Artificial Intelligence II: Deep learning methods

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Lecture 3: Deep Neural Networks

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Overview

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Intro

Radial Basis Function Nets

Consider pairs $(x, y) \in \mathbb{R}^d$.

- 1-layer architecture, which learns means and variances $\forall i \in [0 \dots N-1] \quad (\mu_i, \sigma_i)$ as "weights".

$$\phi(x) = \begin{pmatrix} 1 \\ \exp \frac{-||x-\mu_0||^2}{2\sigma_0^2} \\ \vdots \\ \exp \frac{-||x-\mu_{N-1}||^2}{2\sigma_{N-1}^2} \end{pmatrix}$$

- we model $y = g(w^\top \phi(x))$, where g is called the transfer function
- can be used to solve different problems like: *regression*, *binary classification* and *multi-classification*.

Learning mechanism

- Place the centers and variances randomly and uniformly, by vector quantization (K-means++, GNG, etc.)

2-steps learning

1. fit the centers (μ_i) and variances (σ_i).
2. fit the weights w.

3-steps learning

1. fit the centers (μ_i) and variances (σ_i).
2. fit the weights w.
3. fit everything $(\nabla_\mu \mathcal{L}, \nabla_\sigma \mathcal{L}, \nabla_w \mathcal{L})$, where $\mathcal{L}$ is the cost function.

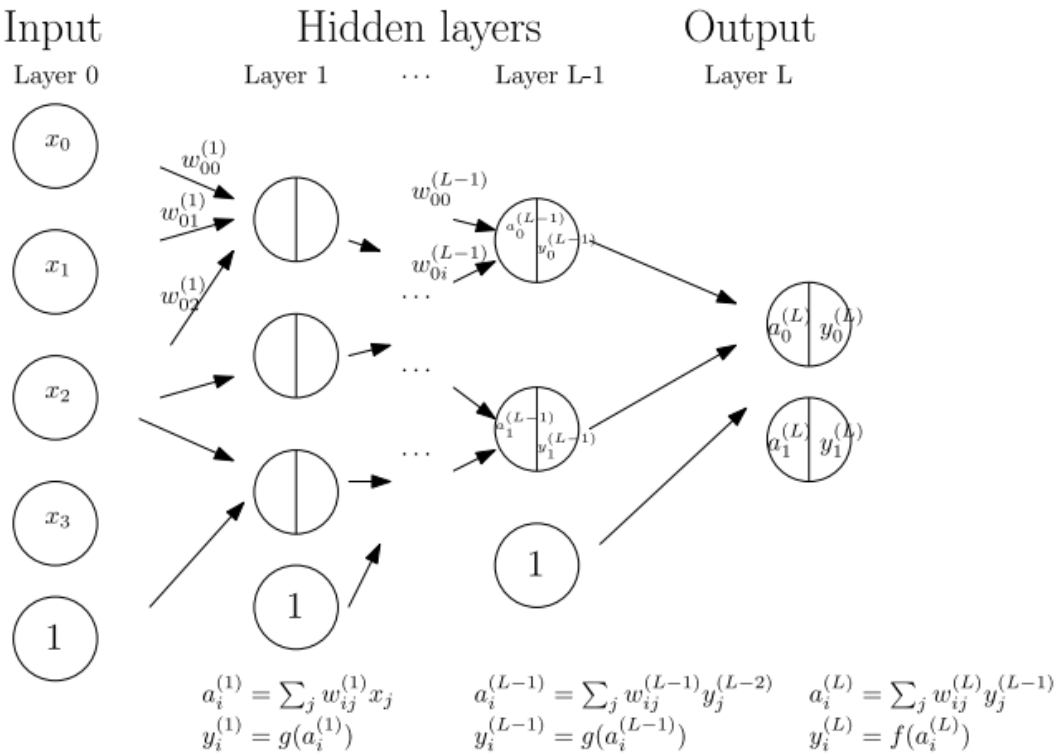
Universal approximator theorem

RBFN are **universal approximators**. Denote $\mathcal{S}$ the family of functions based on RBF in $\mathbb{R}^d$:

$$\mathcal{S} = \{\zeta : \mathbb{R}^d \to \mathbb{R}, \zeta(x) = \sum_i \Theta\left(\frac{x - \mu_i}{\sigma_i}\right), w \in \mathbb{R}^N\},$$

with $\Theta : \mathbb{R}^d \to \mathbb{R}$ continuous (almost everywhere) and $\int_{\mathbb{R}^d} \Omega(x)dx \neq 0$. Then $\mathcal{S}$ is dense in $\ell_p(\mathbb{R})$ for every $p \in [1, \infty)$.

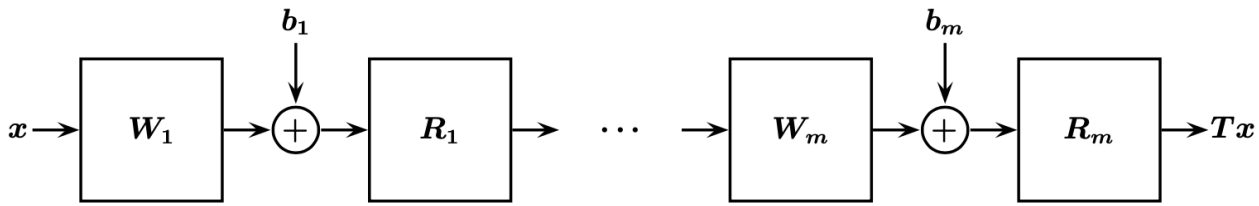
Feedforward Neural Network Architecture



Notations

- **Width** : number of neurons per layer
- **Depth** : number of weight layer
- **Parameters** : weight matrices and bias vector associated with every layer
- **Activation** : a hidden (non-linear) transfer function, denoted with f for layers $l \in \{1 \dots L-1\}$ and g for the last layer L.

Feed-forwars neural networks



An m layers FCN network (T) can be viewed as a composition of elementary functions modelling layers:

$$T = T_m \circ \cdots \circ T_1.$$

$$(\forall i \in \{1, \ldots, m\}) \qquad T_i(x_i) = R_i(W_i^\top x_i + b_i)$$

$x_i \in \mathbb{R}^{N_{i-1}}$ – input of the layer

$W_i \in \mathbb{R}^{N_i \times N_{i-1}}$ – weight matrix,

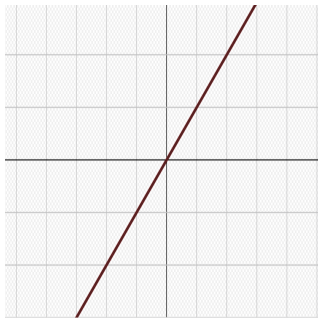
$b_i \in \mathbb{R}^{N_i}$ – bias parameter,

$R_i \colon \mathbb{R}^{N_i} \to \mathbb{R}^{N_i}$ – activation operator.

Dense Neural networks

Classic Activation Operators

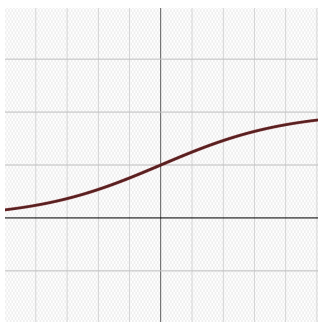
- Identity: $\rho : \mathbb{R} \to \mathbb{R} \quad \rho(x) = x$



- Binary step:

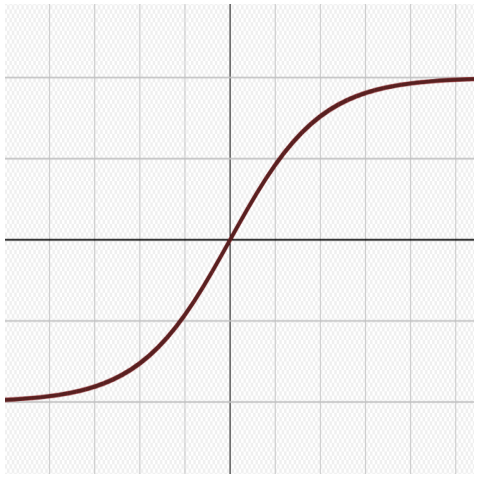
$$\rho : \mathbb{R} \to \{0, 1\} \quad \rho(x) = \begin{cases} 0, & \text{if} \quad x < 0 \\ 1, & \text{if} \quad x \geq 0 \end{cases}$$

