Deep Learning

A course about theory & practice

UNIVERSITÀ DI PAVIA

Learning as Optimization

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About why they did not use Deep Networks from the beginning

Problem: vanishing or exploding Gradients

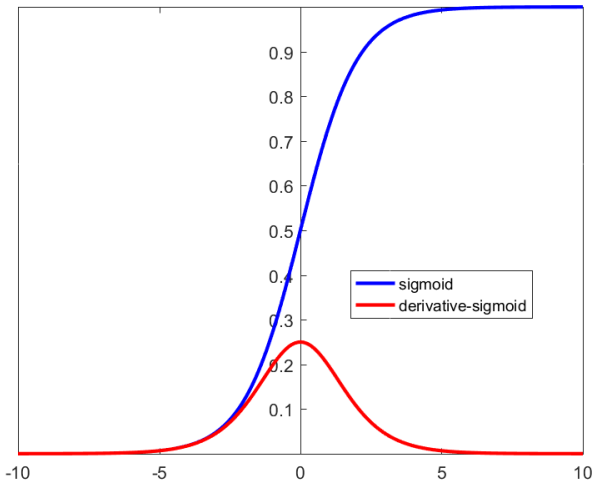
The gradient descent method implies updating the parameters at each step: making sure that the gradient does not either *vanish* or *explode* is not easy

For instance, in

$$\Delta \boldsymbol{W} = -\eta \frac{\partial L}{\partial \boldsymbol{W}}(\tilde{y}^{(i)}, y^{(i)})$$

the gradient contains a multiplicative term $\frac{\partial}{\partial x} g(x)$
which can be $\ll 1.0$

e.g. for the sigmoid function:



Problem: vanishing or exploding Gradients

The gradient descent method implies updating the parameters at each step: making sure that the gradient does not *vanish* or *explode* is not easy ...

Consider a special deep network

$$\tilde{y} = \boldsymbol{w} \cdot g(\boldsymbol{W}^{[k]} \cdots g(\boldsymbol{W}^{[1]}\boldsymbol{x} + \boldsymbol{b}^{[1]}) \cdots + \boldsymbol{b}^{[k]}) + b$$

in which

- g *is the identity function and all* $\boldsymbol{b}^{[i]}$ *and* b *are zero;*
- *all hidden layers have the same size* d *of the input (i.e., al matrices are square);*
- *all* $\boldsymbol{W}^{[i]}$ *are identical and diagonalizable, with eigenbasis* $(\boldsymbol{e}_1, \cdots, \boldsymbol{e}_d)$.

This means that

eigenvalue raised to the k-th power

$$\boldsymbol{W}^{[k]} \ldots \boldsymbol{W}^{[1]}\boldsymbol{x} = \boldsymbol{W}^{k}\boldsymbol{x} = \lambda_1^k(\boldsymbol{e}_1 \cdot \boldsymbol{x})\boldsymbol{e}_1 + \cdots \lambda_d^k(\boldsymbol{e}_d \cdot \boldsymbol{x})\boldsymbol{e}_d$$

$$= \lambda_1^k x_1 \boldsymbol{e}_1 + \cdots \lambda_d^k x_d \boldsymbol{e}_d$$

Moral: any $\lambda_i > 1$ *leads to explosion while any* $\lambda_i < 1$ *leads to vanishing*

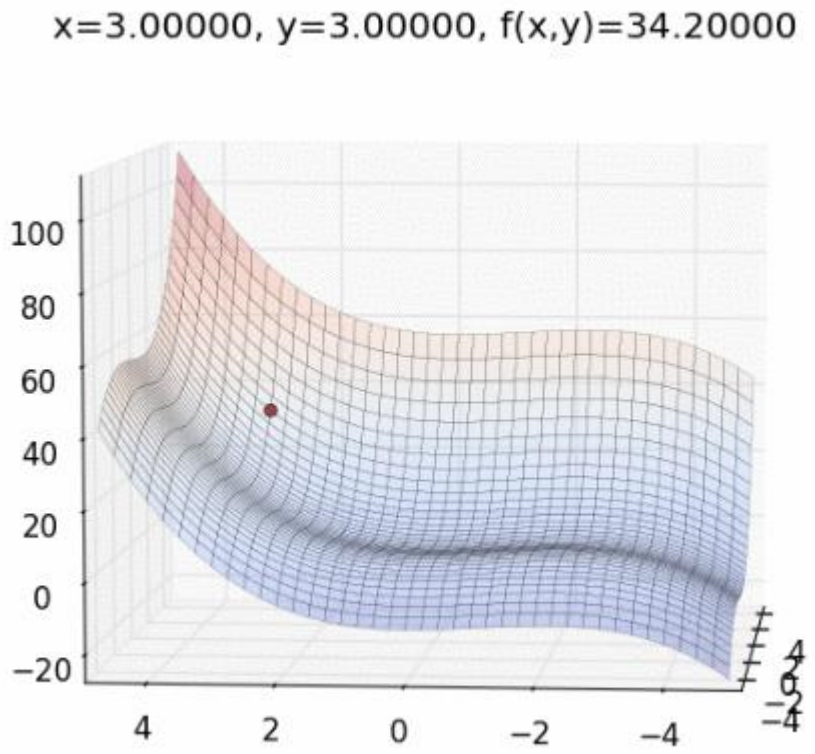
Problem: initial values of the parameters

However, the main problem of training is that of *initial values*…

Gradient Descent can only discover minima that are close to the initial values

Using deep networks
can only make this problem worse:

intuitively, with deeper networks,
the 'surface' can be even rougher…



[Image from http://cpmarkchang.logdown.com/posts/434534-optimization-method-momentum]

Improving optimization

Improving optimization

- ***SGD (or MBGD)***

  Standard, decaying learning rate
  Update step:

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$

decaying learning rate

mini-batch, possibly a singleton

Improving optimization

- **SGD (or MBGD)**

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decaying learning rate

mini-batch, possibly a singleton

Many different ways to improve performance and speed rate:

- add some *momentum*
- take in account *2nd order derivatives*
- make the *learning rate adaptive*

Improving optimization

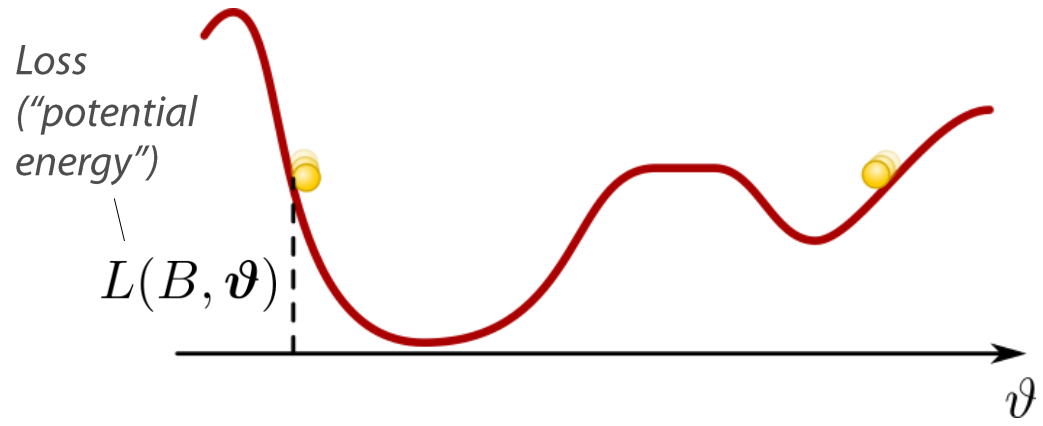
- **SGD (or MBGD)**

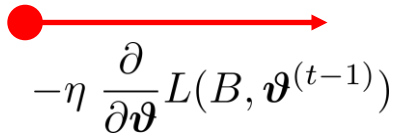
  Standard, decaying learning rate
  Update step:

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$

$$\boldsymbol{\vartheta}^{(t)} - \boldsymbol{\vartheta}^{(t-1)} = -\eta \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$

"velocity"





$$-\eta \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$

"force felt by the ball"

$$\boldsymbol{f} = -\frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta})$$

"acceleration"

$$\boldsymbol{f} = m\boldsymbol{a}$$

$$\boldsymbol{a} \propto -\frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta})$$

... the gradient directly affects the velocity (not the position)

Momentum

- **Momentum**

  "Let the ball run"

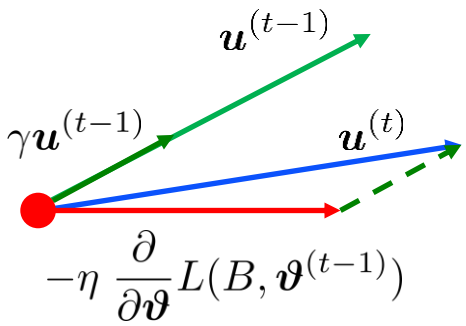
momentum term:
tendency to keep running at the same velocity and direction

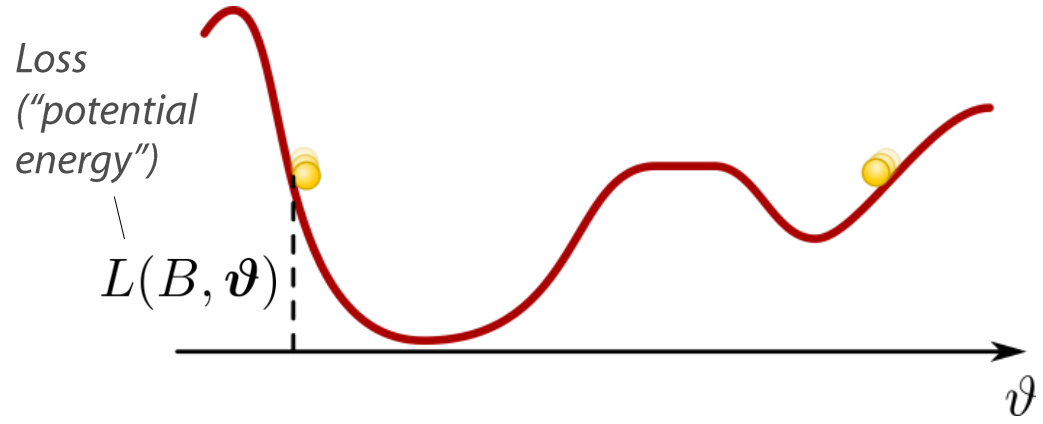
$$\boldsymbol{u}^{(t)} = \gamma \boldsymbol{u}^{(t-1)} - \eta \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)}), \quad \boldsymbol{u}^{(0)} = \mathbf{0}$$

