Università degli Studi di Pavia

Deep Learning

05- Learning as Optimization

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This presentation can be downloaded at:
http://vision.unipv.it/DL

About why they did not use Deep Networks from the beginning

Problem: vanishing or exploding Gradients

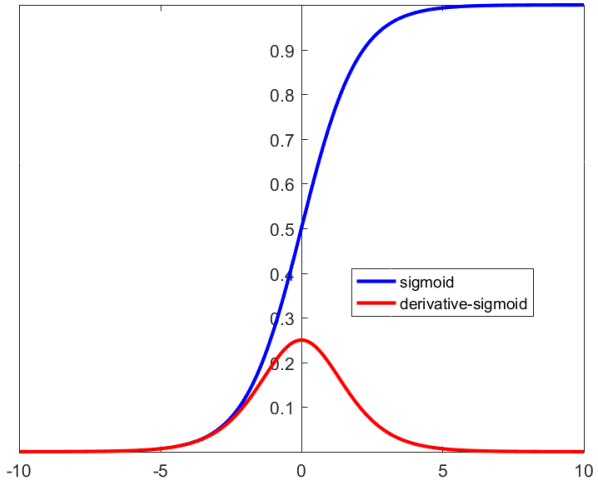
The gradient descent method implies updating the parameters at each step: making sure that the gradient does not either *vanish* or *explode* is not easy

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 either *vanish* or *explode* is not easy

Consider a 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*
- *all hidden layers have the same size* d *of the input*
- *all* $\boldsymbol{W}^{[i]}$ *are identical and diagonalizable, with eigenbasis* $(\boldsymbol{e}_1, \cdots, \boldsymbol{e}_d)$

this means that

i.e. first 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*

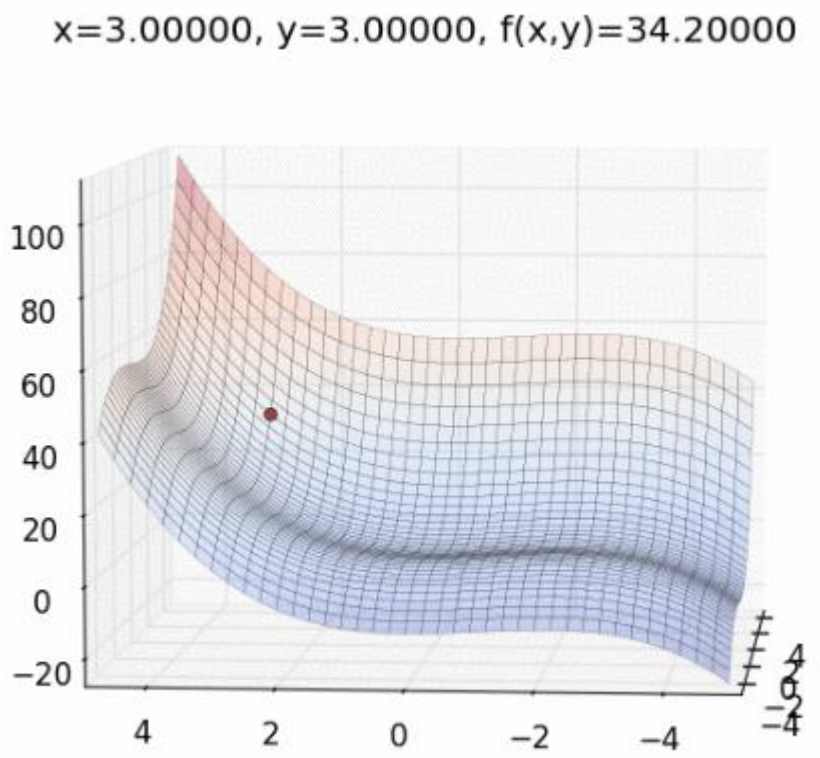
Problem: initial values of the parameters

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)***

  Standard, decaying learning rate
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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*

Momentum

- **Momentum**

  "Let the ball run"

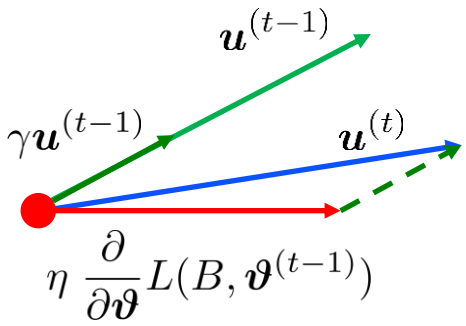
momentum term:
tendency to keep running at the same speed and direction

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

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

$$0 < \gamma < 1$$

"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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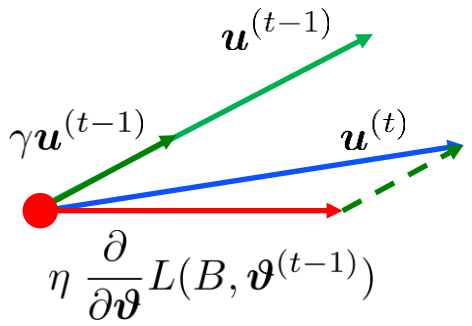
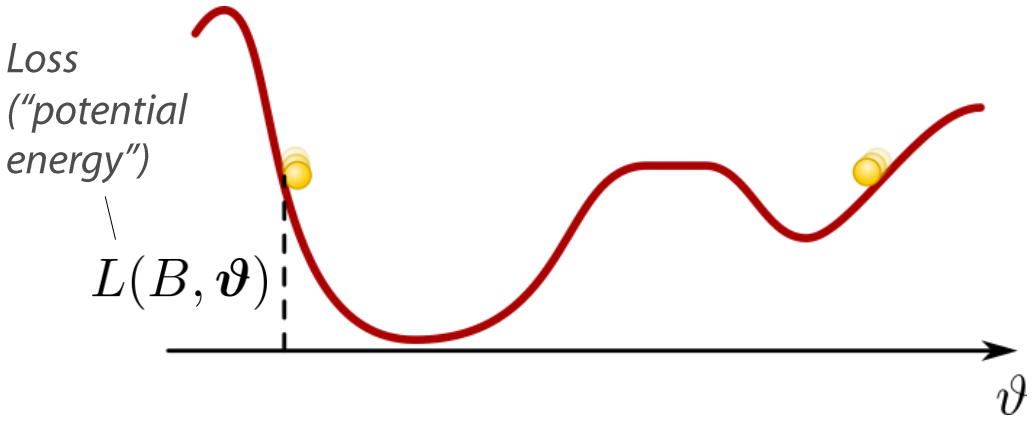




"force felt by the ball"

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

"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)

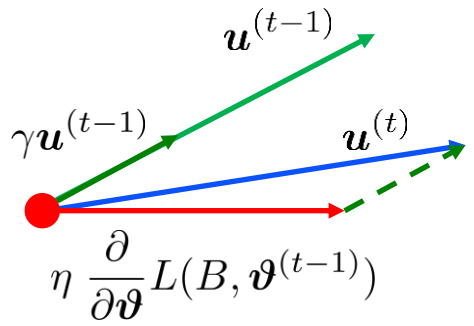
Momentum

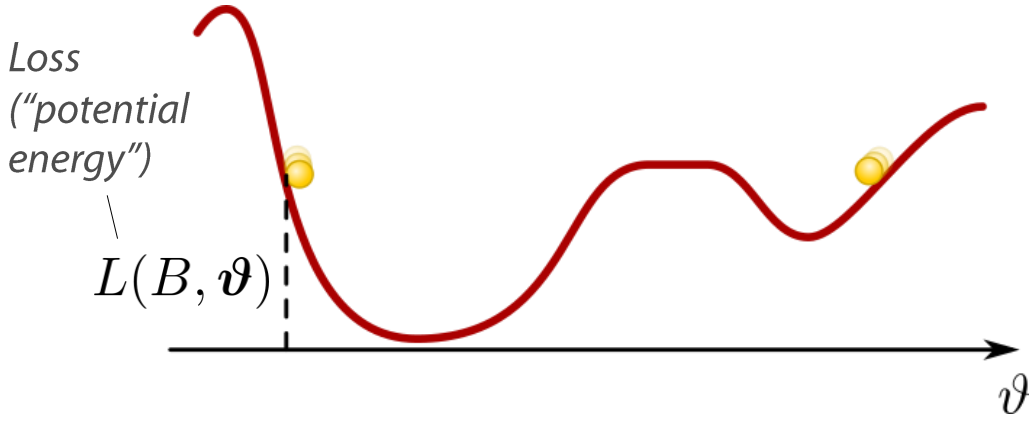
- **Momentum**

  "Let the ball run"