- Sigmoid: $\rho : \mathbb{R} \to (0, 1) \quad \rho(x) = \frac{1}{1+e^{-x}}$

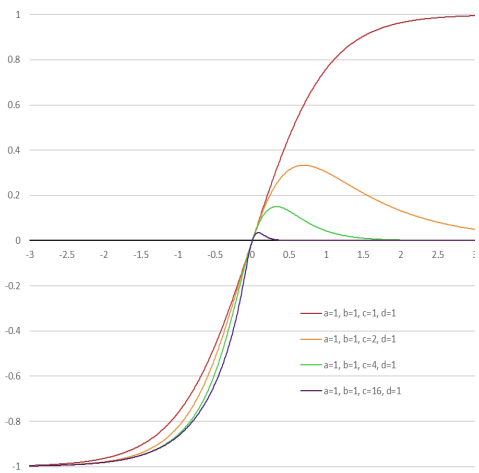


Classic Activation Operators

- Hyperbolic tangent:
  $\rho : \mathbb{R} \to (-1, 1) \quad \rho(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$



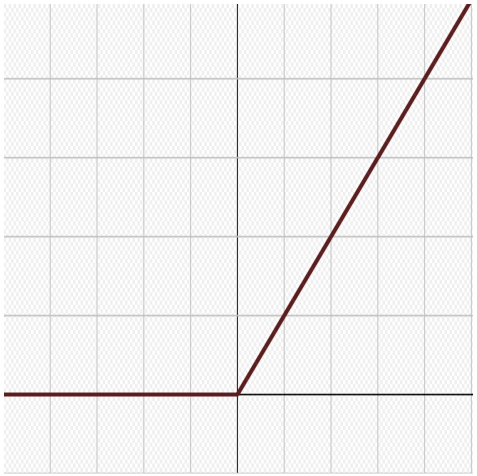
- Soboleva modified hyperbolic tangent:
  $\rho : \mathbb{R} \to (-1, 1) \quad \rho(x) = \frac{e^{ax} - e^{-bx}}{e^{cx} + e^{-dx}}$
  $a, b, c, d \in \mathbb{R}$



Saturating function usually suffer from **vanishing gradient** problem (more on that later).

Modern Activation Operators

- Rectified Linear Unit (ReLU):
  $\rho : \mathbb{R} \to [0, \infty) \quad \rho(x) = \max(0, x)$

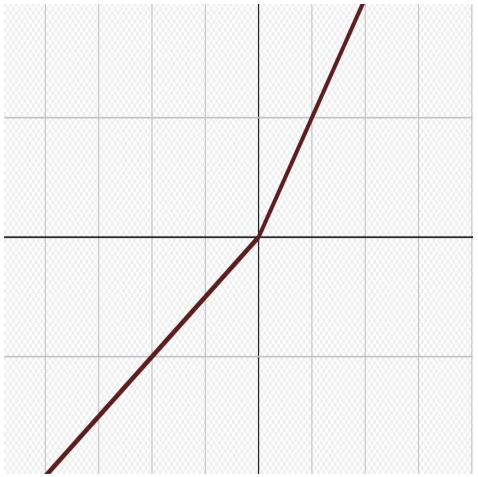


More favorable for the gradient flow, but may suffer from dying ReLU problem.

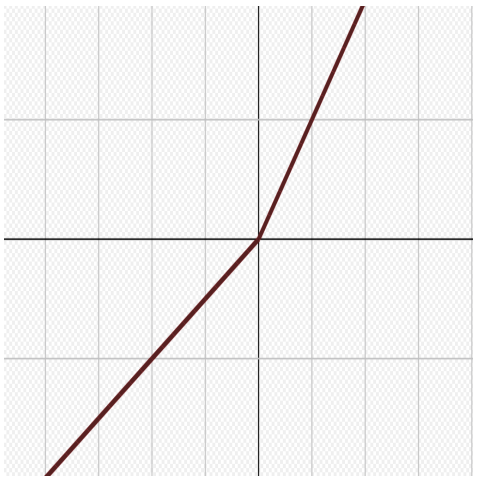
Other variants have been proposed to mitigate this problem, see next slide.

ReLU variants

- Leaky Rectified Linear Unit:
  $\rho : \mathbb{R} \to \mathbb{R}$
  $$\rho(x) = \begin{cases} 0.01x & \text{if} \quad x \leq 0 \\ x & \text{if} \quad x > 0 \end{cases}$$

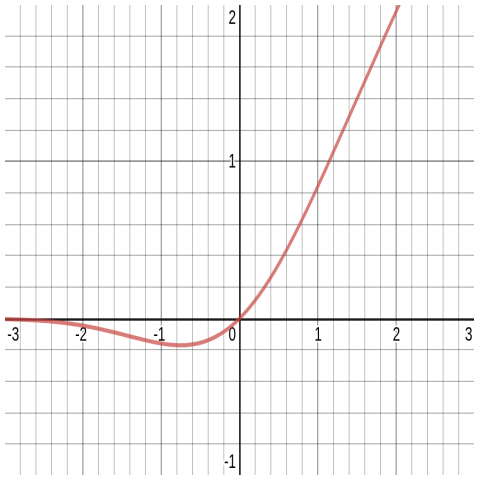


- Parametric Rectified Linear Unit:
  $\rho : \mathbb{R} \to \mathbb{R}$
  $$\rho(x) = \begin{cases} \alpha x & \text{if} \quad x \leq 0 \\ x & \text{if} \quad x > 0, \end{cases}$$
  with $\alpha \in \mathbb{R}^+$.

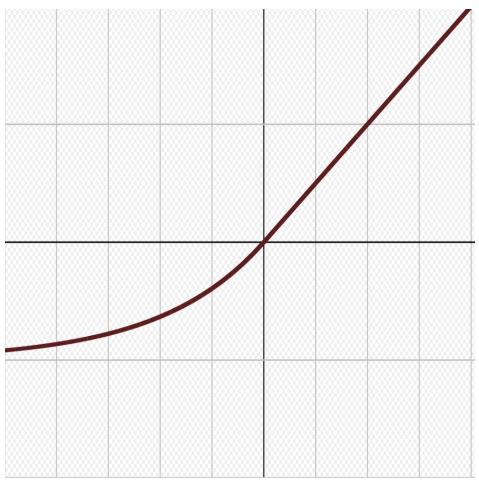


Other ReLU variants

- Gaussian Error Linear Unit (GELU):
  $\rho : \mathbb{R} \to [-0.17, \infty)$
  $\rho(x) = \frac{1}{2}x\left(1 + \text{erf}\left(\frac{x}{\sqrt{2}}\right)\right) = x\Phi(x)$,
  where $\Phi(x) = P(X \leq x), X \approx \mathcal{N}(0,1)$ is the cumulative distribution function of the normal distribution.

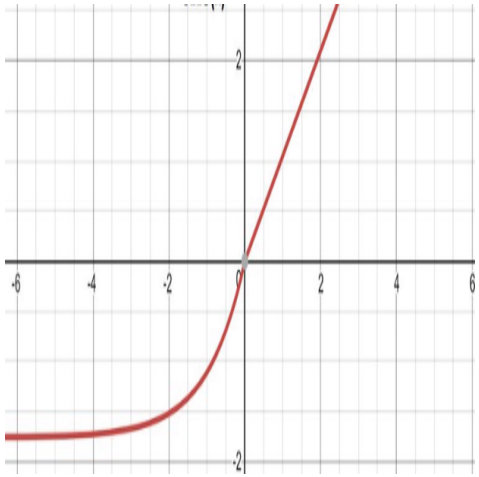


- Exponential Linear Unit (ELU):
  $\rho : \mathbb{R} \to [-\alpha, \infty)$
  $$\rho(x) = \begin{cases} \alpha(e^x - 1) & \text{if} \quad x \leq 0 \\ x & \text{if} \quad x > 0 \end{cases},$$
  where $\alpha \in \mathbb{R}^+$.

