Advanced Machine Learning
Lecture 11

Tricks of the Trade

08.12.2016

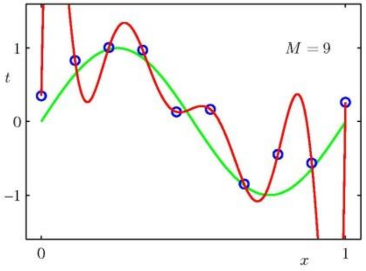
Bastian Leibe
RWTH Aachen
http://www.vision.rwth-aachen.de/

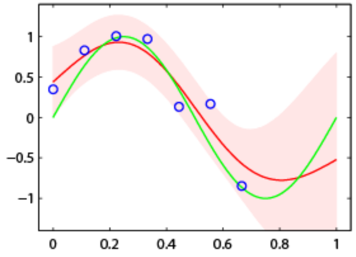
leibe@vision.rwth-aachen.de

This Lecture: *Advanced Machine Learning*

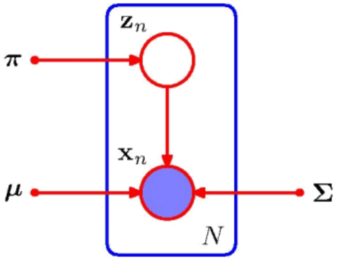
- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
  - Gaussian Processes

$$f : \mathcal{X} \to \mathbb{R}$$

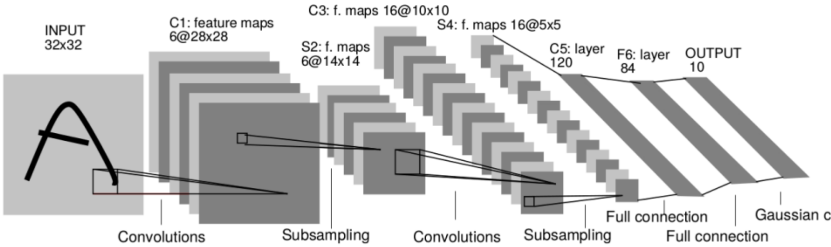




- Approximate Inference
  - Sampling Approaches
  - MCMC



- Deep Learning
  - Linear Discriminants
  - Neural Networks
  - Backpropagation & Optimization
  - CNNs, RNNs, ResNets, etc.



Recap: Learning with Hidden Units

- How can we train multi-layer networks efficiently?
  - Need an efficient way of adapting all weights, not just the last layer.

- Idea: Gradient Descent
  - Set up an error function

$$E(\mathbf{W}) = \sum_n L(t_n, y(\mathbf{x}_n; \mathbf{W})) + \lambda\Omega(\mathbf{W})$$

  with a loss $L(\cdot)$ and a regularizer $\Omega(\cdot)$.

  - E.g., $L(t, y(\mathbf{x}; \mathbf{W})) = \sum_n \left(y(\mathbf{x}_n; \mathbf{W}) - t_n\right)^2$ L_2 loss

$$\Omega(\mathbf{W}) = ||\mathbf{W}||_F^2$$

L_2 regularizer ("weight decay")

$\Rightarrow$ Update each weight $W_{ij}^{(k)}$ in the direction of the gradient $\frac{\partial E(\mathbf{W})}{\partial W_{ij}^{(k)}}$

Gradient Descent

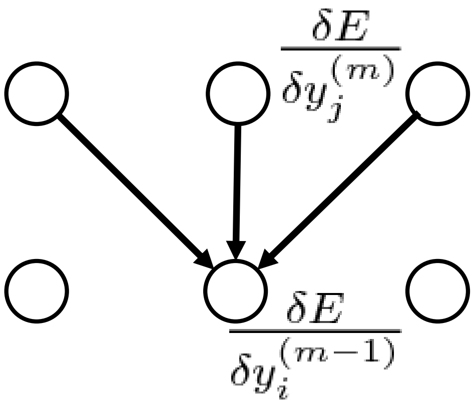
- Two main steps
  1. Computing the gradients for each weight — last lecture
  2. Adjusting the weights in the direction of the gradient — today

Recap: Backpropagation Algorithm

- Core steps
  1. Convert the discrepancy between each output and its target value into an error derivate.
  2. Compute error derivatives in each hidden layer from error derivatives in the layer above.
  3. Use error derivatives *w.r.t.* activities to get error derivatives *w.r.t.* the incoming weights

$$E = \frac{1}{2} \sum_{j \in output} (t_j - y_j)^2$$

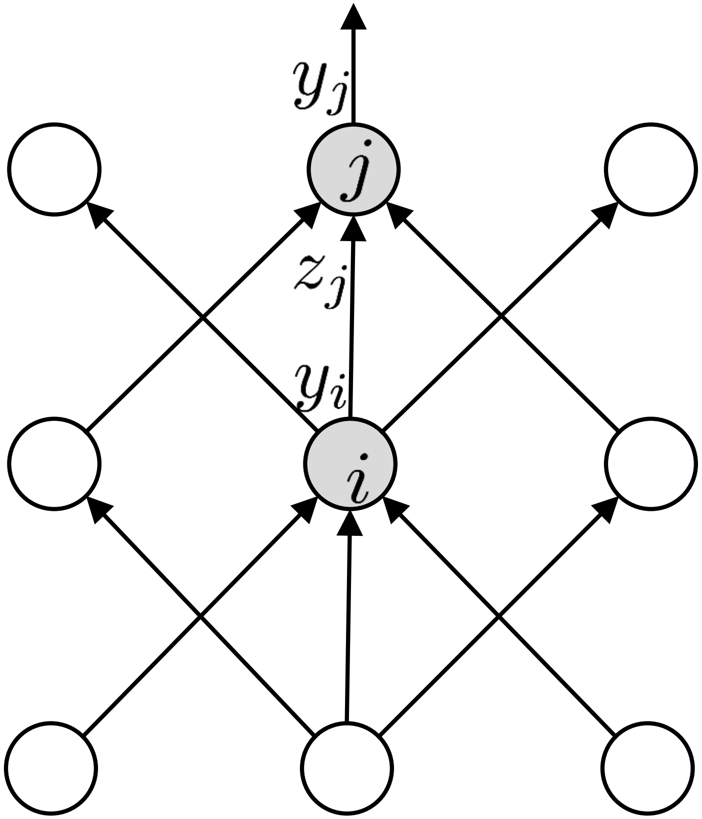
$$\frac{\partial E}{\partial y_j} = -(t_j - y_j)$$


$\frac{\delta E}{\delta y_j^{(m)}}$
$\frac{\delta E}{\delta y_i^{(m-1)}}$

$$\frac{\delta E}{\delta y_j^{(m)}} \longrightarrow \frac{\delta E}{\delta w_{ik}^{(m-1)}}$$

Slide adapted from Geoff Hinton

Recap: Backpropagation Algorithm



$$\frac{\partial E}{\partial z_j} = \frac{\partial y_j}{\partial z_j}\frac{\partial E}{\partial y_j} = y_j(1-y_j)\frac{\partial E}{\partial y_j}$$

$$\frac{\partial E}{\partial y_i} = \sum_j \frac{\partial z_j}{\partial y_i}\frac{\partial E}{\partial z_j} = \sum_j w_{ij}\frac{\partial E}{\partial z_j}$$

$$\frac{\partial E}{\partial w_{ij}} = \frac{\partial z_j}{\partial w_{ij}}\frac{\partial E}{\partial z_j} = y_i\frac{\partial E}{\partial z_j}$$

- **Efficient propagation scheme**
  - y_i **is already known from forward pass! (Dynamic Programming)**
  - ⇒ **Propagate back the gradient from layer j and multiply with y_i.**

Slide adapted from Geoff Hinton

Recap: MLP Backpropagation Algorithm

- **Forward Pass**

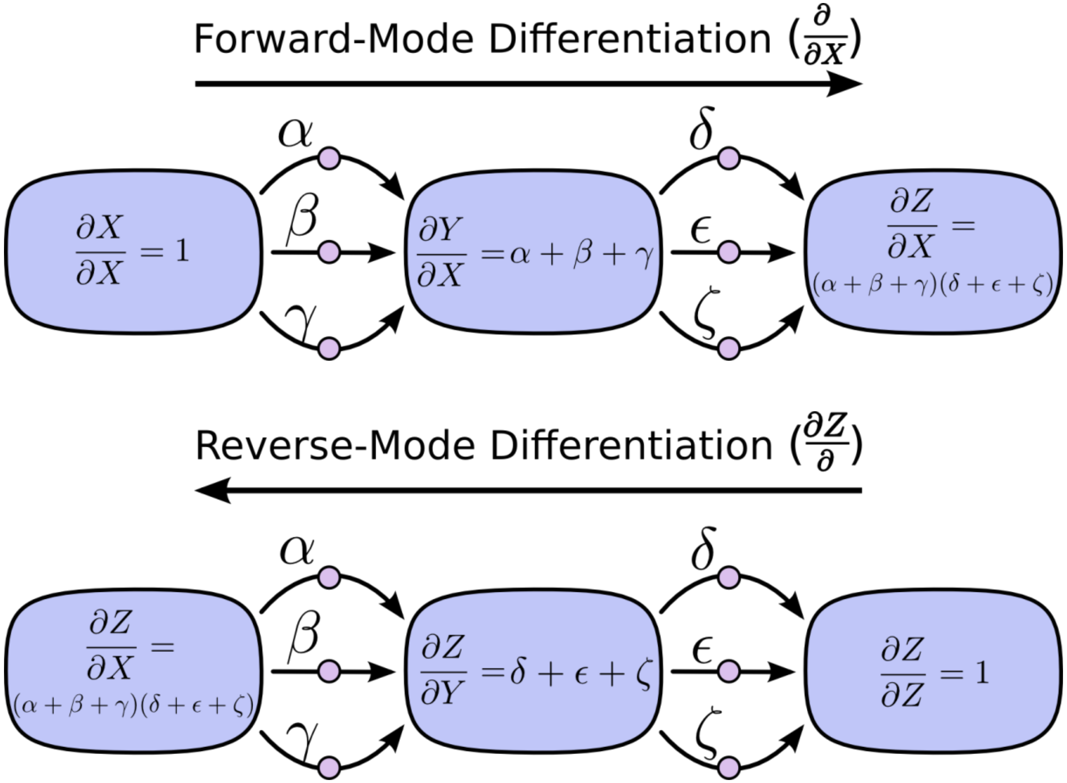
```
$\mathbf{y}^{(0)} = \mathbf{x}$
for $k = 1, ..., l$ do
    $\mathbf{z}^{(k)} = \mathbf{W}^{(k)}\mathbf{y}^{(k-1)}$
    $\mathbf{y}^{(k)} = g_k(\mathbf{z}^{(k)})$
endfor
$\mathbf{y} = \mathbf{y}^{(l)}$
$E = L(\mathbf{t}, \mathbf{y}) + \lambda\Omega(\mathbf{W})$
```

