neural Networks so Hot?

- **Large-Vocabulary Speech Recognition**
  Significant increase in performance (Dahl, Yu, Deng & Acero, 2012)
  - Deep Neural Network : 16-23% relative error rate reduction over the previous state-of-the-art
- **Visual Recognition of 1000 Classes**
  Top results on the ImageNet contest (Krizhevsky, Sutskever & Hinton, 2012), in 1.2 million images
  - Deep Neural Network : 15% top-5 error rate
  - Second best entry: 26% top-5 error rate
- **Face Verification**
  Near human performance, 97.35% accuracy on the Labeled Faces in the Wild (LFW) evaluation, reducing the error of the state of the art at the time by more than 27% (Facebook Research, 2014)
- **Neural Machine Translation**
  Much more accurate translations compared to a strong, highly engineered production grade system at Google

Recent article in Wired & New developments at Facebook

Google Hires Brains that Helped Supercharge Machine Learning

BY ROBERT MCMILLAN 03.13.13 6:30 AM



Geoffrey Hinton (right) Alex Krizhevsky, and Ilya Sutskever (left) will do machine learning work at Google. *Photo: U of T*

Google has hired the man who showed how to make computers learn much like the human brain.

- After winning ImageNet challenge
- Google buys Geoff Hinton's company

facebook

Yann LeCun
December 9, 2013 ·

- Facebook has created a new research lab with the ambitious, long-term goal of bringing about major advances in Artificial Intelligence.
- Simultaneously, Facebook and New York University's Center for Data Science are entering a partnership to carry out research in data science, machine learning, and AI.

An Explosion in Interest

- Lasagne (Library to easily make layers in Theano)
- Tensor Flow (Google – Nov. 2015)
- Computational Network Toolkit (CNTK) Microsoft
- Torch (Facebook)
- Chainer (Japanese effort)

Other related software

- Caffee (Berkeley)

Data Mining

Practical Machine Learning Tools and Techniques

Slides 1-55 for Chapter 10 - Deep learning

of *Data Mining* by I. H. Witten, E. Frank,
M. A. Hall, and C. J. Pal

Introducing Deep Learning

- In recent years, so-called "deep learning" approaches to machine learning have had a major impact on speech recognition and computer vision
- Other disciplines, such as natural language processing, are also starting to see benefits
- A critical ingredient is the use of much larger quantities of data than has heretofore been possible
- Recent successes have arisen in settings involving *high capacity* models—ones with many parameters
- Here, deep learning methods create flexible models that exploit information buried in massive datasets far more effectively than do traditional machine learning techniques using hand-engineered features

Views on machine learning

- One way to view machine learning is in terms of three general approaches:

1. *Classical machine learning* techniques,
   which make predictions directly from a set of features that have been pre-specified by the user;
2. *Representation learning* techniques,
   which transform features into some intermediate representation prior to mapping them to final predictions; and
3. *Deep learning* techniques,
   a form of representation learning that uses multiple transformation steps to create very complex features

The neural network *renaissance* and deep learning *revolution*

- The term "renaissance" captures a massive resurgence of interest in neural networks and deep learning techniques
- Many high-profile media (e.g. *The New York Times*) have documented the striking successes of deep learning techniques on key benchmark problems
- Starting around 2012, impressive results were achieved on long-standing problems in speech recognition and computer vision, and in competitive challenges such as the ImageNet *Large Scale Visual Recognition Challenge* and the *Labeled Faces in the Wild* evaluation

GPUs, graphs and tensors

- The easy availability of high-speed computation in the form of graphics processing units has been critical to the success of deep learning techniques
- When formulated in matrix-vector form, computation can be accelerated using optimized graphics libraries and hardware
- This is why we will study backpropagation in matrix-vector form
  - Readers unfamiliar with manipulating functions that have matrix arguments, and their derivatives are advised to consult Appendix A.1 for a summary of some useful background
- As network models become more complex, some quantities can only be represented using multidimensional arrays of numbers
  - Such arrays are sometimes referred to as tensors, a generalization of matrices that permit an arbitrary number of indices
- Software for deep learning supporting *computation graphs* and *tensors* is therefore invaluable for accelerating the creation of complex network structures and making it easier to learn them

Key developments

The following developments have played a crucial role in the resurgence of neural network methods:

- the proper evaluation of machine learning methods;
- vastly increased amounts of data;
- deeper and larger network architectures;
- accelerated training using GPU techniques

Mixed National Institute of Standards and Technology (MNIST)

- Is a database and evaluation setup for handwritten digit recognition
- Contains 60,000 training and 10,000 test instances of hand-written digits, encoded as 28×28 pixel grayscale images
- The data is a re-mix of an earlier NIST dataset in which adults generated the training data and high school students generated the test set
- Lets compare the performance of different methods

MNIST

Classifier	Test Error Rate (%)	References
Linear classifier (1-layer neural net)	12.0	LeCun et al. (1998)
K-nearest-neighbors, Euclidean (L2)	5.0	LeCun et al. (1998)
2-Layer neural net, 300 hidden units, mean square error	4.7	LeCun et al. (1998)
Support vector machine, Gaussian kernel	1.4	MNIST Website
Convolutional net, LeNet-5 (no distortions)	**0.95**	LeCun et al. (1998)
Methods using distortions		
Virtual support vector machine, deg-9 polynomial, (2-pixel jittered and deskewing)	0.56	DeCoste and Scholkopf (2002)
Convolutional neural net (elastic distortions)	0.4	Simard, Steinkraus, and Platt (2003)
6-Layer feedforward neural net (on GPU) (elastic distortions)	**0.35**	Ciresan, Meier, Gambardella, and Schmidhuber (2010)
Large/deep convolutional neural net (elastic distortions)	**0.35**	Ciresan, Meier, Masci, Maria Gambardella, and Schmidhuber (2011)
Committee of 35 convolutional networks (elastic distortions)	0.23	Ciresan, Meier, and Schmidhuber (2012)

Losses and regularization

- Logistic regression can be viewed as a simple neural network with no hidden units
- The underlying optimization criterion for predicting i=1,…,N labels y_i from features $\mathbf{x}_i$ with parameters θ consisting of a matrix of weights **W** and a vector of biases **b** can be viewed as

$$\sum_{i=1}^{N} -\log p(y_i \mid \mathbf{x}_i; \mathbf{W}, \mathbf{b}) + \lambda \sum_{j=1}^{M} w_j^2 = \sum_{i=1}^{N} L(f_i(\mathbf{x}_i; \theta), y_i) + \lambda R(\theta)$$

- where the first term, $L(f_i(\mathbf{x}_i;\theta), y_i)$, is the negative conditional log-likelihood or *loss*, and
- the second term, $\lambda R(\theta)$, is a weighted *regularizer* used to prevent overfitting

Empirical risk minimization

- This formulation as a loss- and regularizer-based objective function gives us the freedom to choose either probabilistic losses or other loss functions
- Using the *average loss* over the training data, called the *empirical risk*, leads to the following formulation of the optimization problem: minimize the empirical risk plus a regularization term, i.e.

$$\arg\min_{\theta}\left[\frac{1}{N}\sum_{i=1}^{N} L(f_i(\mathbf{x}_i;\theta),\mathbf{y}_i) + \lambda R(\theta)\right].$$

- Note that the factor *N* must be accounted for if one relates the regularization weight here to the corresponding parameter derived from a formal probabilistic model for a distribution on parameters

In practice

- In deep learning we are often interested in examining learning curves that show the loss or some other performance metric on a graph as a function of the number of passes that an algorithm has taken over the data.
- It is much easier to compare the *average* loss over a training set with the *average* loss over a validation set on the same graph, because dividing by *N* gives them the same scale.

Common losses for neural networks

- The final output function of a neural network typically has the form $f_k(\mathbf{x})=f_k(a_k(\mathbf{x}))$, where $a_k(\mathbf{x})$ is just one of the elements of vector fuction $\mathbf{a}(\mathbf{x})=\mathbf{W}\mathbf{h}(\mathbf{x})+\mathbf{b}$
- Commonly used output loss functions, output activation functions, and the underlying distributions from which they derive are shown below

Loss Name, $L(f_i(\mathbf{x}_i;\theta),\mathbf{y}_i)=$	**Distribution Name**, $P(f_i(\mathbf{x}_i;\theta),\mathbf{y}_i)=$	**Output Activation Function**, $f_k(a_k(\mathbf{x}))=$
Squared error, $\sum_{k=1}^{K}(f_k(\mathbf{x})-y_k)^2$	Gaussian, $N(\mathbf{y};\mathbf{f}(\mathbf{x};\theta),\mathbf{I})$	$\frac{1}{(1+\exp(-a_k(\mathbf{x})))}$
Cross entropy, $-\sum_{k=1}^{K}[y_k\log f_k(\mathbf{x})+(1-y_k)\log(1-f_k(\mathbf{x}))]$	Bernoulli, $\text{Bern}(\mathbf{y};\mathbf{f}(\mathbf{x};\theta))$	$\frac{1}{(1+\exp(-a_k(\mathbf{x})))}$
Softmax, $-\sum_{k=1}^{K}y_k\log f_k(\mathbf{x})$	Discrete or Categorical, $\text{Cat}(\mathbf{y};\mathbf{f}(\mathbf{x};\theta))$	$\frac{\exp(a_k(\mathbf{x}))}{\sum_{j=1}^{K}\exp(a_j(\mathbf{x}))}$

Deep neural network architectures

- Compose computations performed by many layers
- Denoting the output of hidden layers by $\mathbf{h}^{(l)}(\mathbf{x})$, the computation for a network with *L* hidden layers is:

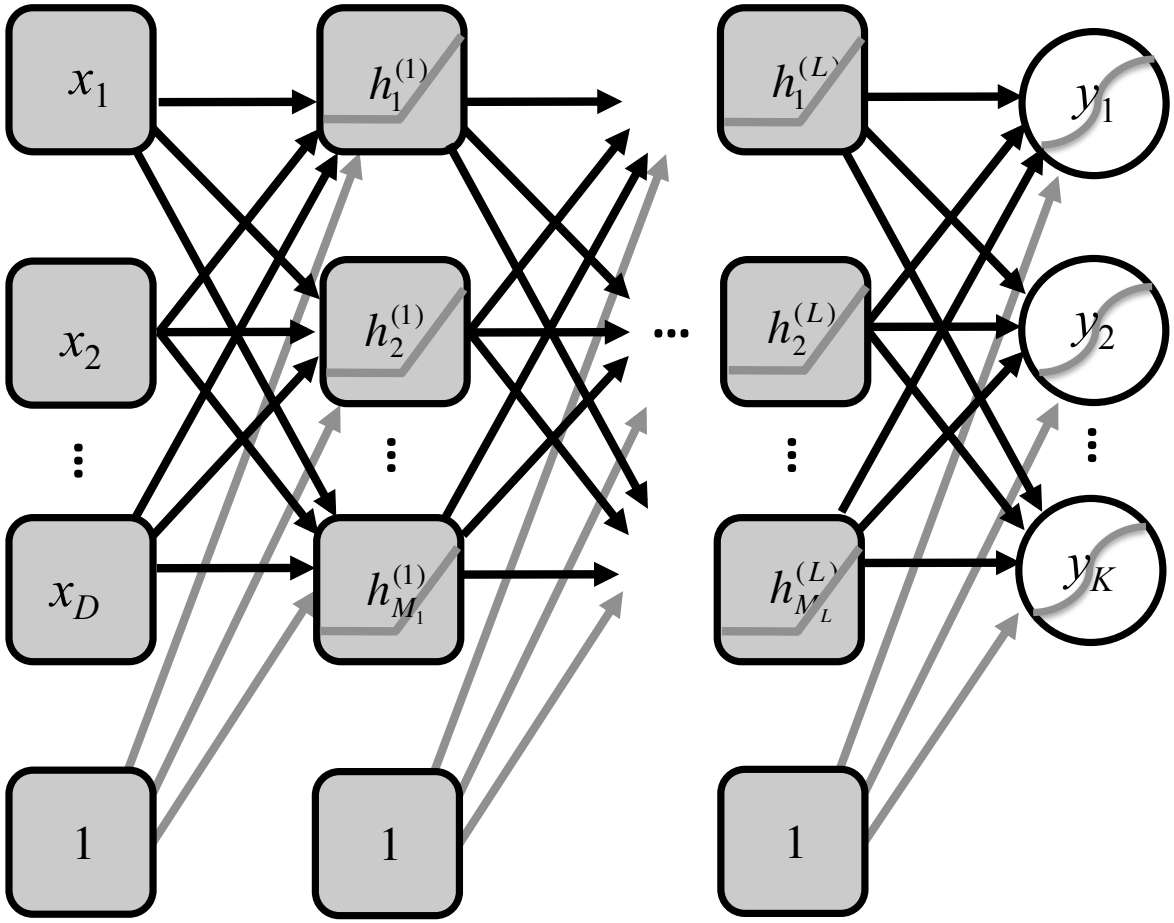
$$\mathbf{f}(\mathbf{x}) = \mathbf{f}\left[\mathbf{a}^{(L+1)}\left(\mathbf{h}^{(L)}\left(\mathbf{a}^{(L)}\left(\ldots\left(\mathbf{h}^{(2)}\left(\mathbf{a}^{(2)}\left(\mathbf{h}^{(1)}\left(\mathbf{a}^{(1)}(\mathbf{x})\right)\right)\right)\right)\right)\right)\right]$$

