RWTH AACHEN UNIVERSITY

Machine Learning – Lecture 14

Deep Learning II

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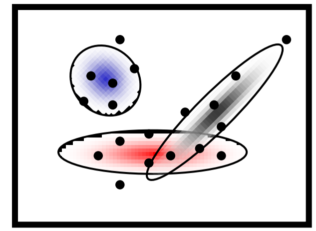
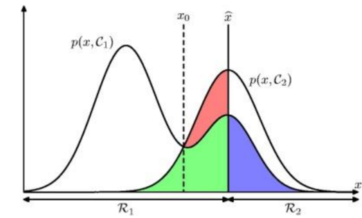
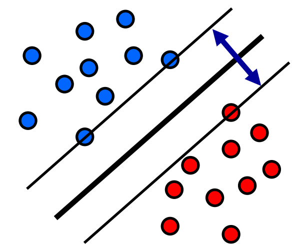
Course Outline

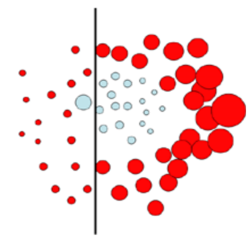
- **Fundamentals (2 weeks)**
  - Bayes Decision Theory
  - Probability Density Estimation



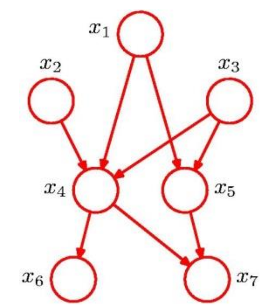


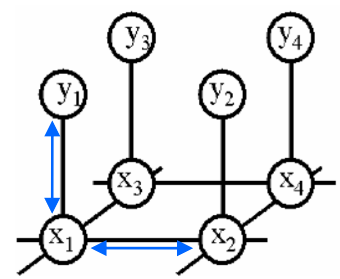
- **Discriminative Approaches (5 weeks)**
  - Linear Discriminant Functions
  - Statistical Learning Theory & SVMs
  - Ensemble Methods & Boosting
  - Randomized Trees, Forests & Ferns
  - Deep Learning





- **Generative Models (4 weeks)**
  - Bayesian Networks
  - Markov Random Fields





Topics of This Lecture

- Recap: Learning Multi-layer Networks
  - Backpropagation
  - Computational graphs
  - Automatic differentiation
- Gradient Descent
  - Stochastic Gradient Descent & Minibatches
  - Data Augmentation
  - Nonlinearities
  - Choosing Learning Rates
  - Momentum
  - RMS Prop
  - Other Optimizers

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

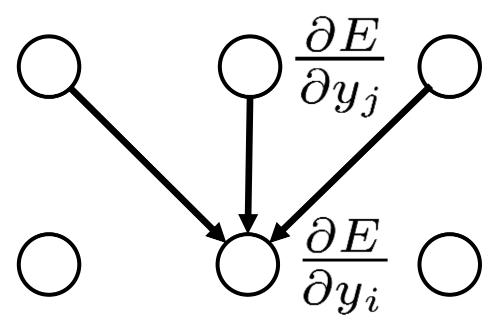
Recap: Backpropagation Algorithm

- Core steps
  1. Convert the discrepancy between each output and its target value into an error derivate.