- **Backward Pass**

```
$\mathbf{h} \leftarrow \frac{\partial E}{\partial \mathbf{y}} = \frac{\partial}{\partial \mathbf{y}} L(\mathbf{t}, \mathbf{y}) + \lambda \frac{\partial}{\partial \mathbf{y}} \Omega$
for $k = l, l\text{-}1, ..., 1$ do
    $\mathbf{h} \leftarrow \frac{\partial E}{\partial \mathbf{z}^{(k)}} = \mathbf{h} \odot g'(\mathbf{y}^{(k)})$
    $\frac{\partial E}{\partial \mathbf{W}^{(k)}} = \mathbf{h}\mathbf{y}^{(k-1)\top} + \lambda \frac{\partial \Omega}{\partial \mathbf{W}^{(k)}}$
    $\mathbf{h} \leftarrow \frac{\partial E}{\partial \mathbf{y}^{(k-1)}} = \mathbf{W}^{(k)\top}\mathbf{h}$
endfor
```

- **Notes**
  - For efficiency, an entire batch of data $\mathbf{X}$ is processed at once.
  - $\odot$ denotes the element-wise product

Recap: Computational Graphs


Forward-Mode Differentiation $(\frac{\partial}{\partial X})$
α
β
γ
δ
ϵ
ζ
$\frac{\partial X}{\partial X} = 1$
$\frac{\partial Y}{\partial X} = \alpha + \beta + \gamma$
$\frac{\partial Z}{\partial X} = (\alpha+\beta+\gamma)(\delta+\epsilon+\zeta)$
Reverse-Mode Differentiation $(\frac{\partial Z}{\partial})$
α
β
γ
δ
ϵ
ζ
$\frac{\partial Z}{\partial X} = (\alpha+\beta+\gamma)(\delta+\epsilon+\zeta)$
$\frac{\partial Z}{\partial Y} = \delta + \epsilon + \zeta$
$\frac{\partial Z}{\partial Z} = 1$

Apply operator $\frac{\partial}{\partial X}$ to every node.

Apply operator $\frac{\partial Z}{\partial}$ to every node.

- **Forward differentiation needs one pass per node. Reverse-mode differentiation can compute all derivatives in one single pass.**

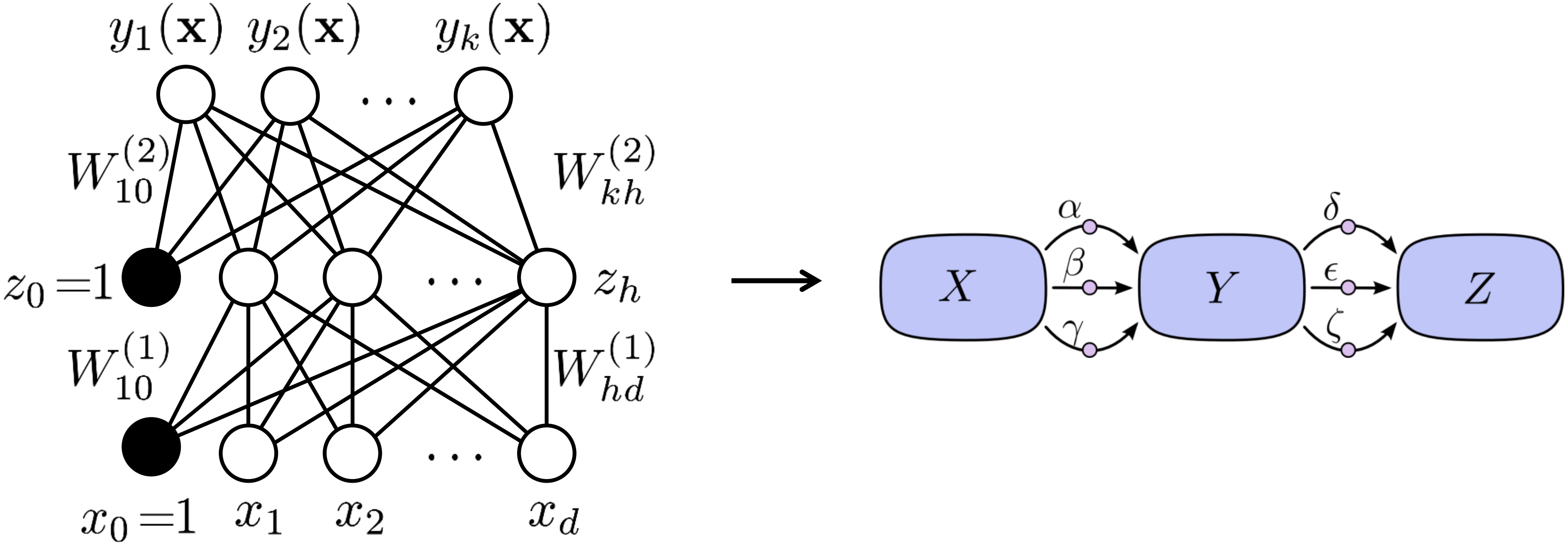
⇒ Speed-up in $\mathcal{O}(\text{\#inputs})$ compared to forward differentiation!

Slide inspired by Christopher Olah

Image source: Christopher Olah, colah.github.io

Recap: Automatic Differentiation

- Approach for obtaining the gradients



  - Convert the network into a computational graph.
  - Each new layer/module just needs to specify how it affects the forward and backward passes.
  - Apply reverse-mode differentiation.

$\Rightarrow$ Very general algorithm, used in today's Deep Learning packages

Image source: Christopher Olah, colah.github.io

Topics of This Lecture

- Gradient Descent Revisited
- Data (Pre-)processing
  - Stochastic Gradient Descent & Minibatches
  - Data Augmentation
  - Normalization
  - Initialization
- Convergence of Gradient Descent
  - Choosing Learning Rates
  - Momentum & Nesterov Momentum
  - RMS Prop
  - Other Optimizers
- Other Tricks
  - Batch Normalization
  - Dropout

Gradient Descent

- Two main steps
  1. Computing the gradients for each weight — last lecture
  2. Adjusting the weights in the direction of the gradient — today

- Recall: Basic update equation

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left. \frac{\partial E(\mathbf{w})}{\partial w_{kj}} \right|_{\mathbf{w}^{(\tau)}}$$

- Main questions
  - On what data do we want to apply this?
  - How should we choose the step size η (the learning rate)?
  - In which direction should we update the weights?

Topics of This Lecture

- Gradient Descent
- Data (Pre-)processing
  - Stochastic Gradient Descent & Minibatches
  - Data Augmentation
  - Normalization
  - Initialization
- Convergence of Gradient Descent
  - Choosing Learning Rates
  - Momentum & Nesterov Momentum
  - RMS Prop
  - Other Optimizers
- Other Tricks
  - Batch Normalization
  - Dropout

Stochastic vs. Batch Learning

- Batch learning
  - Process the full dataset at once to compute the gradient.

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left. \frac{\partial E(\mathbf{w})}{\partial w_{kj}} \right|_{\mathbf{w}^{(\tau)}}$$

- Stochastic learning
  - Choose a single example from the training set.
  - Compute the gradient only based on this example
  - This estimate will generally be noisy, which has some advantages.

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left. \frac{\partial E_n(\mathbf{w})}{\partial w_{kj}} \right|_{\mathbf{w}^{(\tau)}}$$

Stochastiv vs. Batch Learning

- Batch learning advantages
  - Conditions of convergence are well understood.
  - Many acceleration techniques (e.g., conjugate gradients) only operate in batch learning.
  - Theoretical analysis of the weight dynamics and convergence rates are simpler.
- Stochastic learning advantages
  - Usually much faster than batch learning.
  - Often results in better solutions.
  - Can be used for tracking changes.
- Middle ground: Minibatches

Minibatches

- Idea
  - Process only a small batch of training examples together
  - Start with a small batch size & increase it as training proceeds.
- Advantages
  - Gradients will be more stable than for stochastic gradient descent, but still faster to compute than with batch learning.
  - Take advantage of redundancies in the training set.
  - Matrix operations are more efficient than vector operations.
- Caveat
  - Error function should be normalized by the minibatch size, s.t. we can keep the same learning rate between minibatches

$$E(\mathbf{W}) = \frac{1}{N}\sum_n L(t_n, y(\mathbf{x}_n; \mathbf{W})) + \frac{\lambda}{N}\Omega(\mathbf{W})$$

Shuffling the Examples

- Ideas
  - Networks learn fastest from the most unexpected sample.

  ⇒ It is advisable to choose a sample at each iteration that is most unfamiliar to the system.
    - E.g. a sample from a *different class* than the previous one.
    - This means, do not present all samples of class A, then all of class B.

  - A large relative error indicates that an input has not been learned by the network yet, so it contains a lot of information.

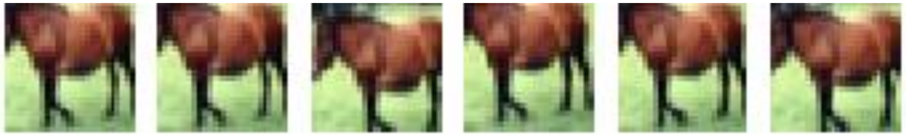
  ⇒ It can make sense to present such inputs more frequently.
    - But: be careful, this can be disastrous when the data are outliers.

- Practical advice
  - When working with stochastic gradient descent or minibatches, make use of shuffling.

