Intro to Deep Learning

Big Data y Machine Learning para Economía Aplicada

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Deep Learning: Intro

- Linear Models may miss the nonlinearities that best approximate $f^*(x)$
- Neural networks are simple models.
- The model has **linear combinations** of inputs that are passed through **nonlinear activation functions** called nodes (or, in reference to the human brain, neurons).

Agenda

1. Recap: SNN
   - Example: XOR
   - Activation Functions
   - Output Functions
2. Training the network
3. Architecture Design
   - Deep Neural Networks
4. When to Use Deep Learning?

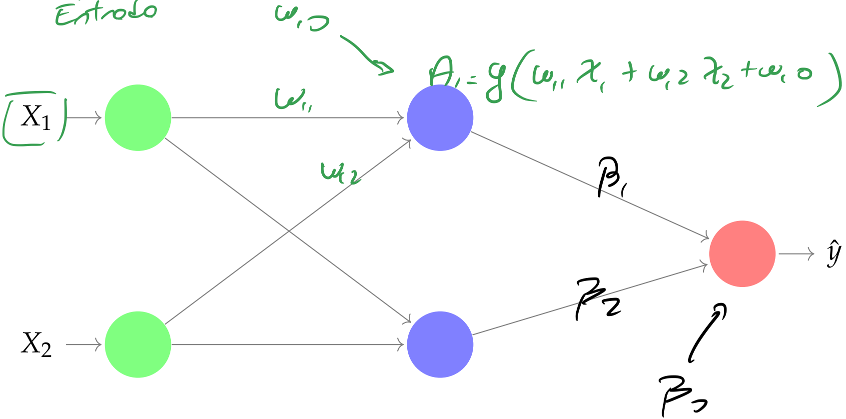
Single Layer Neural Networks

2 Inputs, variables

Capa de Entrada

Capa Oculta

Capa de Salida



Single Layer Neural Networks

- NN are made of **linear combinations** of inputs that are passed through **nonlinear activation functions**

Hiper parámetros

→ # Nodos o Neuronas

→ # g Funcion de Activacion

→ # f capa de salida

- The NN model has the form

$$f(X) = f\left[\beta_0 + \sum_{k=1}^{\boxed{K}} \beta_k A_k\right] \tag{1}$$

$$= f\left[\beta_0 + \sum_{k=1}^{K} \beta_k g\left(w_{k0} + \sum_{j=1}^{p} w_{kj} X_j\right)\right] \tag{2}$$

- where
  - $g(.)$ is a activiation function, the nonlinearity of $g(.)$ is **key**
  - f is the output layer of the network
- both are prespecified

H.w. $g(z) = z$

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Worked Example: The "Exclusive OR (XOR)" Function

- The exclusive disjunction of a pair of propositions, (p, q), is supposed to mean that p is true or q is true, but not both
- It's truth table is:

q	p	q ⊻ p
0	0	0
0	1	1
1	0	1
1	1	0

- When exactly one of these binary values is equal to 1, the XOR function returns 1. Otherwise, it returns 0

Worked Example: The "Exclusive OR (XOR)" Function

- Let's use a linear model

$$y = \overbrace{\beta_0 + \beta_1 q + \beta_2 p}^{f(q,p)} + u \tag{3}$$

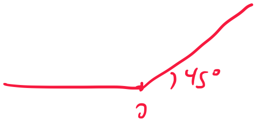
$$X = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{pmatrix} \qquad y = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} \qquad \frac{1}{N} \sum (y - X\beta)^2$$

$$\beta_0 = \frac{1}{2} \qquad \hat{y} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \qquad MSE = 1$$

$$\beta_1 = \beta_2 = 0$$

Worked Example: The "Exclusive OR (XOR)" Function

- Let's use Single Layer NN containing two hidden units
- Activation Funcition: ReLU: $g(z) = max\{0, z\}$
- NN



$$f(X) = \beta_0 + \sum_{k=1}^{2} \beta_k g\left(w_{k0} + \sum_{j=1}^{2} w_{kj} X_j\right) \tag{4}$$