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} + \boldsymbol{u}^{(t)}$$

$0 < \gamma < 1$

"coefficient of friction"





Momentum

- **Momentum**

  "Let the ball run"

$$\boldsymbol{u}^{(t)} = \gamma \boldsymbol{u}^{(t-1)} - \eta \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)}), \quad \boldsymbol{u}^{(0)} = \mathbf{0}$$

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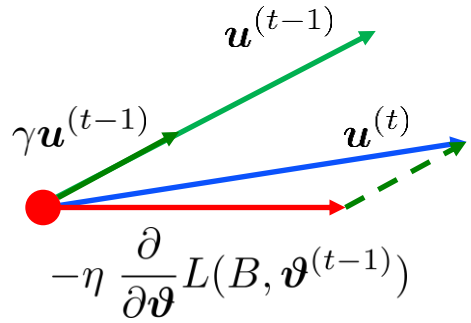
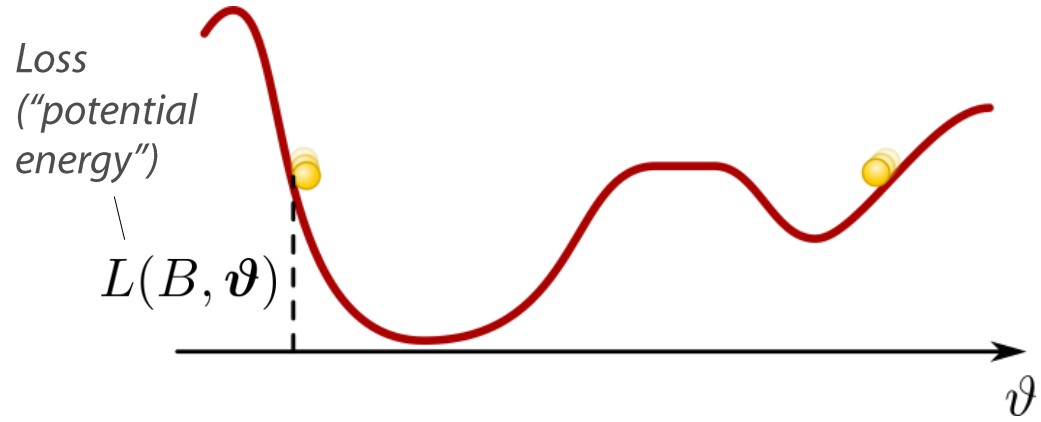




Consider $\boldsymbol{\vartheta}$ *as a position ...*

"velocity"

$$\boldsymbol{u} := \frac{\partial}{\partial t} \boldsymbol{\vartheta} \approx \boldsymbol{\vartheta}^{(t)} - \boldsymbol{\vartheta}^{(t-1)}$$

"acceleration"

$$\boldsymbol{a} \approx \boldsymbol{u}^{(t)} - \boldsymbol{u}^{(t-1)} \propto -\frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta})$$

... the gradient directly affects the velocity (not the position)

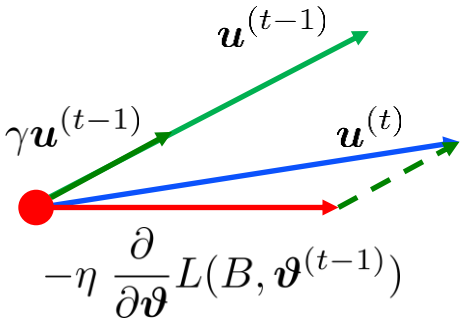
NAG

- ***Momentum***

  "Let the ball run"

$$\boldsymbol{u}^{(t)} = \gamma \boldsymbol{u}^{(t-1)} - \eta \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)}), \quad \boldsymbol{u}^{(0)} = \mathbf{0}$$

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} + \boldsymbol{u}^{(t)}$$

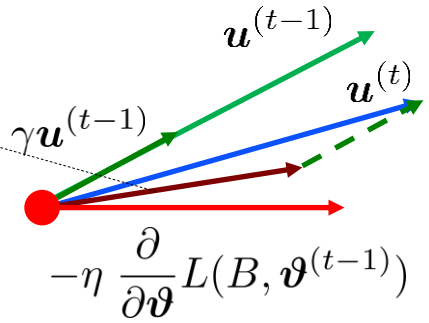


- ***Nesterov Accelerated Gradient (NAG)***

  "Let the ball run but be predictive"

$$\boldsymbol{u}^{(t)} = \gamma \boldsymbol{u}^{(t-1)} - \eta \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)} + \gamma \boldsymbol{u}^{(t-1)})$$

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} + \boldsymbol{u}^{(t)}$$



... the gradient being computed as if the position was a bit forward in time

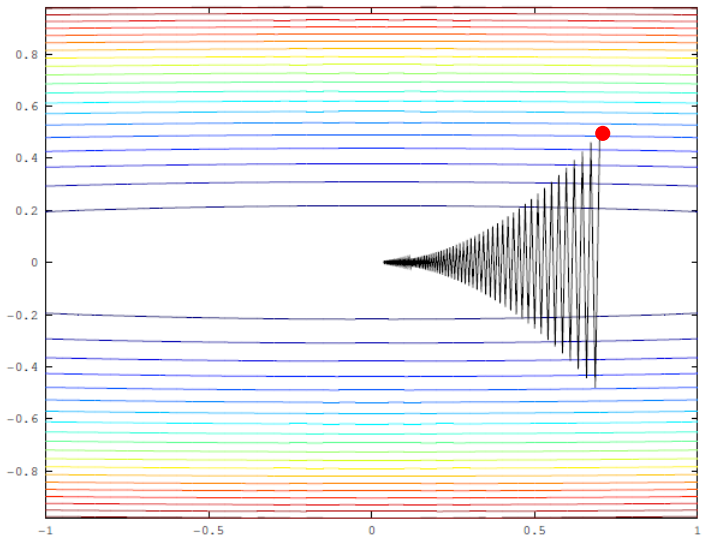
2nd order methods

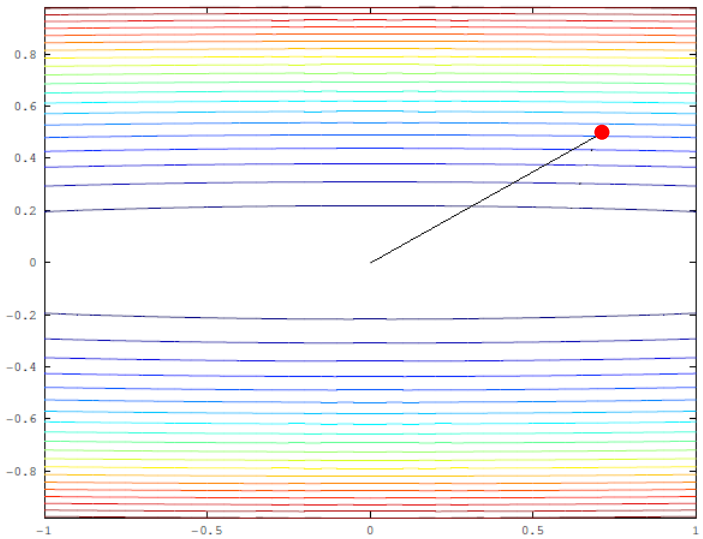
In this example (geometric view)

Gradient Descent

Newton-Raphson

The level curves of a quadratic form in 2D are ellipses centered in the origin





2nd order methods

- **Taylor's expansion**

$$L(B,\boldsymbol{\vartheta}) = L(B,\boldsymbol{\vartheta}^{(t-1)}) + \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B,\boldsymbol{\vartheta}^{(t-1)}) \cdot (\boldsymbol{\vartheta} - \boldsymbol{\vartheta}^{(t-1)}) + \frac{1}{2}(\boldsymbol{\vartheta} - \boldsymbol{\vartheta}^{(t-1)}) \cdot \boldsymbol{H} \; (\boldsymbol{\vartheta} - \boldsymbol{\vartheta}^{(t-1)}) + \ldots$$

The Hessian Matrix

All terms in blue are constant

where:

$$\boldsymbol{H} := \frac{\partial}{\partial \boldsymbol{\vartheta}} \left(\frac{\partial}{\partial \boldsymbol{\vartheta}} L(B,\boldsymbol{\vartheta}^{(t-1)}) \right)$$

The Hessian Matrix

- **Differentiate both sides and take** $\boldsymbol{\vartheta} = \boldsymbol{\vartheta}^*$

The argmin

$$\underline{\frac{\partial}{\partial \boldsymbol{\vartheta}} L(B,\boldsymbol{\vartheta}^*)} = \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B,\boldsymbol{\vartheta}^{(t-1)}) + \boldsymbol{H}(\boldsymbol{\vartheta}^* - \boldsymbol{\vartheta}^{(t-1)})$$

set this equal to 0

then:

$$\boldsymbol{\vartheta}^* - \boldsymbol{\vartheta}^{(t-1)} = -\boldsymbol{H}^{-1} \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B,\boldsymbol{\vartheta}^{(t-1)})$$

2nd order methods

- ***Gradient Descent***

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta \, \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$

- ***Newton-Raphson's optimization method***

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta \, \boldsymbol{H}^{-1} \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$

where:

$$\boldsymbol{H} := \frac{\partial}{\partial \boldsymbol{\vartheta}} \left(\frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)}) \right)$$

Why is the Newton-Raphson's method better than GD?

2nd order methods

- **Newton-Raphson's optimization method**

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta\, \boldsymbol{H}^{-1} \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)}) \qquad \boldsymbol{H} := \frac{\partial}{\partial \boldsymbol{\vartheta}} \left(\frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)}) \right)$$

Example

a quadratic form, centered in the origin

$$L(B, \boldsymbol{\vartheta}) = \boldsymbol{\vartheta} \cdot \boldsymbol{A}\boldsymbol{\vartheta}$$

where;

a diagonal, positive definite matrix (therefore, L is convex)

$$\boldsymbol{A} := \begin{bmatrix} a_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & a_d \end{bmatrix}, \quad a_i > 0 \ \forall i = 1, \dots, d$$

$$\frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}) = 2\boldsymbol{A}\boldsymbol{\vartheta}$$

$$\boldsymbol{H} = \frac{\partial}{\partial \boldsymbol{\vartheta}} \left(\frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}) \right) = 2\boldsymbol{A} \qquad \boldsymbol{H}^{-1} = \frac{1}{2}\boldsymbol{A}^{-1} = \frac{1}{2} \begin{bmatrix} 1/a_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 1/a_d \end{bmatrix}$$

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta\, \frac{1}{2}\boldsymbol{A}^{-1} 2\boldsymbol{A}\boldsymbol{\vartheta}^{(t-1)} = \boldsymbol{\vartheta}^{(t-1)} - \eta\boldsymbol{\vartheta}^{(t-1)} = (1-\eta)\boldsymbol{\vartheta}^{(t-1)}$$

What??