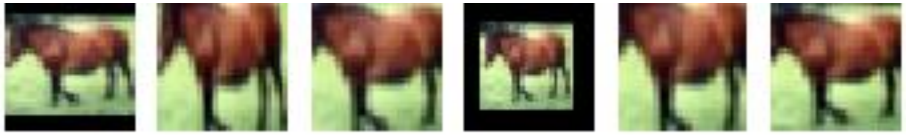
Data Augmentation

- Idea
  - Augment original data with synthetic variations to reduce overfitting

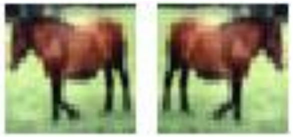
- Example augmentations for images
  - Cropping



  - Zooming



  - Flipping



  - Color PCA

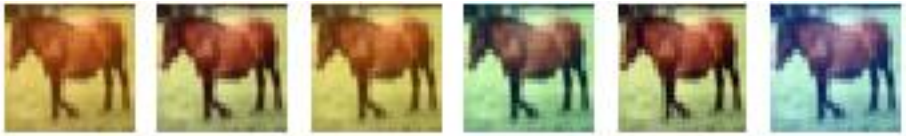
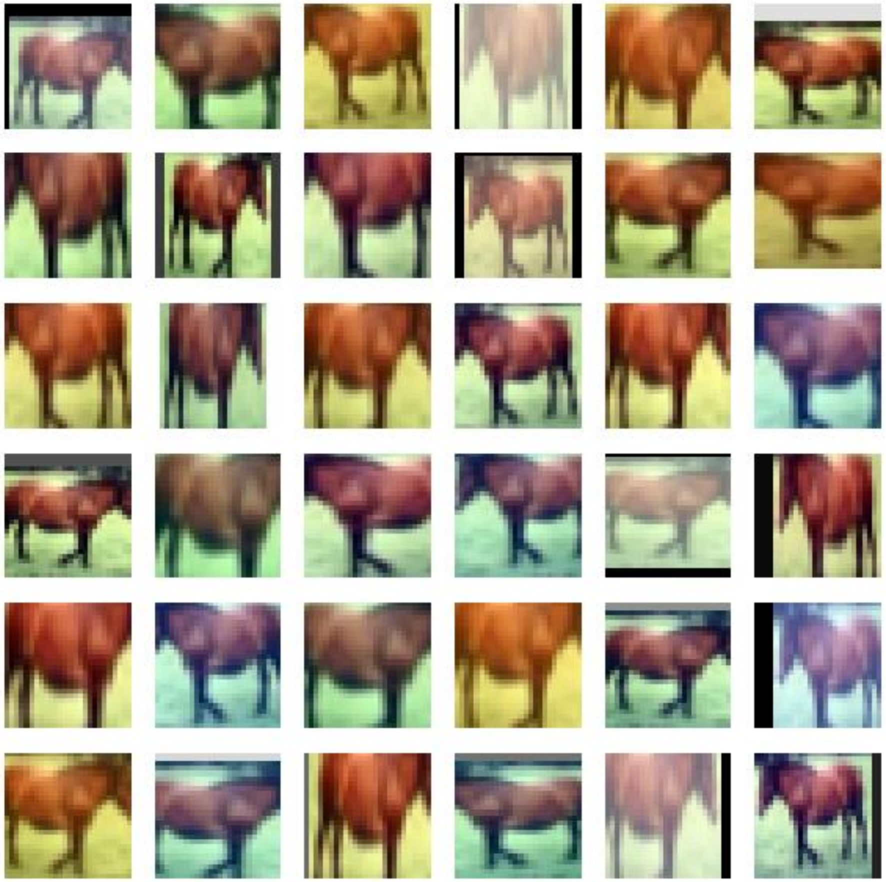


Image source: Lucas Beyer

Data Augmentation

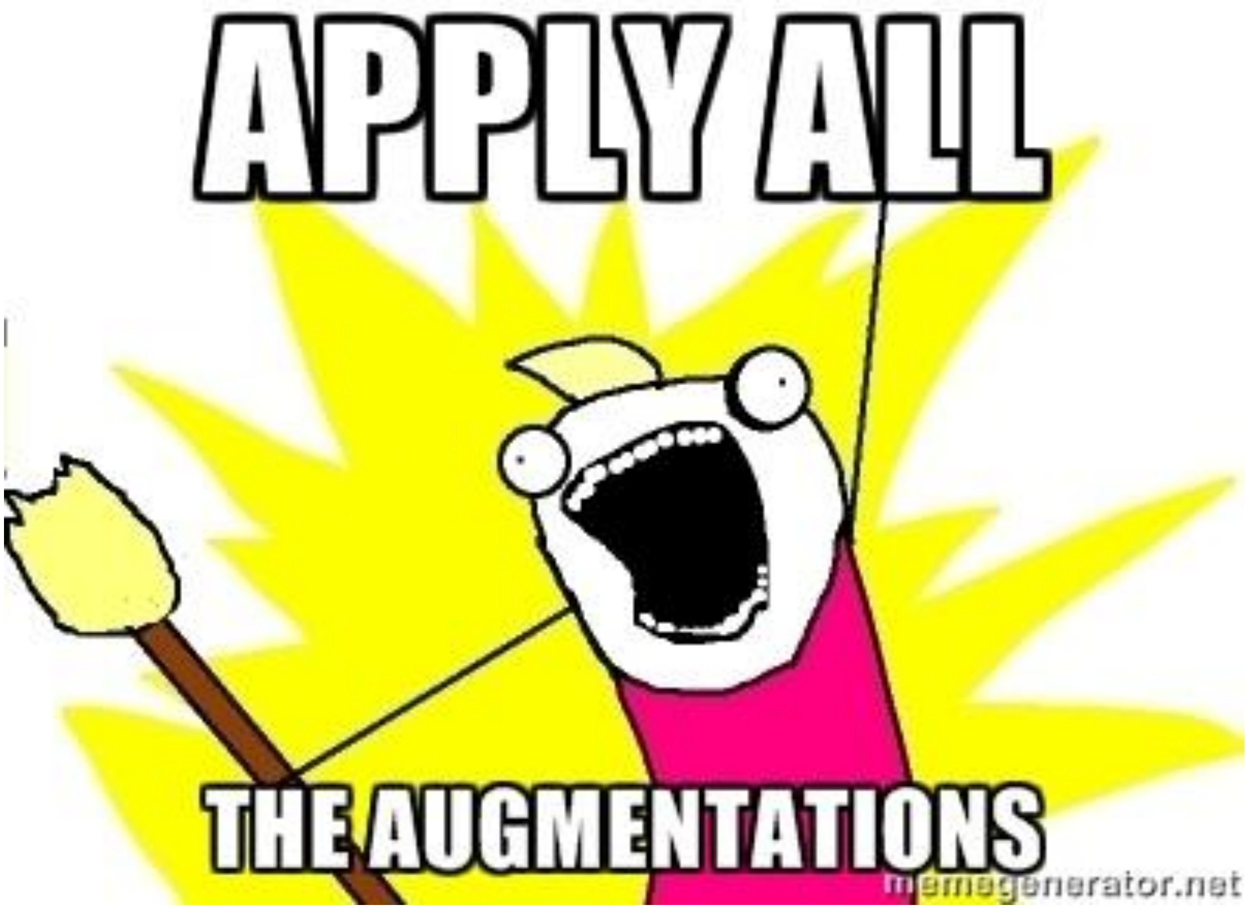
- Effect
  - Much larger training set
  - Robustness against expected variations
- During testing
  - When cropping was used during training, need to again apply crops to get same image size.
  - Beneficial to also apply flipping during test.
  - Applying several ColorPCA variations can bring another ~1% improvement, but at a significantly increased runtime.



Augmented training data (from one original image)

Image source: Lucas Beyer

General Guideline



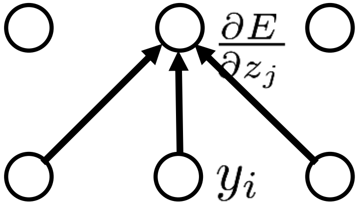
Normalization

- **Motivation**
  - Consider the Gradient Descent update steps

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left. \frac{\partial E(\mathbf{w})}{\partial w_{kj}} \right|_{\mathbf{w}^{(\tau)}}$$

  - From backpropagation, we know that

$$\frac{\partial E}{\partial w_{ij}} = \frac{\partial z_j}{\partial w_{ij}} \frac{\partial E}{\partial z_j} = y_i \frac{\partial E}{\partial z_j}$$



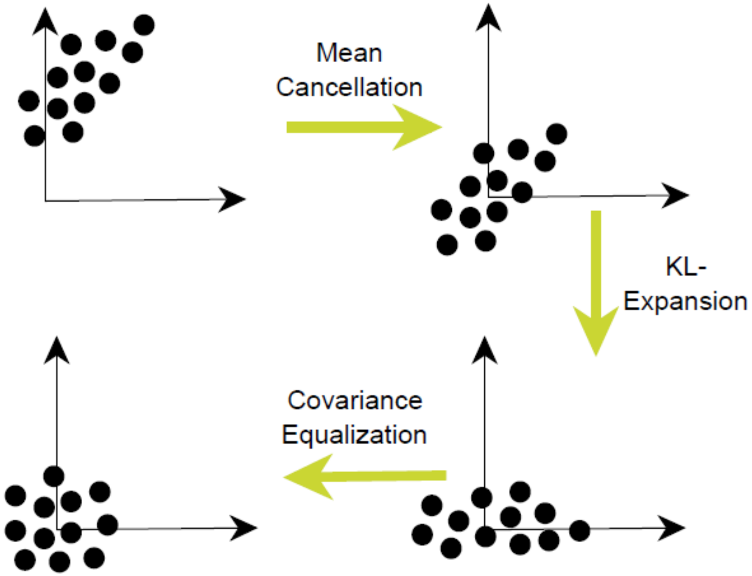
  - When all of the components of the input vector y_i are positive, all of the updates of weights that feed into a node will be of the same sign.

⇒ Weights can only all increase or decrease together.

⇒ Slow convergence

Normalizing the Inputs

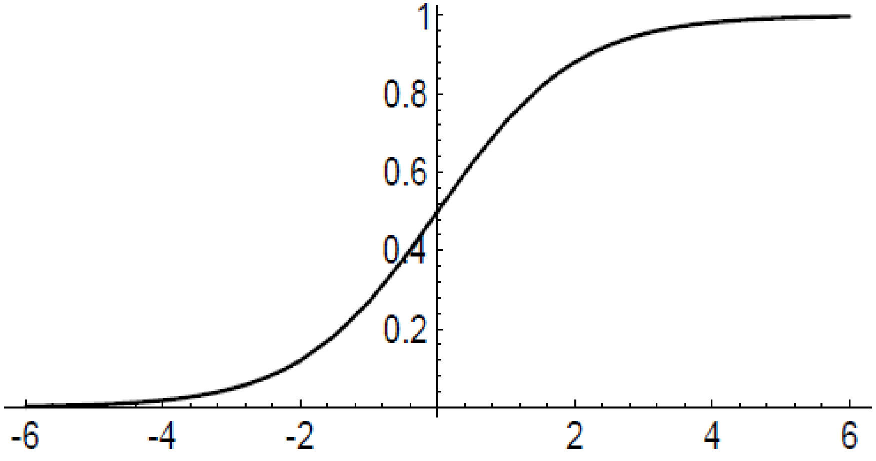
- Convergence is fastest if
  - The mean of each input variable over the training set is zero.
  - The inputs are scaled such that all have the same covariance.
  - Input variables are uncorrelated if possible.