Worked Example: The "Exclusive OR (XOR)" Function

- Suppose this is the solution to the XOR problem

$$f(x) = \underline{max}\{0, XW + W_0\}\,\beta + \beta_0$$

$$W = \begin{array}{c} \begin{array}{cc} w_{11} & 12 \end{array} \\ \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \\ \begin{array}{cc} w_{21} & w_{22} \end{array} \end{array}$$

$$W_0 = \iota_4 \begin{array}{c} \begin{pmatrix} 0 & -1 \end{pmatrix} \\ \begin{array}{cc} w_{01} & w_{02} \end{array} \end{array}$$

$$\beta = \begin{array}{c} \begin{pmatrix} 1 & -2 \end{pmatrix} \\ \begin{array}{cc} \beta_1 & \beta_2 \end{array} \end{array}$$

$$\beta_0 = 0$$

Worked Example: The "Exclusive OR (XOR)" Function

Lets work out the example step by step

$$\begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ -2 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$$

$$\boxed{MSE = 0}$$

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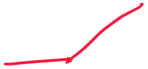
Neural Networks: Activation Functions

HW: como es la derivada de la logística.

- Sigmoid$(x) = \frac{1}{1+\exp(-x)}$ Logística $\mathbb{R} \to [0,1]$

- ReLU$(x) = \max\{x, 0\}$ $\mathbb{R} \to [0, \infty)$



- Among others (see more here)

- Hidden unit design remains an active area of research, and many useful hidden unit types remain to be discovered

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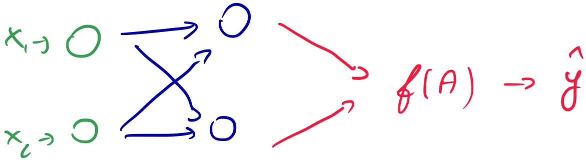
Output Functions



- The choice of output unit is related to the problem at hand

$$\underbrace{z = \beta_0 + \sum_{k=1}^{K} \beta_k A_k}_{\mathbb{R} \;\to\; [0,1]\,?} \qquad \frac{1}{1+e^{-z}} = [0,1]$$

  - Regression
  - Classification
    - Binary → logistic
    - Multiclass → logistica multinomial (softmax)

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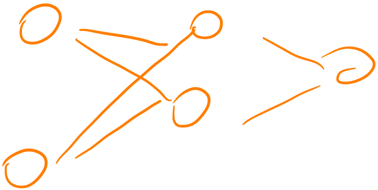
- # Nodos (Final)
- Activation ✓
- Salida ✓

$\boxed{W}$ / $\boxed{B.}$ ✓



Training the network

- El objetivo es

MSE

$$\hat{f} = \underset{f}{\operatorname{argmin}} \left\{ \sum_{i=1}^{n} L(y, f(X; \Theta)) \right\} \tag{5}$$

$\to w, \beta.$

- SNN

$$f(X, \beta, w) = f\left[\beta_0 + \sum_{k=1}^{K} \beta_k g\left(w_{k0} + \sum_{j=1}^{p} w_{kj} X_j\right)\right] \tag{6}$$

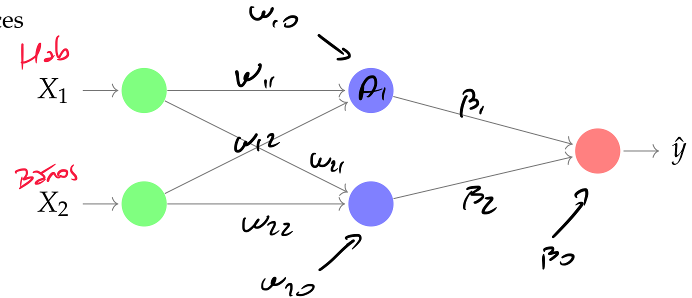
$\beta_0, \beta_1, \beta_2$

w_k

Training the network

2 Nodos ; sigmoidea o logística

Example: House Prices



- Equations
  - Hidden Layer sigmoid (logistic):
    - $A_1 = g(w_{11} \cdot X_1 + w_{12} \cdot X_2 + w_{10})$ 3 param
    - $A_2 = g(w_{21} \cdot X_1 + w_{22} \cdot X_2 + w_{20})$ 3 param.
  - Output Layer, identity output function:
    - $\hat{y}_i = \beta_0 + \beta_1 \cdot A_1 + \beta_2 \cdot A_2$ → 3 param