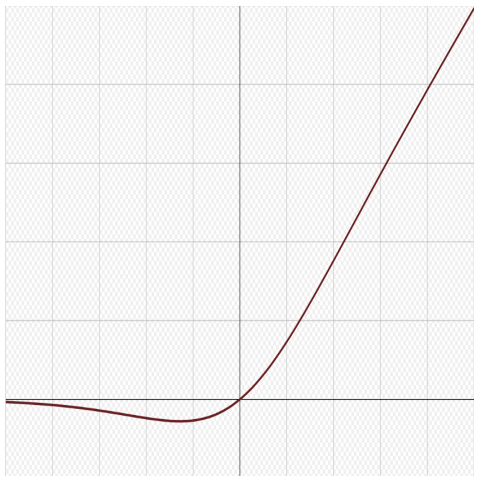


More ReLU activation functions

- Scaled Exponential Linear Unit (SELU):
  $\rho : \mathbb{R} \to [-\alpha\lambda, \infty)$
  $$\rho(x) = \lambda \begin{cases} \alpha(e^x - 1) & \text{if} \quad x \leq 0 \\ x & \text{if} \quad x > 0 \end{cases},$$
  where $\alpha = 1.67326$ and $\lambda = 1.0507$.

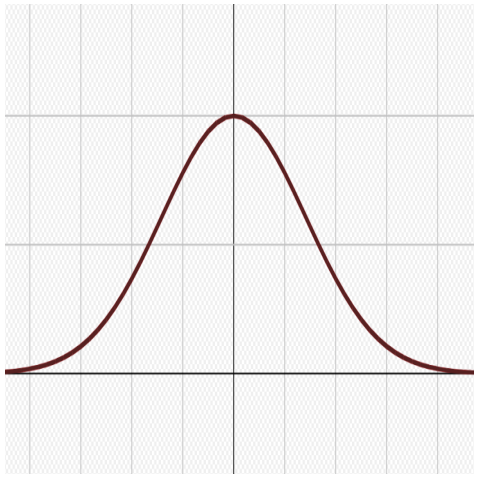


- Sigmoid Linear Unit (SiLU): $\rho : \mathbb{R} \to [-0.278, \infty)$
  $\rho(x) = \frac{x}{1+e^{-x}}$,

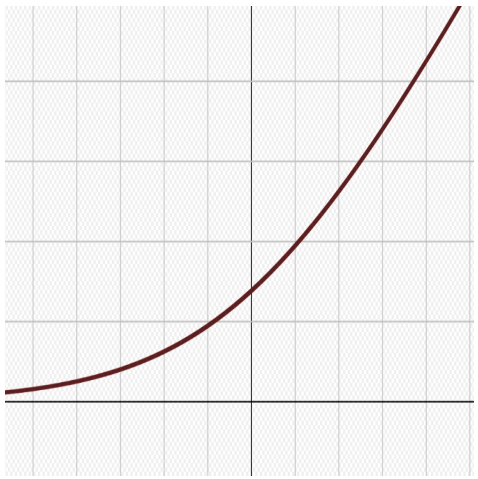


Other activation functions

- Gaussian: $\rho : \mathbb{R} \to [0, 1)\ \rho(x) = e^{-x^2}$



- Softplus: $\rho : \mathbb{R} \to [0, \infty))\ \rho(x) = ln(1 + e^x)$



Output activation functions

- Softmax:
  $\forall x = (x_i)_{1 \geq i \geq J} \quad \rho : \mathbb{R} \to (0,1) \quad \rho_i(x) = \frac{e^{x_i}}{\sum_{j=1}^{J} e^{x_j}}$
  Derivative: $\frac{\partial \rho_i(x)}{\partial x_j} = \rho_i(x)(\delta_{i,j} - \rho_j(x))$,
  where $\delta_{i,j}$ is the Kronecker delta.

- Maxout:
  $\forall x = (x_i)_{1 \geq i \geq J} \quad \rho : \mathbb{R} \to \mathbb{R} \quad \rho_i(x) = \max_i \quad x_i$
  Derivative: $\frac{\partial \rho_i(x)}{\partial x_j} = \begin{cases} 1 & \text{if} \quad j = \text{argmax}_i \quad (x_i) \\ 0 & \text{if} \quad j \neq \text{argmax}_i \quad (x_i) \end{cases}$

The output activation is task-dependent.

Regression
- $\rho \to$ identity
- ℓ_2 loss

Binary classification
- $\rho \to$ sigmoid
- BCE loss

Multi classification
- $\rho \to$ softmax
- CE loss

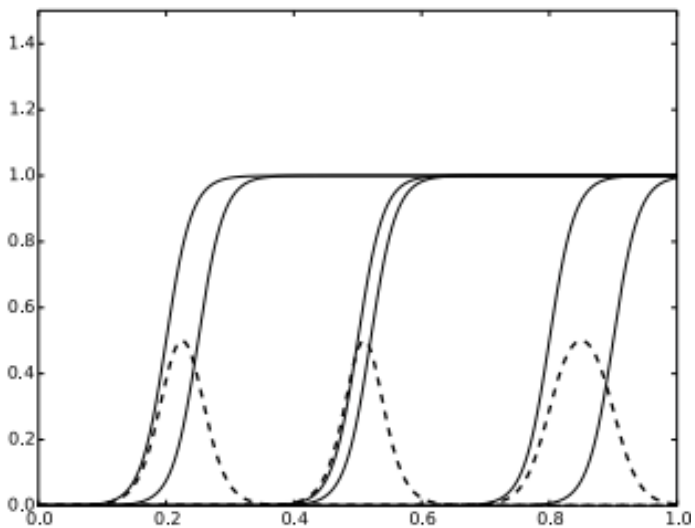
Universal Approximators

Theorem : *Any well behaved function can be arbitrarily approximated with a single layer FNN.*

Proof: A visual proof can be found in here. The original results were presented in (Cybenko, 1989).

Some intuition about this:

- Each layer uses a linear transform : $y = w^\top x$
- We can consider the sigmoid transfer function $\sigma = \rho(y) = \frac{1}{1+e^{-y}}$
- Combine multiple $\sigma-$layer activations to build gaussian kernels.



- subtract and weight consecutive $\sigma-$ layers to obtain RBF kernels, which hold the universal approximation theorem.

Why do we need deep networks?

- It is true that FFNs are universal approximators, but the hidden layer can be arbitrarily large.
- Having a large number of layers $\rightarrow$ explainable networks & helps us to build high level features. Example for an image:
  - first layer: compute contours, texure, rough features ...
  - second layer: learn corners, curves, crosses
  - next layers: build up more complex features.
- Using a shallow network $\rightarrow$ we are not able to compose low features into higher ones, we need to learn all the possibilities at once.

Differntial programming

Error backpropagation

- Training the network is an iterative algorithm, performed by gradient descent (or its variants)
- The algorithm was first introduced by (Werbos, 1981) and then popularized by (Rumelhart and co., 1986).

Training mechanism

1. initialize network parameters (weights and biases - η) at $t = 0$
2. at every iteration t compute: $w_t \leftarrow w_{t-1} - \gamma \nabla_\eta \mathcal{L}$

- Usually a mini-batch version of gradient descent is used (see previous Lecture for details).
- The main question is how do we compute $\frac{\partial \mathcal{L}}{\partial w}$?

Computational graph

Computational graph $\rightarrow$ directed acyclic graph where the nodes may be:

- **variables :** weights, targets, inputs, outputs, ...
- **operators :** Softmax, $w^\top x + b$, ReLU, ℓ_2 normalization, ...

Let us take an example for a graph associated to linear regression in $\mathbb{R}^8 \mapsto \mathbb{R}$, considering a minibatch with $M = 64$ samples (X, y).
In this case, the loss function is defined as follows:

$$\mathcal{L} = \frac{1}{M} \sum_{i=0}^{63} (w_1^\top x_i + b_1 - y_i)^2$$

Computational graph

We denote with η all the variables to be updated in the neural network during training (e.g. weights and biases).

Problem : compute the partial derivatives w.r.t. to η (i.e. $\frac{\partial \mathcal{L}}{\partial \eta}$).

Solution : compute the local derivatives w.r.t. inputs and apply **chain rule**.

We assume **Jacobian (numerator) layout**, e.g. $\frac{\partial \mathcal{L}}{\partial w_1} \in \mathcal{M}_{(1,8)}(\mathbb{R})$.