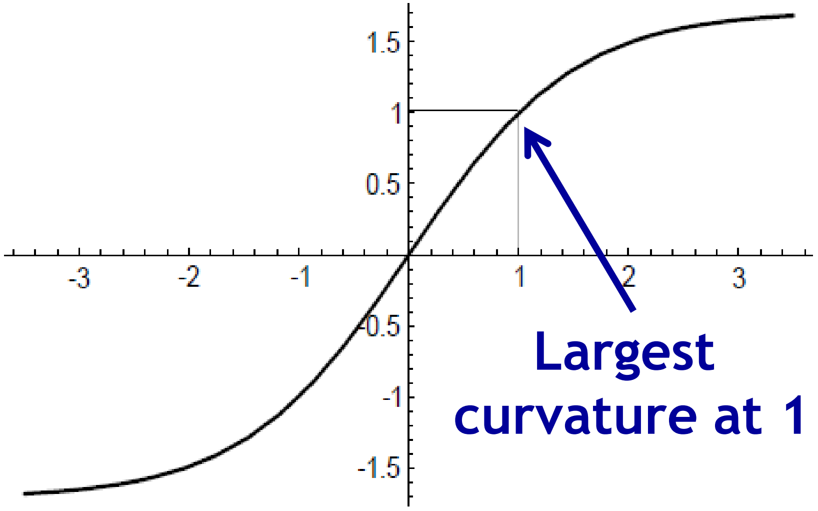


- Advisable normalization steps (for MLPs)
  - Normalize all inputs that an input unit sees to zero-mean, unit covariance.
  - If possible, try to decorrelate them using PCA (also known as Karhunen-Loeve expansion).

Image source: Yann LeCun et al., Efficient BackProp (1998)

Choosing the Right Sigmoid





Largest curvature at 1

- **Normalization is also important for intermediate layers**
  - **Symmetric sigmoids, such as tanh, often converge faster than the standard logistic sigmoid.**
  - **Recommended sigmoid:**

$$f(x) = 1.7159 \tanh\left(\frac{2}{3}x\right)$$

⇒ **When used with transformed inputs, the variance of the outputs will be close to 1.**

Image source: Yann LeCun et al., Efficient BackProp (1998)

Initializing the Weights

- **Motivation**
  - The starting values of the weights can have a significant effect on the training process.
  - Weights should be chosen randomly, but in a way that the sigmoid is primarily activated in its linear region.

- **Guideline (from [LeCun et al., 1998] book chapter)**
  - Assuming that
    - The training set has been normalized
    - The recommended sigmoid $f(x) = 1.7159 \tanh\left(\frac{2}{3}x\right)$ is used

  the initial weights should be randomly drawn from a distribution (e.g., uniform or Normal) with mean zero and variance

$$\sigma_W^2 = \frac{1}{n_{in}}$$

  where n_{in} is the fan-in (#connections into the node).

Historical Sidenote

- Apparently, this guideline was either little known or misunderstood for a long time
  - A popular heuristic (also the standard in Torch) was to use

$$W \sim U\left[-\frac{1}{\sqrt{n_{in}}}, \frac{1}{\sqrt{n_{in}}}\right]$$

  - This looks almost like LeCun's rule. However…

- When sampling weights from a uniform distribution $[a,b]$
  - Keep in mind that the standard deviation is computed as

$$\sigma^2 = \frac{1}{12}(b-a)^2$$

  - If we do that for the above formula, we obtain

$$\sigma^2 = \frac{1}{12}\left(\frac{2}{\sqrt{n_{in}}}\right)^2 = \frac{1}{3}\frac{1}{n_{in}}$$

⇒ Activations & gradients will be attenuated with each layer! (bad)

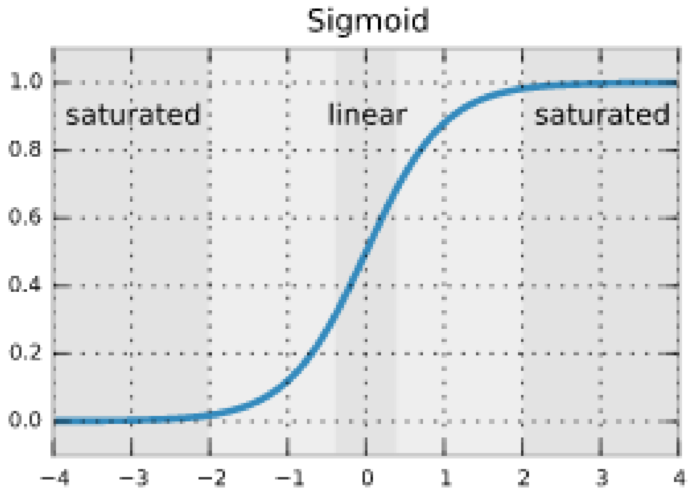
Glorot Initialization

- Breakthrough results
  - In 2010, Xavier Glorot published an analysis of what went wrong in the initialization and derived a more general method for automatic initialization.
  - This new initialization massively improved results and made direct learning of deep networks possible overnight.
  - Let's look at his analysis in more detail...

X. Glorot, Y. Bengio, Understanding the Difficulty of Training Deep Feedforward Neural Networks, AISTATS 2010.

Effect of Sigmoid Nonlinearities

- Effects of sigmoid/tanh function
  - Linear behavior around 0
  - Saturation for large inputs



- If all parameters are too small
  - Variance of activations will drop in each layer
  - Sigmoids are approximately linear close to 0
  - Good for passing gradients through, but...
  - Gradual loss of the nonlinearity

  ⇒ No benefit of having multiple layers

- If activations become larger and larger
  - They will saturate and gradient will become zero

Image source: http://deepdish.io/2015/02/24/network-initialization/

Analysis

- Variance of neuron activations
  - Suppose we have an input X with n components and a linear neuron with random weights W that spits out a number Y.
  - What is the variance of Y?

$$Y = W_1X_1 + W_2X_2 + \cdots + W_nX_n$$

  - If inputs and outputs have both mean 0, the variance is

$$\text{Var}(W_iX_i) = E[X_i]^2\text{Var}(W_i) + E[W_i]^2\text{Var}(X_i) + \text{Var}(W_i)\text{Var}(i_i)$$

$$= \text{Var}(W_i)\text{Var}(X_i)$$

  - If the X_i and W_i are all i.i.d, then

$$\text{Var}(Y) = \text{Var}(W_1X_1 + W_2X_2 + \cdots + W_nX_n) = n\text{Var}(W_i)\text{Var}(X_i)$$

$\Rightarrow$ The variance of the output is the variance of the input, but scaled by $n\ \text{Var}(W_i)$.

Analysis (cont'd)

- Variance of neuron activations
  - if we *want the variance of the input and output of a unit to be the same*, then $n\ \mathrm{Var}(W_i)$ should be 1. This means

$$\mathrm{Var}(W_i) = \frac{1}{n} = \frac{1}{n_{\text{in}}}$$

  - If we do the same for the backpropagated gradient, we get

$$\mathrm{Var}(W_i) = \frac{1}{n_{\text{out}}}$$

  - As a compromise, Glorot & Bengio propose to use

$$\mathrm{Var}(W) = \frac{2}{n_{\text{in}} + n_{\text{out}}}$$

$\Rightarrow$ Randomly sample the weights with this variance. That's it.

Sidenote

- When sampling weights from a uniform distribution $[a,b]$
  - Again keep in mind that the standard deviation is computed as

$$\sigma^2 = \frac{1}{12}(b-a)^2$$

  - Glorot initialization with uniform distribution

$$W \sim U\left[-\frac{\sqrt{6}}{\sqrt{n_{in}+n_{out}}}, \frac{\sqrt{6}}{\sqrt{n_{in}+n_{out}}}\right]$$

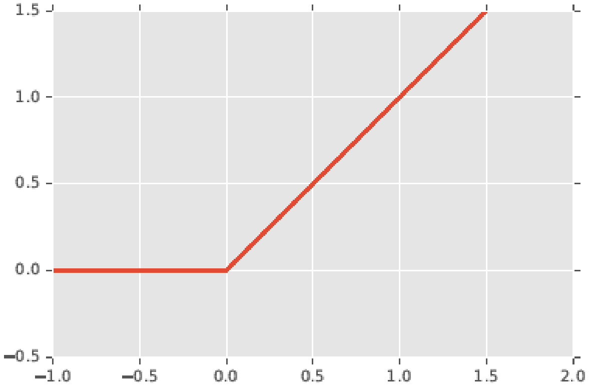
Extension to ReLU

- Another improvement for learning deep models
  - Use Rectified Linear Units (ReLU)

$$g(a) = \max\{0, a\}$$

  - Effect: gradient is propagated with a constant factor

$$\frac{\partial g(a)}{\partial a} = \begin{cases} 1, & a > 0 \\ 0, & \text{else} \end{cases}$$



- We can also improve them with proper initialization
  - However, the Glorot derivation was based on tanh units, linearity assumption around zero does not hold for ReLU.
  - He et al. made the derivations, proposed to use instead

$$\mathrm{Var}(W) = \frac{2}{n_{\text{in}}}$$

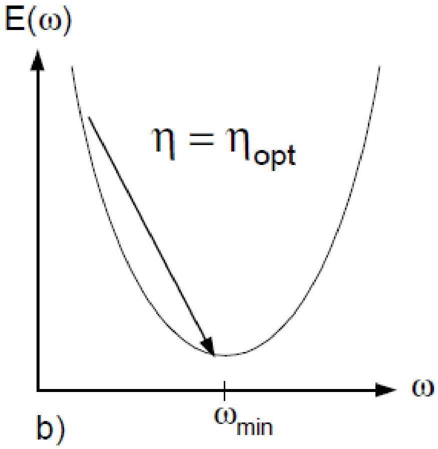
Topics of This Lecture

- Gradient Descent
- Data (Pre-)processing
  - Stochastic Gradient Descent & Minibatches
  - Data Augmentation
  - Normalization
  - Initialization
- Convergence of Gradient Descent
  - Choosing Learning Rates
  - Momentum & Nesterov Momentum
  - RMS Prop
  - Other Optimizers
- Other Tricks
  - Batch Normalization
  - Dropout