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

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

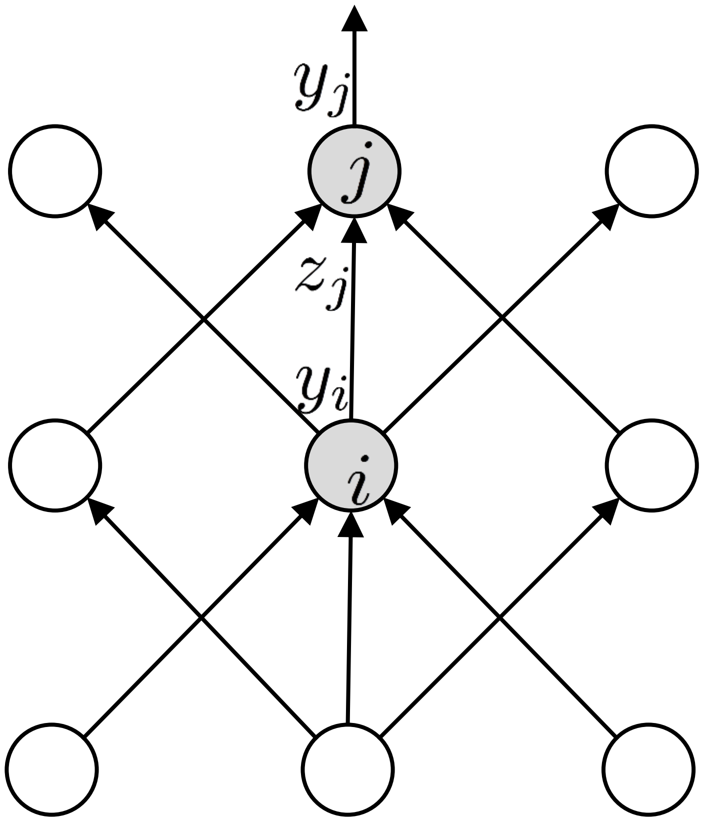
  2. Compute error derivatives in each hidden layer from error derivatives in the layer above.



  3. Use error derivatives *w.r.t.* activities to get error derivatives *w.r.t.* the incoming weights

$$\frac{\partial E}{\partial y_j} \longrightarrow \frac{\partial E}{\partial w_{ik}}$$

Recap: Backpropagation Algorithm



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

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

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

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

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

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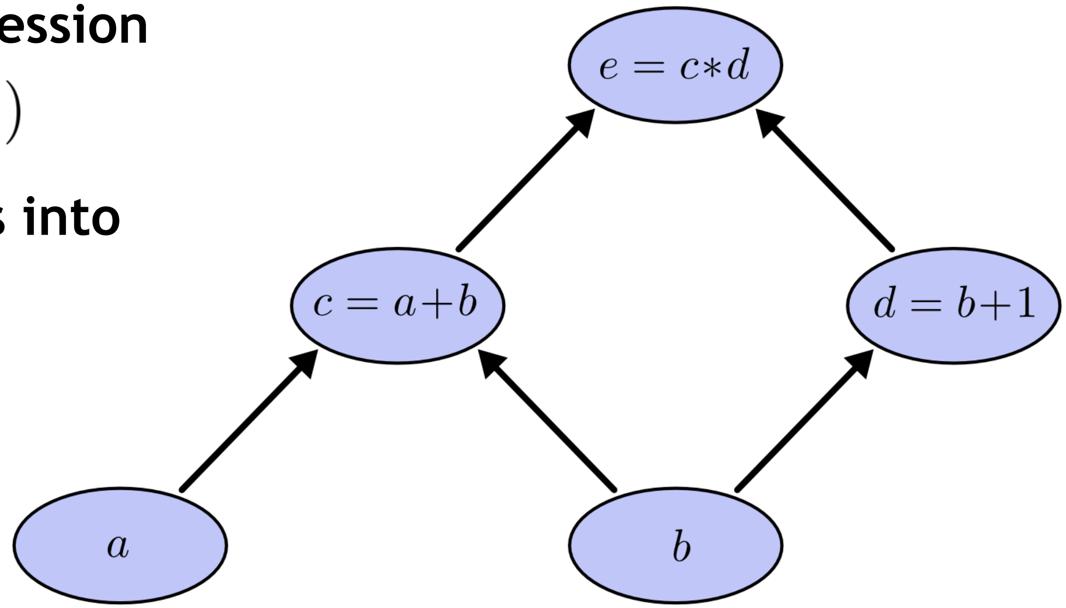
Computational Graphs

- We can think of mathematical expressions as graphs
  - E.g., consider the expression

$$e = (a+b)*(b+1)$$

  - We can decompose this into the operations

$$c = a+b$$
$$d = b+1$$
$$e = c*d$$

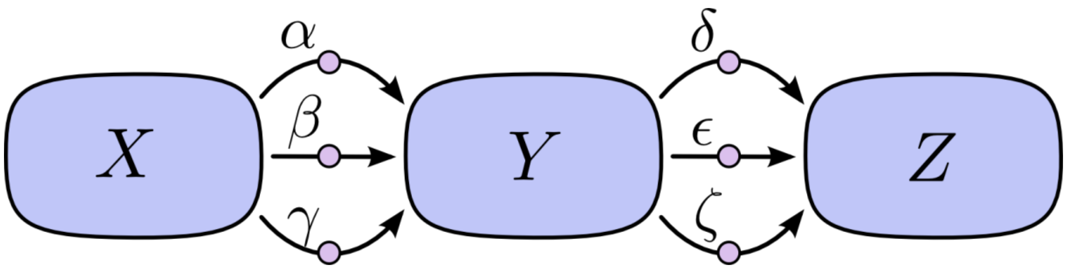


and visualize this as a computational graph.