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

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





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

"velocity"

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

"acceleration"

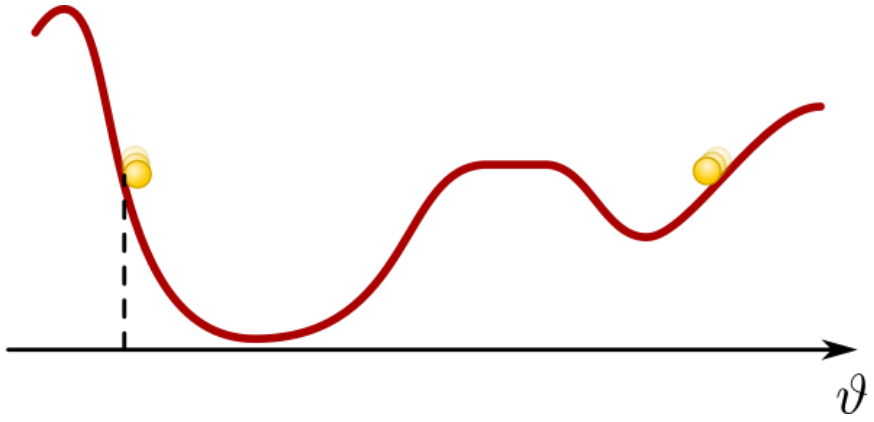
$$\boldsymbol{a} \approx \boldsymbol{u}^{(t)} - \boldsymbol{u}^{(t-1)} \propto -\frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta})$$

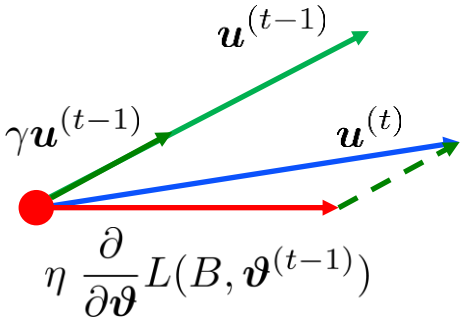
... the gradient directly affects the velocity (not the position)

Momentum

- **Momentum**

  "Let the ball run"





- Update the *velocity* : $\boldsymbol{u}^{(t)} = \gamma \boldsymbol{u}^{(t-1)} + \eta \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)}), \quad \boldsymbol{u}^{(0)} = \mathbf{0}$
- Then the *position*: $\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \boldsymbol{u}^{(t)}$

[See https://cs231n.github.io/neural-networks-3/]

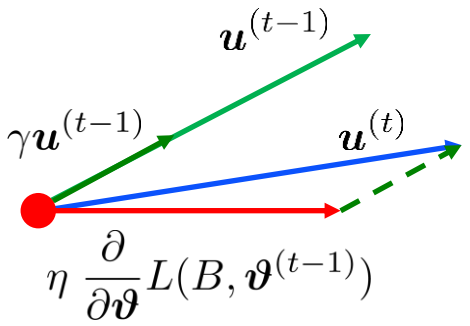
NAG

- **Momentum**

  "Let the ball run"

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

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

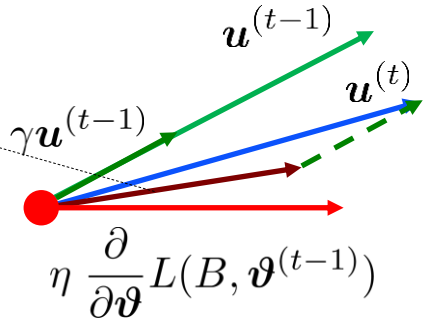


- **Nesterov Accelerated Gradient (NAG)**

  "Let the ball run but be predictive"

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

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



2nd order methods

- **Taylor's expansion**

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

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*

this is 0

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

whence

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

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, does not depend on B

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

where

a diagonal, positive definite matrix (whence 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

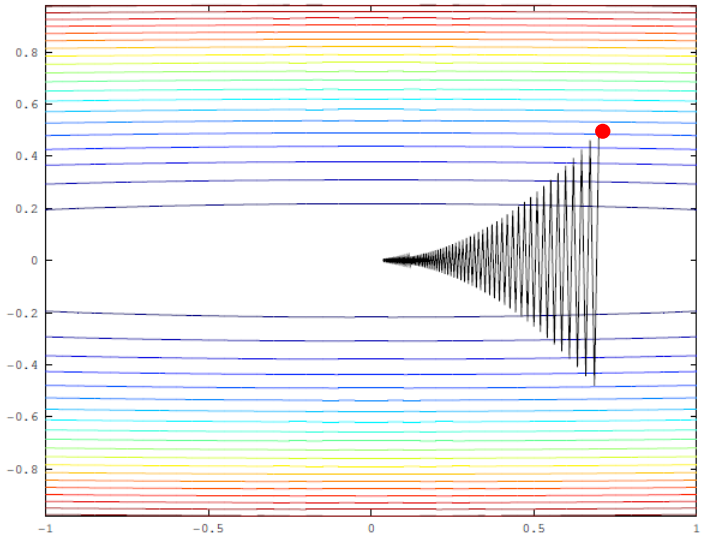
In this example (geometric view)

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

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

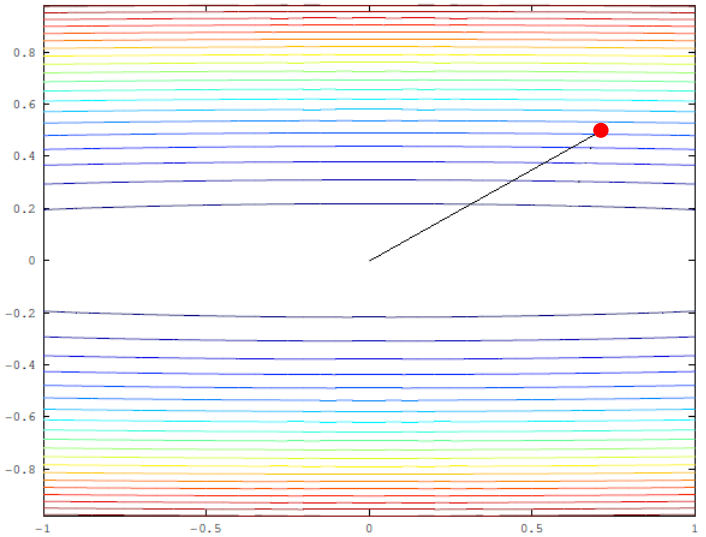
Gradient Descent

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



Newton-Raphson

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



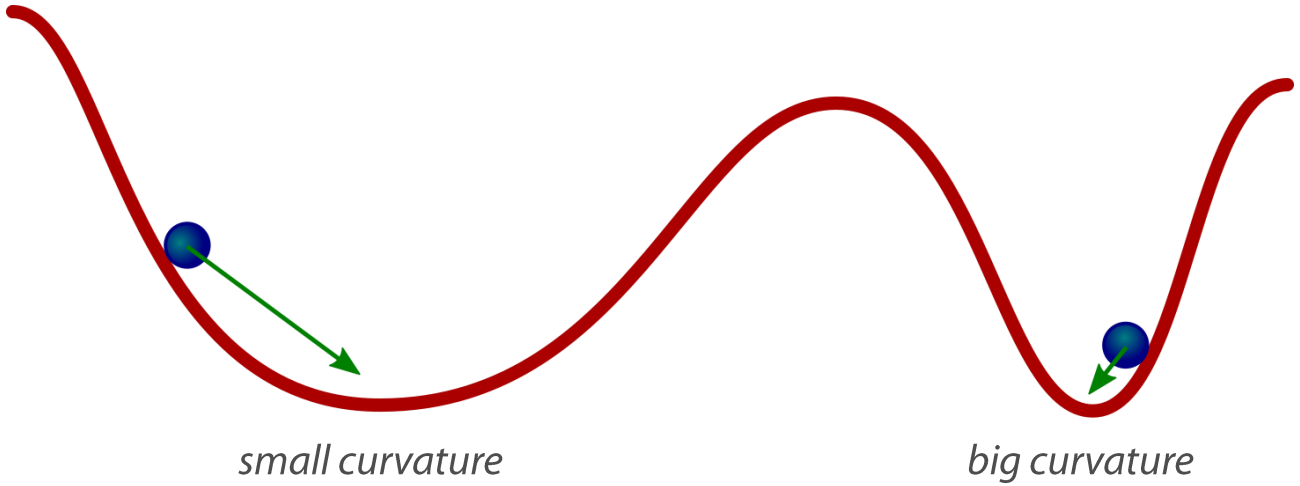
2nd order methods

- ***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 takes into account also the curvature