Choosing the Right Learning Rate

- **Analyzing the convergence of Gradient Descent**
  - **Consider a simple 1D example first**

$$W^{(\tau-1)} = W^{(\tau)} - \eta \frac{\mathrm{d}E(W)}{\mathrm{d}W}$$



  - **What is the optimal learning rate η_{opt}?**
  - **If E is quadratic, the optimal learning rate is given by the inverse of the Hessian**

$$\eta_{\text{opt}} = \left(\frac{\mathrm{d}^2 E(W^{(\tau)})}{\mathrm{d}W^2} \right)^{-1}$$

  - ***What happens if we exceed this learning rate?***

Image source: Yann LeCun et al., Efficient BackProp (1998)

Choosing the Right Learning Rate

- **Behavior for different learning rates**

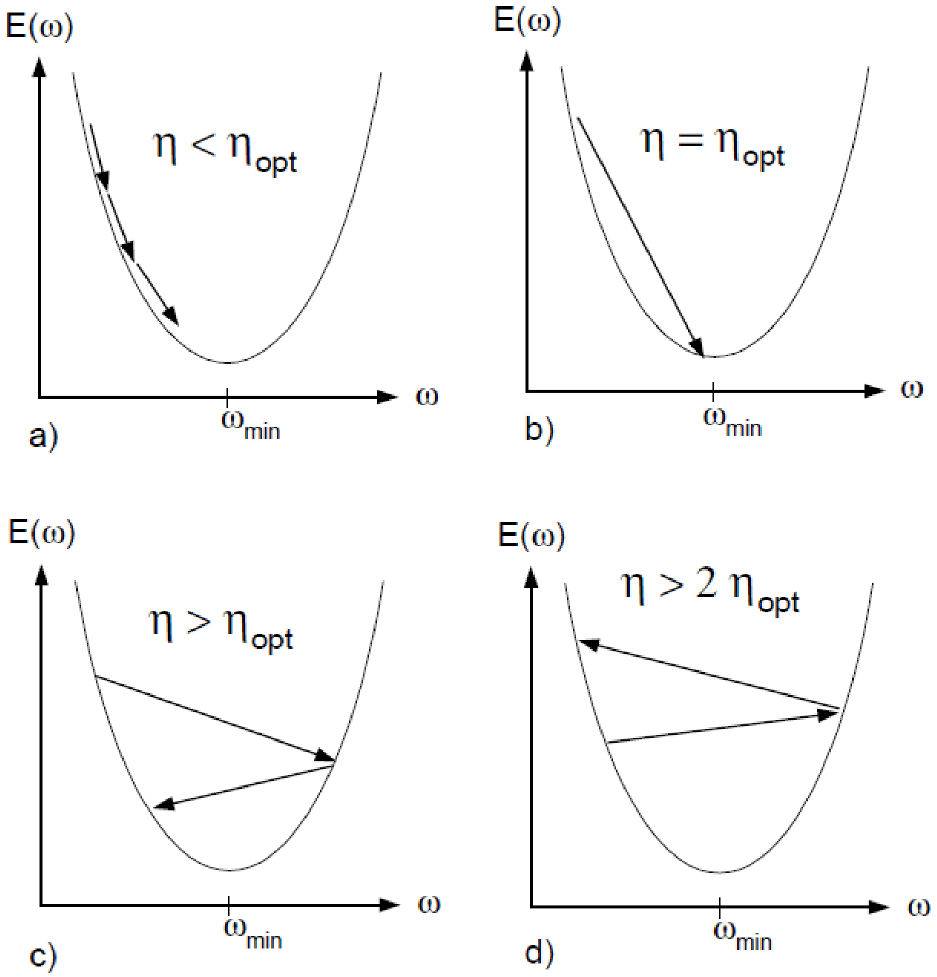
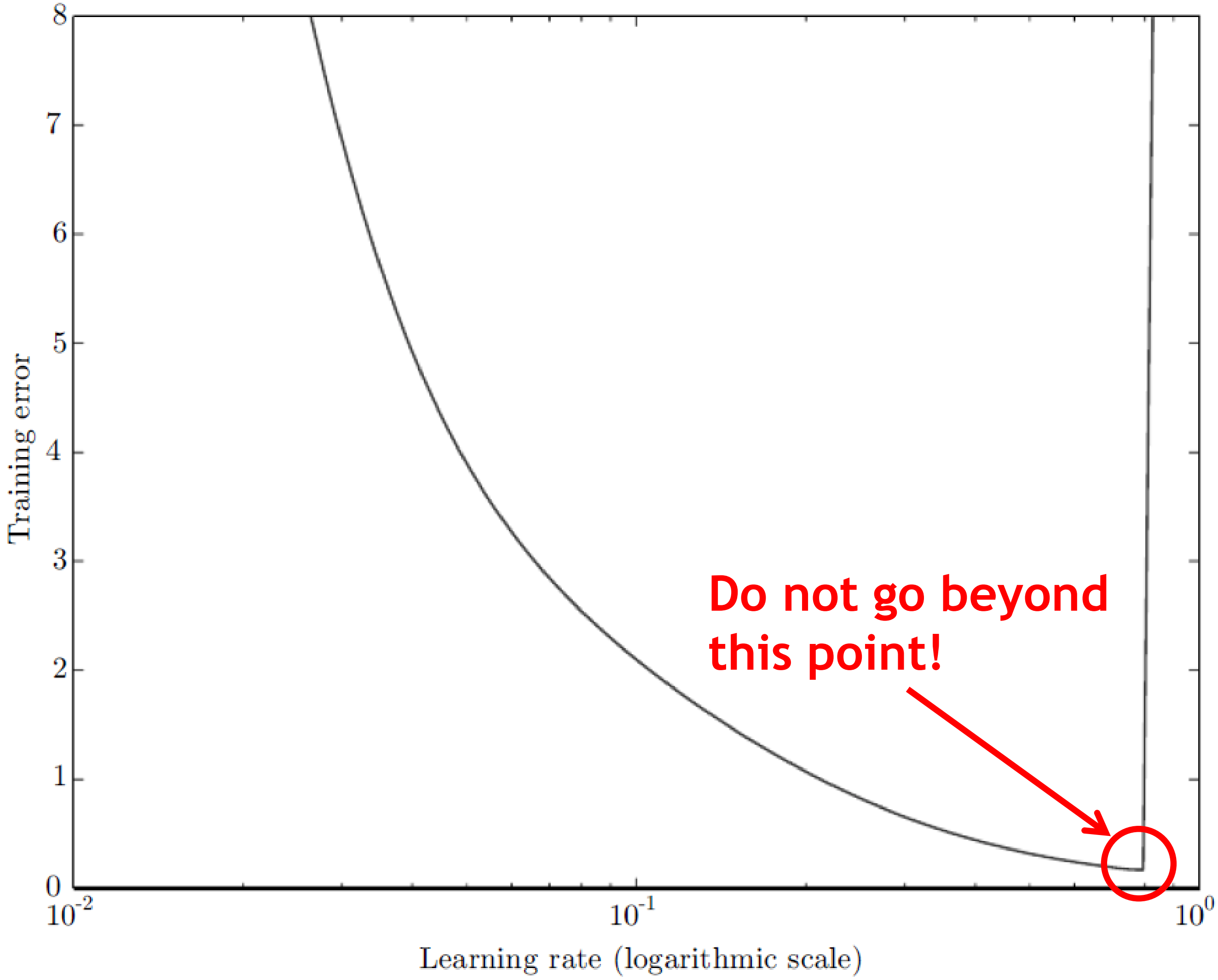


Image source: Yann LeCun et al., Efficient BackProp (1998)

Advanced Machine Learning Winter’16

Learning Rate vs. Training Error

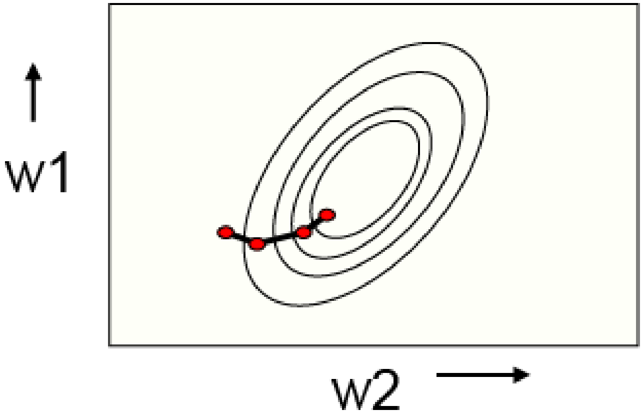


Do not go beyond this point!

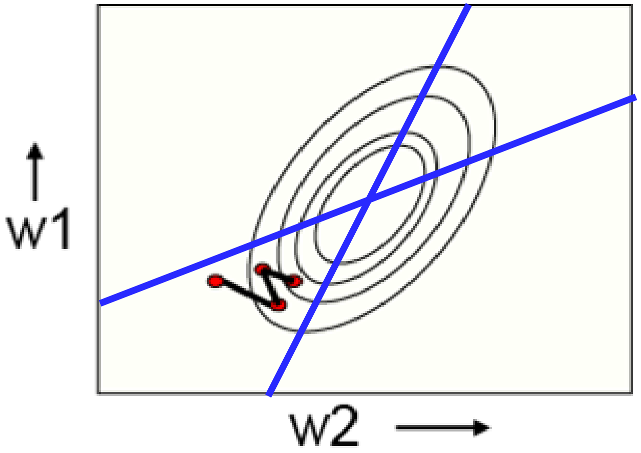
Image source: Goodfellow & Bengio book

Batch vs. Stochastic Learning

- Batch Learning
  - Simplest case: steepest decent on the error surface.
  - ⇒ Updates perpendicular to contour lines



- Stochastic Learning
  - Simplest case: zig-zag around the direction of steepest descent.
  - ⇒ Updates perpendicular to constraints from training examples.

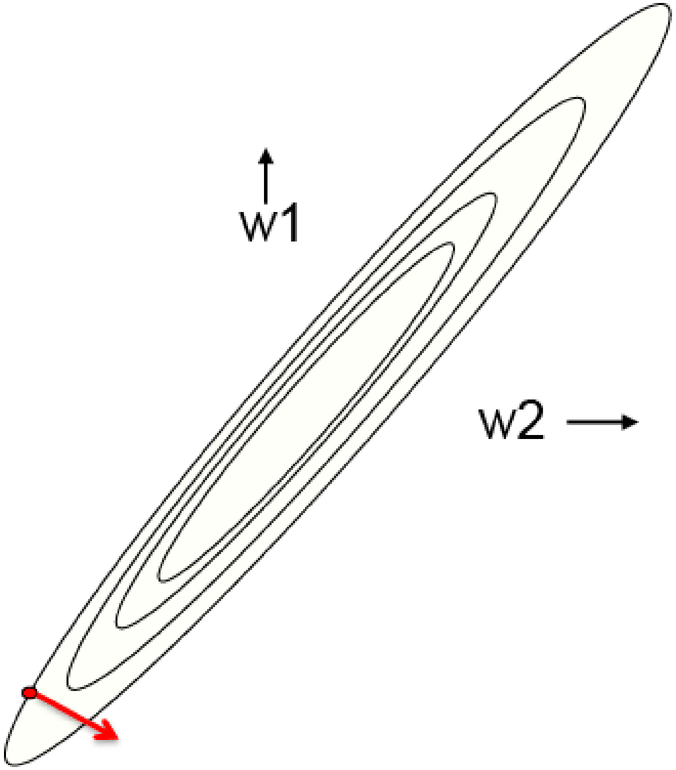


Slide adapted from Geoff Hinton

Image source: Geoff Hinton

Why Learning Can Be Slow

- If the inputs are correlated
  - The ellipse will be very elongated.
  - The direction of steepest descent is almost perpendicular to the direction towards the minimum!