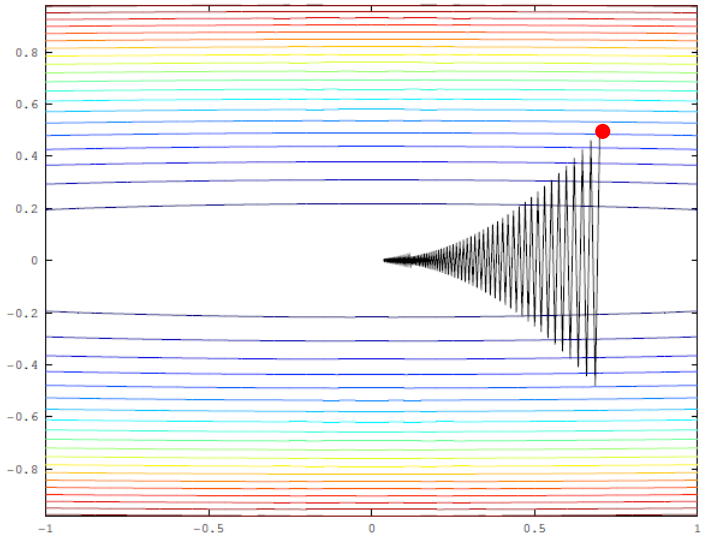
2nd order methods

In this example (geometric view)

$$L(B, \boldsymbol{\vartheta}) = \boldsymbol{\vartheta} \cdot \boldsymbol{A}\boldsymbol{\vartheta} \qquad \text{with} \qquad \boldsymbol{A} := \begin{bmatrix} a_1 & 0 \\ 0 & a_2 \end{bmatrix}, \; a_1 \ll a_2$$

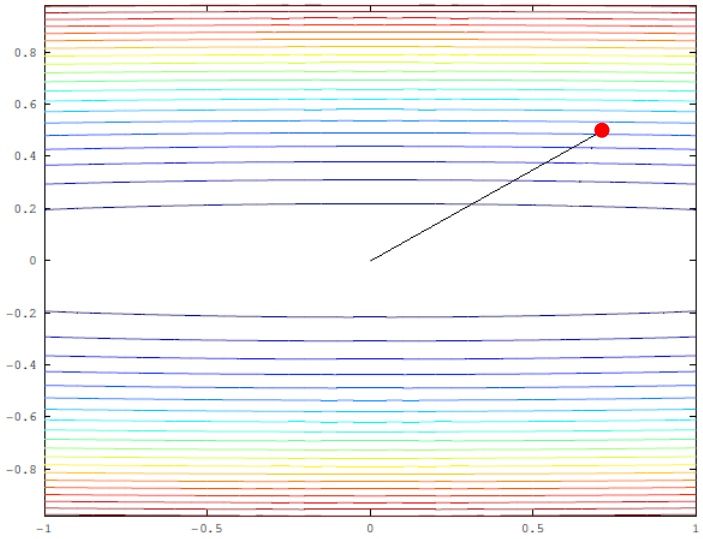
Gradient Descent

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta 2\boldsymbol{A}\boldsymbol{\vartheta}^{(t-1)}$$



Newton-Raphson

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta\boldsymbol{\vartheta}^{(t-1)}$$



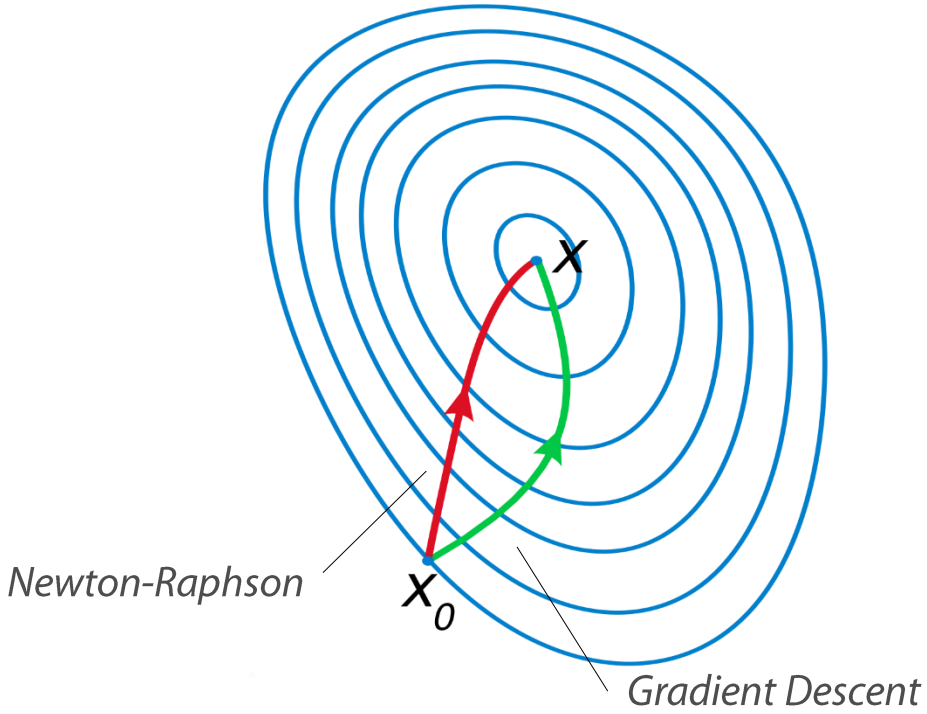
The level curves of a quadratic form in 2D are ellipses centered in the origin

2nd order methods

- ***Newton-Raphson's optimization method***

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta\, \boldsymbol{H}^{-1} \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)}) \qquad \boldsymbol{H} := \frac{\partial}{\partial \boldsymbol{\vartheta}} \left(\frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)}) \right)$$

The (inverse of the) Hessian Matrix considers the curvature



AdaGrad

- ***Newton-Raphson's optimization method***

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta\, \boldsymbol{H}^{-1} \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)}) \qquad \boldsymbol{H} := \frac{\partial}{\partial \boldsymbol{\vartheta}} \left(\frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)}) \right)$$

However

- Computing the inverse Hessian matrix is not easy, in general
- It requires $\mathcal{O}(d^3)$ time versus $\mathcal{O}(d)$ of the gradient — *d is the number of parameters*

AdaGrad

- ***Newton-Raphson's optimization method***

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta\, \boldsymbol{H}^{-1} \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)}) \qquad \boldsymbol{H} := \frac{\partial}{\partial \boldsymbol{\vartheta}} \left(\frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)}) \right)$$

However

- Computing the inverse Hessian matrix is not easy, in general
- It requires $\mathcal{O}(d^3)$ time versus $\mathcal{O}(d)$ of the gradient — *d is the number of parameters*

- ***AdaGrad approximation***

$$G_i^{(t)} := \sqrt{\sum_{j=1}^{t} \left(\frac{\partial}{\partial \vartheta_i} L(B, \boldsymbol{\vartheta}^{(j)}) \right)^2} \qquad \boldsymbol{G}^{(t)} := \begin{bmatrix} G_1^{(t)} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & G_d^{(t)} \end{bmatrix}$$

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta\, (\boldsymbol{G}^{(t-1)})^{-1} \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$

AdaGrad

Gradient Descent

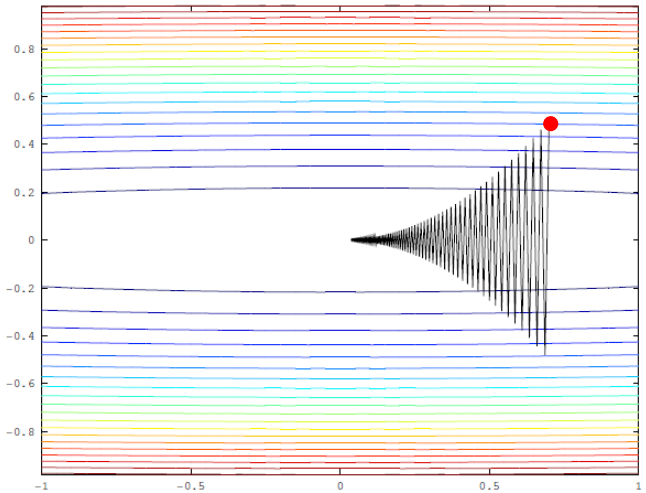
$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta \, \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$

Newton-Raphson

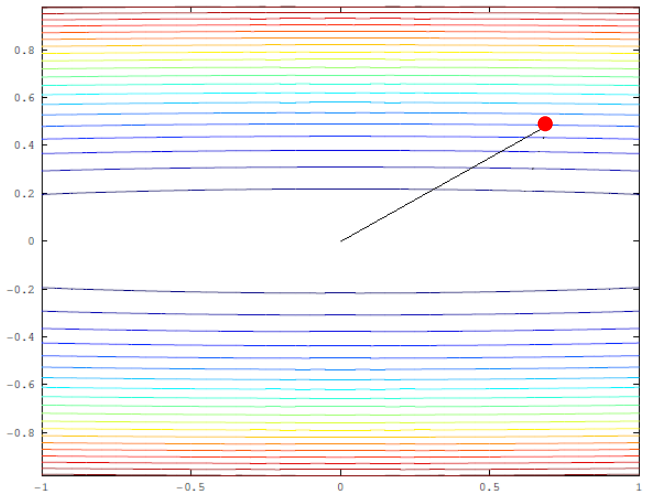
$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta \, \boldsymbol{H}^{-1} \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$