- A smaller curvature leads to a bigger update step



- ***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

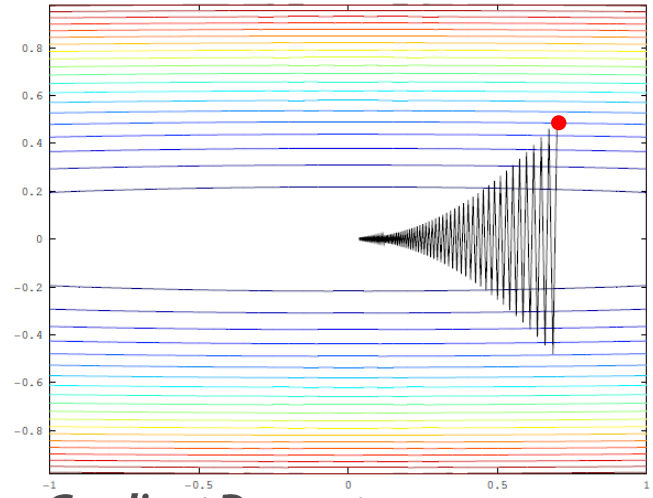
$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$

Newton-Raphson

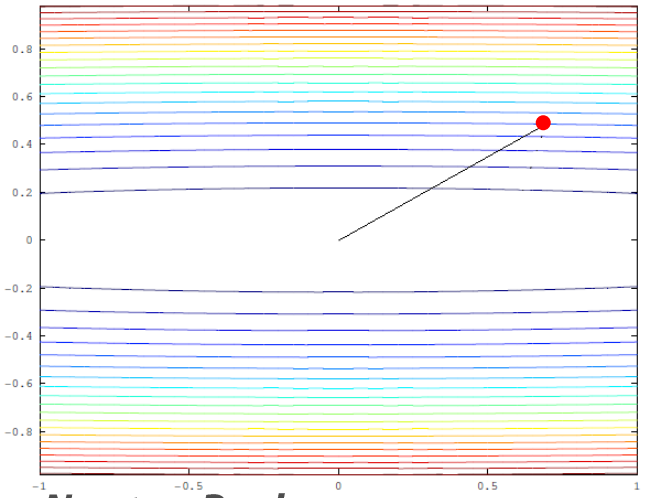
$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta \, \boldsymbol{H}^{-1} \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$

AdaGrad

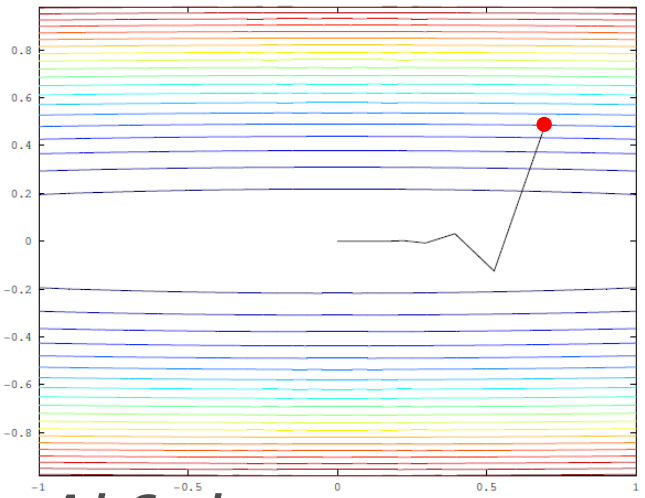
$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta \, (\boldsymbol{G}^{(t-1)})^{-1} \frac{\partial}{\partial \boldsymbol{\vartheta}} L(B, \boldsymbol{\vartheta}^{(t-1)})$$



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***

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

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

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

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***

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

'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

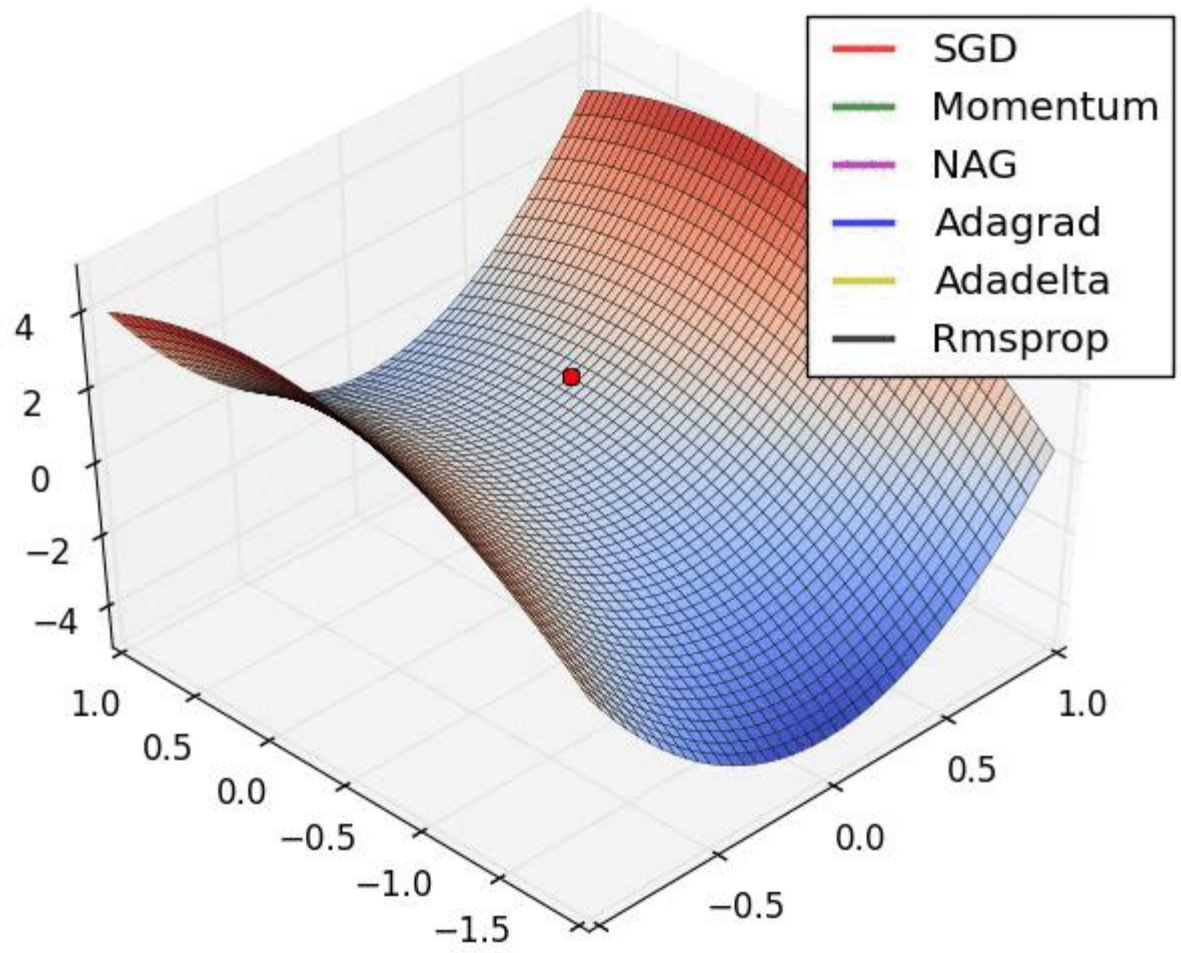
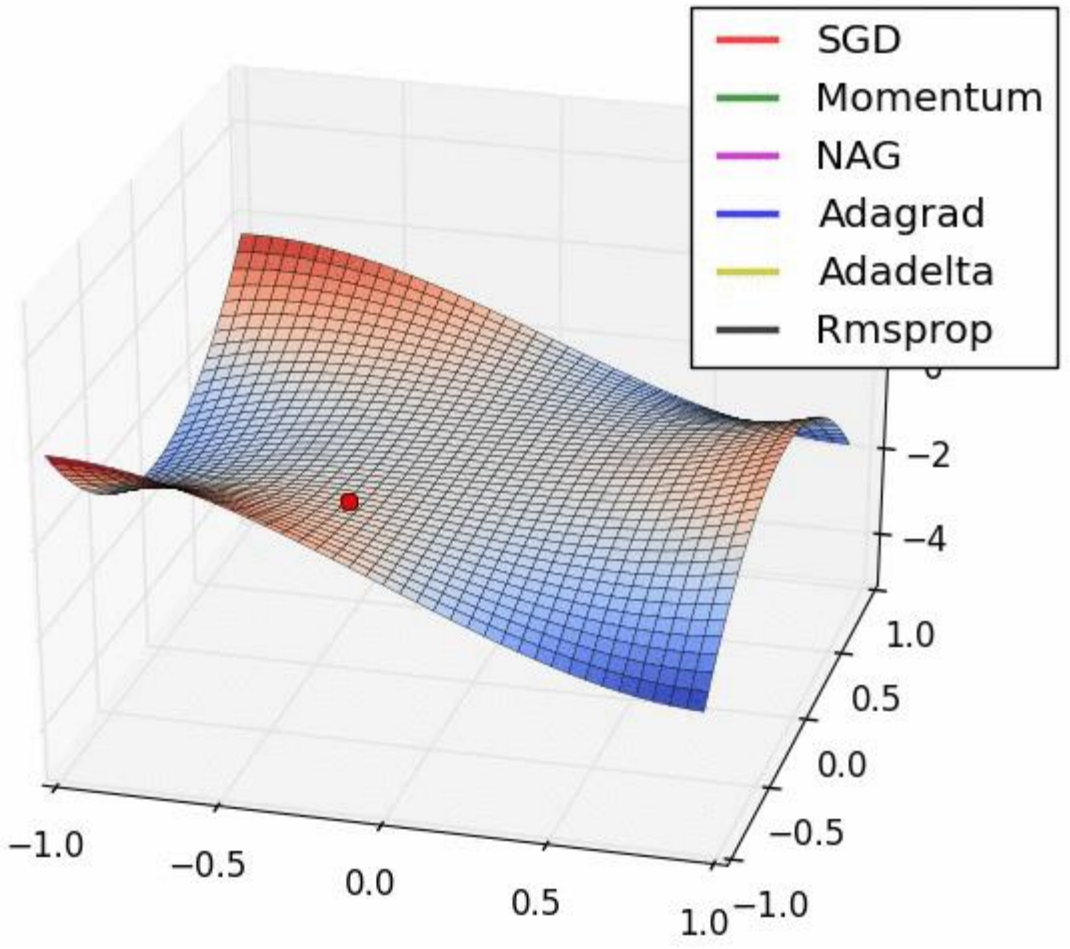