Otherwise, we transpose and reverse the jacobian product order. This is called the denominator (hessian) layout.

The chain rule

General rule : The derivative of a scalar w.r.t. a vector is a **row vector**:

$$y \in \mathbb{R}, \quad x \in \mathbb{R}^n, \quad \frac{dy}{dx} \in \mathcal{M}_{1,n}(\mathbb{R})$$

The derivative of a vector function $y : \mathbb{R}^{n_x} \mapsto \mathbb{R}^{n_y}$ w.r.t. input (Jacobian) is an $n_y \times n_x$ matrix:

$$x \in \mathbb{R}^{n_x}, \quad y(x) \in \mathbb{R}^{n_y}, \quad \frac{dy}{dx}(x) = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \dots & \frac{\partial y_1}{\partial x_{n_x}} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \dots & \frac{\partial y_2}{\partial x_{n_x}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_{n_y}}{\partial x_1} & \frac{\partial y_{n_y}}{\partial x_2} & \dots & \frac{\partial y_{n_y}}{\partial x_{n_x}} \end{bmatrix}(x)$$

The Chain Rule

- If we only got a single path chain of vector functions $y_1 \in \mathbb{R}^{n_1}, y_2 \in \mathbb{R}^{n_2}, \cdots y_n \in \mathbb{R}^{n_y}$, then

$$y_1 \to y_2 = \rho_1(y_1) \to y_3 = \rho_2(y_2) \cdots y_n = \rho_{n-1}(y_{n-1}),$$

and

$$\frac{\partial y_n}{\partial y_1} = \frac{\partial y_n}{\partial y_{n-1}} \frac{\partial y_{n-1}}{\partial y_{n-2}} \cdots \frac{\partial y_2}{\partial y_1}.$$

Let us compute for our example: $\frac{\partial \mathcal{L}}{\partial w_1} = \ldots$

In the case of matrix-like variables, things are a little more complex. We highly suggest you follow Jeremy's course for more details about multivariate calculus. Another useful insight about Tensor derivatives can be found here.

Multiple paths

To obtain the final result, we sum over all the possible paths. For example :

$$\frac{\partial y}{\partial x} = \sum_{i=3,4} \frac{\partial y}{\partial y_i} \frac{\partial y_i}{\partial x} = y_4 \frac{\partial y_3}{\partial x} + y_3 \frac{\partial y_4}{\partial x} = ...$$

For a reasonably large network, this is very computationally expensive:

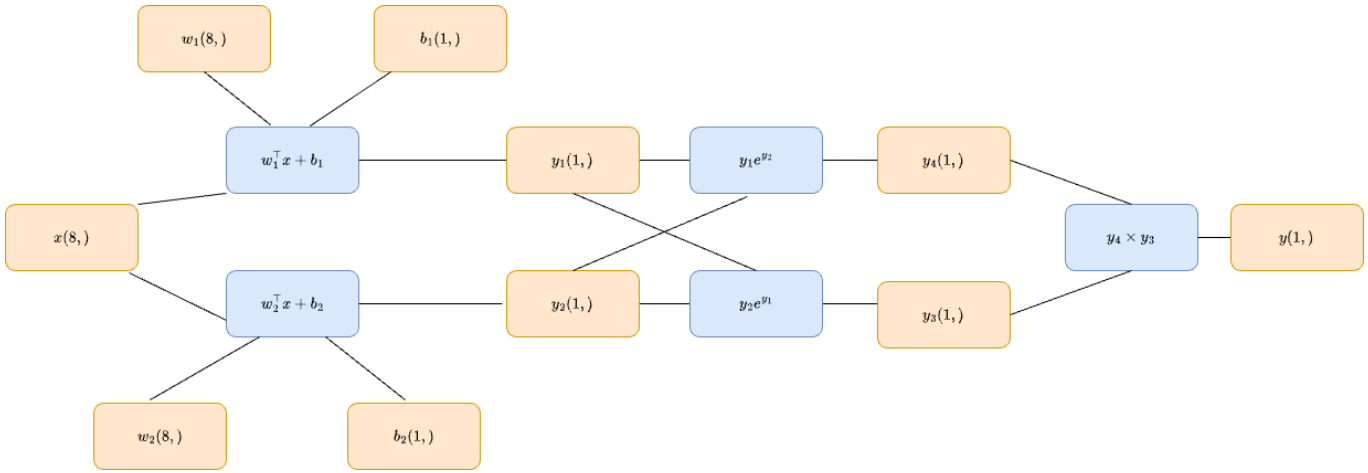
- The total number of paths : m layers and N neurons $\rightarrow N^m$ possible paths.
- This process must be repeated for each variable w.r.t. we have to differentiate
- some computations can be factored

We need to find a way to make it more efficient!!

Automatic differentiation

- Is a computational technique used to calculate the derivative of a function w.r.t its input variables.
- Unlike traditional methods such as symbolic differentiation or numerical differentiation, automatic differentiation leverages the chain rule of calculus to recursively break down a function into elementary operations and their derivatives.
- By automatically propagating these derivatives through the computation graph, automatic differentiation can provide accurate and efficient gradients for complex functions.
- Is has two modes: **forward** and **reverse** differentiation.
- Using it is particularly useful for training neural networks and optimizing machine learning algorithms.
- Check out Margossian's paper for more details about this domain that has revolutionized the field of computational mathematics.

Automatic differentiation - example



- Forward mode differentiation : compute $\frac{\partial y}{\partial x}$ forward propagate $\frac{\partial}{\partial x}$

$$\frac{\partial y}{\partial x} = y_3 e^{y_1}[w_2^\top + y_2 w_1^\top] + y_4 e^{y_2}[w_1^\top + y_1 w_2^\top]$$

- Reverse mode differentiation : compute $\frac{\partial y}{\partial x}$ by propagating backwards $\frac{\partial y}{\partial}$

$$\frac{\partial y}{\partial x} = (y_4 y_1 e^{y_2} + y_3 e^{y_1})w_2^\top + (y_3 y_2 e^{y_1} + y_4 e^{y_2})w_1^\top$$

This is more efficient when we have more inputs than outputs!

Error backpropagation

- Let us consider an $m = 2$ layer feedforward neural network, propagating one real sample x. Let $n_1, n_2, n_x \in \mathbb{N}^+$ be the number of neurons on each layer and the input dimension, respectively.
- In this case, the loss, assuming scalar, can be written as follows:

$$\mathcal{L} = \phi\left(y_i, \begin{bmatrix} \quad W_2(n_2 \times n_1) \quad \end{bmatrix} \rho\left(\begin{bmatrix} \quad W_1(n_1 \times n_x) \quad \end{bmatrix} \begin{bmatrix} x_i \end{bmatrix}\right)\right) \in \mathbb{R},$$

  where ϕ is the loss function, which is task dependent.
- For example, for a regression problem, we have $n_2 = 1$ and ϕ a squared error. For a classification problem, we can use CE loss and $n_2 > 1$ is the number of classes.
- We neglect the *bias* operator for this example.

Modelling example

Let us denote some intermediate results, as follows:
$z_1 = W_1 x_i, \qquad z_2 = W_2 \rho(z_1)$

Consider each error: $\delta_i = \frac{\partial \mathcal{L}}{\partial z_i} \in \mathbb{R}^{n_i}$. Then:

$$\delta_2 = \frac{\partial \mathcal{L}}{\partial z_2} = \frac{\partial \phi(y_i, z_2)}{\partial x_i}$$

$$\delta_1 = \frac{\partial \mathcal{L}}{\partial z_1} = \frac{\partial \mathcal{L}}{\partial z_2} \frac{\partial z_2}{\partial z_1}$$

The errors are integrated through the matrix used for forward pass.

Practical example using PyTorch

- Most deep learning frameworks compute all the derivatives automatically with `autograd`.
- The computational graphs can be build static or dynamically (eager mode)
- The leraning process has 2 phases: forward pass (eval. of outputs) and reverse-mode differentiation (backward pass)
- The reverse-mode differentiation uses the variables computed in the forward pass $\rightarrow$ learning through SGD!

```
optimizer = optim.Adam(model.parameters())

for e in range(epochs):
    for X,y in train_dataloader:
        optimizer.zero_grad()
        ...
        loss.backward()
        optimizer.step()
```

Gradient descent algorithms

Why do we use it in deep learning

- Neural networks $\rightarrow$ **non-convex optimization**
- Using Gradient Descent $\rightarrow$ guarantee to get a **local minima**
- *Can we do better?*

  Maybe yes, but for large/deep nets it has been proven (empirically though) that most local minima are close (in performance) with the global one.
- Saddle points are critical!!