AdaGrad

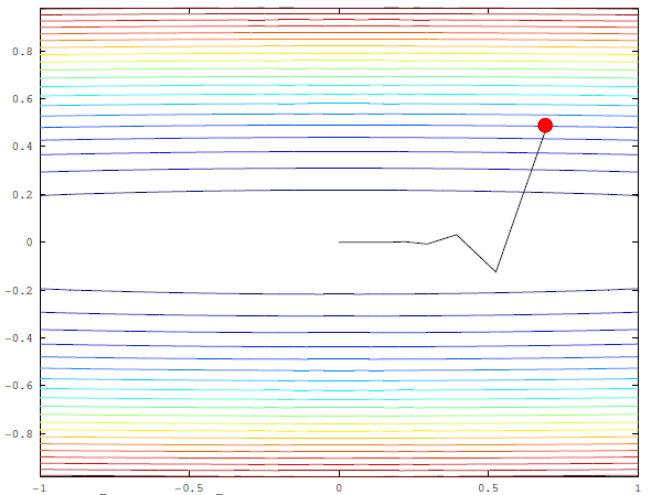
$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta \, (\boldsymbol{G}^{(t-1)})^{-1} \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$



Gradient Descent



Newton-Raphson



AdaGrad

RMSprop

- **AdaGrad approximation**

$$G_i^{(t)} := \sqrt{\sum_{j=1}^{t} \left(\frac{\partial}{\partial \vartheta_i} L(B, \boldsymbol{\vartheta}^{(j)}) \right)^2}$$

- **RMSprop approximation**

The overall sum is replaced by the exponential moving average (EMA)

$$g_i^{(t)} := \frac{\partial}{\partial \vartheta_i} L(B, \boldsymbol{\vartheta}^{(t)})$$

$$\mathrm{EMA}(g_i^2)^{(t)} := \gamma (g_i^{(t)})^2 + (1-\gamma)\mathrm{EMA}(g_i^2)^{(t-1)}$$

$$G_i^{(t)} := \sqrt{\mathrm{EMA}(g_i^2)^{(t)}}$$

$$\boldsymbol{G}^{(t)} := \begin{bmatrix} G_1^{(t)} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & G_d^{(t)} \end{bmatrix}$$

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta \, (\boldsymbol{G}^{(t-1)})^{-1} \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$

AdaDelta

- ***RMSprop approximation***

$$g_i^{(t)} := \frac{\partial}{\partial \vartheta_i} L(B, \boldsymbol{\vartheta}^{(t)})$$

$$\text{EMA}(g_i^2)^{(t)} := \gamma (g_i^{(t)})^2 + (1-\gamma)\text{EMA}(g_i^2)^{(t-1)}$$

$$G_i^{(t)} := \sqrt{\text{EMA}(g_i^2)^{(t)}}$$

Hessian approximation

$$\boldsymbol{G}^{(t)} := \begin{bmatrix} G_1^{(t)} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & G_d^{(t)} \end{bmatrix}$$

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta \, (\boldsymbol{G}^{(t-1)})^{-1} \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$

- ***AdaDelta approximation***

$$D_i^{(t)} := \sqrt{\text{EMA}(\Delta \vartheta_i^2)^{(t)}}$$

'momentum' factor

$$\boldsymbol{D}^{(t)} := \begin{bmatrix} D_1^{(t)} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & D_d^{(t)} \end{bmatrix}$$

$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta \, \boldsymbol{D}^{(t-1)} (\boldsymbol{G}^{(t-1)})^{-1} \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$

Improving optimization

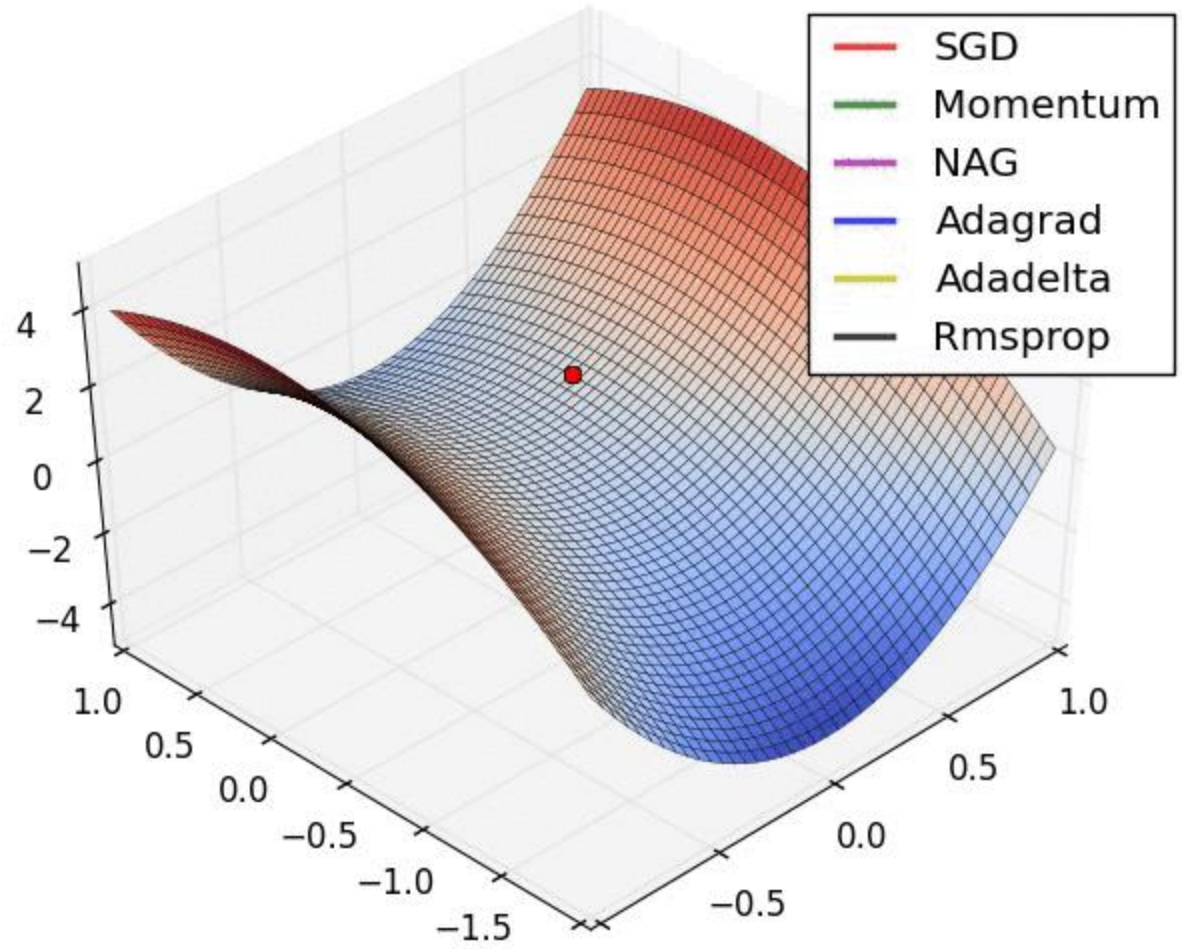
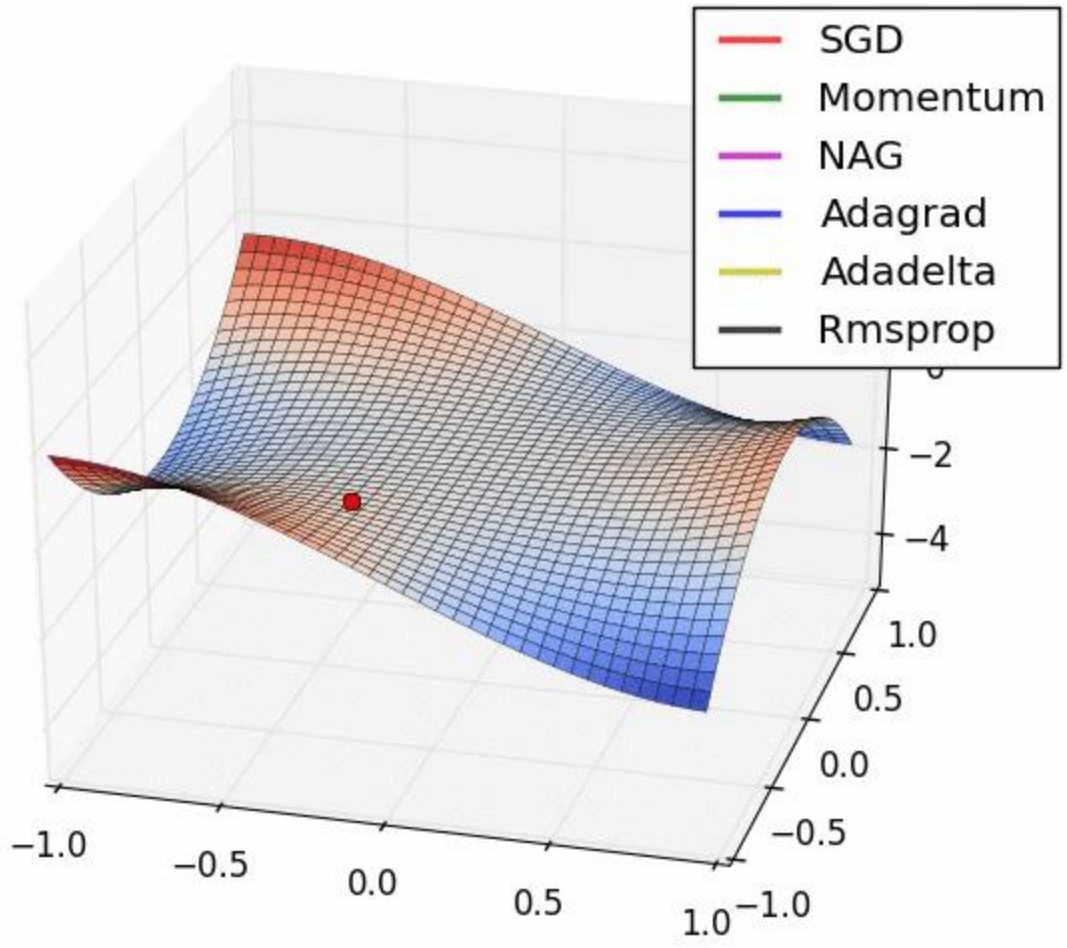