Image from https://imgur.com/a/Hqolp

Improving optimization



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Improving optimization

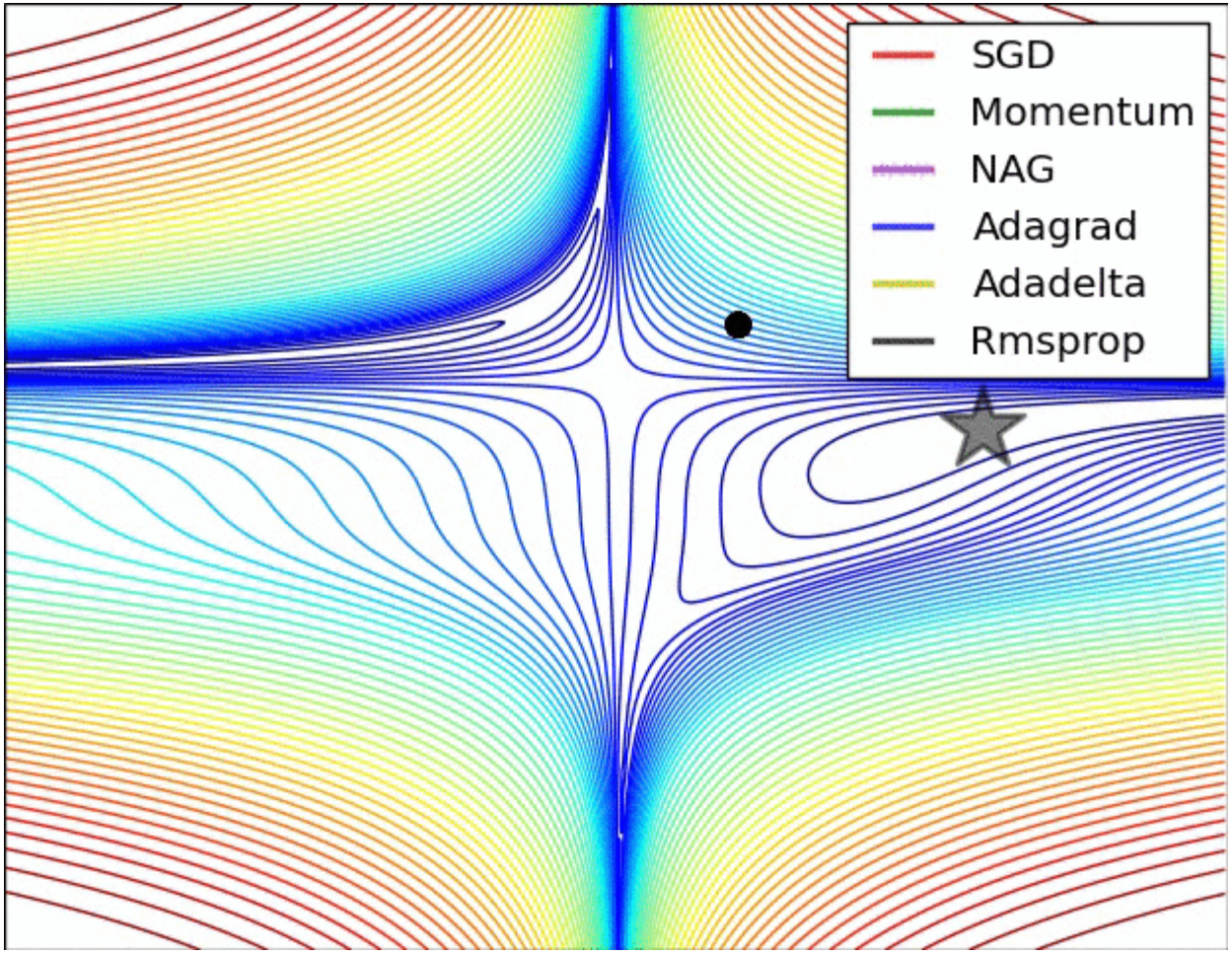


Image from https://imgur.com/a/Hqolp

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)