- Where *pre-activation functions* $\mathbf{a}^{(l)}(\mathbf{x})$ are typically linear, of the form $\mathbf{a}^{(l)}(\mathbf{x}) = \mathbf{W}^{(l)}\mathbf{x} + \mathbf{b}^{(l)}$ with matrix $\mathbf{W}^{(l)}$ and bias $\mathbf{b}^{(l)}$
- This formulation can be expressed using a single parameter matrix θ with the trick of defining $\hat{\mathbf{x}}$ as x with a 1 appended to the end of the vector; we then have

$$\mathbf{a}^{(l)}(\hat{\mathbf{x}}) = \boldsymbol{\theta}^{(l)}\hat{\mathbf{x}} \qquad , l = 1$$

$$\mathbf{a}^{(l)}(\hat{\mathbf{h}}^{(l-1)}) = \boldsymbol{\theta}^{(l)}\hat{\mathbf{h}}^{(l-1)} \qquad , l > 1$$

Deep feedforward networks

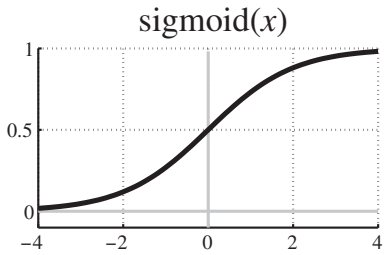
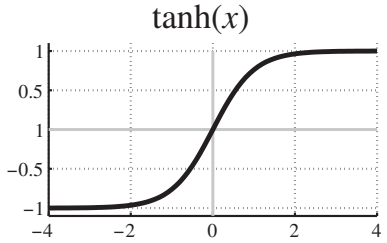
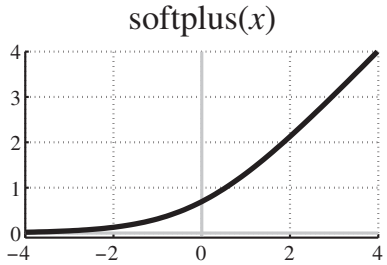
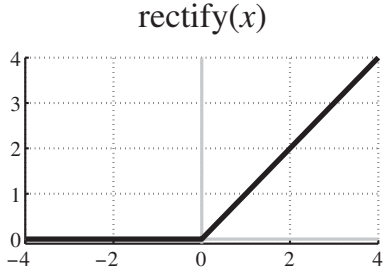


- Unlike Bayesian networks the hidden units here are *intermediate deterministic computations* not random variables, which is why they are not represented as circles
- However, the output variables y_k are drawn as circles because they can be formulated probabilistically

Activation functions

- Activation functions, $\mathbf{h}^{(l)}(\mathbf{x})$ generally operate on the pre-activation vectors in an *element-wise* fashion
- While sigmoid functions have been popular, the hyperbolic tangent function is sometimes preferred, partly because it has a steady state at 0
- More recently the *rectify*() function or rectified linear units (ReLUs) have been found to yield superior results in many different settings
  - Since ReLUs are 0 for negative argument values, some units in the model will yield activations that are 0, giving a sparseness property that is useful in many contexts
  - The gradient is particularly simple—either 0 or 1
  - This helps address the *exploding gradient problem*
- A number of software packages make it easy to use a variety of activation functions, determining gradients automatically using symbolic computations

Activation functions

Name and Graph	Function	Derivative
	$h(x) = \frac{1}{1 + \exp(-x)}$	$h'(x) = h(x)[1 - h(x)]$
	$h(x) = \frac{\exp(x) - \exp(-x)}{\exp(x) + \exp(-x)}$	$h'(x) = 1 - h(x)^2$
	$h(x) = \log(1 + \exp(x))$	$h'(x) = \frac{1}{1 + \exp(-x)}$
	$h(x) = \max(0, x)$	$h'(x) = \begin{cases} 1 \text{ if } x \geq 0 \\ 0 \text{ if } x < 0 \end{cases}$

Bibliographic Notes & Further Reading

- The backpropagation algorithm has been known in close to its current form since Werbos (1974)'s PhD thesis
- In his extensive literature review of deep learning, Schmidhuber (2015) traces key elements of the algorithm back even further.
  - He also traces the idea of "deep networks" back to the work of Ivakhnenko and Lapa (1965).
- The popularity of neural network techniques has gone through several cycles and while some factors are social, there are important technical reasons behind the trends.
- A single-layer neural network cannot solve the XOR problem, a failing that was derided by Minsky and Papert (1969) and which stymied neural network development in the following decades.

Bibliographic Notes & Further Reading

- It is well known that networks with one additional layer can approximate any function (Cybenko, 1989; Hornik, 1991), and Rumelhart et al. (1986)'s influential work re-popularized neural network methods for a while.
- By the early 2000s neural network methods had fallen out of favor again – kernel methods like SVMs yielded state of the art results on many problems and were convex
- Indeed, the organizers of NIPS, the *Neural Information Processing Systems* conference, which was (and still is) widely considered to be the premier forum for neural network research, found that the presence of the term "neural networks" in the title was highly correlated with the paper's rejection!
  - A fact that is underscored by citation analysis of key neural network papers during this period.
- In this context, the recent resurgence of interest in deep learning really does feel like a "revolution."

Bibliographic Notes & Further Reading

- It is known that most complex Boolean functions require an exponential number of two-step logic gates for their representation (Wegener, 1987).
- The solution appears to be greater depth: according to Bengio (2014), the evidence strongly suggests that "functions that can be compactly represented with a depth-*k* architecture could require a very large number of elements in order to be represented by a shallower architecture".

Backpropagation revisited in vector matrix form

Backpropagation in matrix vector form

- Backpropagation is based on the chain rule of calculus
- Consider the loss for a single-layer network with a softmax output (which corresponds exactly to the model for multinomial logistic regression)
- We use multinomial vectors **y**, with a single dimension $y_k = 1$ for the corresponding class label and whose other dimensions are 0
- Define $\mathbf{f} = [\ f_1(\mathbf{a}),\ \ldots,\ f_K(\mathbf{a})\ ]^T$, and $a_k(\mathbf{x};\boldsymbol{\theta}_k) = \boldsymbol{\theta}_k^{\mathrm{T}}\mathbf{x}$, $\mathbf{a}(\mathbf{x};\boldsymbol{\theta}) = [\ a_1(\mathbf{x};\boldsymbol{\theta}_1),\ \ldots,\ a_K(\mathbf{x};\boldsymbol{\theta}_K)\ ]^T$ where $\boldsymbol{\theta}_k$ is a column vector containing the k^{th} row of the parameter matrix
- Consider the softmax loss for **f**(**a**(**x**))

Logistic regression and the chain rule

- Given loss $L = -\sum_{k=1}^{K} y_k \log f_k(\mathbf{x}), \quad f_k(\mathbf{x}) = \dfrac{\exp(a_k(\mathbf{x}))}{\sum_{c=1}^{K} \exp(a_c(\mathbf{x}))}.$
- Use the chain rule to obtain

$$\frac{\partial L}{\partial \boldsymbol{\theta}_k} = \frac{\partial \mathbf{a}}{\partial \boldsymbol{\theta}_k} \frac{\partial \mathbf{f}}{\partial \mathbf{a}} \frac{\partial L}{\partial \mathbf{f}} = \frac{\partial \mathbf{a}}{\partial \boldsymbol{\theta}_k} \frac{\partial L}{\partial \mathbf{a}}.$$

- Note the order of terms - in vector matrix form terms build from right to left

$$\frac{\partial L}{\partial a_j} = \frac{\partial}{\partial a_j}\left[-\sum_{k=1}^{K} y_k \left[a_k - \log\left[\sum_{c=1}^{K} \exp(a_c)\right]\right]\right]$$

$$= -\left[y_{k=j} - \frac{\exp(a_{k=j})}{\sum_{c=1}^{K} \exp(a_c)}\right] = -\left[y_j - p(y_j \mid \mathbf{x})\right] = -\left[y_j - f_j(\mathbf{x})\right],$$

Matrix vector form of gradient

- We can write $$\frac{\partial L}{\partial \mathbf{a}} = -\left[\mathbf{y} - \mathbf{f}(\mathbf{x})\right] \equiv -\Delta$$

  and since $$\frac{\partial a_j}{\partial \boldsymbol{\theta}_k} = \begin{cases} \dfrac{\partial}{\partial \boldsymbol{\theta}_k} \boldsymbol{\theta}_k^{\mathrm{T}} \mathbf{x} = \mathbf{x} & , j = k \\ 0 & , j \neq k \end{cases}$$

  we have $$\frac{\partial \mathbf{a}}{\partial \boldsymbol{\theta}_k} = \mathbf{H}_k = \begin{bmatrix} 0 & x_1 & 0 \\ \vdots & \vdots & \vdots \\ 0 & x_n & 0 \end{bmatrix}$$

- Notice that we avoid working with the partial derivative of the vector **a** with respect to the matrix θ, because it cannot be represented as a matrix — it is a multidimensional array of numbers (a tensor).

A compact expression for the gradient

- The gradient (as a column vector) for the vector in the *k*th row of the parameter matrix

$$\frac{\partial L}{\partial \boldsymbol{\theta}_k} = \frac{\partial \mathbf{a}}{\partial \boldsymbol{\theta}_k}\frac{\partial L}{\partial \mathbf{a}} = -\begin{bmatrix} 0 & x_1 & 0 \\ \vdots & \vdots & \vdots \\ 0 & x_n & 0 \end{bmatrix}\big[\mathbf{y} - \mathbf{f}(\mathbf{x})\big]$$

$$= -\mathbf{x}(y_k - f_k(x)).$$

- With a little rearrangement the gradient for the entire matrix of parameters can be written compactly:

$$\frac{\partial L}{\partial \boldsymbol{\theta}} = -\big[\mathbf{y} - \mathbf{f}(\mathbf{x})\big]\mathbf{x}^{\mathrm{T}} = -\Delta\mathbf{x}^{\mathrm{T}}.$$

Consider now a multilayer network

- Using the same activation function for all L hidden layers, and a softmax output layer
- The gradient of the k^{th} parameter vector of the $L+1^{\text{th}}$ matrix of parameters is

$$\frac{\partial L}{\partial \boldsymbol{\theta}_k^{(L+1)}} = \frac{\partial \mathbf{a}^{(L+1)}}{\partial \boldsymbol{\theta}_k^{(L+1)}} \frac{\partial L}{\partial \mathbf{a}^{(L+1)}}, \qquad \frac{\partial L}{\partial \mathbf{a}^{(L+1)}} = -\Delta^{(L+1)}$$

$$= -\frac{\partial \mathbf{a}^{(L+1)}}{\partial \boldsymbol{\theta}_k^{(L+1)}} \Delta^{(L+1)}$$

$$= -\mathbf{H}_k^L \Delta^{(L+1)} \quad \Rightarrow \quad \frac{\partial L}{\partial \boldsymbol{\theta}^{(L+1)}} = -\Delta^{(L+1)} \tilde{\mathbf{h}}_{(L)}^{\mathrm{T}}.$$

where $\mathbf{H}_k^L$ is a matrix containing the activations of the corresponding hidden layer, in column k

Backpropagating errors

- Consider the computation for the gradient of the k^{th} row of the L^{th} matrix of parameters
- Since the bias terms are constant, it is unnecessary to backprop through them, so

$$\frac{\partial L}{\partial \, \boldsymbol{\theta}_k^{(L)}} = \frac{\partial \, \mathbf{a}^{(L)}}{\partial \, \boldsymbol{\theta}_k^{(L)}} \frac{\partial \, \mathbf{h}^{(L)}}{\partial \, \mathbf{a}^{(L)}} \frac{\partial \, \mathbf{a}^{(L+1)}}{\partial \, \mathbf{h}^{(L)}} \frac{\partial \, L}{\partial \, \mathbf{a}^{(L+1)}}$$

$$= -\frac{\partial \, \mathbf{a}^{(L)}}{\partial \, \boldsymbol{\theta}_k^{(L)}} \frac{\partial \, \mathbf{h}^{(L)}}{\partial \, \mathbf{a}^{(L)}} \frac{\partial \, \mathbf{a}^{(L+1)}}{\partial \, \mathbf{h}^{(L)}} \Delta^{(L+1)}, \qquad \Delta^{(L)} \equiv \frac{\partial \, \mathbf{h}^{(L)}}{\partial \, \mathbf{a}^{(L)}} \frac{\partial \, \mathbf{a}^{(L+1)}}{\partial \, \mathbf{h}^{(L)}} \Delta^{(L+1)}$$

$$= -\frac{\partial \, \mathbf{a}^{(L)}}{\partial \, \boldsymbol{\theta}_k^{(L)}} \Delta^{(L)}$$

- Similarly, we can define $\Delta^{(l)}$ recursively in terms of $\Delta^{(l+1)}$

Backpropagating errors

- The backpropagated error can be written as simply

$$\Delta^{(l)} = \frac{\partial\, \mathbf{h}^{(l)}}{\partial\, \mathbf{a}^{(l)}} \frac{\partial\, \mathbf{a}^{(l+1)}}{\partial\, \mathbf{h}^{(l)}} \Delta^{(l+1)}, \qquad \frac{\partial\, \mathbf{h}^{(l)}}{\partial\, \mathbf{a}^{(l)}} = \mathbf{D}^{(l)}, \qquad \frac{\partial\, \mathbf{a}^{(l+1)}}{\partial\, \mathbf{h}^{(l)}} = \mathbf{W}^{\mathrm{T}(l+1)},$$

$$\Delta^{(l)} = \mathbf{D}^{(l)} \mathbf{W}^{\mathrm{T}(l+1)} \Delta^{(l+1)}$$

  where $\mathbf{D}^{(l)}$ contains the partial derivatives of the hidden-layer activation function with respect to the pre-activation input.