Image from https://imgur.com/a/Hqolp

Improving optimization



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Improving optimization

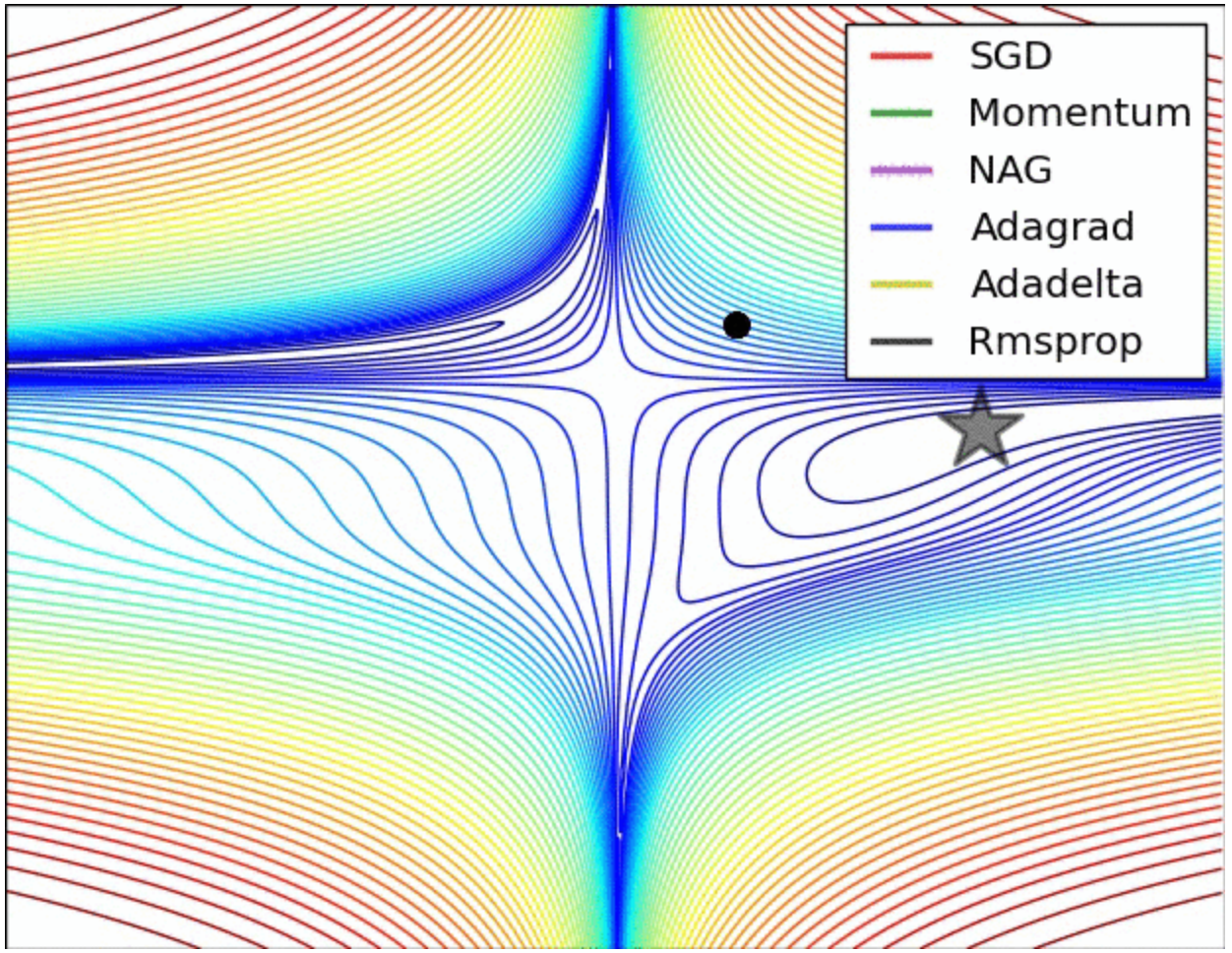


Image from https://imgur.com/a/Hqolp

Adam

- ***Replace components with their EMAs …***

$$m_i^{(t)} := \beta_1(g_i^{(t)}) + (1-\beta_1)m_i^{(t-1)} \qquad \boldsymbol{m}^{(t)} := \begin{bmatrix} m_1^{(t)} \\ \vdots \\ m_d^{(t)} \end{bmatrix}$$

EMA of the gradient

$$r_i^{(t)} := \beta_2(g_i^{(t)})^2 + (1-\beta_2)r_i^{(t-1)} \qquad \boldsymbol{r}^{(t)} := \begin{bmatrix} r_1^{(t)} \\ \vdots \\ r_d^{(t)} \end{bmatrix}$$

EMA of the Hessian approximation (vector form)

$$\hat{\boldsymbol{m}}^{(t)} := \frac{\boldsymbol{m}^{(t)}}{1-(1-\beta_1)^t}$$

$$\hat{\boldsymbol{r}}^{(t)} := \frac{\boldsymbol{r}^{(t)}}{1-(1-\beta_2)^t}$$

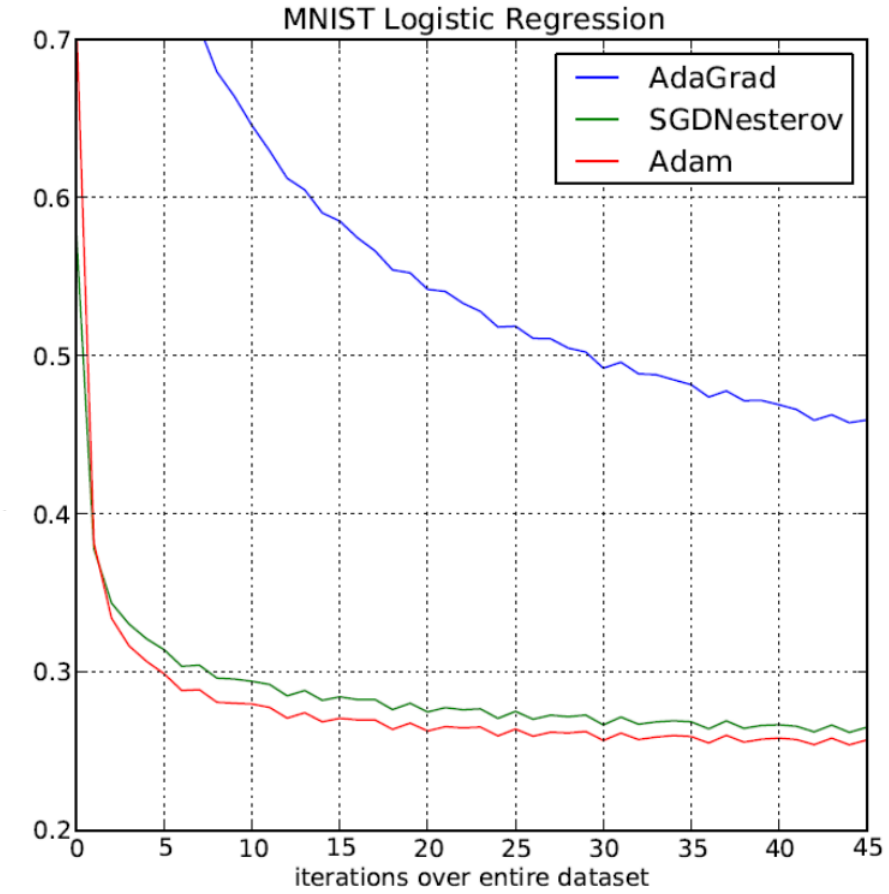
bias corrections (decay with time)

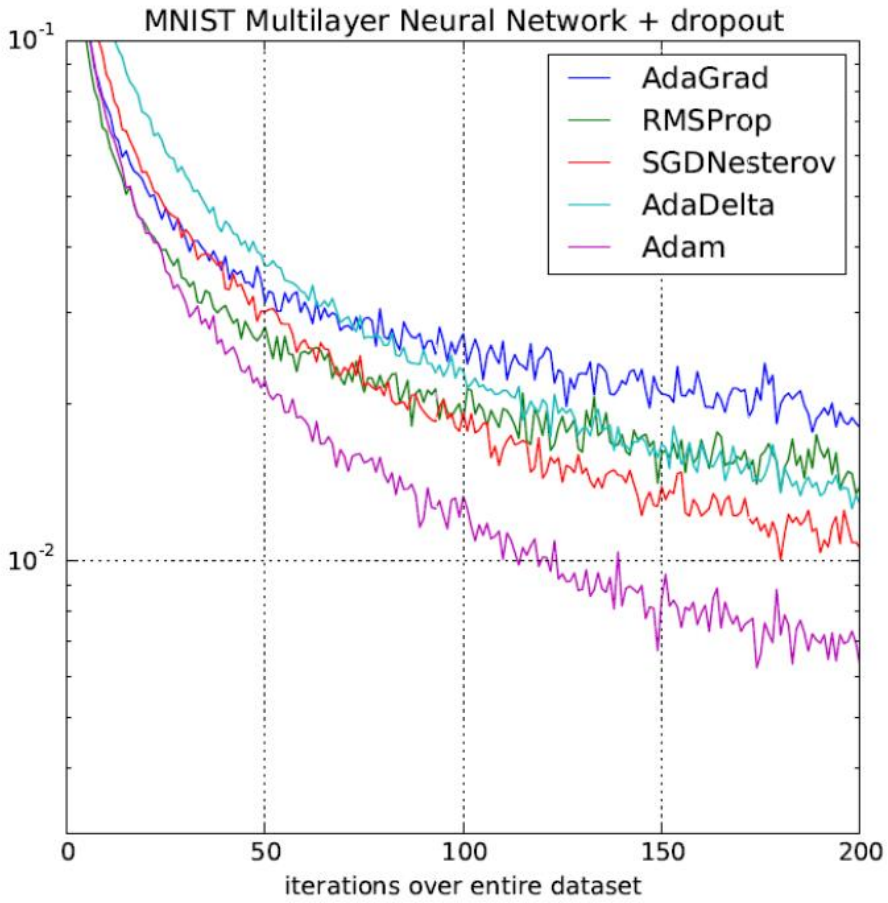
$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta \, \frac{\hat{\boldsymbol{m}}^{(t-1)}}{\sqrt{\hat{\boldsymbol{r}}^{(t-1)}}}$$

(elementwise)

Adam

- ***Experimentally***





Improving optimization

- ***Messages to take home***

  - Improved optimizers adopt a combination of intuition and mathematical modeling
  - In particular, some of them are *approximators* to 2nd order optimization methods
  - As such, there is no formal guarantee that they will be effective in *all* cases

  Moral: in general, their effectiveness will depend on the optimization problem and the representation being used