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

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

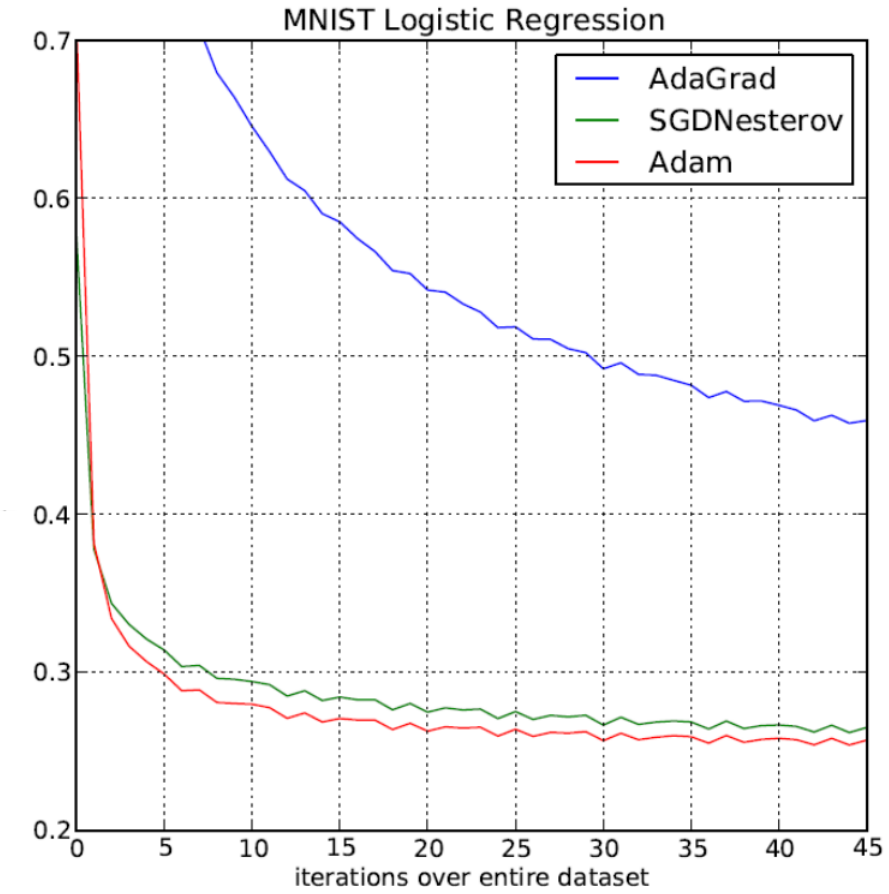
bias corrections (decay with time)

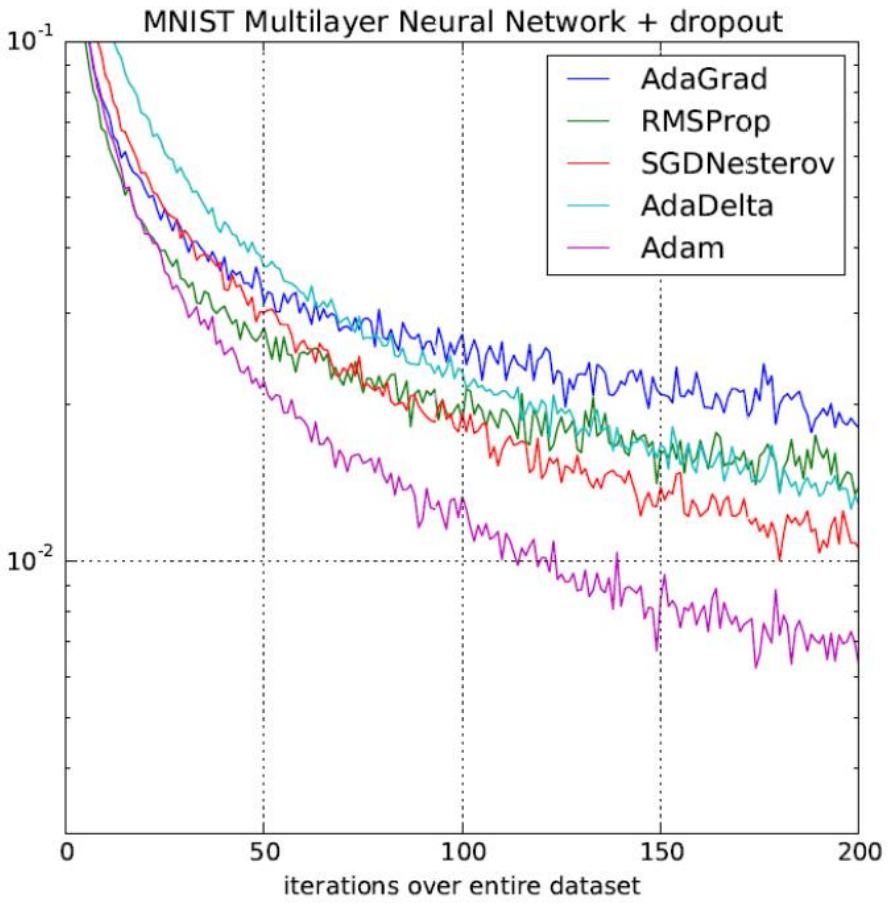
$$\boldsymbol{\vartheta}^{(t)} = \boldsymbol{\vartheta}^{(t-1)} - \eta \, \frac{\hat{\boldsymbol{m}}^{(t-1)}}{\sqrt{\hat{\boldsymbol{r}}^{(t-1)}}}$$

(elementwise)

Adam

- ***Experimentally***





A bag of wonderful tricks

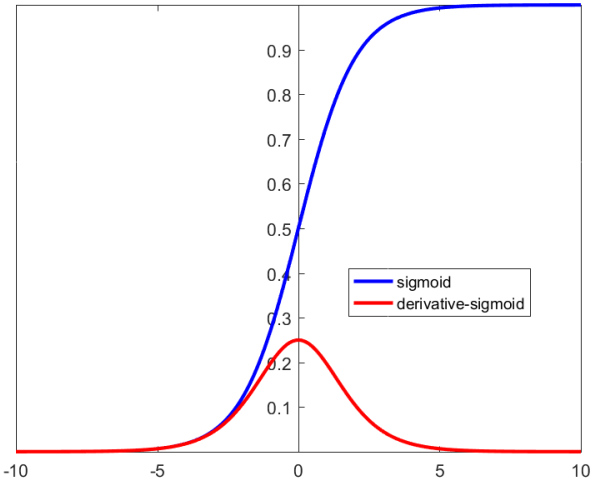
Why ReLU is better (sometimes)

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

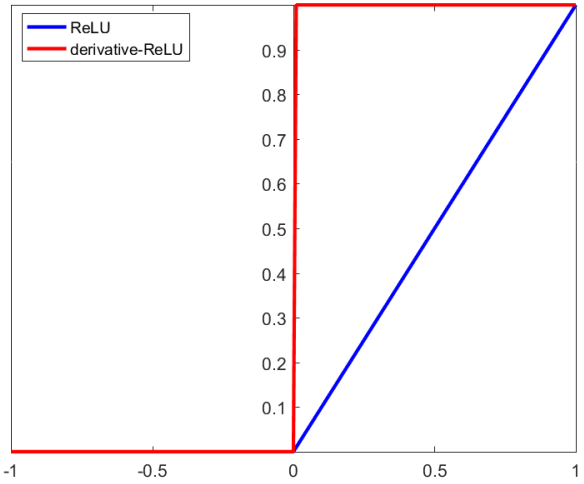
For instance, in

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

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



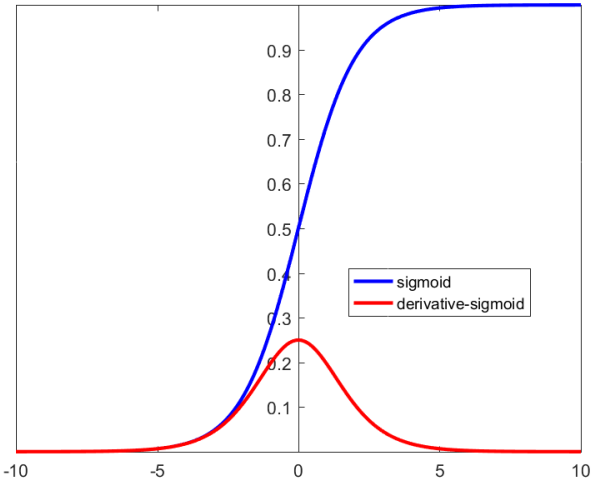
In general, the derivative of ReLU does not suffer from the same problem