- $\mathbf{D}^{(l)}$ is generally diagonal, because activation functions usually operate on an elementwise basis
- $\mathbf{W}^{\mathrm{T}(l+1)}$ arises from the fact that $\mathbf{a}^{(l+1)}(\mathbf{h}^{(l)}) = \mathbf{W}^{(l+1)}\mathbf{h}^{(l)} + \mathbf{b}^{(l+1)}$

A general form for gradients

- The gradients for the k^{th} vector of parameters of the l^{th} network layer can therefore be computed using products of matrices of the following form

$$\frac{\partial L}{\partial \boldsymbol{\theta}_k^{(l)}} = -\mathbf{H}_k^{(l-1)} \mathbf{D}^{(l)} \mathbf{W}^{\mathrm{T}(l+1)} \cdots \mathbf{D}^{(L)} \mathbf{W}^{\mathrm{T}(L+1)} \Delta^{(L+1)}, \qquad \frac{\partial L}{\partial \boldsymbol{\theta}^{(l)}} = -\Delta^{(l)} \hat{\mathbf{h}}_{(l-1)}^{\mathrm{T}}$$

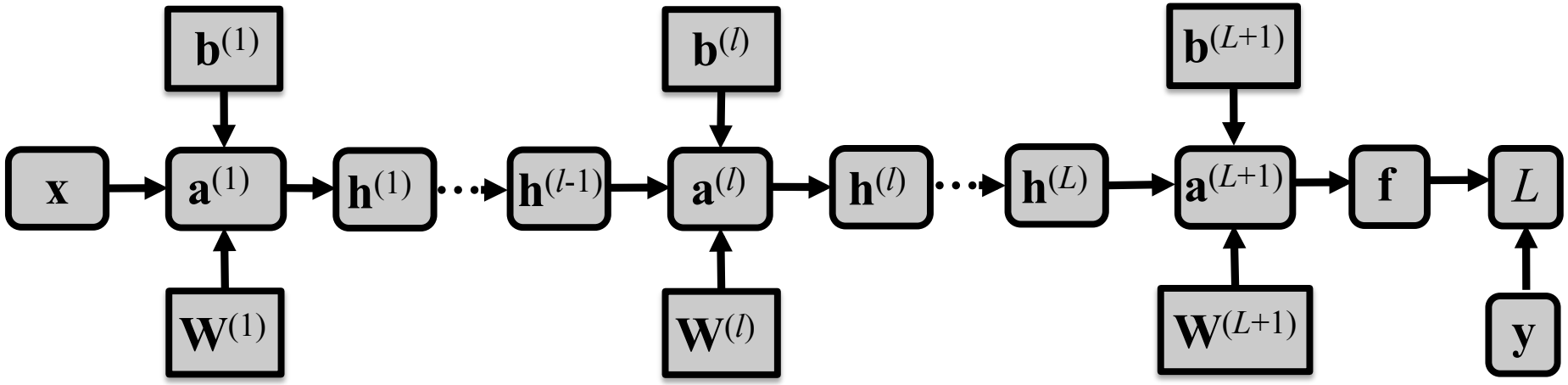
- When l=1, $\hat{\mathbf{h}}_{(0)} = \hat{\mathbf{x}}$, the input data with a 1 appended
- Note: since **D** is usually diagonal the corresponding matrix-vector multiply can be transformed into an element-wise product $\circ$ by extracting the diagonal for **d**

$$\Delta^{(l)} = \mathbf{D}^{(l)} (\mathbf{W}^{\mathrm{T}(l+1)} \Delta^{(l+1)}) = \mathbf{d}^{(l)} \circ (\mathbf{W}^{\mathrm{T}(l+1)} \Delta^{(l+1)})$$

Visualizing backpropagation

$$\mathbf{a}^{(1)} = \mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)} \qquad \mathbf{a}^{(l)} = \mathbf{W}^{(l)}\mathbf{h}^{(l-1)} + \mathbf{b}^{(l)} \qquad \mathbf{a}^{(L+1)} = \mathbf{W}^{(L+1)}\mathbf{h}^{(L)} + \mathbf{b}^{(L+1)}$$

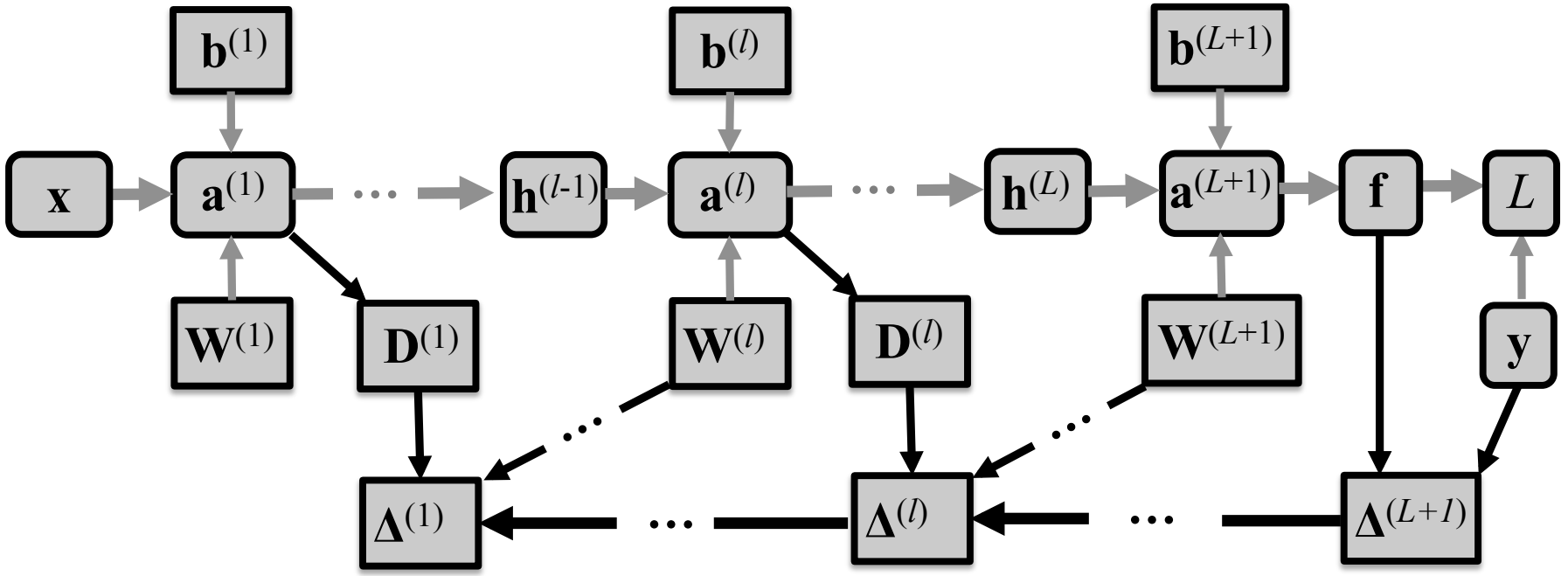
$$\mathbf{h}^{(1)} = \text{act}(\mathbf{a}^{(1)}) \qquad \mathbf{h}^{(l)} = \text{act}(\mathbf{a}^{(l)}) \qquad \mathbf{f} = \text{out}(\mathbf{a}^{(L+1)})$$



- In the forward propagation phase we compute terms of the form above
- The figure above is a type of computation graph, (which is different from the probability graphs we saw earlier)

Visualizing backpropagation

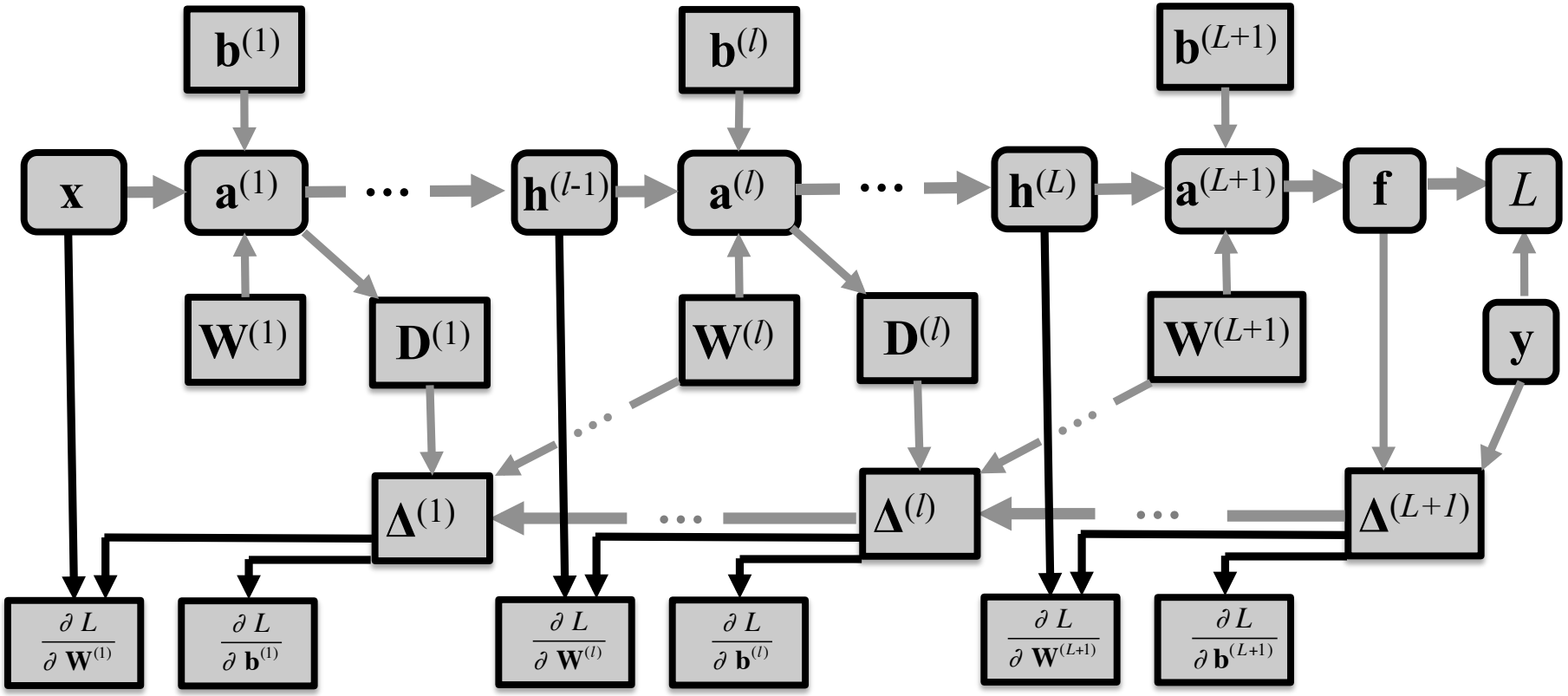
- In the backward propagation phase we compute terms of the form below



$$\boldsymbol{\Delta}^{(l)} = \mathbf{D}^{(l)}\mathbf{W}^{\mathrm{T}(l+1)}\boldsymbol{\Delta}^{(l+1)} \qquad \frac{\partial\, \mathbf{h}^{(l)}}{\partial\, \mathbf{a}^{(l)}} = \mathbf{D}^{(l)} \qquad \frac{\partial\, \mathbf{a}^{(l+1)}}{\partial\, \mathbf{h}^{(l)}} = \mathbf{W}^{\mathrm{T}(l+1)} \qquad \frac{\partial\, L}{\partial\, \mathbf{a}^{(L+1)}} = -\left[\mathbf{y} - \mathbf{f}(\mathbf{x})\right] = -\boldsymbol{\Delta}^{(L+1)}$$