A bag of wonderful tricks

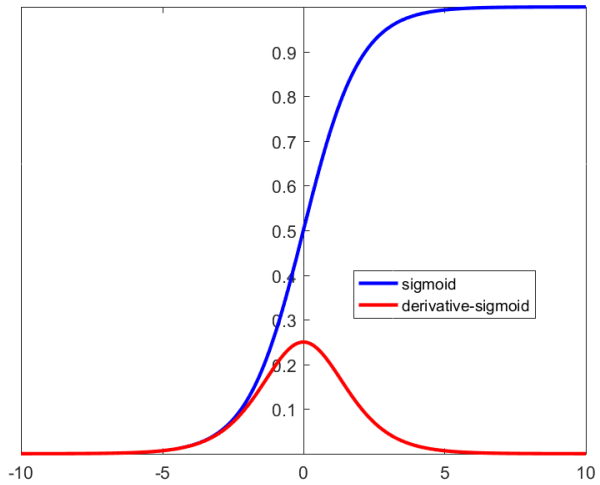
Why ReLU is better (sometimes)

The gradient descent method implies updating the parameters at each step: making sure that the gradient does not either *vanish* or *explode* is not easy

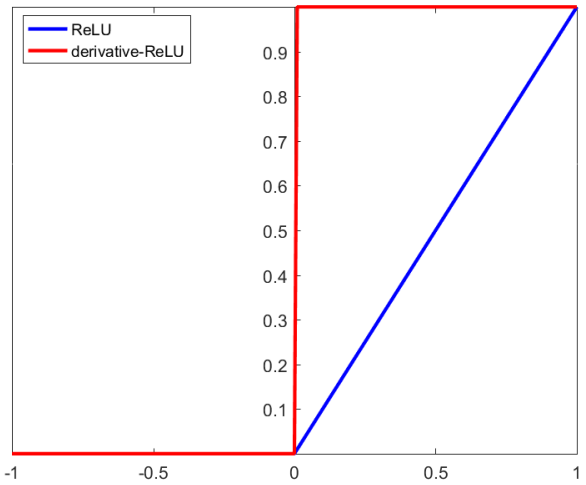
For instance, in

$$\Delta \boldsymbol{W} = -\eta \frac{\partial L}{\partial \boldsymbol{W}}(\tilde{y}^{(i)}, y^{(i)})$$

the gradient contains a multiplicative term $\frac{\partial}{\partial x} g(x)$
which can be $\ll 1.0$



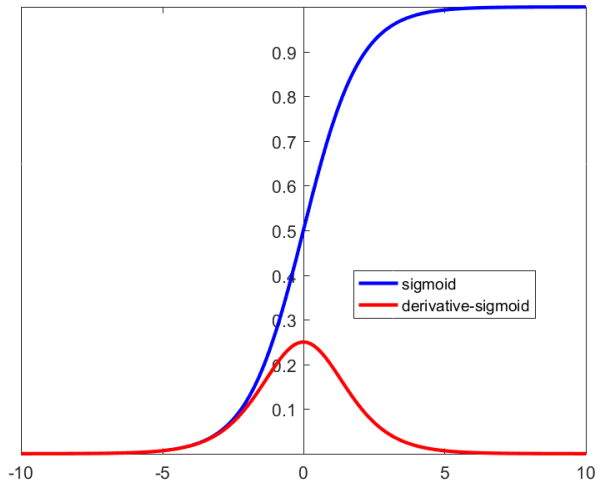
In general, the derivative of ReLU does not suffer from the same problem



Why ReLU is better (sometimes)

In experimental practice (*sometimes*):

- ReLU alleviates the problem of initial values
  (i.e. when initial values are too far away and cause sigmoid or tanh to saturate)



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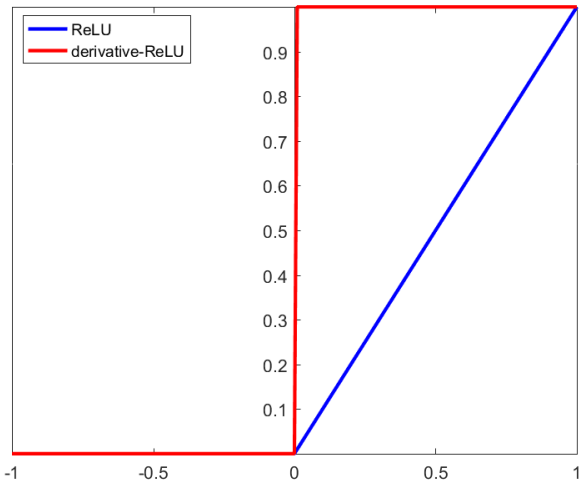


Why ReLU is better (sometimes)

In experimental practice (*sometimes*):

- ReLU alleviates the problem of initial values
  (i.e. when initial values are too far away and cause sigmoid or tanh to saturate)
- ReLU may accelerate the training process

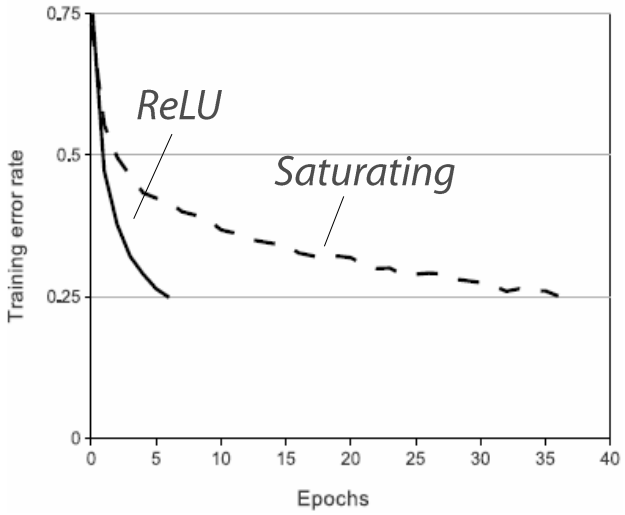
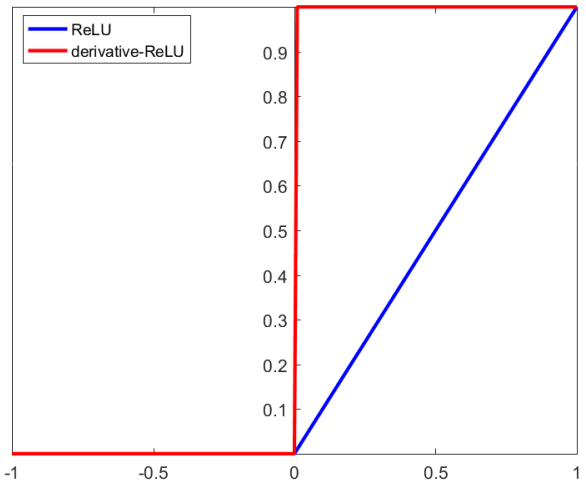


Image from [Krizhevsky, Sutskever & Hinton, 2012]



Xavier (Glorot) Initialization

- ***The problem of initialization***

  Have a look to the demo at: https://www.deeplearning.ai/ai-notes/initialization/index.html

  See what happens when the initial weights are either too small or too large

- ***Objectives***

  1. *The mean of the activations should be zero*
  2. *The variance of the activations should stay the same across layers*

- ***Strategy***

$$\boldsymbol{W}^{[l]} \sim \mathcal{N}\left(0, \frac{1}{h^{[l-1]}}\right) \quad \text{or} \quad \boldsymbol{W}^{[l]} \sim \mathcal{N}\left(0, \frac{2}{h^{[l-1]} + h^{[l]}}\right)$$

$$\boldsymbol{b}^{[l]} = 0$$

where: $\boldsymbol{W}^{[l]} \in \mathbb{R}^{h^{[l]} \times h^{[l-1]}}$

Under some simplifying assumptions, this makes all layers have the same variance

(see the link above for a complete mathematical justification)

Input Normalization

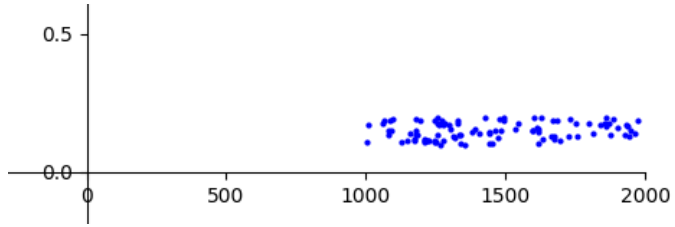
- ***Intuition***

  Consider the (very simple) layer

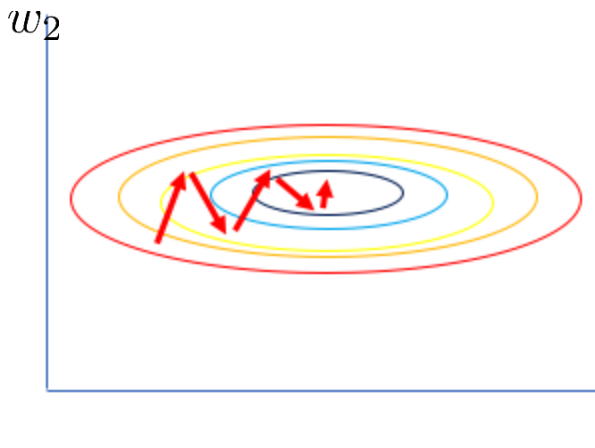
$$h(\boldsymbol{x}) := g(\boldsymbol{w}\boldsymbol{x} + b) = g(w_1 x_1 + w_2 x_2 + b)$$

  and suppose $x_1 \in [1000, 2000],\ x_2 \in [0.1, 0.2]$

  x_1 and x_2 are in completely different scales



  - w_1 influences h a lot more than w_2
  - training w_2 is challenging and slow



level curves of loss function (during training)