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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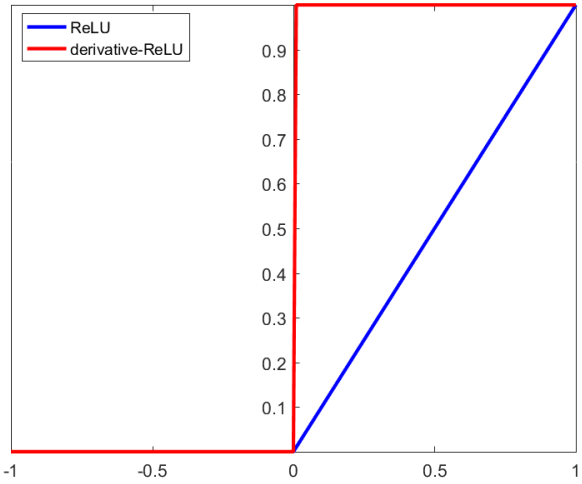


Why ReLU is better (sometimes)

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

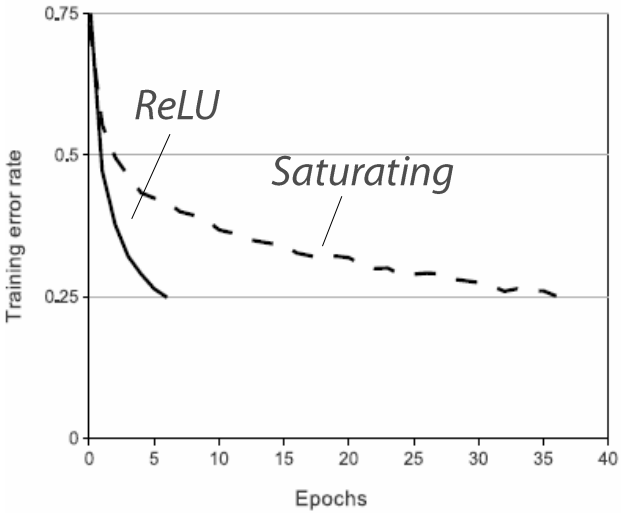
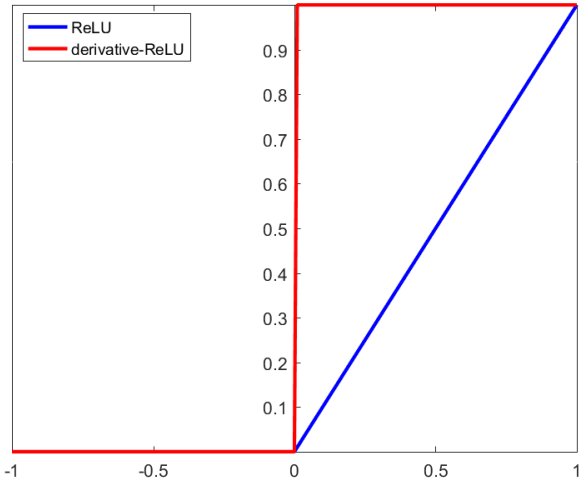


Image from [Krizhevsky, Sutskever & Hinton, 2012]



Overfitting

When the training process becomes too specific to the training set

- ***Training set, validation set***

  Splitting the dataset

  $$D = D_{train} \cup D_{val}$$

  $$\{(\boldsymbol{x}^{(i)}, y^{(i)})\}_{i=1}^{N} = \{(\boldsymbol{x}^{(j)}, y^{(j)})\}_{j=1}^{N_{train}} \cup \{(\boldsymbol{x}^{(i)}, y^{(i)})\}_{i=1}^{N_{val}}$$

  $$N_{train} \gg N_{val}$$

  Training is made on D_{train} only

  At each *epoch* — *when the whole D_{train} has been processed*

  the loss function is evaluated on D_{val}

  After some epochs, the performance on D_{val} might get worse

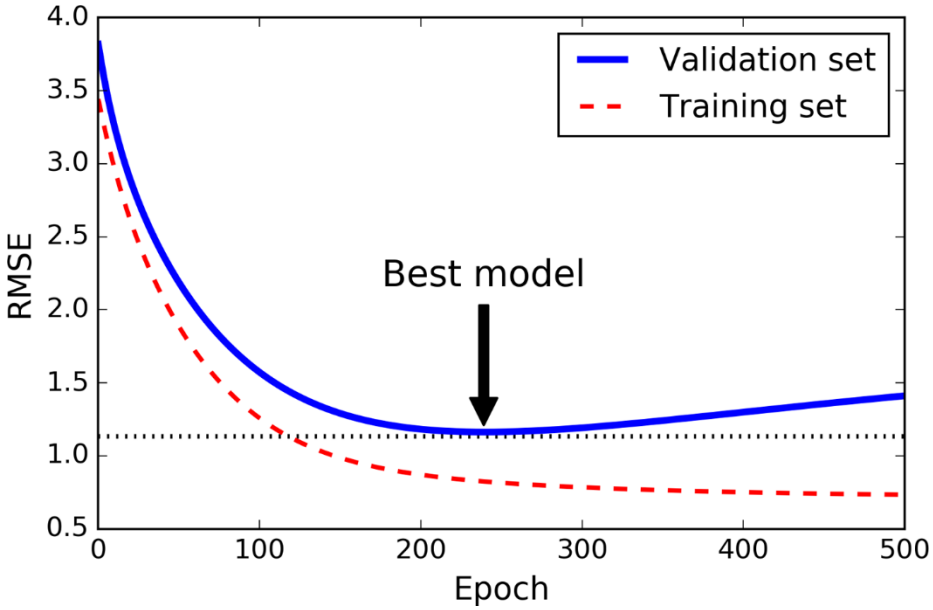
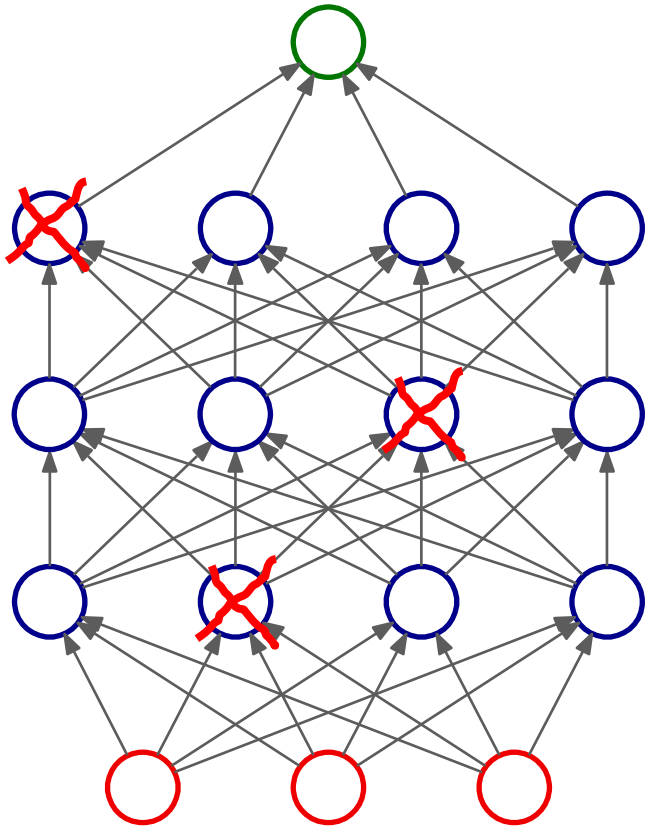


Image from https://www.safaribooksonline.com/library/view/hands-on-machine-learning/9781491962282/ch04.html