Mini-batch gradient descent

Algorithm 1: Minibatch Gradient Descent

Input: Learning rate α, minibatch size M, training dataset pairs (x_i, y_i)
Output: Updated model parameters θ

for *every minibatch* $B \subseteq D$ *of size* M **do**
  initialize (randomly) parameters θ_0;
  for *iteration* $t = 0 \dots$ **do**
    $\theta_{t+1} = \theta_t - \alpha \nabla_\theta \mathcal{L}(\theta_t)$;
    $\mathcal{L}(\theta) = \frac{1}{M} \sum_i \phi(\theta, x_i, y_i)$

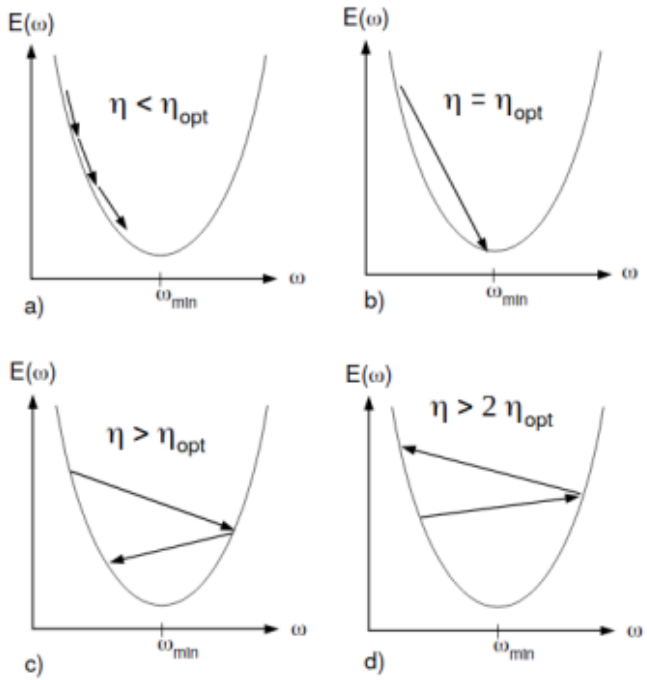
Taylor series expansion : $\mathcal{L}(\theta_{t+1}) \approx \mathcal{L}(\theta_t) + (\theta_{t+1} - \theta_t)^\top \nabla_\theta \mathcal{L}(\theta_t)$

Is the size of M important?

- If $(M = 1)$ Stochastic Gradient Descent : noisy estimate, not GPU friendly
- If $(M = N > 1)$ Batch Gradient Descent : generalization gap and local minima problem.

How about the learning rate?

The model may converge very slowly or even diverge if α is not appropriately chosen! So, what is the optimal learning rate?



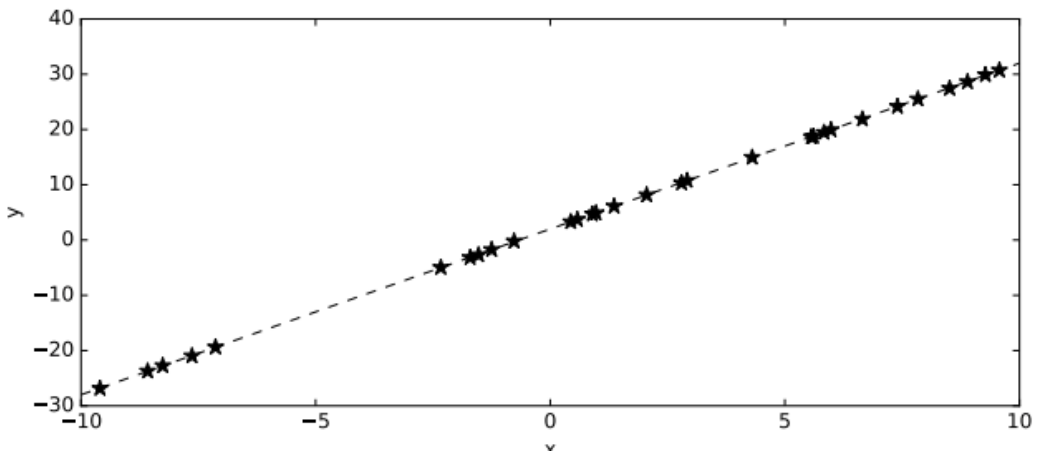
Efficient Backprop, LeCun et al., 1998

- Y.Bengio : *"The optimal learning rate is usually close to the largest learning rate that does not cause divergence of the training criterion."*
- Karpathy : *"0.0003 is the best learning rate for Adam, hands down."*

Let us take a simple example

Let us consider a **regression problem** having the following setup

- $N = 30$ samples generated with : $y = 3x + 2 + \mathcal{U}(-0.1, 0.1)$
- Model: $\rho(x) = \theta^\top \begin{bmatrix} 1 \\ x \end{bmatrix}$,
- ℓ_2 loss :$\mathcal{L}(y_i, \rho(x_i)) = (y_i - \rho(x_i))^2$

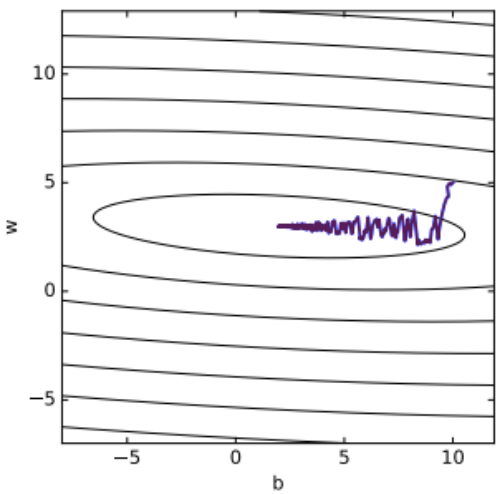


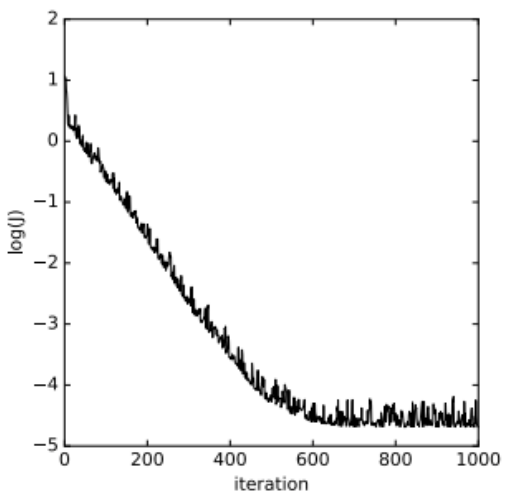
SGD minimization

Consider:

- learning rate : $\alpha = 0.005$,
- Initial parameters : $\theta_0 = \begin{bmatrix} 10 \\ 5, \end{bmatrix}$
- $t = 1000$ iterations.

Obtained solution : $\theta_{1000} = \begin{bmatrix} 1.9882 \\ 2.9975 \end{bmatrix}$





SGD with Momentum

Idea : Dampen the oscillations in the optimization path using a low pass filter on ∇_θ.