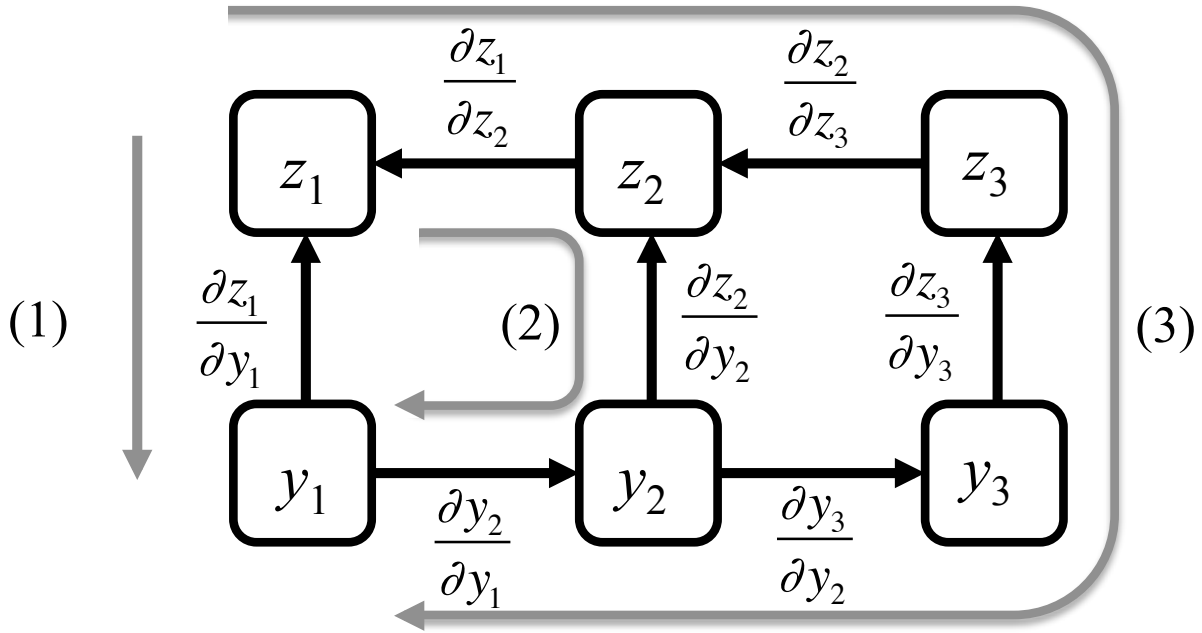
Visualizing backpropagation

- We update the parameters in our model using the simple computations below



$$\frac{\partial L}{\partial \mathbf{W}^{(1)}} = -\Delta^{(1)}\mathbf{x}^{\mathrm{T}} \qquad \frac{\partial L}{\partial \mathbf{b}^{(1)}} = -\Delta^{(1)} \qquad \frac{\partial L}{\partial \mathbf{W}^{(l)}} = -\Delta^{(l)}\mathbf{h}_{(l-1)}^{\mathrm{T}} \qquad \frac{\partial L}{\partial \mathbf{b}^{(l)}} = -\Delta^{(l)}$$

Computation graphs



- For more complicated computations, computation graphs can help us keep track of how computations decompose, ex. $z_1 = z_1(y_1, z_2(y_2(y_1), z_3(y_3(y_2(y_1)))))$

$$\frac{\partial z_1}{\partial y_1} = \underbrace{\frac{\partial z_1}{\partial y_1}}_{(1)} + \underbrace{\frac{\partial z_1}{\partial z_2}\frac{\partial z_2}{\partial y_2}\frac{\partial y_2}{\partial y_1}}_{(2)} + \underbrace{\frac{\partial z_1}{\partial z_2}\frac{\partial z_2}{\partial z_3}\frac{\partial z_3}{\partial y_3}\frac{\partial y_3}{\partial y_2}\frac{\partial y_2}{\partial y_1}}_{(3)}$$

Checking an implementation of backpropagation and software tools

- An implementation of the backpropagation algorithm can be checked for correctness by comparing the analytic values of gradients with those computed numerically
- For example, one can add and subtract a small perturbation to each parameter and then compute the symmetric finite difference approximation to the derivative of the loss:

$$\frac{\partial L}{\partial \theta} \approx \frac{L(\theta+\varepsilon)-L(\theta-\varepsilon)}{2\varepsilon}$$

- Many software packages use computation graphs to allow complex networks to be more easily defined and optimized
- Examples include: Theano, TensorFlow, Keras and Torch

Reminder About Stochastic Gradient Descent (SGD)

Mini-batch based stochastic gradient descent (SGD)

- Stochastic gradient descent updates model parameters according to the gradient computed from one example
- The mini-batch variant uses a small subset of the data and bases updates to parameters on the average gradient over the examples in the batch
- This operates just like the regular procedure: initialize the parameters, enter a parameter update loop, and terminate by monitoring a validation set
- Normally these batches are randomly selected disjoint subsets of the training set, perhaps shuffled after each epoch, depending on the time required to do so

Mini-batch based SGD

- Each pass through a set of mini-batches that represent the complete training set is an *epoch*
- Using the empirical risk plus a regularization term as the objective function, updates are

$$\boldsymbol{\theta}^{\text{new}} \leftarrow \boldsymbol{\theta} - \eta_t \left[\frac{1}{B_k} \sum_{i \in \mathrm{I}} \left[\frac{\partial}{\partial \boldsymbol{\theta}} L(f(\mathbf{x}_i; \boldsymbol{\theta}), \mathbf{y}_i) \right] + \frac{B_k}{N} \lambda \frac{\partial}{\partial \boldsymbol{\theta}} R(\boldsymbol{\theta}) \right]$$

- η_t is the learning rate and may depend on the epoch t
- The batch is represented by a set of indices I=I(t,k) into the original data; the kth batch has B_k examples
- N is the size of the training set
- $L(f(\mathbf{x}_i;\theta),\mathbf{y}_i)$ is the loss for example $\mathbf{x}_i$, label $\mathbf{y}_i$, params θ
- R(θ) is the regularizer, with weight λ

Mini-batches

- Typically contain two to several hundred examples
  - For large models the choice may be constrained by resources
- Batch size often influences the stability and speed of learning; some sizes work particularly well for a given model and data set.
- Sometimes a search is performed over a set of potential batch sizes to find one that works well, before doing a lengthy optimization.
- The mix of class labels in the batches can influence the result
  - For unbalanced data there may be an advantage in pre-training the model using mini-batches in which the labels are balanced, then fine-tuning the upper layer or layers using the unbalanced label statistics.

Momentum

- As with regular gradient descent, 'momentum' can help the optimization escape plateaus in the loss
- Momentum is implemented by computing a moving average: $\Delta\theta = -\eta\nabla_\theta L(\theta) + \alpha\Delta\theta^{\text{old}}$
  - where the first term is the current gradient of the loss times a learning rate
  - the second term is the previous update weighted by $\alpha \in [0,1]$
- Since the mini- batch approach operates on a small subset of the data, this averaging can allow information from other recently seen mini-batches to contribute to the current parameter update
- A momentum value of 0.9 is often used as a starting point, but it is common to hand-tune it, the learning rate, and the schedule used to modify the learning rate during the training process

Learning rate schedules

- The learning rate is a critical choice when using mini-batch based stochastic gradient descent.
- Small values such as 0.001 often work well, but it is common to perform a logarithmically spaced search, say in the interval [10^{-8}, 1], followed by a finer grid or binary search.
- The learning rate may be adapted over epochs *t* to give a learning rate schedule, ex. $\eta_t = \eta_0 (1 + \varepsilon t)^{-1}$
- A fixed learning rate is often used in the first few epochs, followed by a decreasing schedule
- Many other options, ex. divide the rate by 10 when the validation error rate ceases to improve

Mini-batch SGD pseudocode

$\theta = \theta_o$ // initialize parameters

$\Delta\theta = 0$

$t = 0$

while converged == FALSE

$\{I_1, \ldots, I_K\} = \text{shuffle}(X)$ // create K mini-batches

for $k = 1 \ldots K$

$$\mathbf{g} = \frac{1}{B_k} \sum_{i \in I_k} \left[\frac{\partial}{\partial \theta} L(f(\mathbf{x}_i; \theta), \mathbf{y}_i) \right] + \frac{B_k}{N} \lambda \frac{\partial}{\partial \theta} R(\theta)$$

$$\Delta\theta \leftarrow -\eta_t \mathbf{g} + \alpha \Delta\theta$$

$$\theta \leftarrow \theta + \Delta\theta$$

end

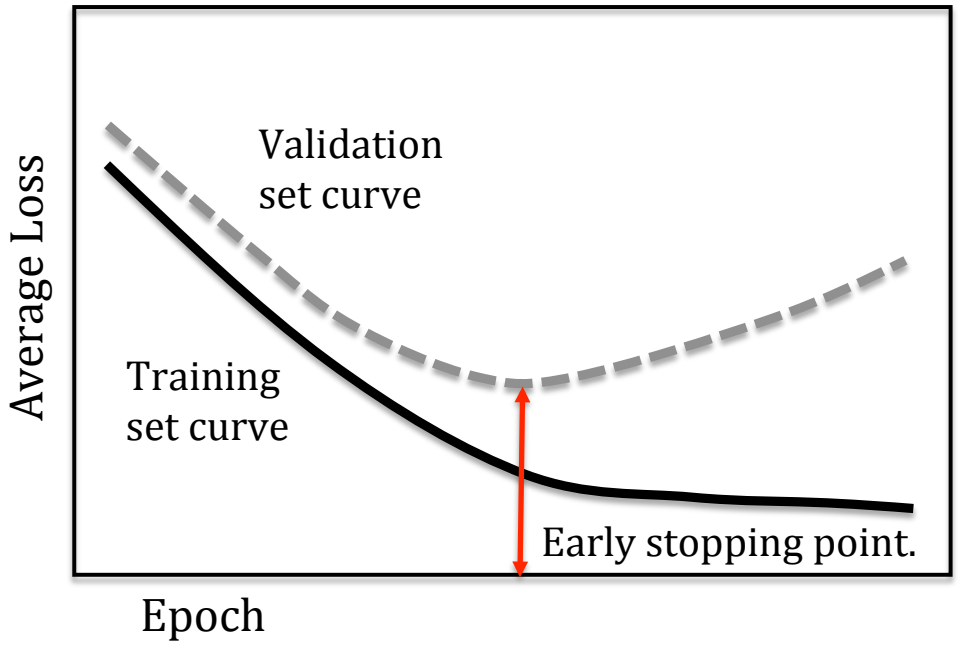
$t = t + 1$

end

Early stopping

- Deep learning involves high capacity architectures, which are susceptible to overfitting even when data is plentiful,
- Early stopping is standard practice even when other methods to reduce overfitting are employed, ex. regularization and dropout
- The idea is to monitor learning curves that plot the average loss for the training and validation sets as a function of epoch
- The key is to find the point at which the validation set average loss begins to deteriorate

Early stopping



- In practice the curves above can be more noisy due to the use of stochastic gradient descent
- As such, it is common to keep the history of the validation set curve when looking for the minimum – even if it goes back up it might come back down