Dropout

- **Knocking-out at random**

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



Training: mini-batch 1

Dropout

- **Knocking-out at random**

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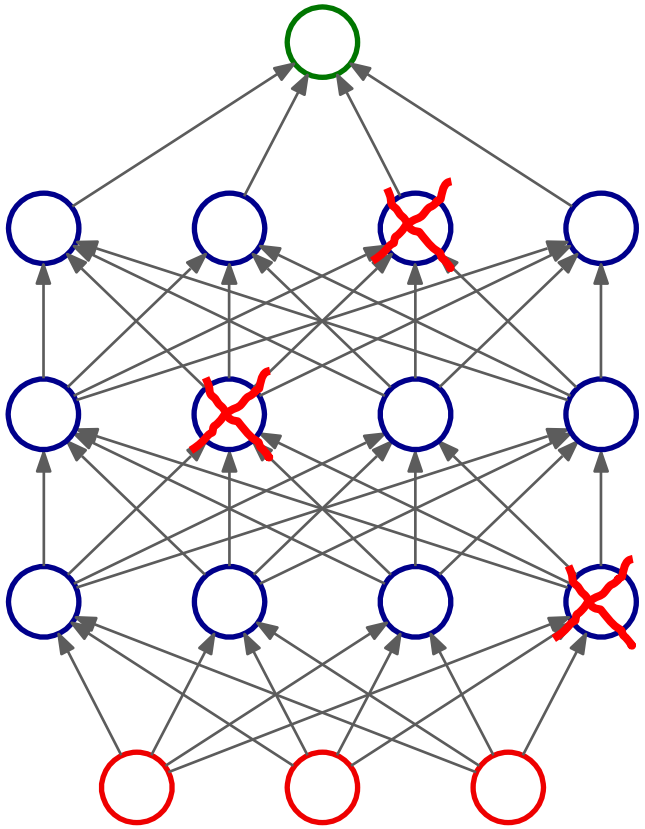
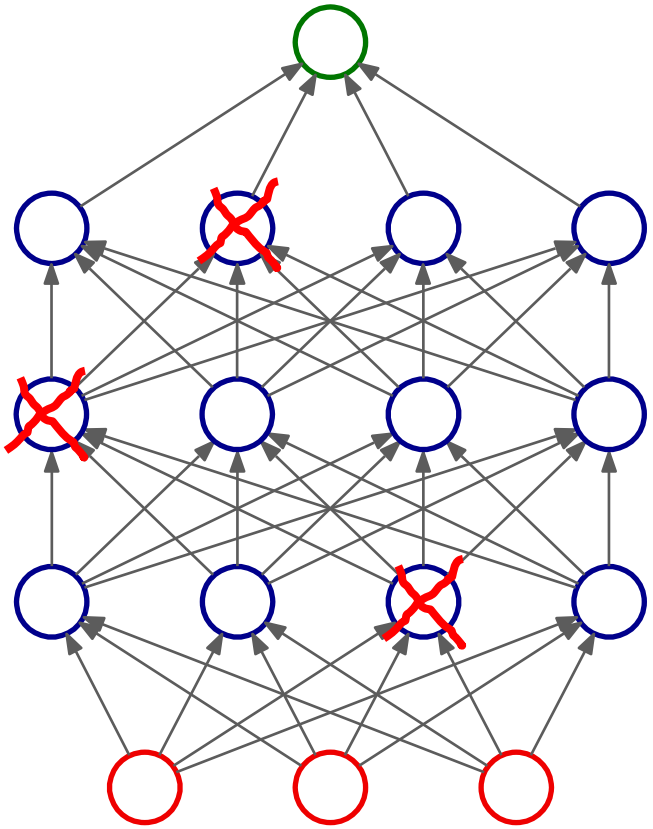


Training: mini-batch 2

Dropout

- **Knocking-out at random**

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

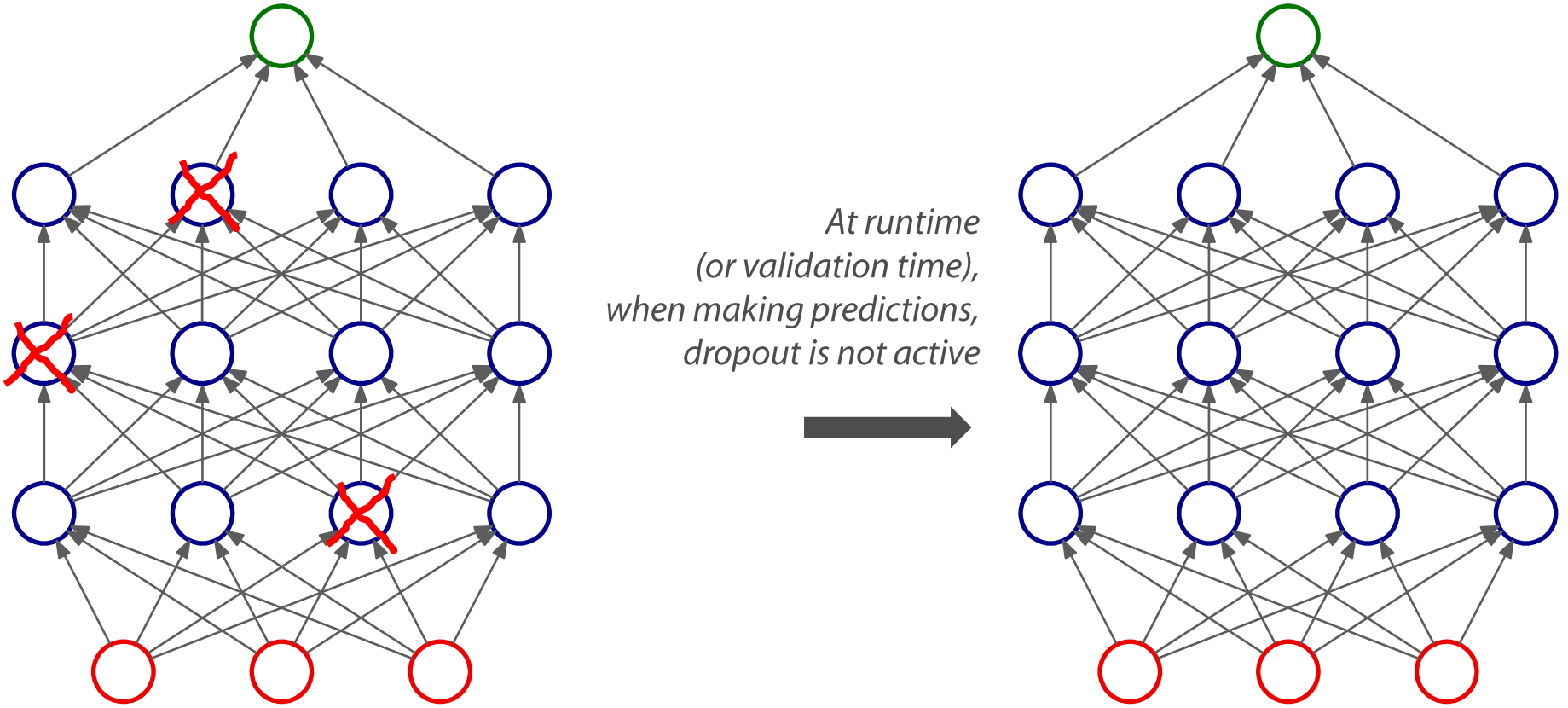


Training: mini-batch 3

Dropout

- **Knocking-out at random**

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



Training ***Prediction***

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

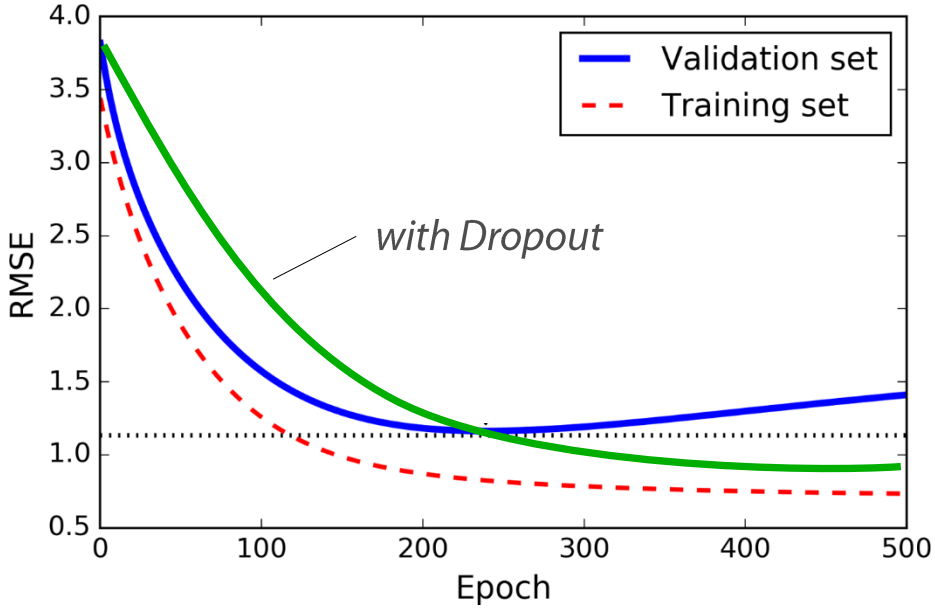


Image from https://www.safaribooksonline.com/library/view/hands-on-machine-learning/9781491962282/ch04.html