9 parametros

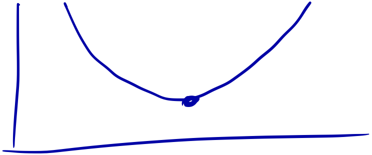
- Loss Function ⇒ MSE: $\frac{1}{n} \sum_i^n (y_i - \hat{y}_i)^2$

Training the network

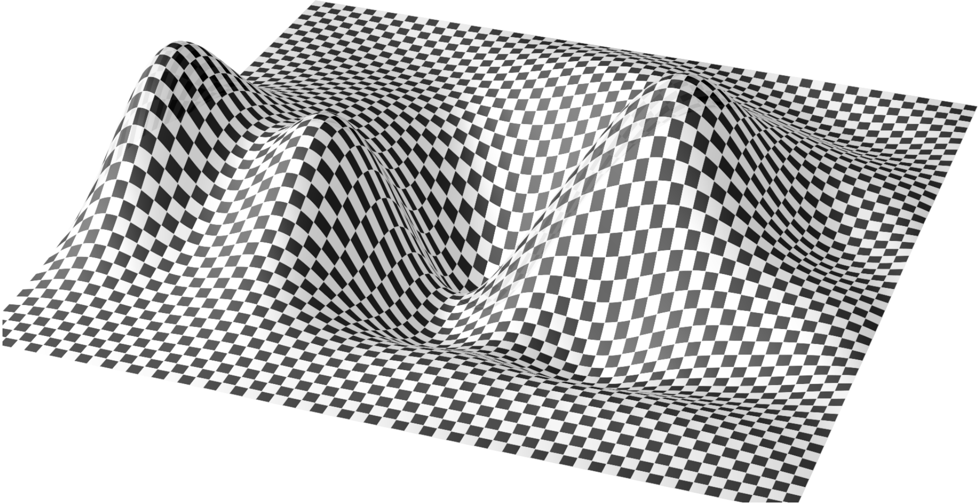
- El objetivo es

$$\hat{f} = \underset{w,\beta}{\operatorname{argmin}} \left\{ \sum_{i=1}^{n} L\left(y, f\left[\beta_0 + \sum_{k=1}^{K} \beta_k g\left(w_{k0} + \sum_{j=1}^{p} w_{kj} X_j\right)\right]\right) \right\} \tag{7}$$

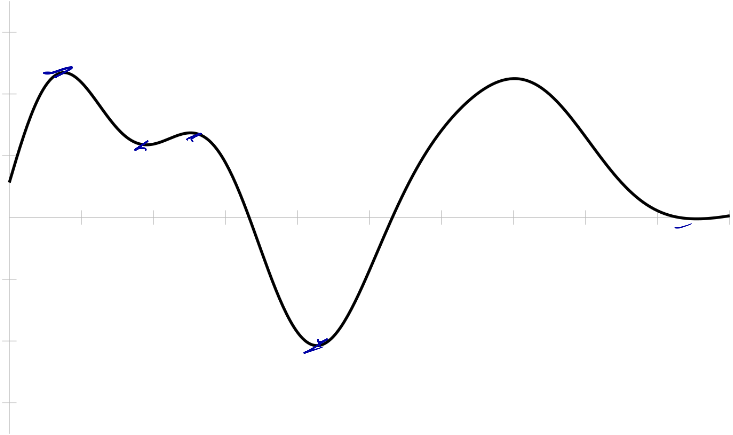
$$w, \beta \Rightarrow \frac{1}{N} \sum_{i=1}^{n} \left(y - \beta_0 - \sum_{k=1}^{2} \beta_k g \left(w_{k0} + \sum_{j=}^{2} w_{kj} x \right) \right)^2$$