Algorithm 2: Minibatch Stochastic Gradient Descent with Momentum

Input: Learning rate α, momentum parameter β, minibatch size M, training dataset pairs (x_i, y_i)

Output: Updated model parameters θ

initialize parameters θ_0; initialize momentum vector $v_0 = 0$;
for *every minibatch* $B \subseteq D$ *of size* M **do**
  for *every iteration* $t = 0 \dots$ **do**
    $v_{t+1} = \beta v_t - \alpha \nabla_\theta J(\theta_t)$;
    $\theta_{t+1} = \theta_t + v_{t+1}$;

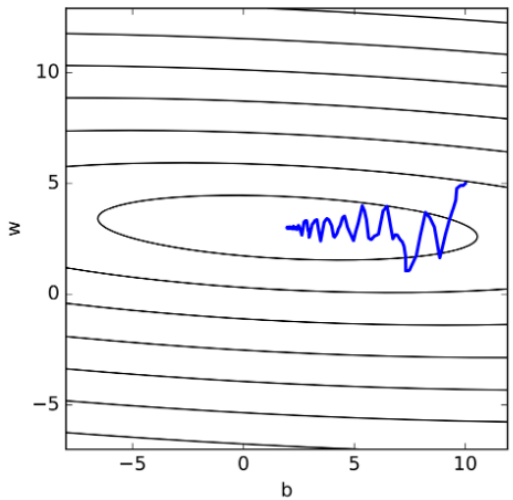
Here-above, $\beta \in \mathbb{R}$ is a hyper-parameter, usually ≈ 0.9.

- The purpose is to accelerate the learning rate in constant directions and low curvature.
- Check this link for more details about this.

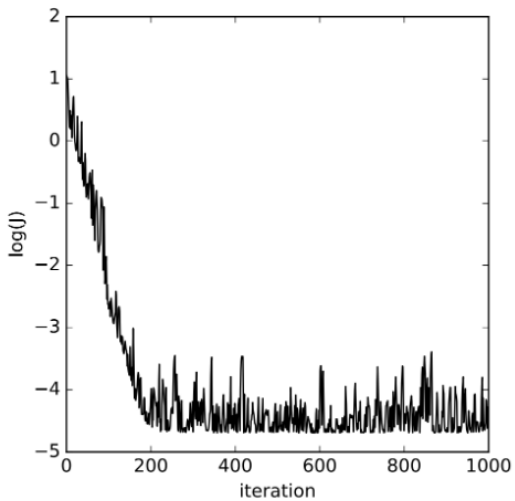
Back to our example

Parameters: $\alpha = 0.005,\ \beta = 0.6,\ \theta_0 = \begin{bmatrix} 10 \\ 5 \end{bmatrix}$

Solution : $\theta_{1000} = \begin{bmatrix} 1.9837 \\ 2.9933 \end{bmatrix}$



The optimization path



The value of the function

Gradient descent with Nesterov momentum

Idea : Based on Nesterov Accelerated Gradient. Look ahead to correct the update.

Algorithm 3: Minibatch Stochastic Gradient Descent with Nesterov Momentum

Input: Learning rate α, momentum parameter β, minibatch size M, training dataset pairs (x_i, y_i)

Output: Updated model parameters θ

initialize parameters θ_0; initialize momentum vector $v_0 = 0$;

for *every minibatch* $B \subseteq D$ *of size* M **do**

  for *every iteration* $t = 0 \dots$ **do**

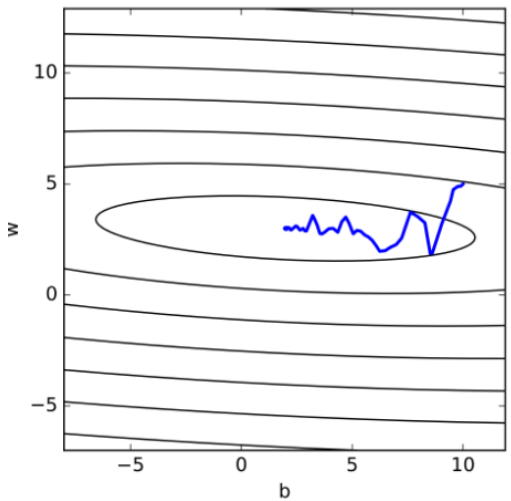
    $v_{t+1} = \beta v_t - \alpha \nabla_\theta J(\theta_t + \beta v_t)$; (Nesterov lookahead update)

    $\theta_{t+1} = \theta_t + v_{t+1}$;

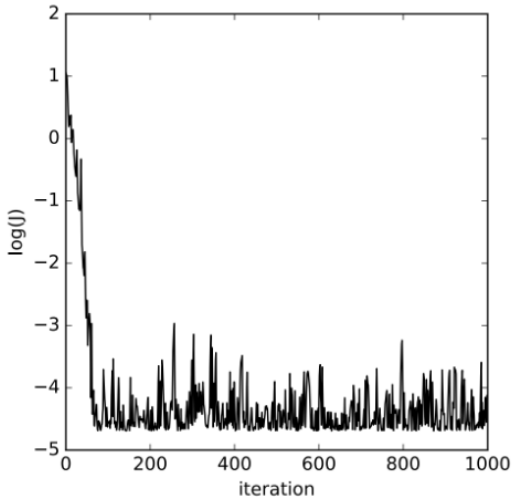
Back to our example

Parameters: $\alpha = 0.005,\ \beta = 0.8,\ \theta_0 = \begin{bmatrix} 10 \\ 5 \end{bmatrix}$

Solution : $\theta_{1000} = \begin{bmatrix} 1.9738 \\ 2.9914 \end{bmatrix}$

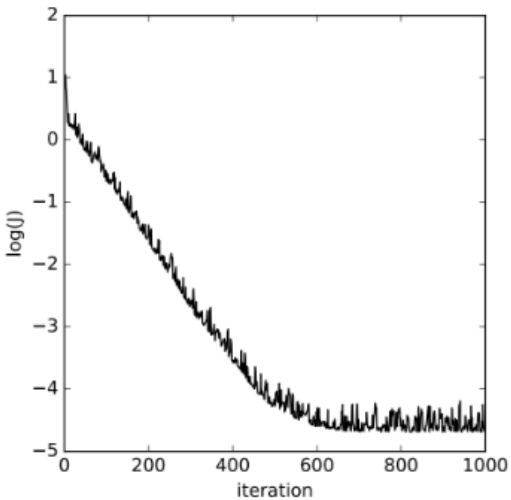


The optimization path

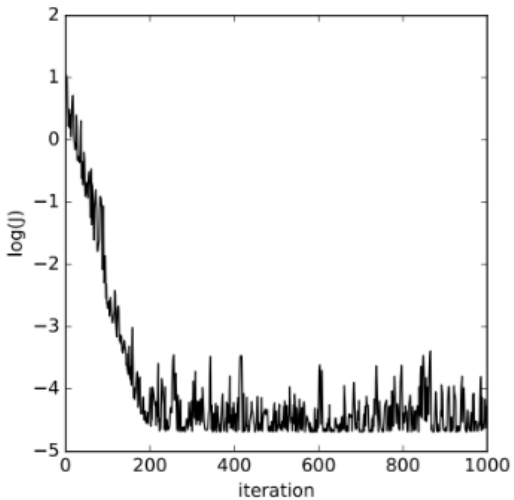


The value of the function

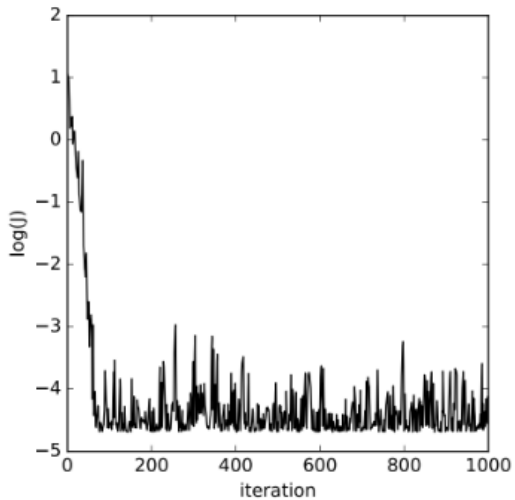
Comparison



SGD



Momentum



Nesterov

Adaptive Learning rate

Idea : Modify the learning rate during the training phase

Decreasing the learning rate – Robbins Monro conditions

- Linear decrease from α_0 to α_f
- Halve the learning rate when the validation error stops improving
- Halve the learning rate on a fixed schedule

More recent approaches are not advocating for decreasing the learning rate

Increasing learning rate

- The 1-cycle policy
- Stochastic Gradient Descent with Warm Restart

Adaptive first order : ADAGRAD

Adagrad - Adaptive gradient proposed in 2011

- Accumulate the square of the gradient

$$r_{t+1} = r_t + \nabla_\theta J(\theta_t) \odot \nabla_t J(\theta_t)$$

- Scale individually the learning rates

$$\theta_{t+1} = \theta_t - \frac{\alpha}{\delta + \sqrt{r_{t+1}}} \odot \nabla_\theta J(\theta_t),$$

where $\delta \approx 1e^{-8}$

- Small gradients $\rightarrow$ bigger learning rate for moving fast along flat directions
- High gradients $\rightarrow$ smaller learning rate to calm down on high curvature

RMSProp

Idea : using an exponential moving average when accumulating the gradient.