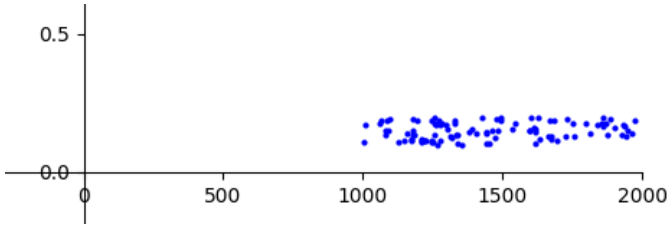
Input Normalization

- ***Intuition***

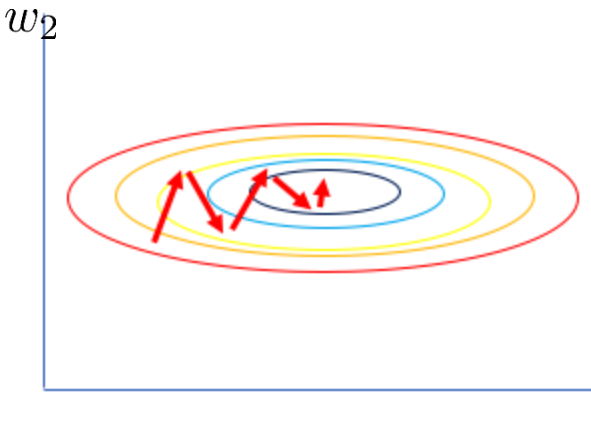
  Consider the (very simple) layer

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

  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***

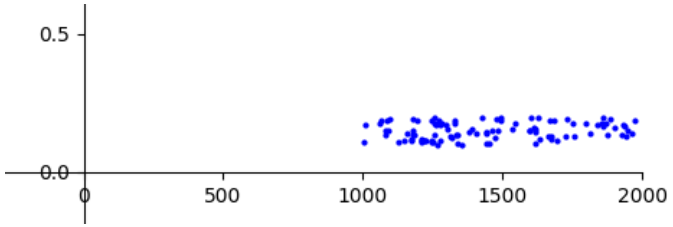
1) compute **mean** $\boldsymbol{\mu}$ and (*component-wise*) **variance** $\boldsymbol{\sigma}^2$ of inputs over dataset D

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

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



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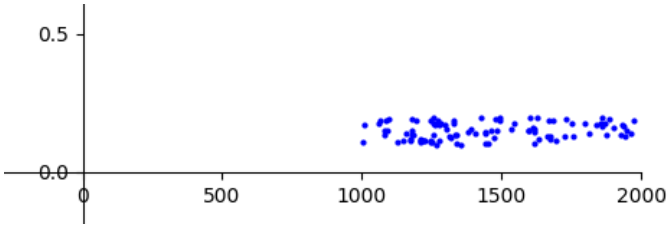
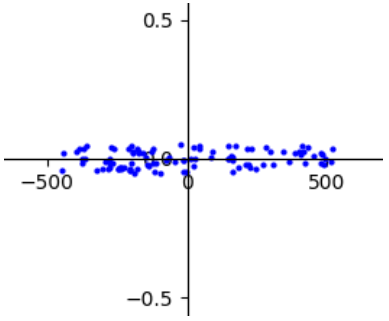
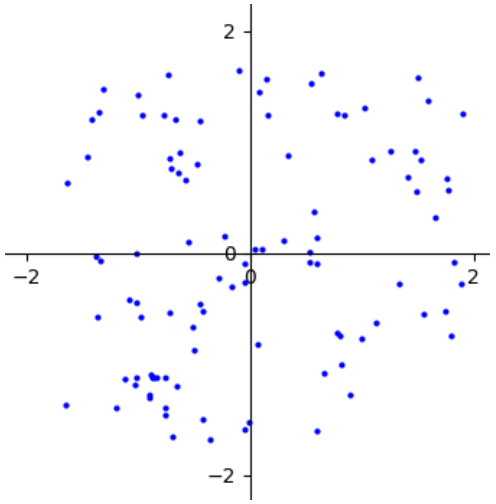


shift by $\boldsymbol{\mu}$



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



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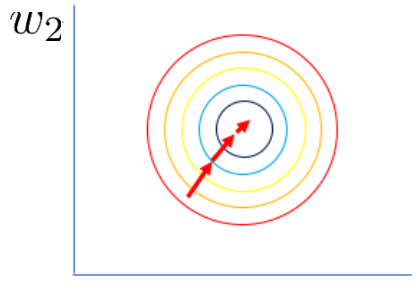
3) apply $h(\hat{\boldsymbol{x}}) := g(\boldsymbol{w}\hat{\boldsymbol{x}} + b) = g(w_1\hat{x}_1 + w_2\hat{x}_2 + b)$

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



level curves of the loss function (during training)

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

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

  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*
  - *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***

  It will be performed for fewer inputs, possibly just one

Batch Normalization

- ***Training***
  - at step : $\boldsymbol{\mu}_{B^{(t)}}$ 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*
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- ***Inference***

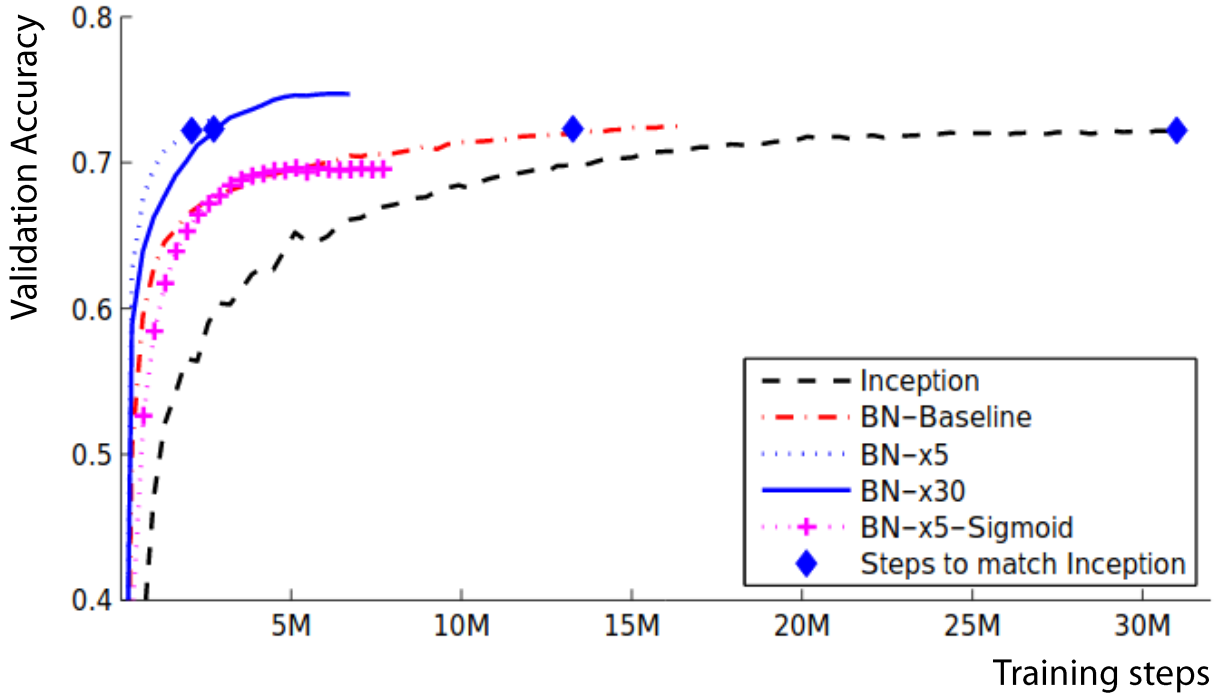
  Normalize using the moving averages collected *during training*

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

  as collected during the training process

Batch Normalization

- ***Does it work?***



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

Image from [Ioffe and Szegedy 2015]