Image from https://https://www.jeremyjordan.me/batch-normalization/

Input Normalization

- ***Input normalization***

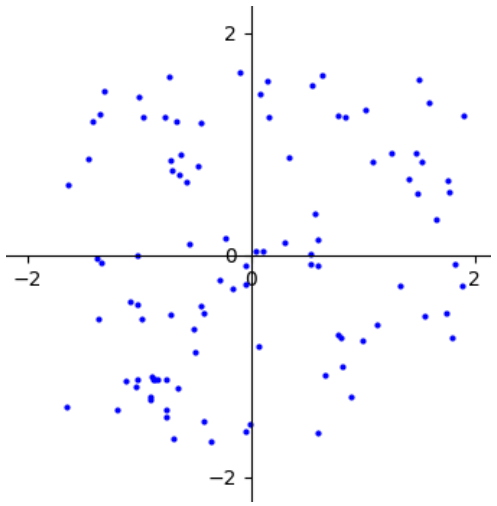
1) compute **mean** $\boldsymbol{\mu}$ and (*component-wise*) **variance** $\boldsymbol{\sigma}^2$ of inputs over dataset D

$$\boldsymbol{\mu} := \frac{1}{|D|} \sum_{\boldsymbol{x} \in D} \boldsymbol{x} \qquad \boldsymbol{\sigma}^2 := (\sigma_1^2, \ldots, \sigma_d^2,) \quad \text{with } \sigma_i^2 := \frac{1}{|D|} \sum_{\boldsymbol{x} \in D} (x_i - \mu_i)^2$$

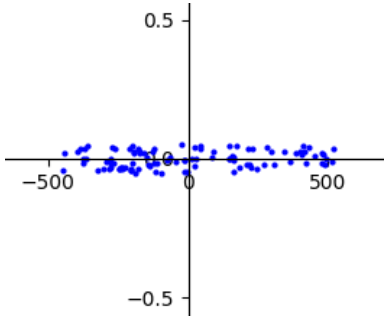
2) normalize all inputs, component-wise

$$\hat{\boldsymbol{x}} := (\hat{x}_1, \ldots, \hat{x}_d), \quad \text{with } \hat{x}_i := \frac{x_i - \mu_i}{\sqrt{\sigma_i^2 + \epsilon}}$$

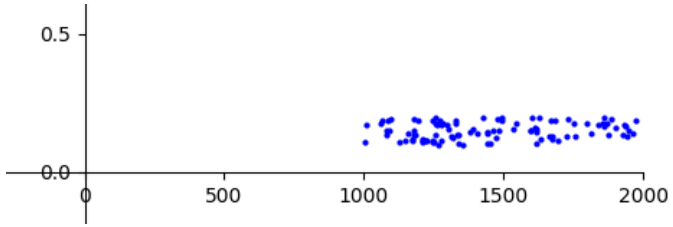
to avoid division by zero



rescale each component by $\frac{1}{\sqrt{\sigma_i^2 + \epsilon}}$



shift by $\boldsymbol{\mu}$



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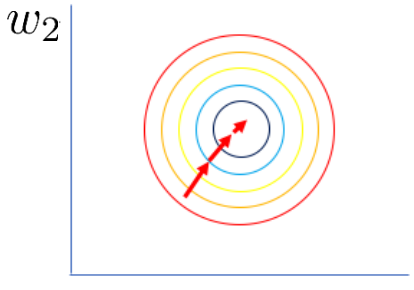
- training becomes
  faster and *more stable*
  (also allowing higher learning rates)



level curves of the loss function (during training)

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Batch Normalization

- ***Normalizing in between layers***

  In a *DNN*

$$\tilde{\boldsymbol{y}} = \boldsymbol{h}^{[n]}(\boldsymbol{h}^{[n-1]}(\ldots(\boldsymbol{h}^{[2]}(\boldsymbol{h}^{[1]}(\boldsymbol{x})))\ldots))$$

  each layer $\boldsymbol{h}^{[i]}$ has an input of its own, which should be *normalized*

  How?

Batch Normalization

- ***Normalizing in between layers***

  In a *DNN*

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  Normalizing in between layers during training would require:

  - pre-computing the input to each layer, for *each data item* in D
  - applying normalization before proceeding further upwards
  - doing it again after *each* updating the DNN parameters

  Moral: *it's impossible*

Batch Normalization

- **For each mini-batch:**

$$B = \left\{ \boldsymbol{x}^{(i)} \right\}_{i=1}^{m}$$

(all operations are performed element-wise)

$$\mathrm{BN}_{\boldsymbol{\beta},\boldsymbol{\gamma}}(\boldsymbol{x}^{(i)}) := \boldsymbol{\gamma}\hat{\boldsymbol{x}}^{(i)} + \boldsymbol{\beta}$$

trainable parameters

$$\hat{\boldsymbol{x}}^{(i)} = \frac{\boldsymbol{x}^{(i)} - \boldsymbol{\mu}_B}{\sqrt{\boldsymbol{\sigma}_B^2 + \epsilon}}$$

avoid division by zero

$$\boldsymbol{\sigma}_B^2 = \frac{1}{m}\sum_{i=1}^{m}(\boldsymbol{x}^{(i)} - \boldsymbol{\mu}_B)$$

$$\boldsymbol{\mu}_B = \frac{1}{m}\sum_{i=1}^{m}\boldsymbol{x}^{(i)}$$

Batch Normalization

- ***Training***
  - at step t: $\boldsymbol{\mu}_{B^{(t)}}$ and $\boldsymbol{\sigma}^2_{B^{(t)}}$ are computed over the *current* mini-batch $B^{(t)}$
  - parameters $\boldsymbol{\gamma}$ and $\boldsymbol{\beta}$ (for each BN-layer) are trained *in the same way as the other parameters in the DNN*
  - *exponential moving averages* of mean and variance of the mini-batches $B^{(t)}$ are *collected*

$$\mathrm{MA}(\boldsymbol{\mu})^{(t)} := \delta \cdot \boldsymbol{\mu}_{B^{(t)}} + (1-\delta) \cdot \mathrm{MA}(\boldsymbol{\mu})^{(t-1)}, \qquad \mathrm{MA}(\boldsymbol{\mu})^{(1)} := \boldsymbol{\mu}_{B^{(1)}}$$
$$\mathrm{MA}(\boldsymbol{\sigma}^2)^{(t)} := \delta \cdot \boldsymbol{\sigma}^2_{B^{(t)}} + (1-\delta) \cdot \mathrm{MA}(\boldsymbol{\sigma}^2)^{(t-1)}, \qquad \mathrm{MA}(\boldsymbol{\sigma}^2)^{(1)} := \boldsymbol{\sigma}^2_{B^{(1)}}$$

- ***Inference***

  Inference is typically performed for fewer inputs, possibly just one ...

Batch Normalization

- ***Training***
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- ***Inference***

  Normalize using the moving averages collected *during training*

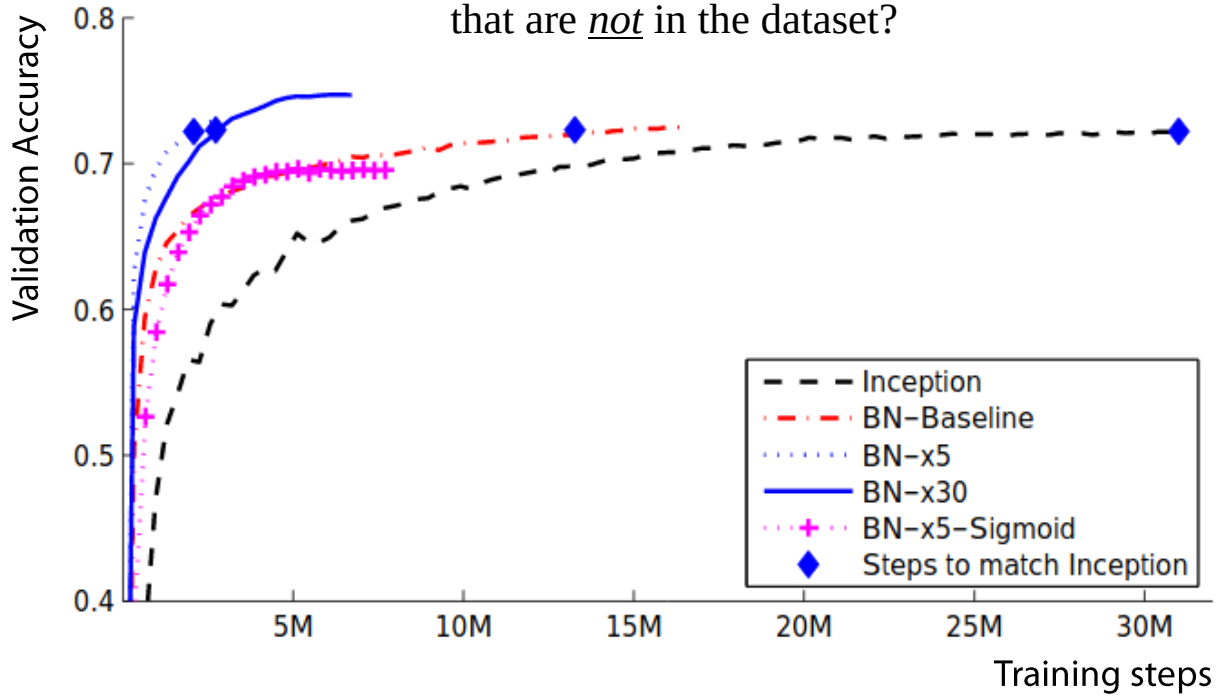
  - $\boldsymbol{\mu} := \mathrm{MA}(\boldsymbol{\mu})^{(T)}$
  - $\boldsymbol{\sigma}^2 := \mathrm{MA}(\boldsymbol{\sigma}^2)^{(T)}$

  as collected during the training process

Batch Normalization

- ***Does it work?***

How good is the approximator when applied to data items that are *not* in the dataset?