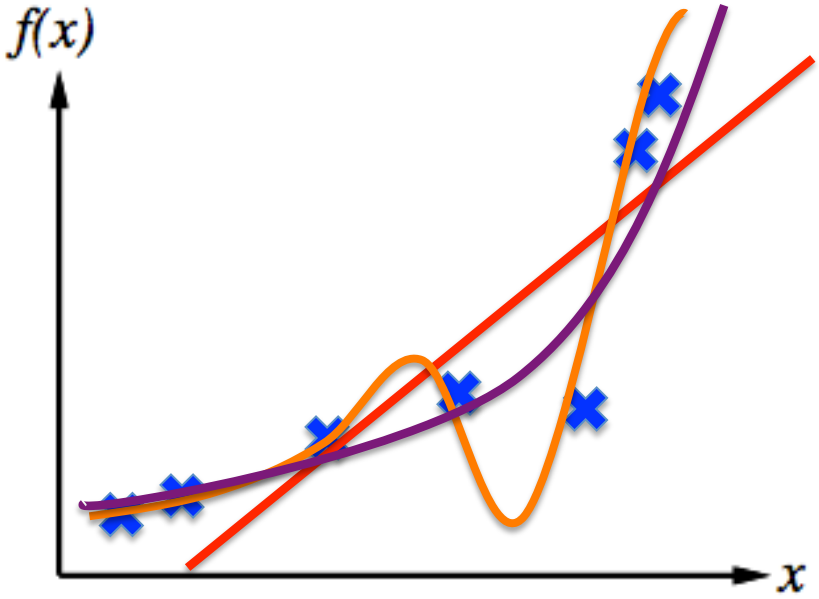
Bibliographic Notes & Further Reading

- Many neural network books (Haykin, 1994; Bishop, 1995; Ripley, 1996) do not formulate backpropagation in vector-matrix terms.
- However, recent online courses (e.g. by Hugo Larochelle), and Rojas (1996)'s text, do adopt this formulation, as we have done here

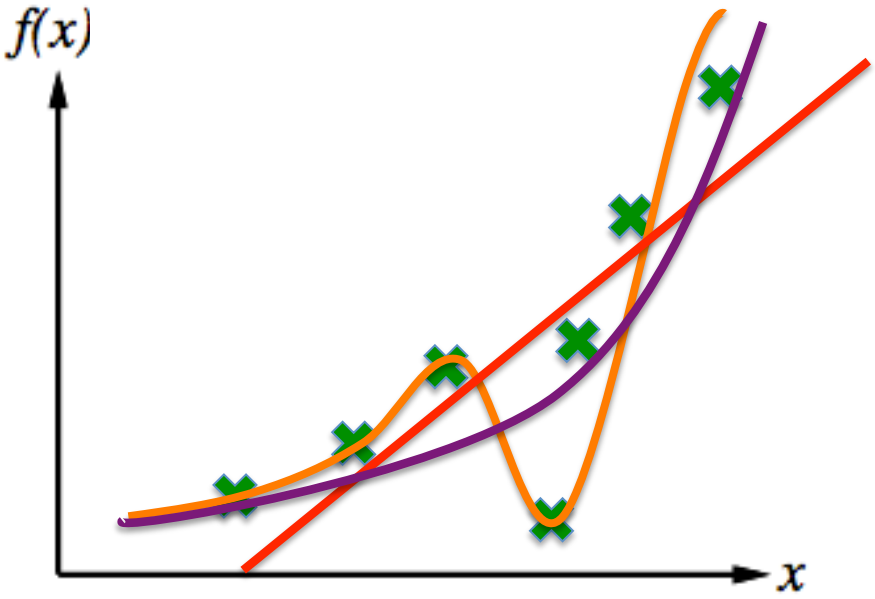
Le choix du modèle et l'ajustement des hyperparamètres

Exemple

- Sélection de la complexité du modèle
- *Utilisez l'ensemble de validation pour choisir l'ordre du polynôme. Q: Comment exactement?*



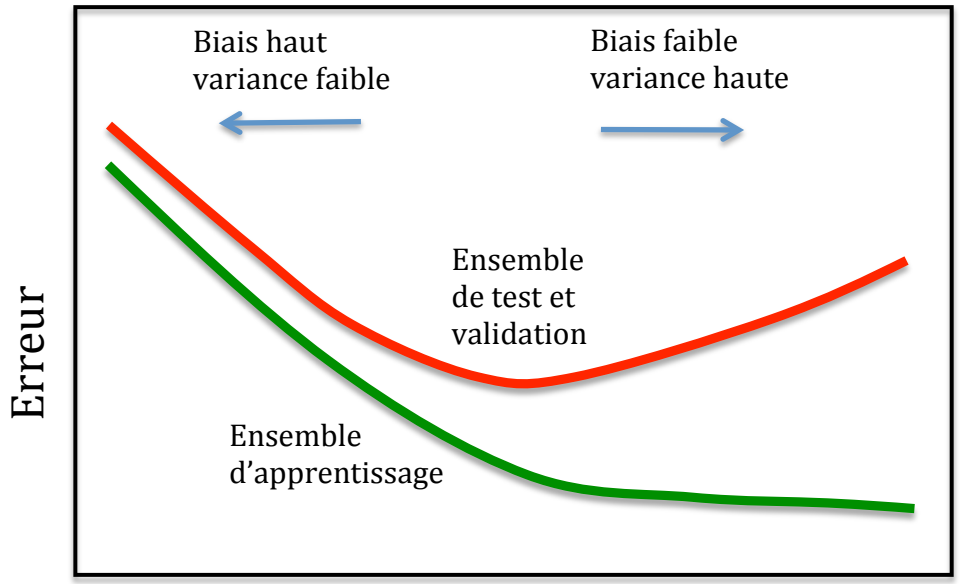
Ensemble d'apprentissage



Ensemble de validation

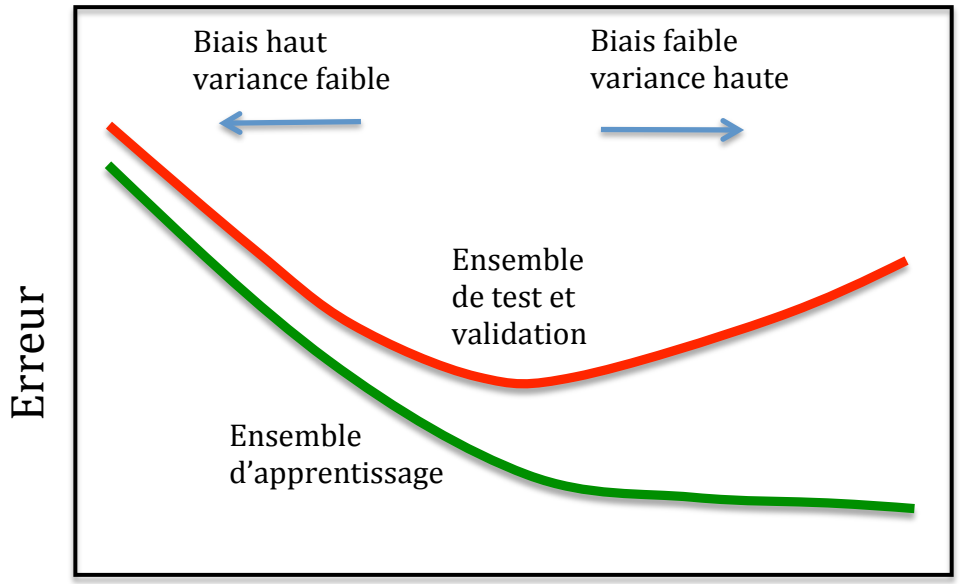
La compromise entre le biais et la variance

- En général, il existe un compromis entre des hypothèses complexes qui approchent bien les données d'apprentissage et des hypothèses plus simples qui peuvent mieux généraliser



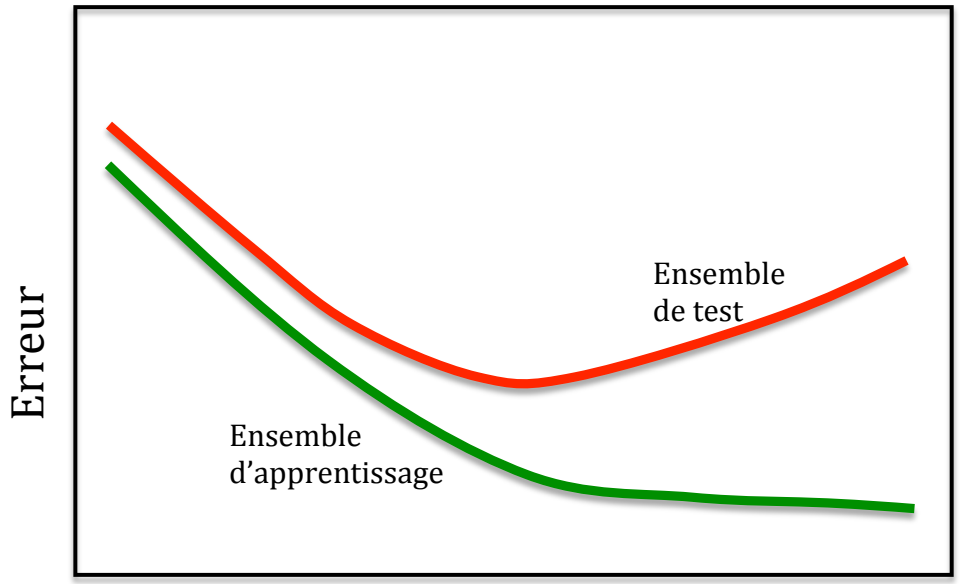
Le compromis entre le biais et la variance

- Exercice: faire une recherche sur les hyperparameters pour sélectionner le modèle le plus performant sur l'ensemble de validation
- Pourriez-vous expliquer cette recherche en termes de ce compromis?



Surapprentissage

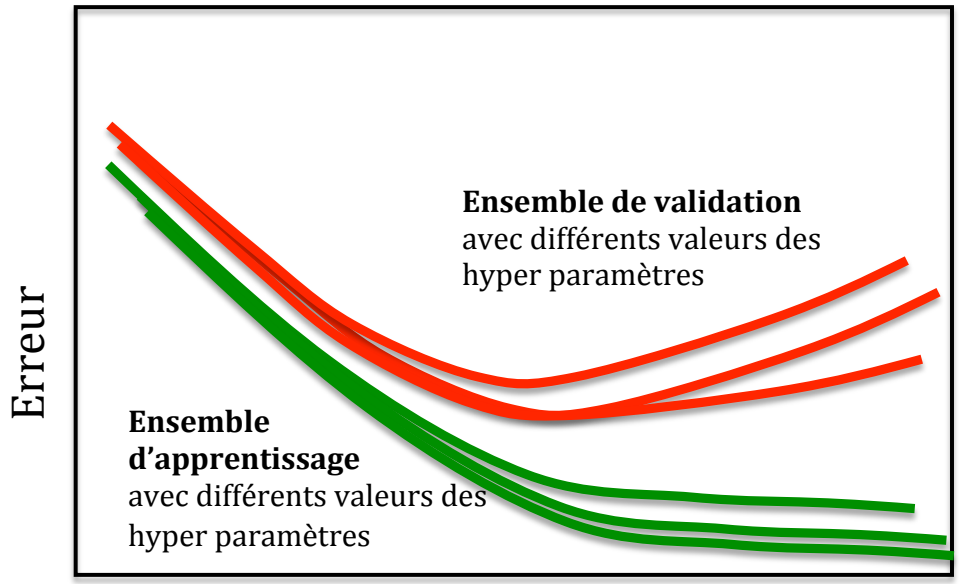
- Avec plusieurs itérations d'apprentissage, (ex. utilisant un réseau de neurones), on peut obtenir un modèle trop spécialisée pour notre ensemble d'apprentissage



Stratégies pour minimiser les effets de « surapprentissage »

- Il est typique à utiliser une distribution gaussienne (moyenne zéro) sur les paramètres pour les régressions logistique
- Avec des réseaux neuronales on utilise « early stopping »
- De plus, souvent il existe des hyper paramètres (par exemple la variance d'une gaussienne sur les paramètres),

- donc, en pratique on utilise un troisième ensemble : l'ensemble de validation avec une validation croisée « hold-out »
- Cependant, un but des méthodes plus bayésiens comme BIC est à évider le besoin pour cette phase



Training and evaluating deep networks

Part I

Validation sets and hyperparameters

- In deep learning hyperparameters are tuned by identifying what settings lead to best performance on the validation set, using early stopping
- Common hyperparameters include the strength of parameter regularization, but also model complexity in terms of the number of hidden units and layers and their connectivity, the form of activation functions, and parameters of the learning algorithm itself.
- Because of the many choices involved, performance monitoring on validation sets assumes an even more central role than it does with traditional machine learning methods.