- Accumulate the square of the gradient:

$$r_{t+1} = \rho r_t + (1-\rho)\nabla_\theta J(\theta_t) \odot \nabla_\theta J(\theta_t)$$

- Scale each learning rate accordingly:

$$\theta_{t+1} = \theta_t - \frac{\alpha}{\delta + \sqrt{r_{t+1}}} \odot \nabla_\theta J(\theta_t),$$

where ρ is a training parameter, $\rho \approx 0.9$

ADAM algorithm

Idea : Use Adaptive Moments of past gradients

- Store running averages of past gradients:

$$m_{t+1} = \beta_1 m_t + (1 - \beta_1)\nabla_\theta J(\theta_t)$$

$$v_{t+1} = \beta_2 v_t + (1 - \beta_2)\nabla_\theta J(\theta_t) \odot \nabla_\theta J(\theta_t),$$

$m(t)$ and $v(t)$ are the first and second (uncentred) moments of $\nabla_\theta J$.
Correct the bias $\hat{m}_t$ and $\hat{v}_t$:

$$\theta_{t+1} = \theta_t - \frac{\alpha}{\delta + \sqrt{\hat{v}_{t+1}}}\hat{m}_{t+1}$$

Some references

- Overview of gradient descent
- Recent gradient descent algorithms

First order methods summary

Goodfellow, Bengio, & Courville – " There is currently no consensus [. . .] no single best algorithm has emerged [. . .] "

- The most popular and actively in use include SGD, SGD with momentum, RMSprop, RMSprop with momentum, Adadelta and Adam
- It is task-specific mostly.

Second order methods

Idea : use the second derivative, and Taylor series expansion

$$J(\theta_t) \approx J(\theta_0) + (\theta - \theta_0)^\top \nabla_\theta J(\theta_0) + \frac{1}{2}(\theta - \theta_0)^\top \nabla_\theta^2 J(\theta_0)(\theta - \theta_0),$$

where $H = \nabla^2 J$ - Hessian matrix

Methods

- Conjugate gradient : using line search along $\nabla_\theta J(\theta_k)$
- Newton : just to find critical points
- Quasi Newton : BFGS (approximating H^{-1}), L-BFGS, and saddle-free versions

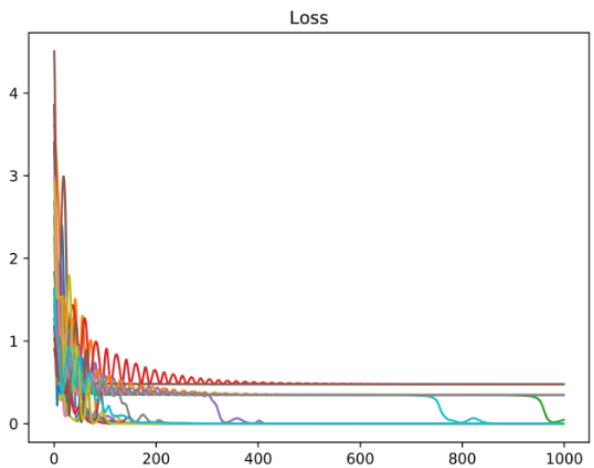
Initialization mechanisms

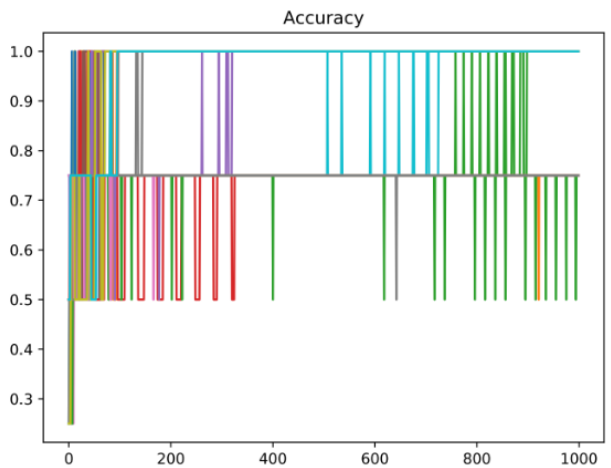
Does the starting point matter?

Problem : XOR classification

Model architecture :

- Layers: 3 Dense (2-4-1); Activation: Sigmoid
- Init: $\mathcal{U}(-10, 10)$, bias $= 0$
- Loss: BCE
- SGD ($\alpha = 0.1$, momentum $= 0.99$)
- $n = 1000$ epochs





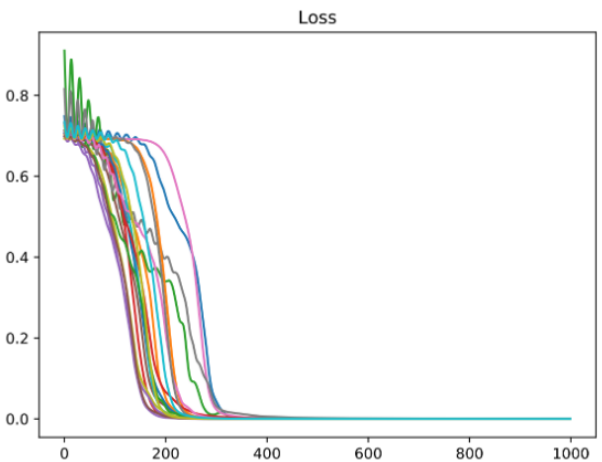
It fails 6/20 times.

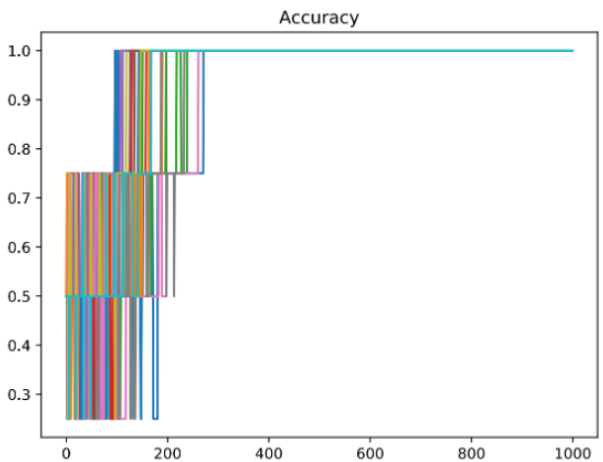
Does the starting point matter?

Problem : XOR classification

Model architecture :

- Layers: 3 Dense (2-4-1); Activation: Sigmoid
- Init: $\mathcal{N}(0, \frac{1}{\sqrt{fan_{in}}})$, bias $= 0$
- Loss: BCE
- SGD ($\alpha = 0.1$, momentum $= 0.99$)
- $n = 1000$ epochs





It fails 0/20 times.

Standardization

- The starting point of a gradient descent has a dramatic impact.
- All gradient-based algorithms converge faser is the data are normalized and decorrelated.
- Several strategies are currently used, depending on the task.

Let x be you input data.