- Batch normalization acts as a *reparametrization* of the optimization process that
  1. makes the loss function smoother
  2. allows higher learning rates
  3. reduces chances to getting stuck into local minima

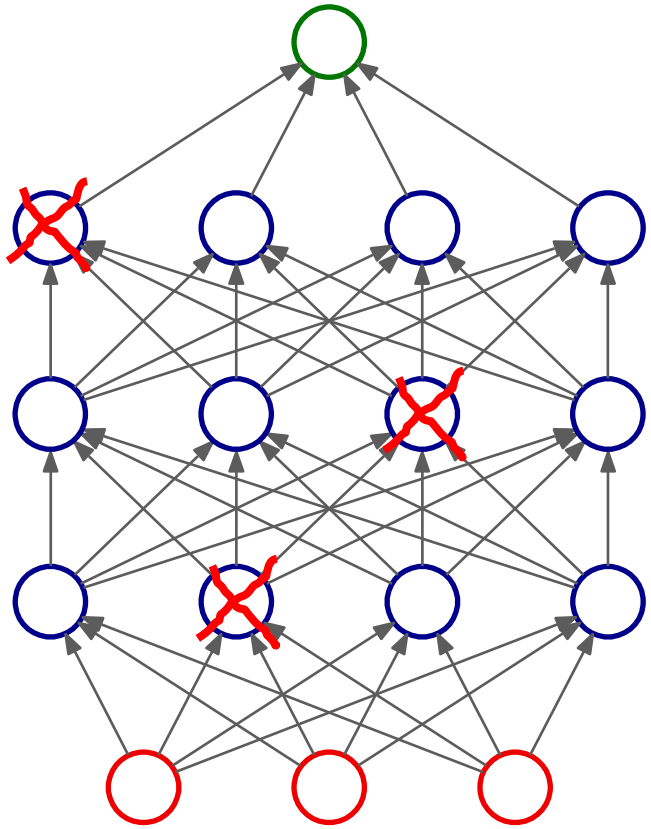
Image from [Ioffe and Szegedy 2015]

Fighting Overfitting

Dropout

- **Knocking-out at random**

  For each mini-batch, a small percentage of 'units' is de-activated



Training: mini-batch 1

Dropout

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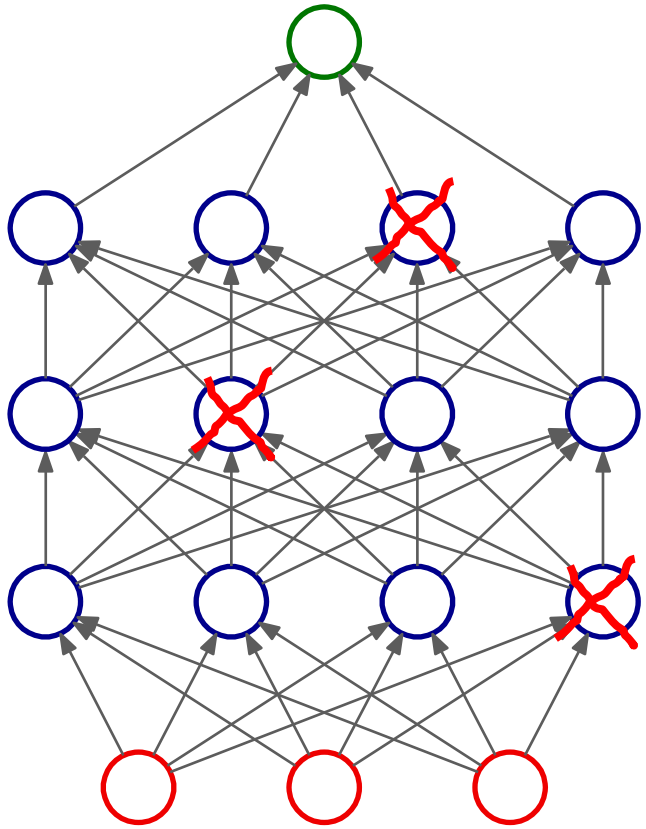
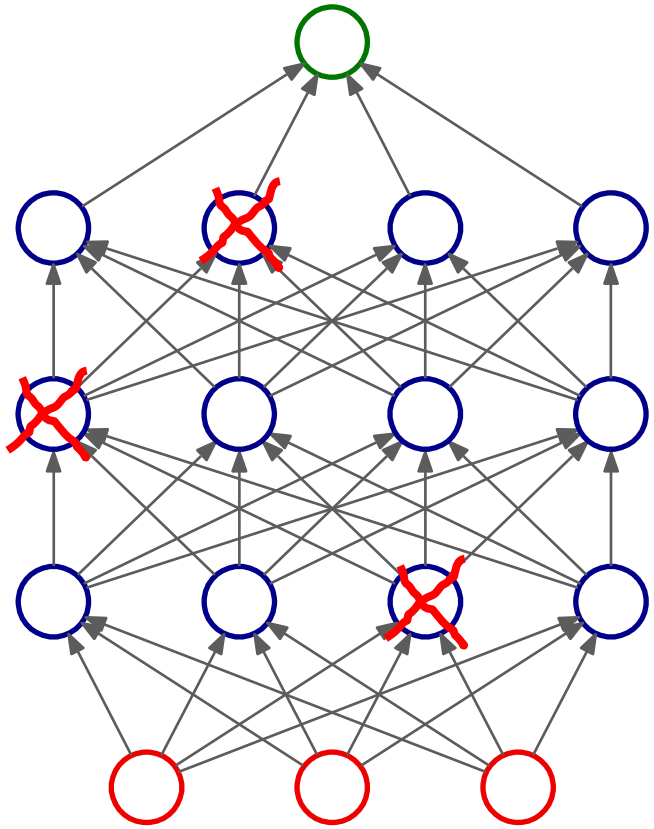


Training: mini-batch 2

Dropout

- **Knocking-out at random**

  For each mini-batch, a small percentage of 'units' is de-activated



Training: mini-batch 3

Dropout

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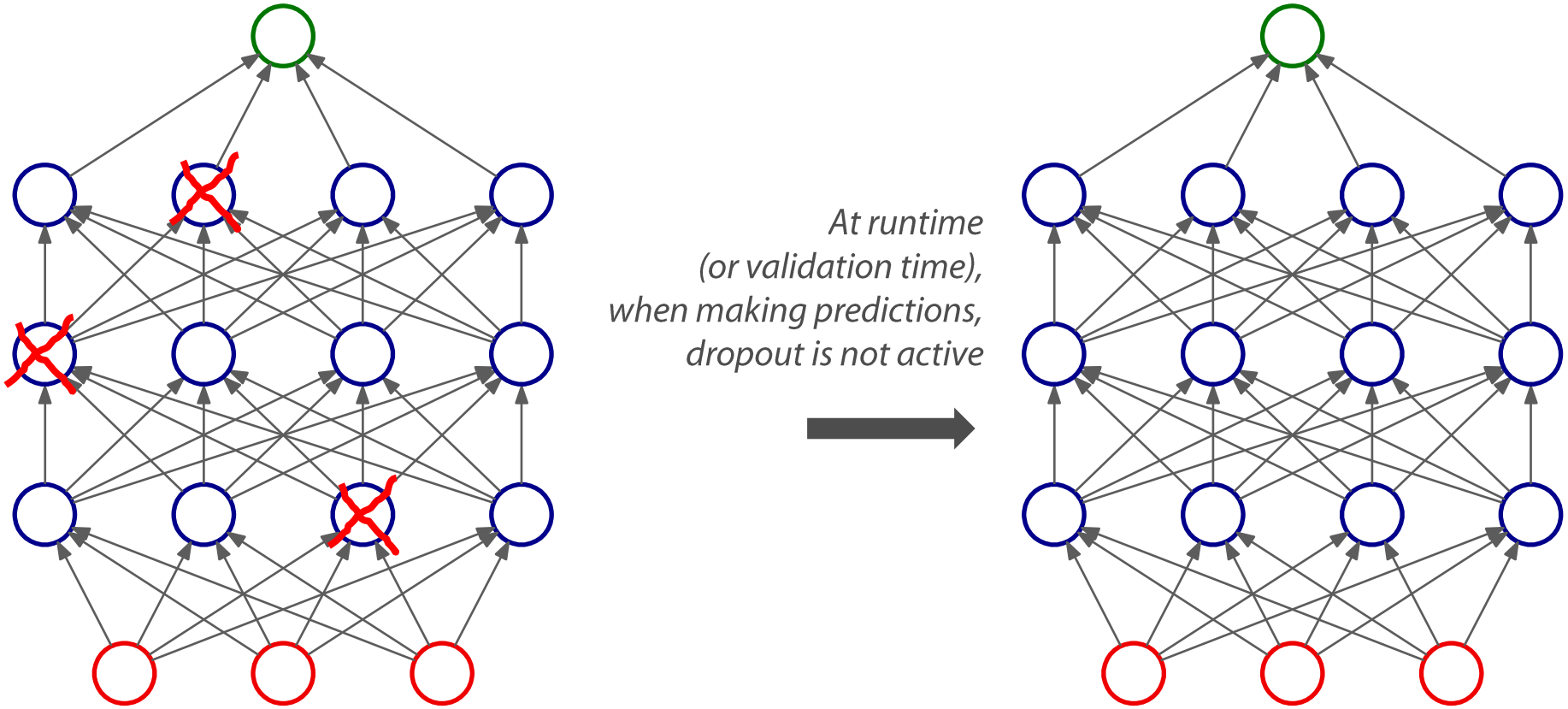

Contrasting Overfitting

- ***Applying Dropout***

  In a typical experiment
  - initially, the performance on D_{val} improves slowly
  - then it becomes better and more resilient to *overfitting* *(to be explained next)*

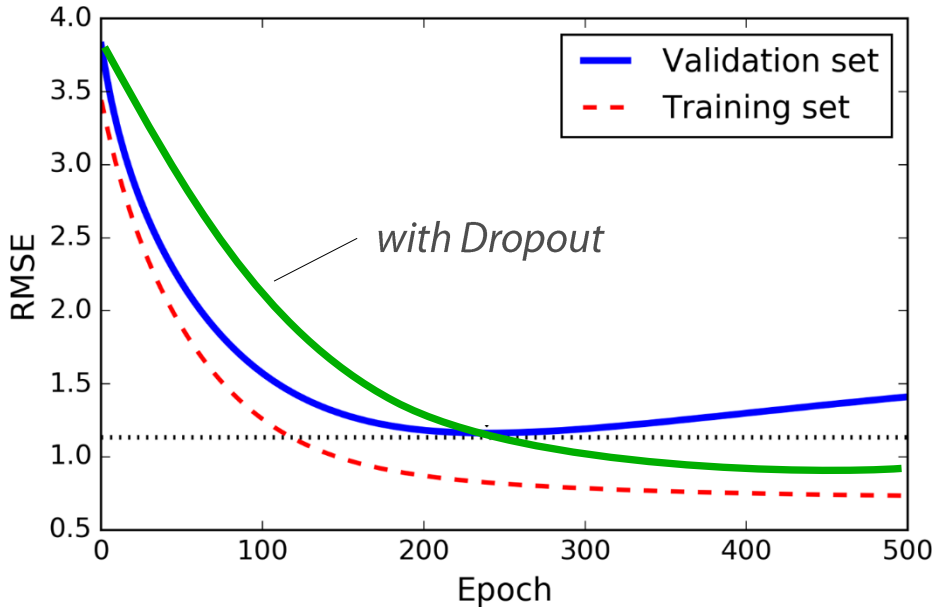

Image from https://www.safaribooksonline.com/library/view/hands-on-machine-learning/9781491962282/ch04.html