Test sets

- *Should be set aside for a truly final evaluation*
- Repeated rounds of experiments using test set data give misleading (ex. optimistic) estimates of performance on fresh data
- For this reason, the research community has come to favor public challenges with hidden test-set labels, a development that has undoubtedly helped gauge progress in the field
- Controversy arises when participants submit multiple entries, and some favor a model where participants submit code to a competition server, so that the test data itself is hidden

Validation sets vs. cross-validation

- The use of a validation set is different from using *k*-fold cross-validation to evaluate a learning technique or to select hyperparameters.
- Cross-validation involves creating multiple training and testing partitions.
- Datasets for deep learning tend to be so massive that a single large test set adequately represents a model's performance, reducing the need for cross-validation
  - Since training often takes days or weeks, even using GPUs, cross-validation is often impractical anyway.
- If you do use cross validation you need to have an intern validation set *for each fold* to adjust hyperparameters or perform cross validation only using the training set

Validation set data and the 'end game'

- To obtain the best possible results, one needs to tune hyperparameters, usually with a single validation set extracted from the training set.
- However, there is a dilemma: omitting the validation set from final training can reduce performance in the test.
- It is advantageous to train on the combined training and validation data, but this risks overfitting.
- One solution is to stop training after the same number of epochs that led to the best validation set performance; another is to monitor the average loss over the combined training set and stop when it reaches the level it was at when early stopping was performed using the validation set.
- One can use cross validation within the training set, treating each fold as a different validation set, then train the final model on the entire training data with the identified hyperparameters to perform the final test

Hyperparameter tuning

- A weighted combination of L_2 and L_1 regularization is often used to regularize weights
- Hyperparameters in deep learning are often tuned heuristically by hand, or using grid search
- An alternative is random search, where instead of placing a regular grid over hyperparameter space, probability distributions are specified from which samples are taken
- Another approach is to use machine learning and Bayesian techniques to infer the next hyperparameter configuration to try in a sequence of experimental runs
- Keep in mind even things like the learning rate schedule (discussed below) are forms of hyperparameters and you need to be careful not to tune them on the test set

Training and evaluating deep networks

Part II

Parameter initialization

- Can be deceptively important!
- Bias terms are often initialized to 0 with no issues
- Weight matrices more problematic, ex.
  - If initialized to all 0s, can be shown that the tanh activation function will yield zero gradients
  - If the weights are all the same, hidden units will produce same gradients and behave the same as each other (wasting params)
- One solution: initialize all elements of weight matrix from uniform distribution over interval [–b, b]
- Different methods have been proposed for selecting the value of b, often motivated by the idea that units with more inputs should have smaller weights
- Weight matrices of rectified linear units have been successfully initialized using a zero-mean isotropic Gaussian distribution with standard deviation of 0.01

Unsupervised pre-training

- Idea: model the distribution of unlabeled data using a method that allows the parameters of the learned model to inform or be somehow transferred to the network
- Can be an effective way to both initialize and regularize a feedforward network
- Particularly useful when the volume of labeled data is small relative to the model's capacity.
- The use of activation functions such as rectified linear units (which improve gradient flow in deep networks), along with good parameter initialization techniques, can mitigate the need for sophisticated pre-training methods

Data augmentation

- Can be critical for best results
- As seen in MNIST table, augmenting even a large dataset with transformed data can increase performance
- A simple transformation is simply to jiggle the image
- If the object to be classified can be cropped out of a larger image, random bounding boxes can be placed around it, adding small translations in the vertical and horizontal directions
- Can also use rotations, scale changes, and shearing
- There is a hierarchy of rigid transformations that increase in complexity as parameters are added which can be used

Batch normalization

- A way of accelerating training for which many studies have found to be important to obtain state-of-the-art results
- Each element of a layer is normalized to zero mean and unit variance based on its statistics within a mini-batch
  - This can change the network's representational power
- Each activation has learned scaling and shifting parameter
- Mini-batch based SGD is modified by calculating the mean μ_j and variance σ_j^2 over the batch for each hidden unit h_j in each layer, then normalize the units, scale them using the learned scaling parameter γ_j and shift them by the learned shifting parameter β_j such that

$$\hat{h}_j \leftarrow \gamma_j \frac{h_j - \mu_j}{\sqrt{\sigma_j^2 + \varepsilon}} + \beta_j.$$

- To update the γ_j and β_j one needs to backpropagate the gradient of the loss through these additional parameters

Dropout

- A form of regularization that randomly deletes units and their connections during training
- Intention: reducing hidden unit co-adaptation & combat over-fitting
- Has been argued it corresponds to sampling from an exponential number of networks with shared parameters & missing connections
- One averages over models at test time by using original network without dropped-out connections, but with scaled-down weights
- If a unit is retained with probability *p* during training, its outgoing weights are rescaled or multiplied by a factor of *p* at test time
- By performing dropout a neural network with *n* units can be made to behave like an ensemble of 2^n smaller networks
- One way to implement it is with a binary mask vector $\mathbf{m}^{(l)}$ for each hidden layer *l* in the network: the dropped out version of $\mathbf{h}^{(l)}$ masks out units from the original version using element-wise multiplication, $\mathbf{h}_d^{(l)} = \mathbf{h}^{(l)} \odot \mathbf{m}^{(l)}$
- If the activation functions lead to diagonal gradient matrices, the backpropagation update is $\boldsymbol{\Delta}^{(l)} = \mathbf{d}^{(l)} \odot \mathbf{m}^{(l)} \odot (\mathbf{W}^{(l+1)} \boldsymbol{\Delta}^{(l+1)})$.

Bibliographic Notes & Further Reading

- Bergstra and Bengio (2012) give empirical and theoretical justification for the use of random search for hyperparameter settings.
- Snoek et al. (2012) propose the use of Bayesian learning methods to infer the next hyperparameter setting to explore, and their Spearmint software package performs Bayesian optimizations of both deep network hyperparameters and general machine learning algorithm hyperparameters.
- Stochastic gradient descent methods go back at least as far as Robbins and Monro (1951).

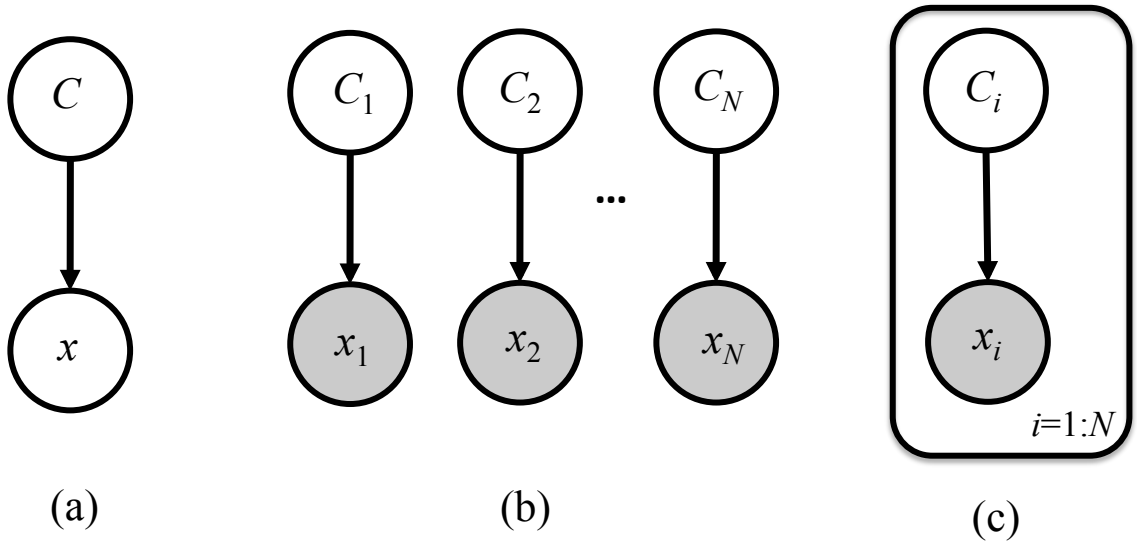
Bibliographic Notes & Further Reading

- Bottou (2012) is an excellent source of tips and tricks for learning with stochastic gradient descent, while Bengio (2012) gives further practical recommendations for training deep networks.
- Glorot and Bengio (2010) cover various weight matrix initialization heuristics, and how the concepts of fan-in and fan-out can be used to justify them for networks with different kinds of activation functions.
- The origins of dropout and more details about it can be found in Srivastava et al. (2014).
- Ioffe and Szegedy (2015) proposed batch normalization and give more details on its implementation.

Probability Models, Plate Notation and the Gaussian Mixture Model

Plate notation

- A “plate” is simply a box around a Bayesian network that denotes a certain number of replications of it, one for each data instance
- The plate below indicates i=1…N networks, each with an observed value for x_i and hidden variable C_i
- Plate notation captures a model for the joint probability of the entire data with a simple picture.



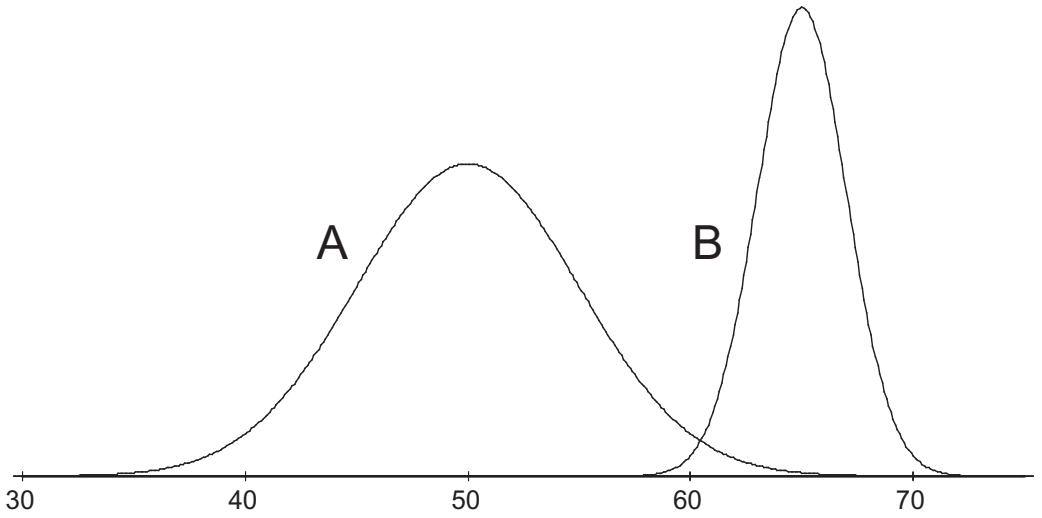
Clustering with a Gaussian Mixture

- Given the data on the left *without the labels A and B*, we wish to estimate a model for a two class Gaussian Mixture Model (GMM) on the right

Data

A 51	A 46	B 65
A 43	B 64	A 46
B 62	A 51	A 39
B 64	A 52	B 62
A 45	B 62	B 64
A 42	A 49	A 52
A 46	A 48	B 63
A 45	B 62	B 64
A 45	A 43	A 48
B 62	A 40	B 64
A 47	A 48	A 48
A 52	B 64	A 51
B 64	A 51	A 48
A 51	B 63	B 64
B 65	A 43	A 42
A 48	B 65	A 48
A 49	B 66	A 41

Model



μ_A=50, σ_A =5, p_A=0.6 μ_B=65, σ_B =2, p_B=0.4

Clustering and probability density estimation

- If we had data belonging to two known classes A and B, each having a normal distribution with means and standard deviations μ_A and σ_A for class A, and μ_B and σ_B for class B
- We could define a model whereby samples are taken from these distributions, using cluster A with probability p_A and cluster B with probability p_B (where $p_A + p_B = 1$),
- Sampling we might obtain the data in the next slide
- Now, imagine given the dataset without the classes—just the numbers—and being asked to determine the five parameters that characterize the model: μ_A, σ_A, μ_B, σ_B, and p_A (the parameter p_B can be calculated directly from p_A)

Estimating Gaussian parameters

- If we knew which of the two distributions each instance came from, finding the five parameters would be easy—just estimate the mean and standard deviation for $n=n_A$ or $n=n_B$ samples x_1, x_2, …, x_n for each cluster, A and B

$$\mu = \frac{x_1 + x_2 + \ldots + x_n}{n}$$

$$\sigma^2 = \frac{(x_1 - \mu)^2 + (x_2 - \mu)^2 + \ldots + (x_n - \mu)^2}{n - 1}$$

- To estimate the fifth parameter p_A, just take the proportion of the instances that are in the A cluster, then $p_B=1-p_A$.