Min-Max scaling

$$x' = \frac{x - \text{min (x)}}{\text{max}(x) - \text{min}(x)}$$

Z-score scaling

$$x' = \frac{x - \mu_x}{\sigma_x + \epsilon},$$

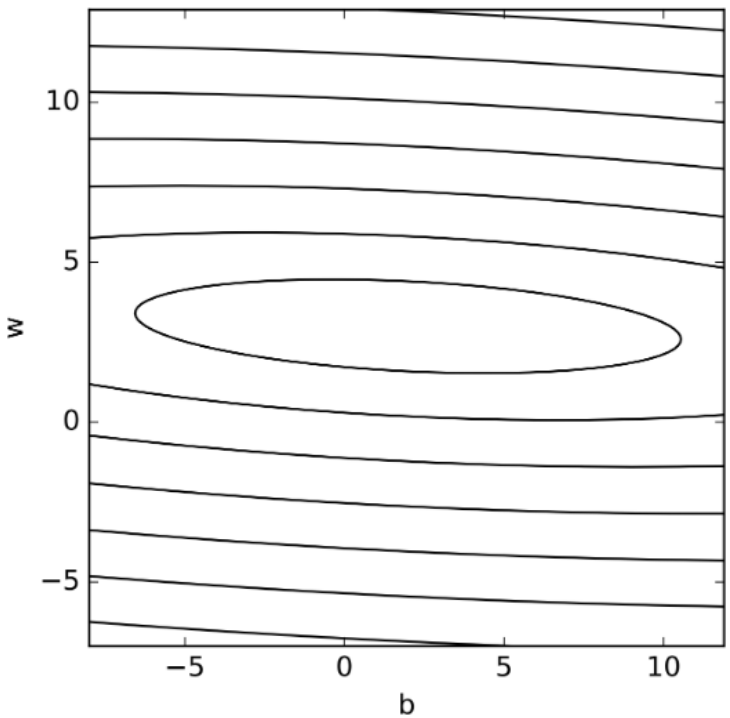
where μ_x, σ_x andϵ are the mean, the standard deviation and a small constant, respectively.

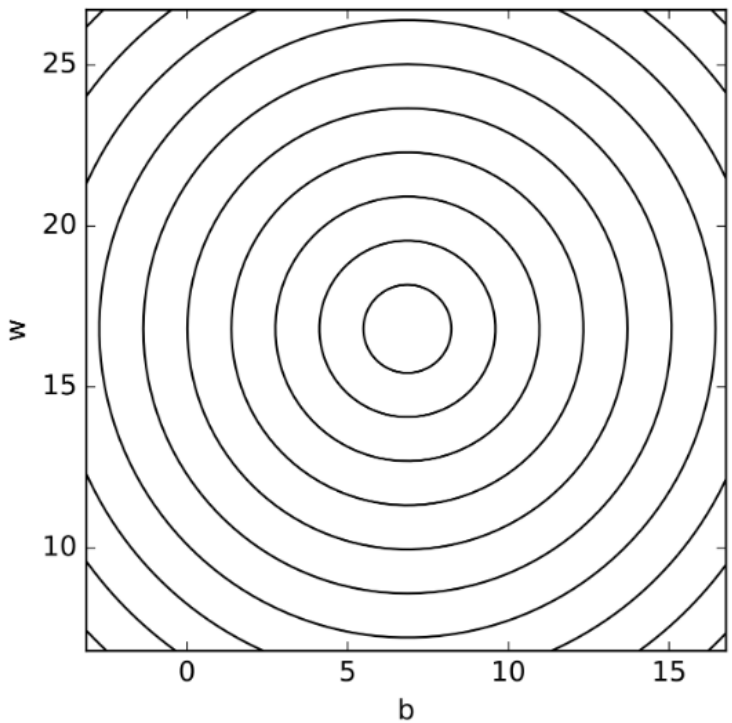
ZCA whitening

$$X' = WX, W = \frac{1}{\sqrt{n-1}}(X'X^\top)^{(-1/2)}$$

The effect of standardization

Problem: $y = 3x + 2 + \mathcal{U}(-0.1, 0.1)$





How to chose a good initialization

- An effective initialization strategy should disrupt symmetry within the neural network; constant initialization methods tend to lead units to learn identical patterns.
- A favorable initialization should commence optimization from a region of limited capacity, e.g. linear neural networks.
- An ideal initialization scheme should maintain the distribution of both activations and gradients, guarding against issues such as exploding or vanishing gradients.

Exploding and vanishing gradients

- **The Fundamental Deep Learning Problem** – the gradient can either vanish or explode, especially in deep networks.
- The deeper the network ($m \rightarrow$ large), the more chances that through backprop the gradients either explode or vanish.
- Problems with activations such as *sigmoid*, *ReLU*.

Preventing vanishing/ exploding gradients

- ensure a good flow of gradient – use appropriate activation functions (e.g. ReLu, PreLu, etc..) or some architectural elements (e.g. skip-connections, constant error loops (LSTMs))
- use *clipping* methods $\rightarrow$ only for exploding gradients problem

Initialization of Y. LeCun

First introduced in Gradient-Based Learning Aplied to Document Recognition
Goal : Initialize parameters such that the activation operator ρ stays in its linear part by using more layers:

- use symmetric transfer operations : R_i is symmetric, which means there exist $(c_i, d_i) \in (\mathbb{R}^{N_i})^2$ such that

$$(\forall x \in \mathbb{R}^{N_i}) \quad R_i(x) - d_i = -R_i(-x + c_i).$$

  e.g. $R_i = 1.7159\text{tanh}(\frac{2}{3}x)$
- initialize the biases with 0 and the weights drawn randomly from $\mathcal{N}(\mu = 0, \sigma^2 = \frac{1}{fan_{N_i}})$
  If $x \in \mathbb{R}^n$ is $\mathcal{N}(0, \Sigma = I_d)$ and $w \in \mathbb{R}^n$ is $\mathcal{N}(0, \Sigma = \frac{1}{n} I_d)$. Assume x_i, w_i pair wise independent, then:

$$E[w^\top x + b] = E[w^\top x] = \sum_i E[w_i x_i] \sum_i E[w_i] E[x_i] = 0$$

$$\begin{aligned} \text{var}[w^\top x + b] &= \text{var}[w^\top x] \\ &= \sum_i \sigma_{w_i}^2 \sigma_{x_i}^2 + \sigma_{w_i}^2 \mu {x_i}^2 + \mu {w_i}^2 \sigma_{x_i}^2 \\ &= \sum_i \sigma_{w_i}^2 \sigma_{x_i}^2 = \frac{1}{n} \sum_i \sigma_{x_i}^2 = 1 \end{aligned}$$

Glorot Initialization

Goal : preserve the same distribution along the forward and backward pass, which prevents saturating transfer functions.

$$T = R_m(W_m \dots R_1(W_1(W_0 x + b_0) + b_1) \cdots + b_m)$$

Glorot (Xavier) initialization

- Input data should be centered, normalized and decorrelated
- Symmetric activation functions should be used, with $R_i'(0) = 1$

Assuming the linear regime $R_i'() = 1$ for the network:

- Forward prop. var. constraint : $\forall i, fan_{in_i} \sigma^2_{W_i} = 1$
- Backward prop. var. constraint : $\forall i, fan_{out_i} \sigma^2_{W_i} = 1$

Compromise: $\forall i, \frac{1}{\sigma^2_{W_i}} = \frac{fan_{in} + fan_{out}}{2}$

- Glorot Uniform: $\mathcal{U}\left(-\frac{\sqrt{6}}{\sqrt{fan_{in}+fan_{out}}}, \frac{\sqrt{6}}{\sqrt{fan_{in}+fan_{out}}}\right)$ and $b = 0$
- Glorot Normal: $\mathcal{N}\left(0, \frac{\sqrt{2}}{\sqrt{fan_{in}+fan_{out}}}\right)$ and $b = 0$

He Initialization

Goal : preserve the same distribution along the forward and backward pass for rectifiers.

$$T = R_m(W_m \dots R_1(W_1(W_0 x + b_0) + b_1) \cdots + b_m)$$

- input dimensions should be centered, normalized, uncorrelated
- use ReLU operators: $\forall i \in \{1, \dots, m\} \quad R_i(x) = \max(0, x)$
- weights are initialized with symmetric distribution, zero-mean, independently
- biases are set to 0
- the components of x are assumed i.i.d.

Forward prop. var. constraint : $\forall i, \frac{1}{2} fan_{in_i} \sigma^2_{W_i} = 1$
Backward prop. var. constraint : $\forall i, \frac{1}{2} fan_{out_i} \sigma^2_{W_i} = 1$

Compromise: use one of them, e.g. $\sigma^2_{W_i} = \frac{2}{fan_{out}}$

- He Uniform: $\mathcal{U}\left(-\frac{\sqrt{6}}{\sqrt{fan_{in}}}, \frac{\sqrt{6}}{\sqrt{fan_{in}}}\right)$ and $b = 0$
- He Normal: $\mathcal{N}\left(0, \frac{\sqrt{2}}{\sqrt{fan_{in}}}\right)$ and $b = 0$