Training the network



Training the network

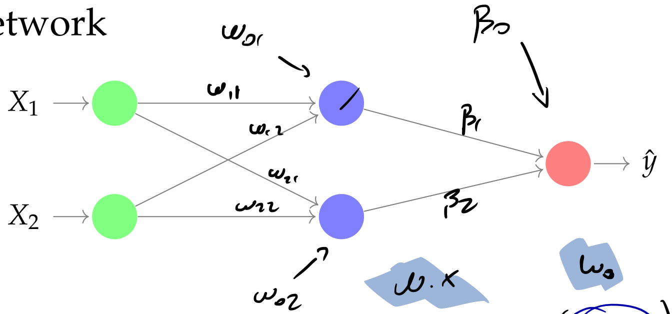


Training the network

Example: House Prices

Training the network

9 parametros

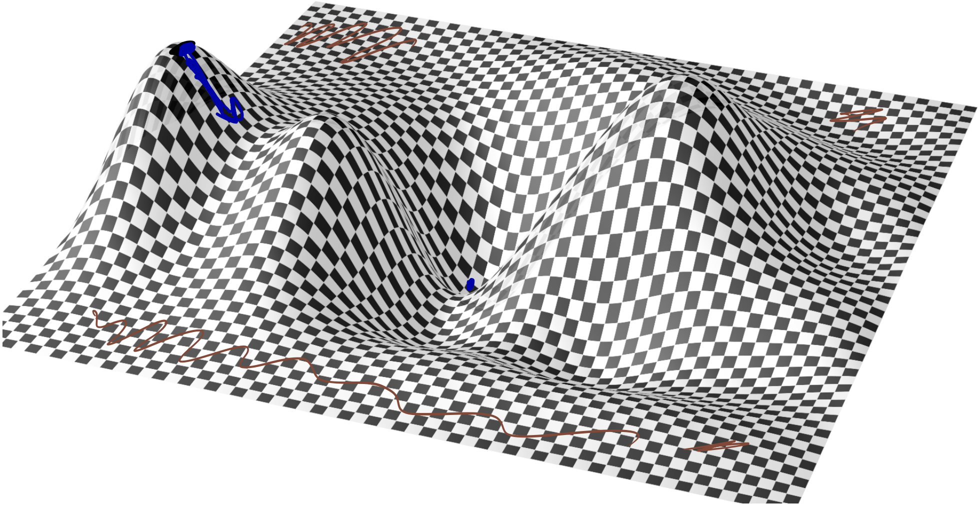


$$w = \begin{pmatrix} 2{,}17 & 2{,}57 \\ \cancel{2{,}84} & 4{,}34 \end{pmatrix} \begin{pmatrix} 1 \\ 3 \end{pmatrix} = \underbrace{\begin{pmatrix} 9{,}98 \\ 15{,}88 \end{pmatrix}}_{w.X} + \underbrace{\begin{pmatrix} 1{,}87 \\ 2{,}09 \end{pmatrix}}_{w_0} = \begin{pmatrix} 11{,}85 \\ 11{,}97 \end{pmatrix}$$

$X \to$ primera obs

$$sig\left(w.X + w_0\right) = \begin{pmatrix} 0{,}98 \\ 0{,}99 \end{pmatrix} \cdot \begin{pmatrix} 28{,}33 \\ 60{,}17 \end{pmatrix} + 59 = 142.905 \quad 215$$

Training the network



Training the network

Backpropagation

$$\theta' = \theta - \epsilon \cdot \nabla_\theta \mathcal{L}(\theta)$$

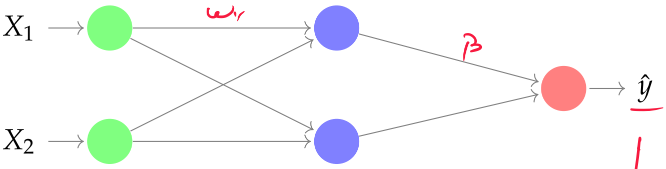
Funcion de Perdida

depende de capas

Training the network

Forward pass

Example: House Prices



Back prop.