Motivating the EM algorithm

- If you knew the five parameters, finding the (posterior) probabilities that a given instance comes from each distribution would be easy
- Given an instance x_i, the probability that it belongs to cluster A is

$$P(\mathrm{A}|x_i) = \frac{P(x_i \mid \mathrm{A}) \cdot P(\mathrm{A})}{P(x_i)} = \frac{N(x_i;\mu_\mathrm{A},\sigma_\mathrm{A})p_\mathrm{A}}{N(x_i;\mu_\mathrm{A},\sigma_\mathrm{A})p_\mathrm{A} + N(x_i;\mu_\mathrm{B},\sigma_\mathrm{B})p_\mathrm{B}}$$

where $N()$ is the normal or Gaussian distribution

$$N(x;\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

The EM algorithm for a GMM

- Start with a random (but reasonable) assignment to the parameters
- Compute the posterior distribution for the cluster assignments for each example
- Update the parameters based on the expected class assignments - where probabilities act like weights.
- If w_i is the probability that instance *i* belongs to cluster A, the mean and std. dev. are

$$\mu_A = \frac{w_1 x_1 + w_2 x_2 + \ldots + w_n x_n}{w_1 + w_2 + \ldots + w_n}$$

$$\sigma_A^2 = \frac{w_1 (x_1 - \mu)^2 + w_2 (x_2 - \mu)^2 + \ldots + w_n (x_n - \mu)^2}{w_1 + w_2 + \ldots + w_n}$$

The EM algorithm

- Optimizes the marginal likelihood, obtained by marginalizing over the two components of the Gaussian mixture
- The marginal likelihood is a measure of the "goodness" of the clustering and it increases at each iteration of the EM algorithm.
- In practice we use the log marginal likelihood

$$\log \prod_{i=1}^{n} P(x_i) = \sum_{i=1}^{n} \log \sum_{c_i} P(x_i \mid c_i) \cdot P(c_i)$$

$$= \sum_{i=1}^{n} \log \left[N(x_i; \mu_{\mathrm{A}}, \sigma_{\mathrm{A}}) p_{\mathrm{A}} + N(x_i; \mu_{\mathrm{B}}, \sigma_{\mathrm{B}}) p_{\mathrm{B}} \right]$$

Extending the mixture Model

- The Gaussian distribution generalizes to n-dimensions
- Consider a two-dimensional model consisting of independent Gaussian distributions for each dimension
- We can transform from scalar to matrix notation for a two dimensional Gaussian distribution as follows:

$$P(x_1, x_2) = \frac{1}{\sqrt{2\pi}\sigma_1}\exp\left[-\frac{(x_1-\mu_1)^2}{2\sigma_1^2}\right]\frac{1}{\sqrt{2\pi}\sigma_2}\exp\left[-\frac{(x_2-\mu_2)^2}{2\sigma_2^2}\right]$$

$$= (2\pi)^{-1}\left(\sigma_1^2\sigma_2^2\right)^{-1/2}\exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\begin{bmatrix}\sigma_1^2 & 0\\ 0 & \sigma_2^2\end{bmatrix}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

$$= (2\pi)^{-1}|\boldsymbol{\Sigma}|^{-1/2}\exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\},$$

- $\boldsymbol{\Sigma}$ is the covariance *matrix,* $|\boldsymbol{\Sigma}|$ is its determinant, the vector $\mathbf{x} = [x_1\ x_2]^T$, and the mean *vector* $\boldsymbol{\mu} = [\mu_1\ \mu_2]^T$

The multivariate Gaussian distribution

- Can be written in the following general form

$$P(x_1, x_2, \ldots, x_d) = (2\pi)^{-d/2} |\boldsymbol{\Sigma}|^{-1/2} \exp\left\{ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right\}.$$

- The equation for estimating the covariance matrix is

$$\boldsymbol{\Sigma} = \frac{1}{N} \sum_{i=1}^{N} (\mathbf{x}_i - \boldsymbol{\mu})(\mathbf{x}_i - \boldsymbol{\mu})^T.$$

- The mean is simply

$$\boldsymbol{\mu} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{x}_i.$$

Markov Random Fields

Undirected Graphical Models

Markov random fields (MRFs)

- A clique is a group of nodes in an undirected graph where all nodes are connected to one another
- MRFs define another factorized model for a set of random variables X, where clique sets are given by X_c and a factor $\Psi_c(X_c)$ is defined for each clique such that

$$P(X) = \frac{1}{Z}\prod_{c=1}^{C}\Psi_c(X_c),$$

- The partition function Z normalizes the result to form a probability distribution

$$Z = \sum_{x\in X}\prod_{c=1}^{C}\Psi_c(X_c).$$

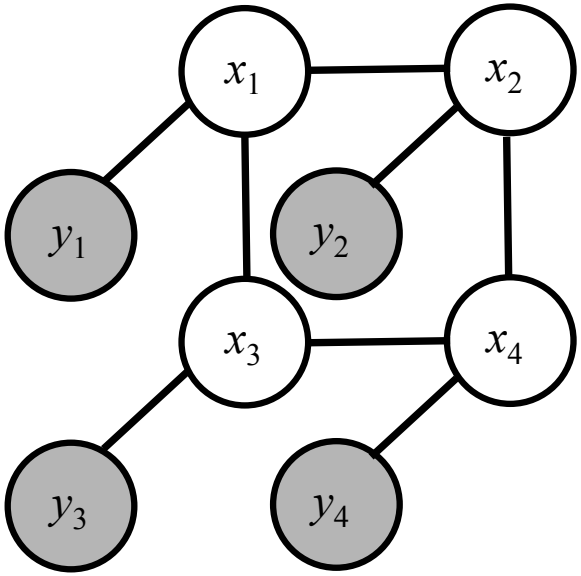
Markov random field example

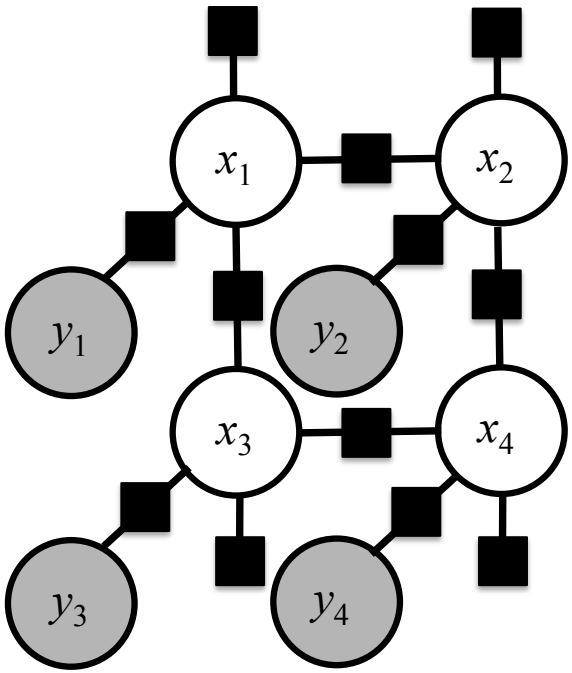
$$P(x_1, x_2, x_3, x_4) = \frac{1}{Z} \prod_{u=1}^{U} \phi_u(X_u) \prod_{v=1}^{V} \Psi_v(X_v)$$

$$= \frac{1}{Z} f_A(x_1) f_B(x_2) f_C(x_1) f_D(x_2) f_E(x_1, x_2) f_F(x_2, x_3) f_G(x_3, x_4) f_H(x_4, x_1)$$

- Note we used unary and pairwise potentials

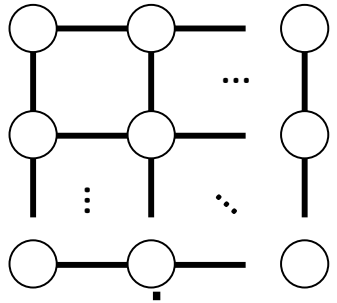
An MRF using a traditional MRF style undirected graph





An MRF as a factor graph

MRFs and energy functions



- An MRF lattice is often repeated over an imag
- MRFs can be expressed in terms of an energy function $F(X)$, where

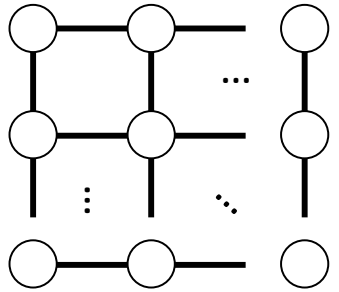
$$F(X) = \sum_{u=1}^{U} U(X_u) + \sum_{v=1}^{V} V(X_v), \qquad \text{and}$$

$$P(X) = \frac{1}{Z}\exp(-F(X)) = \frac{1}{Z}\exp\left(-\sum_{u=1}^{U} U(X_u) - \sum_{v=1}^{V} V(X_v)\right).$$

- Since Z is constant for any assignment of the variables X we have

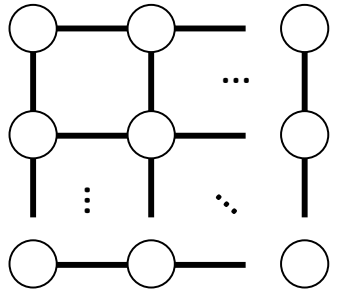
$$-\log P(x_1, x_2, x_3, x_4) \propto \sum_{u=1}^{U} U(X_u) + \sum_{v=1}^{V} V(X_v)$$

Minimizing MRF energies



- A commonly used strategy for tasks such as image segmentation and entity resolution in text documents is to minimizing an energy function of the form in the previous slide
- When such energy functions are “sub-modular”, an exact minimum can be found using algorithms based on graph-cuts; otherwise methods such as tree-reweighted message passing can be used.

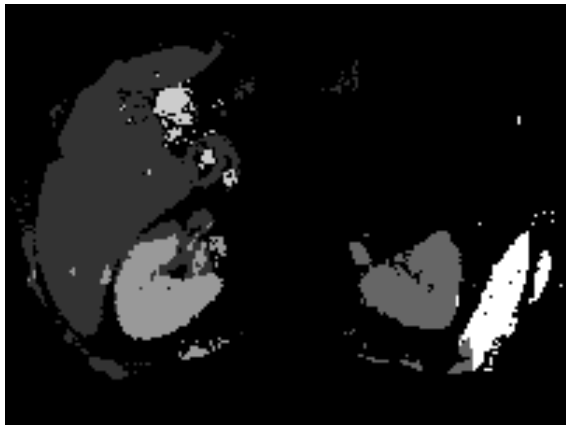
Example: Image Segmentation



- Given a labeled dataset of medical imagery, such as a computed tomography or CT image
- A well known approach is to learn a Markov Random Field model to segment that image into classes of interest, ex. anatomical structures or tumors
- Image features are combined with spatial context

Original Image

Ground truth



MRF segmentation

From Bhole et al.

Bibliographic Notes & Further Reading

Graphical Probabilty Models (GPMs) and Inference

- Plate notation has been widely used in artificial intelligence (Buntine, 1994), machine learning (Blei et al., 2003) and computational statistics (Lunn et al., 2000) to define complex probabilistic graphical models,
- GPMs form the basis of the BUGS (Bayesian inference Using Gibbs Sampling) software project (Lunn et al., 2000)
- Our presentation of factor graphs and the sum-product algorithm follows their origins in Kschischang et al. (2001) and Frey (1998)
- Bayesian networks and other models that contain cycles can be manipulated into a structure known as a *junction tree* by clustering variables, and Lauritzen and Spiegelhalter (1988)'s junction tree algorithm permits exact inference

Bibliographic Notes & Further Reading

Graphical Probabilty Models and Inference

- Ripley (1996) covers the junction tree algorithm, with practical examples
- Huang and Darwiche (1996)'s procedural guide is an excellent resource for those who need to implement the algorithm
- Probability propagation in a junction tree yields exact results, but is sometimes infeasible because the clusters become too large—in which case one must resort to sampling or variational methods

Classical Simple Statistical Models as Conditional Probability Models

Conditional continuous probability models

- Consider a model where the conditional probability for y_i given x_i is a Gaussian with mean given by a linear function of x:

$$p(y_i \mid x_i) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{\left\{ y_i - (\theta_0 + \theta_1 x_i) \right\}^2}{2\sigma^2} \right],$$

- The conditional distribution for N y_is given the corresponding x_is can be defined as

$$p(y_1, \ldots, y_N \mid x_1, \ldots, x_N) = \prod_{i=1}^{N} p(y_i \mid x_i).$$

Linear regression as a probability model

- The log-likelihood of our linear model is:

$$L_{y|x} = \log \prod_{i=1}^{N} p(y_i \mid x_i) = \sum_{i=1}^{N} \log p(y_i \mid x_i).$$

$$L_{y|x} = \sum_{i=1}^{N} \log \left\{ \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{\left\{ y_i - (\theta_0 + \theta_1 x_i) \right\}^2}{2\sigma^2} \right] \right\}$$

$$= -N \log\left[\sigma\sqrt{2\pi}\right] - \sum_{i=1}^{N} \frac{\left\{ y_i - (\theta_0 + \theta_1 x_i) \right\}^2}{2\sigma^2}.$$