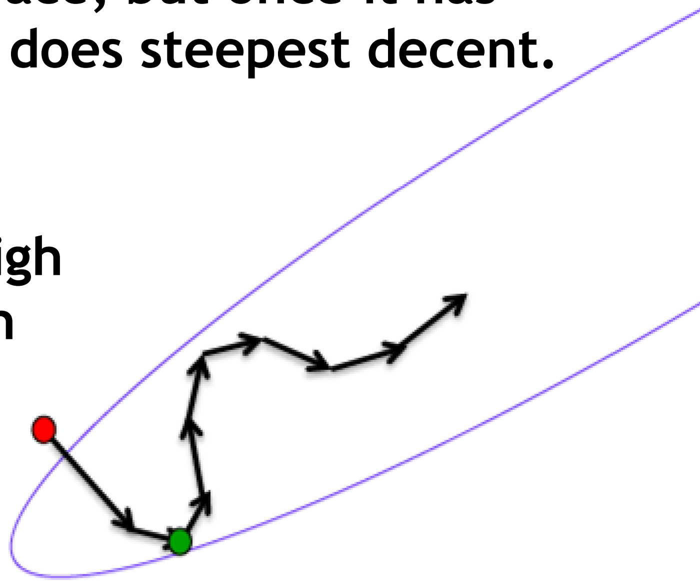
This is just the opposite of what we want!

Image source: Geoff Hinton

Slide adapted from Geoff Hinton

The Momentum Method

- Idea
  - Instead of using the gradient to change the position of the weight "particle", use it to change the velocity.
- Intuition
  - Example: Ball rolling on the error surface
  - It starts off by following the error surface, but once it has accumulated momentum, it no longer does steepest decent.
- Effect
  - Dampen oscillations in directions of high curvature by combining gradients with opposite signs.
  - Build up speed in directions with a gentle but consistent gradient.



Slide credit: Geoff Hinton

Image source: Geoff Hinton

The Momentum Method: Implementation

- Change in the update equations
  - Effect of the gradient: increment the previous velocity, subject to a decay by $\alpha < 1$.

$$\mathbf{v}(t) = \alpha \mathbf{v}(t-1) - \varepsilon \frac{\partial E}{\partial \mathbf{w}}(t)$$

  - Set the weight change to the current velocity

$$\begin{aligned} \Delta \mathbf{w} &= \mathbf{v}(t) \\ &= \alpha \mathbf{v}(t-1) - \varepsilon \frac{\partial E}{\partial \mathbf{w}}(t) \\ &= \alpha \Delta \mathbf{w}(t-1) - \varepsilon \frac{\partial E}{\partial \mathbf{w}}(t) \end{aligned}$$

Slide credit: Geoff Hinton

The Momentum Method: Behavior

- **Behavior**
  - If the error surface is a tilted plane, the ball reaches a terminal velocity

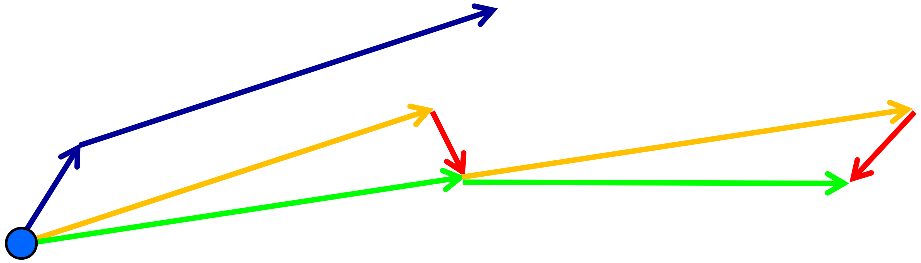
$$\mathbf{v}(\infty) = \frac{1}{1-\alpha}\left(-\varepsilon\frac{\partial E}{\partial \mathbf{w}}\right)$$

    - If the momentum α is close to 1, this is much faster than simple gradient descent.
  - At the beginning of learning, there may be very large gradients.
    - Use a small momentum initially (e.g., $\alpha = 0.5$).
    - Once the large gradients have disappeared and the weights are stuck in a ravine, the momentum can be smoothly raised to its final value (e.g., $\alpha = 0.90$ or even $\alpha = 0.99$).

$\Rightarrow$ This allows us to learn at a rate that would cause divergent oscillations without the momentum.

Slide credit: Geoff Hinton

Improvement: Nesterov-Momentum



Standard Momentum

Jump

Correction

Accumulated gradient

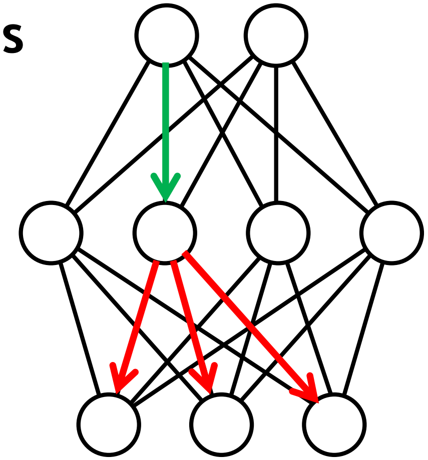
- Standard Momentum method
  - First compute the gradient at the current location
  - Then jump in the direction of the updated accumulated gradient
- Improvement [Sutskever 2012]
  - (Inspiration: Nesterov method for optimizing convex functions.)
  - First jump in the direction of the previous accumulated gradient
  - Then measure the gradient where you end up and make a correction.

⇒ *Intuition: It's better to correct a mistake after you've made it.*

Slide adapted from Geoff Hinton

Separate, Adaptive Learning Rates

- Problem
  - In multilayer nets, the appropriate learning rates can vary widely between weights.
  - The magnitudes of the gradients are often very different for the different layers, especially if the initial weights are small.
    - ⇒ Gradients can get very small in the early layers of deep nets.

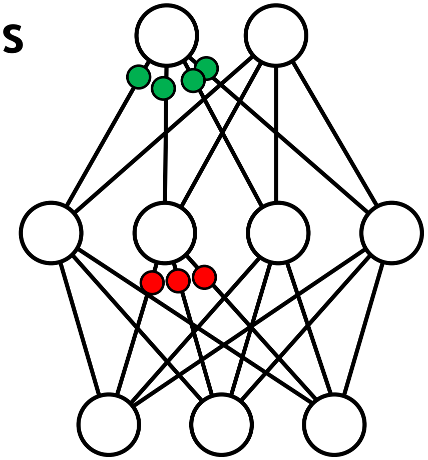


Slide adapted from Geoff Hinton

Separate, Adaptive Learning Rates

- Problem
  - In multilayer nets, the appropriate learning rates can vary widely between weights.
  - The magnitudes of the gradients are often very different for the different layers, especially if the initial weights are small.

    ⇒ Gradients can get very small in the early layers of deep nets.
  - The fan-in of a unit determines the size of the "overshoot" effect when changing multiple weights simultaneously to correct the same error.
    - The fan-in often varies widely between layers



- Solution
  - Use a global learning rate, multiplied by a local gain per weight (determined empirically)

Slide adapted from Geoff Hinton

Adaptive Learning Rates

- One possible strategy
  - Start with a local gain of 1 for every weight
  - Increase the local gain if the gradient for the weight does not change the sign.
  - Use small additive increases and multiplicative decreases (for mini-batch)

$$\Delta w_{ij} = -\varepsilon g_{ij} \frac{\partial E}{\partial w_{ij}}$$

$$\text{if} \quad \left(\frac{\partial E}{\partial w_{ij}}(t) \frac{\partial E}{\partial w_{ij}}(t-1) \right) > 0$$

$$\text{then } g_{ij}(t) = g_{ij}(t-1) + 0.05$$

$$\text{else} \quad g_{ij}(t) = g_{ij}(t-1) * 0.95$$

⇒ Big gains will decay rapidly once oscillation starts.

Slide adapted from Geoff Hinton

Better Adaptation: RMSProp

- **Motivation**
  - The magnitude of the gradient can be very different for different weights and can change during learning.
  - This makes it hard to choose a single global learning rate.
  - For batch learning, we can deal with this by only using the sign of the gradient, but we need to generalize this for minibatches.

- **Idea of RMSProp**
  - Divide the gradient by a running average of its recent magnitude

$$MeanSq(w_{ij}, t) = 0.9 MeanSq(w_{ij}, t-1) + 0.1 \left(\frac{\partial E}{\partial w_{ij}}(t) \right)^2$$

  - Divide the gradient by $\mathrm{sqrt}(MeanSq(w_{ij},t))$.