- Equations
  - Hidden Layer sigmoid (logistic):
    - $A_1 = \sigma(w_{11} \cdot X_1 + w_{12} \cdot X_2 + w_{10})$
    - $A_2 = \sigma(w_{21} \cdot X_1 + w_{22} \cdot X_2 + w_{20})$
  - Output Layer, identity output function:
    - $\hat{y}_i = \beta_0 + \beta_1 \cdot A_1 + \beta_2 \cdot A_2$
- Loss Function $\Rightarrow$ MSE: $\frac{1}{n} \sum_i^n (y_i - \hat{y}_i)^2$ $= d$

How does backpropagation work?

Updating a single weight

- For simplicity let's focus on updating w_{11}

$$w_{11}' = w_{11} - \varepsilon \underbrace{\frac{\partial \mathcal{L}}{\partial w_{11}}}$$

$$\frac{\partial A_1}{\partial w_{11}} = \sigma'(\cdot)\, x_1$$

$$= \sigma(\cdot) \cdot [1-\sigma(\cdot)] \cdot x_1$$

$$\underbrace{\frac{\partial \mathcal{L}}{\partial w_{11}}} = \frac{\partial \mathcal{L}}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial A_1} \cdot \frac{\partial A_1}{\partial w_{11}} \cdot \frac{\partial}{\partial}$$

$$\frac{\partial \hat{y}}{\cancel{\partial A_1}} = \hat{\beta}_1$$

H.W. derivada de la relu?

$$(y-\hat{y})^2 \rightarrow \frac{\partial \mathcal{L}}{\partial \hat{y}} = 2(y-\hat{y}) \cdot (-1)$$

215 - 147

Training the network

Updating a weight in the output layer

- Now let's update one of the weights from the hidden layer to the output layer, β_1

$$\beta_1' = \beta_1 - \varepsilon \frac{\partial \mathcal{L}}{\partial \beta_1}$$

$$\frac{\partial \mathcal{L}}{\partial \beta_1} = \frac{\partial \mathcal{L}}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \beta_1} = -2(y-\hat{y}) A_1$$

- Notice that this formula involves calculations over the full data set, at each Gradient Descent step!
- This is why the algorithm is called Batch Gradient Descent: it uses the whole batch of training data at every step.
- As a result it is terribly slow on very large data sets.

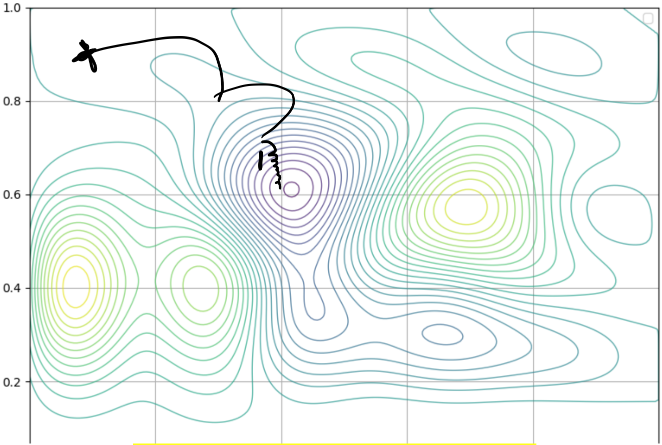
Training the network

Stochastic Gradient-Based Optimization

- Stochastic Gradient Descent just picks a random observation at every step and computes the gradients based only on that single observation.