- To maximize the log-likelihood it suffices to find the parameters that minimize the squared error

$$\arg\max_{\theta_0\,\theta_1}\left(L_{y|x}\right) = \arg\min_{\theta_0\,\theta_1}\left(\sum_{i=1}^{N}\left\{ y_i - (\theta_0 + \theta_1 x_i) \right\}^2\right).$$

  i.e. this probability model is simply linear

Priors on parameters, Gaussians, ridge regression and weight decay

- Placing a zero mean Gaussian prior on the parameters **w** leads to the method of *ridge regression,* also called *weight decay*
- Consider a linear regression that uses a *D* dimensional vector **x** to make predictions
- The regression's bias term can be represented by appending a constant feature = 1 as an additional final dimension of **x** for every example
- The prior is frequently omitted from the bias
- The underlying probability model can be written

$$\prod_{i=1}^{N} p(y_i \mid x_i;\theta)p(\theta;\tau) = \left[\prod_{i=1}^{N} N(y_i;\mathbf{w}^{\mathrm{T}}x_i,\sigma^2)\right]\left[\prod_{d=1}^{D} N(w_d;0,\tau^2)\right]$$

Priors on parameters, L_2 and L_1 regularization

- Maximum a posteriori parameter estimation based on the log conditional likelihood with a zero mean Gaussian prior on weights is equivalent to minimizing a squared error loss function plus an L_2 based regularization term

$$F(\mathbf{w}) = \sum_{i=1}^{N} \left\{ y_i - \mathbf{w}^{\mathrm{T}} x_i \right\}^2 + \lambda R_{L_2}(\mathbf{w}), \quad R_{L_2}(\mathbf{w}) = \mathbf{w}^{\mathrm{T}}\mathbf{w} = \left\| \mathbf{w} \right\|_2^2$$

- Using a Laplace prior for the distribution over weights and taking the log of the likelihood function yields an L_1 based regularization term

$$R_{L_1}(\mathbf{w}) = \left\| \mathbf{w} \right\|_1$$

Laplace, L_1 regularization the LASSO and the Elastic Net approach

- The Laplace distribution with params μ and b is

$$P(w;\mu,b) = L(w;\mu,b) = \frac{1}{2b}\exp\left(-\frac{|w-\mu|}{b}\right)$$

- Modeling the log of the prior probability for each weight by a Laplace distribution with $\mu=0$ yields

$$-\log\left[\prod_{d=1}^{D} L(w_d;0,b)\right] = \log(2b) + \frac{1}{b}\sum_{d=1}^{D}|w_d| \propto \|\mathbf{w}\|_1$$

- The use of L_1 regularization is also know as the LASSO, "Least Absolute Shrinkage and Selection Operator".
- An alternative (convex!) approach known as the *elastic net* combines L_1 and L_2 regularization techniques using

$$\lambda_1 R_{L_1}(\boldsymbol{\theta}) + \lambda_2 R_{L_2}(\boldsymbol{\theta}) = \lambda_1 \|\mathbf{w}\|_1 + \lambda_2 \|\mathbf{w}\|_2^2$$

Matrix vector form of regression

- Linear regression can be written in matrix form

$$\sum_{i=1}^{N}\{y_i-(\theta_0+\theta_1 x_i)\}^2=\left(\begin{bmatrix}y_1\\ \vdots\\ y_N\end{bmatrix}-\begin{bmatrix}1 & x_1\\ \vdots & \vdots\\ 1 & x_N\end{bmatrix}\begin{bmatrix}\theta_0\\ \theta_1\end{bmatrix}\right)^T\left(\begin{bmatrix}y_1\\ \vdots\\ y_N\end{bmatrix}-\begin{bmatrix}1 & x_1\\ \vdots & \vdots\\ 1 & x_N\end{bmatrix}\begin{bmatrix}\theta_0\\ \theta_1\end{bmatrix}\right)$$

$$=(\mathbf{y}-\mathbf{A}\mathbf{w})^T(\mathbf{y}-\mathbf{A}\mathbf{w}),$$

- Taking the partial derivative with respect to **w** and setting the result to zero yields a *closed form* expression for the parameters:

$$\frac{\partial}{\partial \mathbf{w}}(\mathbf{y}-\mathbf{A}\mathbf{w})^{\mathrm{T}}(\mathbf{y}-\mathbf{A}\mathbf{w})=0 \quad \Rightarrow \mathbf{A}^{\mathrm{T}}\mathbf{A}\mathbf{w}=\mathbf{A}^{\mathrm{T}}\mathbf{y}, \quad \mathbf{w}=(\mathbf{A}^{\mathrm{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathrm{T}}\mathbf{y}$$

$\mathbf{A}^{\mathrm{T}}\mathbf{A}\mathbf{w}=\mathbf{A}^{\mathrm{T}}\mathbf{y}$ are the famous "normal equations"

$\mathbf{A}^{+}=(\mathbf{A}^{\mathrm{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathrm{T}}$

Linear regression with regularization

- For ridge regression our objective function becomes

$$F(\mathbf{w}) = (\mathbf{y} - \mathbf{A}\mathbf{w})^T (\mathbf{y} - \mathbf{A}\mathbf{w}) + \lambda \mathbf{w}^{\mathrm{T}} \mathbf{w}$$

- We get a closed form solution for the result

$$\frac{\partial}{\partial \mathbf{w}} F(\mathbf{w}) = 0$$

$$\Rightarrow \mathbf{A}^{\mathrm{T}} \mathbf{A}\mathbf{w} + \lambda \mathbf{w} = \mathbf{A}^{\mathrm{T}} \mathbf{y}$$

$$\mathbf{w} = (\mathbf{A}^{\mathrm{T}} \mathbf{A} + \lambda \mathbf{I})^{-1} \mathbf{A}^{\mathrm{T}} \mathbf{y}$$

- This modification to the pseudoinverse equation is very useful, allowing solutions to be found when they would otherwise not exist, often using a very small λ
- The extension to multidimensional inputs **x** can still be formulated using these matrix forms

Polynomial regression and kernels

- We can create a model for non-linear predictions using polynomials of x
- The estimation problem remains linear!

$$\sum_{i=1}^{N}\left\{y_i - (\theta_0 + \theta_1 x_i + \theta_2 x_i^2 + \ldots + \theta_K x_i^K)\right\}^2$$

$$= \left(\begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} - \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^K \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & x_N & x_N^2 & & x_N^K \end{bmatrix} \begin{bmatrix} \theta_0 \\ \vdots \\ \theta_K \end{bmatrix}\right)^{\mathbf{T}} \left(\begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} - \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^K \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & x_N & x_N^2 & & x_N^K \end{bmatrix} \begin{bmatrix} \theta_0 \\ \vdots \\ \theta_K \end{bmatrix}\right)$$

$$= (\mathbf{y} - \mathbf{A}\mathbf{c})^T (\mathbf{y} - \mathbf{A}\mathbf{c}).$$

- A similar trick for transforming a linear model into a non-linear model is based on using basis functions $\boldsymbol{\phi}(\mathbf{x})$, where $p(y \mid \mathbf{x}) = N(y; \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}), \sigma^2)$

Generalized linear models

- Linear regression and logistic regression are special cases of a family of conditional probability models known in statistics as "generalized linear models" (GLMs)
- Idea: unify and generalize linear and logistic regression
- Data can be thought of in terms of response variables y_i and explanatory variables organized as vectors $\mathbf{x}_i$, i=1,…,n.
- Response variables could be expressed in different ways, ranging from binary to categorical or ordinal data
- A model is then defined where μ or the expected value of the distribution used for the response variable consists of an initial linear prediction which is then subjected to a smooth, invertible and potentially non-linear transformation using the *mean function* g^{-1}, i.e.

$$\mu_i = \mathrm{E}[y_i] = g^{-1}(\boldsymbol{\beta}^T \mathbf{x}_i)$$

- The mean function is the inverse of the *link function, g*

GLMs

- In GLMs the entire set of explanatory variables for all the observations is often arranged as a nxp matrix **X**, so that a vector of linear predictions for the entire data set is $\boldsymbol{\eta} = \mathbf{X}\boldsymbol{\beta}$
- The variance of the underlying distribution can also be modeled; typically as a function of the mean
- Different distributions, link functions and corresponding mean functions give a great deal of flexibility in defining probabilistic models, see examples below

Link Name	**Link Function** $\eta = \beta^T \mathbf{x} = g(\mu)$	**Mean Function** $\mu = g^{-1}(\beta^T \mathbf{x}) = g^{-1}(\eta)$	**Typical Distribution**
Identity	$\eta = \mu$	$\mu = \eta$	Gaussian
Inverse	$\eta = \mu^{-1}$	$\mu = \eta^{-1}$	Exponential
Log	$\eta = \log_e \mu$	$\mu = \exp(\eta)$	Poisson
Log-log	$\eta = -\log(-\log_e \mu)$	$\mu = \exp(-\exp(-\eta))$	Bernoulli
Logit	$\eta = \log_e \frac{\mu}{1-\mu}$	$\mu = \frac{1}{1+\exp(-\eta)}$	Bernoulli
Probit	$\eta = \Phi^{-1}(\mu)$	$\mu = \Phi(\eta)$	Bernoulli

Note: $\Phi(\cdot)$ *is the cumulative normal distribution.*

Predictions for ordered classes

- To define a model with *M* ordinal categories, *M*–1 *cumulative* probability models of the form $P(Y_i \leq j)$ can be used where the random variable Y_i represents the category of a given instance *i*
- Models for $P(Y_i = j)$ can then be obtained using differences between the cumulative distribution models
- Here we will use complementary cumulative probabilities, known as *survival functions,* of the form $P(Y_i > j) = 1 - P(Y_i \leq j)$
- They sometimes simplify the interpretation of parameters
- The class probabilities can be obtained from:

$$P(Y_i = 1) = 1 - P(Y_i > 1)$$

$$P(Y_i = j) = P(Y_i > j - 1) - P(Y_i > j)$$

$$P(Y_i = M) = P(Y_i > M - 1).$$

- For binary predictions the following model is popular

$$\text{logit}(\gamma_{ij}) = \log \frac{\gamma_{ij}}{1 - \gamma_{ij}} = b_j + \mathbf{w}^T \mathbf{x}_i$$

Conditional probability models based on kernels

- Linear models can be transformed into non-linear ones by applying the "kernel trick"
- Suppose the features **x** are replaced by the vector **k**(**x**) whose elements are determined using a kernel function $k(\mathbf{x},\mathbf{x}_j)$ for every training example:

$$\mathbf{k}(\mathbf{x}) = \begin{bmatrix} k(\mathbf{x},\mathbf{x}_1) \\ \vdots \\ k(\mathbf{x},\mathbf{x}_V) \\ 1 \end{bmatrix}$$

- A "1" has been appended to this vector to implement the bias term in the parameter matrix
- Kernelized regression

$$p(y \mid \mathbf{x}) = N(y; \mathbf{w}^{\mathrm{T}}\mathbf{k}(\mathbf{x}), \sigma^2)$$

- Kernelized classification

$$p(\mathbf{y} \mid \mathbf{x}) = \frac{\exp\left(\mathbf{y}^T \boldsymbol{\theta}\mathbf{k}(\mathbf{x})\right)}{\sum_{\mathbf{y}} \exp\left(\mathbf{y}^T \boldsymbol{\theta}\mathbf{k}(\mathbf{x})\right)}$$

Training and evaluating deep networks

Bibliographic Notes & Further Reading

Logistic Regression, GLMs and Regularized Regression

- Logistic regression is sometimes referred to as the workhorse of applied statistics; Hosmer and Lemeshow (2004) is a great reference
- Nelder and Wedderburn (1972)'s work led to the generalized linear modeling framework
- McCullagh (1980)'s developed proportional odds models for ordinal regression, which are sometimes called ordered logit models because they use the generalized logit function
- Frank and Hall (2001) showed how to adapt arbitrary machine learning techniques to ordered predictions
- McCullagh and Nelder (1989)'s widely cited monograph is another good source for details on the framework of GLMs
- Tibshirani (1996) developed the famous "Least Absolute Shrinkage and Selection Operator," also known as the LASSO
- Zou and Hastie (2005) developed the "elastic net" regularization approach which combines L_1 and L_2 regularization

Bibliographic Notes & Further Reading

Kernel Logistic Regression, and Various Vector Machines

- Kernel logistic regression transforms a linear classifier into a non-linear one, and probabilistic sparse kernel techniques are attractive alternatives to support vector machines
- Tipping (2001) proposed a "relevance vector machine" that manipulates priors on parameters in a way that encourages kernel weights to become zero during learning
- Lawrence, Seeger, and Herbrich (2003) proposed an "informative vector machine," which treats the problem as a fast, sparse Gaussian process method in the sense of Williams and Rasmussen (2006)
- Zhu and Hastie (2005) formulated sparse kernel logistic regression as an "import vector machine" that uses greedy search methods
- None of these methods approach the popularity of Cortes and Vapnik (1995)'s support vector machines, perhaps because their objective functions are not convex, in contrast to the underlying SVM (and L2 regularized kernel logistic regression)
- When probabilities are needed from an SVM, Platt (1999) shows how to fit a logistic regression to the classification scores.