Slide adapted from Geoff Hinton

Other Optimizers (Lucas)

- AdaGrad [Duchi '10]

- AdaDelta [Zeiler '12]

- Adam [Ba & Kingma '14]

- Notes
  - All of those methods have the goal to make the optimization less sensitive to parameter settings.
  - Adam is currently becoming the quasi-standard

Behavior in a Long Valley

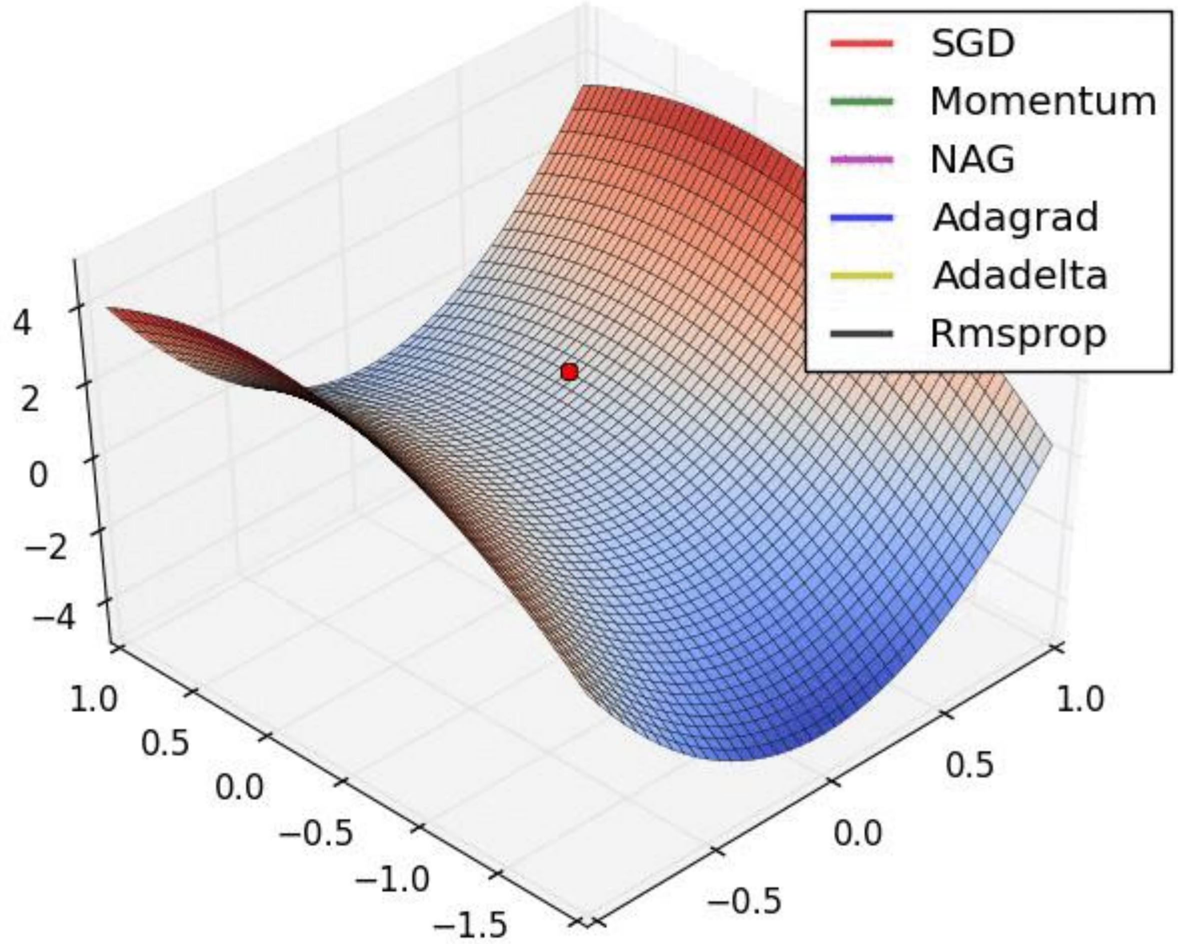


Image source: Aelc Radford, http://imgur.com/a/Hqolp

Behavior around a Saddle Point

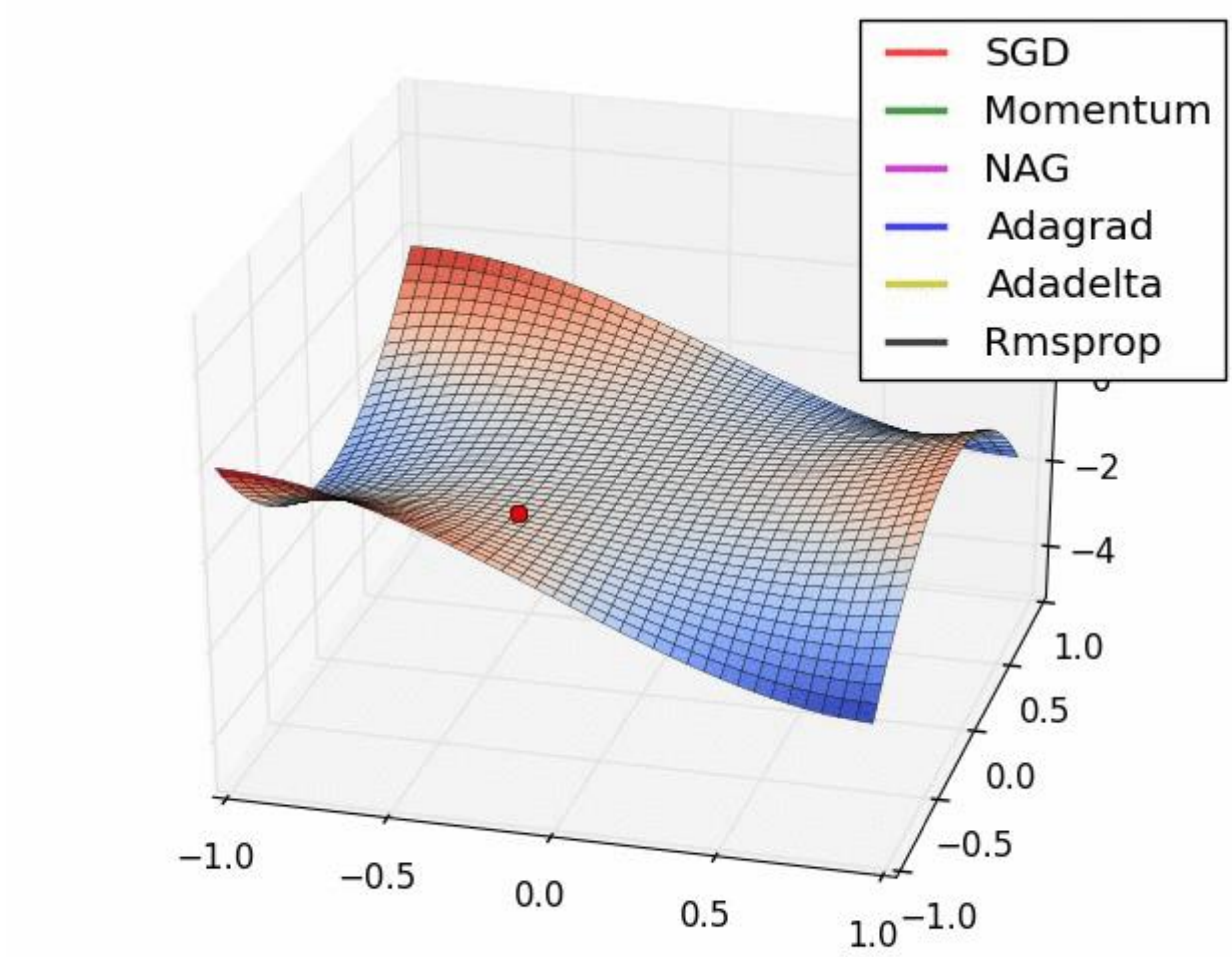


Image source: Aelc Radford, http://imgur.com/a/Hqolp

Visualization of Convergence Behavior

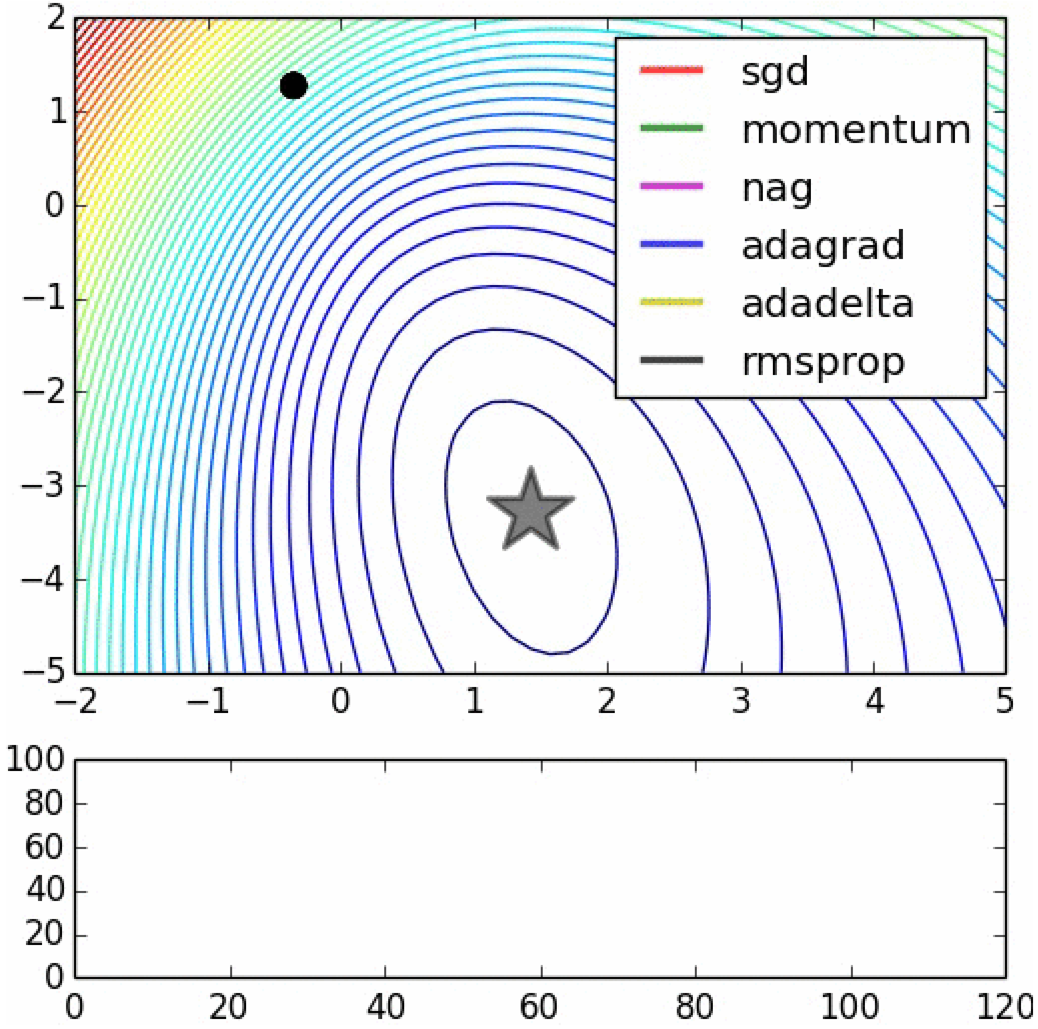
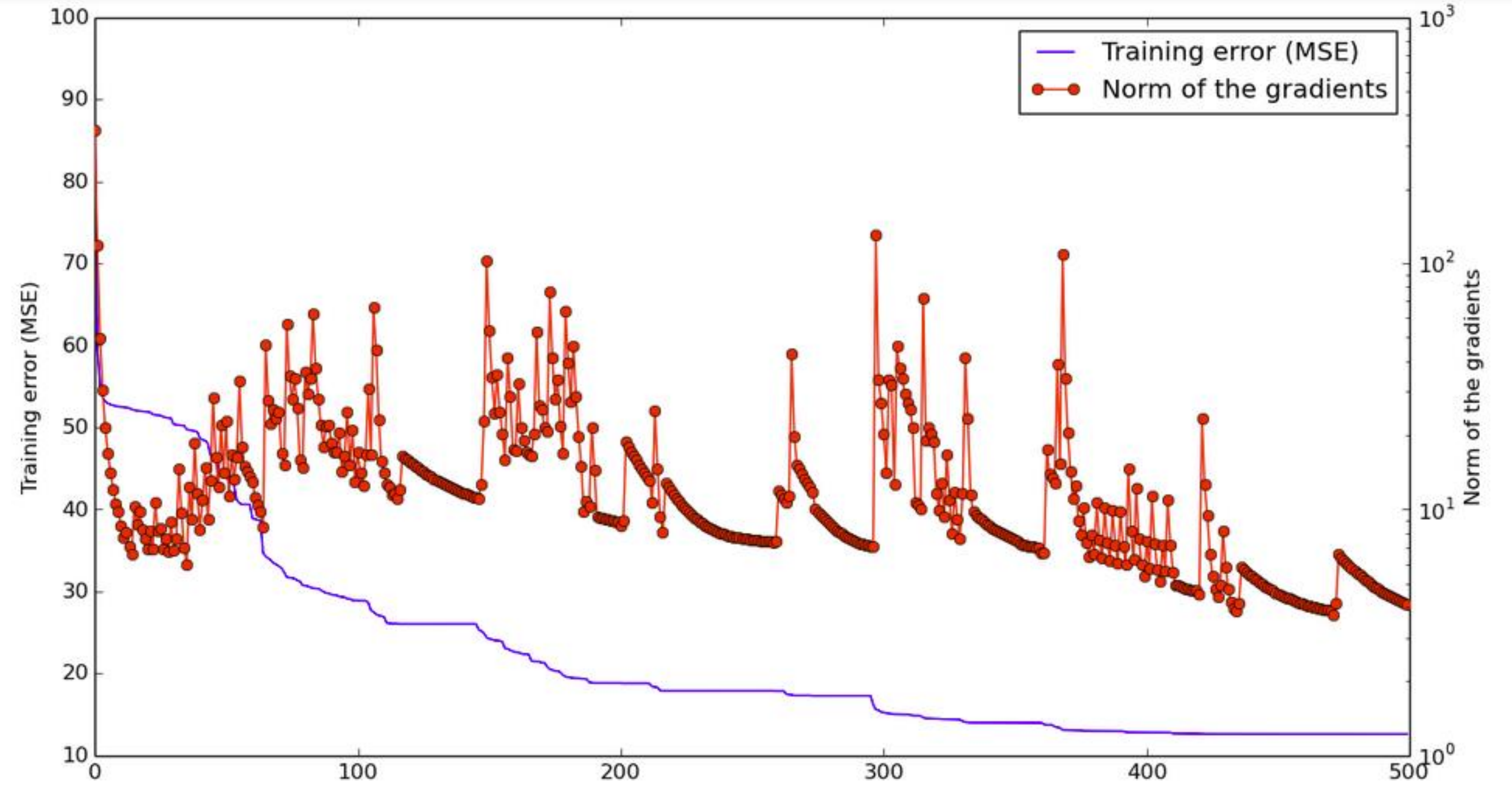