$\underline{\mathcal{E}}$

Gradiente



Training the network

Mini-batch Gradient Descent

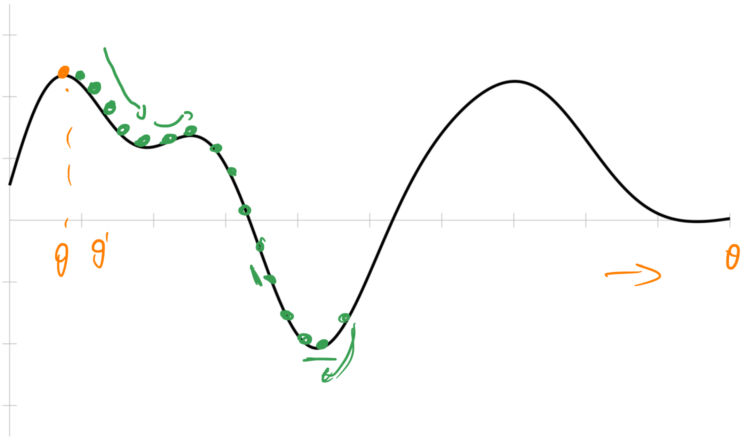
- Batch Gradient Descent involves calculations over the full data set
- Stochastic Gradient Descent just picks one random observation at every step
- At each step, mini- batch GD computes the gradients on small random sets of observations called mini- batches.

Training the network

$$\theta' = \theta - \varepsilon \nabla_\theta \mathcal{L}(\theta)$$

(-) (-)

sgd (mini batch)



Training the network

SGD + Momentum, Polyak, 1964

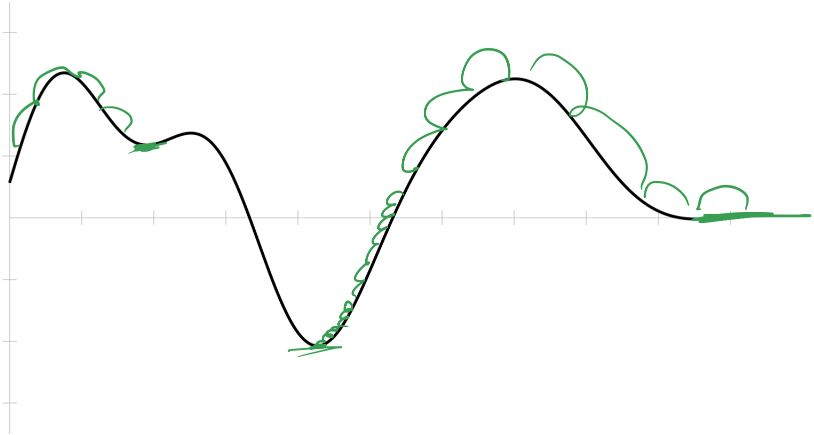
0,9

$$v' = \gamma v - \epsilon \cdot \nabla_\theta \mathcal{L}(\theta)$$

$$\theta' = \theta + v'$$

- Agrega una "inercia" al gradiente.
- Permite acumular dirección $\rightarrow$ suaviza la trayectoria.
- Ayuda a escapar de mínimos poco profundos.

Training the network



Training the network

RMSProp, Tieleman and Hinton, 2012

$$\frac{\epsilon}{[\ \ ]}\uparrow\downarrow \quad \downarrow \quad \uparrow$$

$$E[\nabla_\theta \mathcal{L}(\theta)^2] = \overset{0,9}{\rho} E[\nabla_\theta \mathcal{L}(\theta)^2]_{iter-1} + (1-\rho)\nabla_\theta \mathcal{L}(\theta)^2$$

$$\theta' = \theta - \frac{\epsilon}{\underbrace{\sqrt{E[\nabla_\theta \mathcal{L}(\theta)^2] + \eta}}_{\downarrow\ 0}} \cdot \nabla_\theta \mathcal{L}(\theta)_t$$

η ↪ constante

Training the network

Adam, Kingma and Ba, 2014

0,99 0,9

$$m = \beta_1 m_{iter-1} + (1-\beta_1)\nabla_\theta \mathcal{L}(\theta)$$

$$v = \beta_2 v_{iter-1} + (1-\beta_2)\nabla_\theta \mathcal{L}(\theta)^2$$

$$\hat{m} = \frac{m}{1-\beta_1^{iter}}, \quad \hat{v} = \frac{v}{1-\beta_2^{iter}}$$

$$\boxed{\theta' = \theta - \epsilon \cdot \frac{\hat{m}}{\sqrt{\hat{v}} + \eta}}$$

10^{-8}

- Combina Momentum + RMSProp.
- Corrige sesgo en los primeros pasos.
- Muy popular por su robustez y rapidez.

Training the network

Which one to use? Zhou et al., 2020

- Aunque Adam converge más rápido, SGD suele encontrar soluciones que generalizan mejor.
- Zhou et al., 2020 modela ambos métodos
- SGD: Puede
  - Escapar más fácilmente de mínimos locales.
  - Alcanzar soluciones que generalizan mejor.
- Adam: quedar atrapado en mínimos subóptimos.

Conclusión: El ruido inherente al SGD actúa como una forma de regularización que favorece la generalización.

Training the network

Example: MNIST

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Architecture Design

- A key design consideration for neural networks is determining the architecture.
- The word architecture refers to the overall structure of the network: how many units it should have and how these units should be connected to each other.
- The universal approximation theorem (Hornik et al., 1989; Cybenko, 1989) guarantees that regardless of what function we are trying to learn, a sufficiently large MLP will be able to represent this function.

Architecture Design

- A key design consideration for neural networks is determining the architecture.
- The word architecture refers to the overall structure of the network: how many units it should have and how these units should be connected to each other.
- The universal approximation theorem (Hornik et al., 1989; Cybenko, 1989) guarantees that regardless of what function we are trying to learn, a sufficiently large MLP will be able to represent this function.
- However, learning can fail for two different reasons.
  1. The optimization algorithm used for training may not be able to find the value of the parameters that corresponds to the desired function.
  2. The training algorithm might choose the wrong function as a result of overfitting

Architecture Design

- Using deeper models can reduce the number of units required to represent the desired function and can reduce the amount of generalization error.
- The ideal network architecture for a task must be found via experimentation guided by monitoring the validation set error

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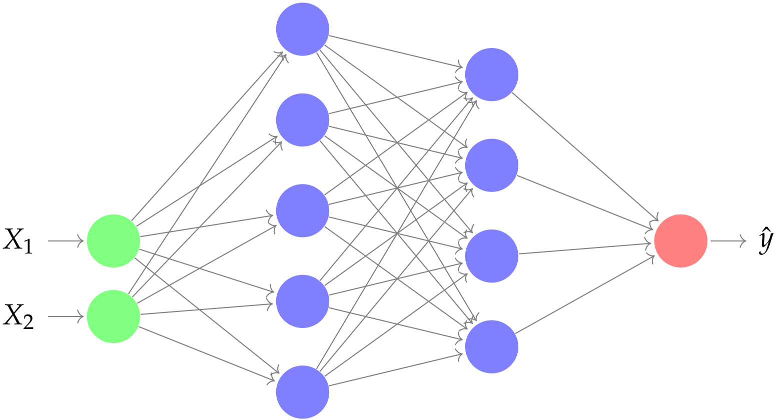
Architecture Design

Multilayer Neural Networks

- Modern neural networks typically have more than one hidden layer, and often many units per layer.
- In theory a single hidden layer with a large number of units has the ability to approximate most functions.
- However, the learning task of discovering a good solution is made much easier with multiple layers each of modest size.

Architecture Design

Multilayer Neural Networks



Architecture Design

Network Tuning

- Training networks requires a number of choices that all have an effect on the performance:
  - The number of hidden layers,
  - The number of units per layer
  - Details of stochastic gradient descent. → SGD, → RMSProp, → Adam } Hiperparametros (tweek)
  - Regularization of parameters → Dropout rate, → L1 → λ, → L2 → λ

→ Funcion de Activacion

- This is an active research area that involves a lot of trial and error, and overfitting is a latent danger at each step.

Training the network

Example: MNIST

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When to Use Deep Learning?

- The performance of deep learning ussually is very impressive.
- The question that then begs an answer is: should we discard all our older tools, and use deep learning on every problem with data?

When to Use Deep Learning?