Image source: Aelc Radford, http://imgur.com/SmDARzn

Trick: Patience

- Saddle points dominate in high-dimensional spaces!

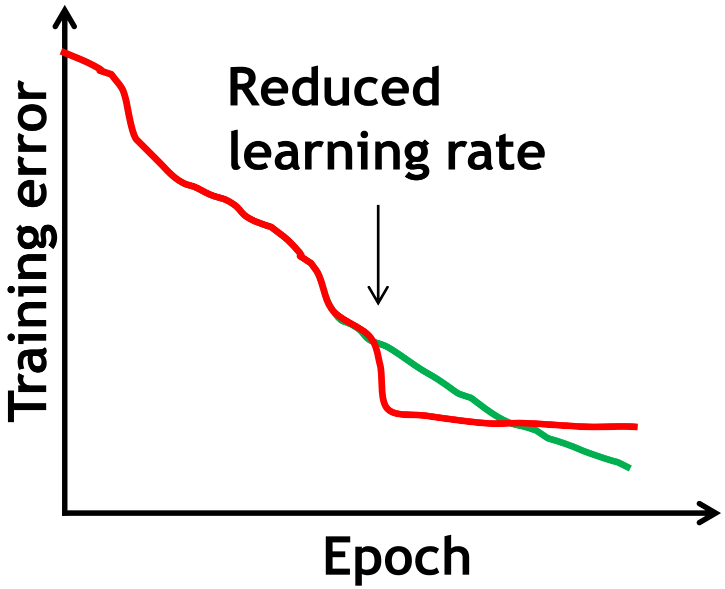


⇒ Learning often doesn't get stuck, you just may have to wait...

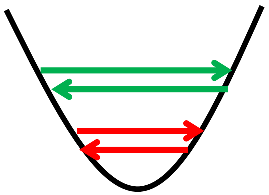
Image source: Yoshua Bengio

Reducing the Learning Rate

- Final improvement step after convergence is reached
  - Reduce learning rate by a factor of 10.
  - Continue training for a few epochs.
  - Do this 1-3 times, then stop training.



- Effect
  - Turning down the learning rate will reduce the random fluctuations in the error due to different gradients on different minibatches.



- *Be careful: Do not turn down the learning rate too soon!*
  - Further progress will be much slower after that.

Slide adapted from Geoff Hinton

Topics of This Lecture

- Gradient Descent
- Data (Pre-)processing
  - Stochastic Gradient Descent & Minibatches
  - Data Augmentation
  - Normalization
  - Initialization
- Convergence of Gradient Descent
  - Choosing Learning Rates
  - Momentum & Nesterov Momentum
  - RMS Prop
  - Other Optimizers
- **Other Tricks**
  - **Batch Normalization**
  - **Dropout**

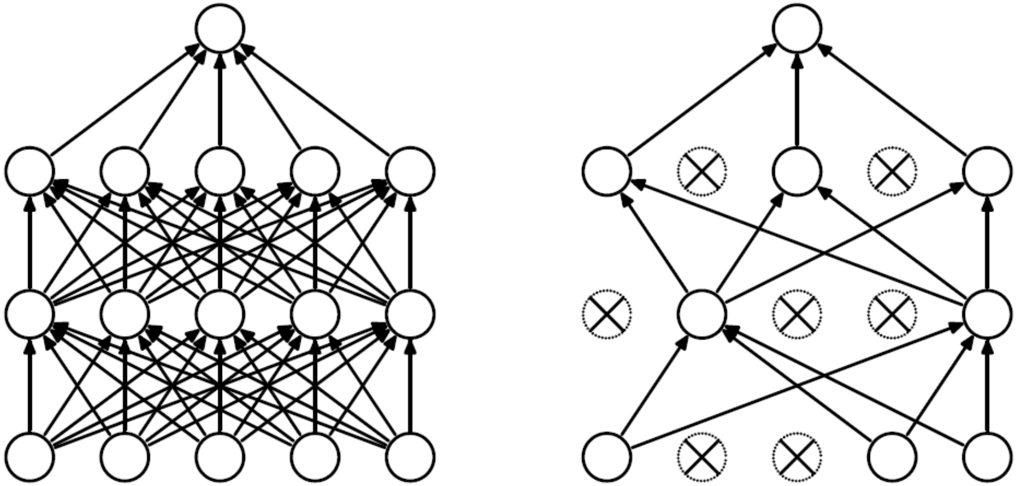
Batch Normalization [Ioffe & Szegedy '14]

- Motivation
  - Optimization works best if all inputs of a layer are normalized.

- Idea
  - Introduce intermediate layer that centers the activations of the previous layer per minibatch.
  - I.e., perform transformations on all activations and undo those transformations when backpropagating gradients

- Effect
  - Much improved convergence

Dropout [Srivastava, Hinton '12]



(a) Standard Neural Net (b) After applying dropout.

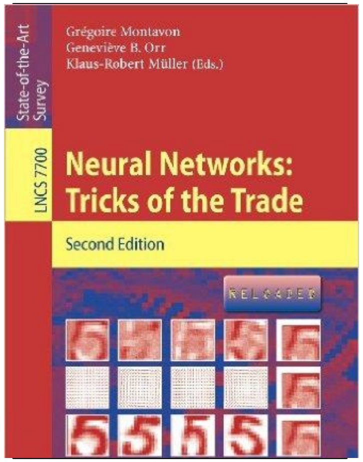
- **Idea**
  - Randomly switch off units during training.
  - Change network architecture for each data point, effectively training many different variants of the network.
  - When applying the trained network, multiply activations with the probability that the unit was set to zero.

  ⇒ Greatly improved performance

References and Further Reading

- More information on many practical tricks can be found in Chapter 1 of the book

G. Montavon, G. B. Orr, K-R Mueller (Eds.)
Neural Networks: Tricks of the Trade
Springer, 1998, 2012



Yann LeCun, Leon Bottou, Genevieve B. Orr, Klaus-Robert Mueller
Efficient BackProp, Ch.1 of the above book., 1998.

References

- ReLu
  - X. Glorot, A. Bordes, Y. Bengio, Deep sparse rectifier neural networks, AISTATS 2011.

- Initialization
  - X. Glorot, Y. Bengio, Understanding the difficulty of training deep feedforward neural networks, AISTATS 2010.
  - K. He, X.Y. Zhang, S.Q. Ren, J. Sun, Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification, ArXiV 1502.01852v1, 2015.
  - A.M. Saxe, J.L. McClelland, S. Ganguli, Exact solutions to the nonlinear dynamics of learning in deep linear neural networks, ArXiV 1312.6120v3, 2014.

References and Further Reading

- Batch Normalization
  - S. Ioffe, C. Szegedy, Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift, ArXiV 1502.03167, 2015.
- Dropout
  - N. Srivastava, G. Hinton, A. Krizhevsky, I. Sutskever, R. Salakhutdinov, Dropout: A Simple Way to Prevent Neural Networks from Overfitting, JMLR, Vol. 15:1929-1958, 2014.