- Evaluating partial derivatives $\frac{\partial Y}{\partial X}$ in such a graph
  - General rule: sum over all possible paths from Y to X and multiply the derivatives on each edge of the path together.

Factoring Paths

- Problem: Combinatorial explosion
  - Example:



  - There are 3 paths from X to Y and 3 more from Y to Z.
  - If we want to compute $\frac{\partial Z}{\partial X}$, we need to sum over 3×3 paths:

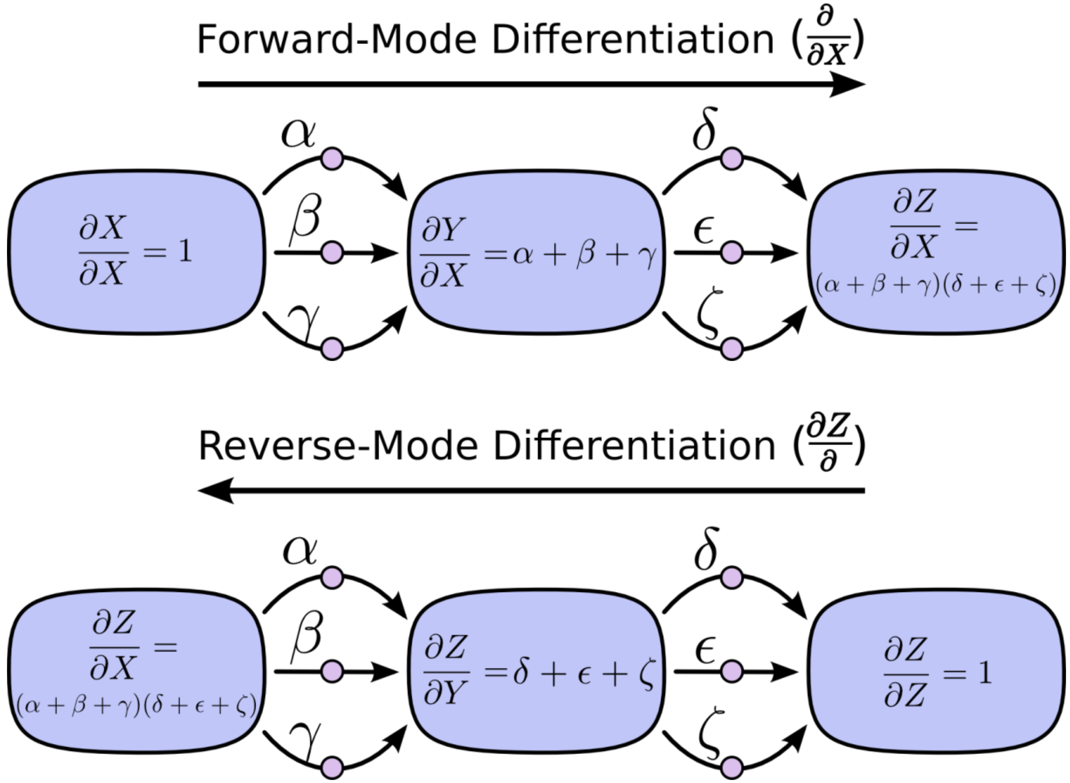
$$\frac{\partial Z}{\partial X} = \alpha\delta + \alpha\epsilon + \alpha\zeta + \beta\delta + \beta\epsilon + \beta\zeta + \gamma\delta + \gamma\epsilon + \gamma\zeta$$

  - Instead of naively summing over paths, it's better to factor them

$$\frac{\partial Z}{\partial X} = (\alpha + \beta + \gamma) * (\delta + \epsilon + \zeta)$$

Image source: Christopher Olah, colah.github.io

Efficient Factored Algorithms



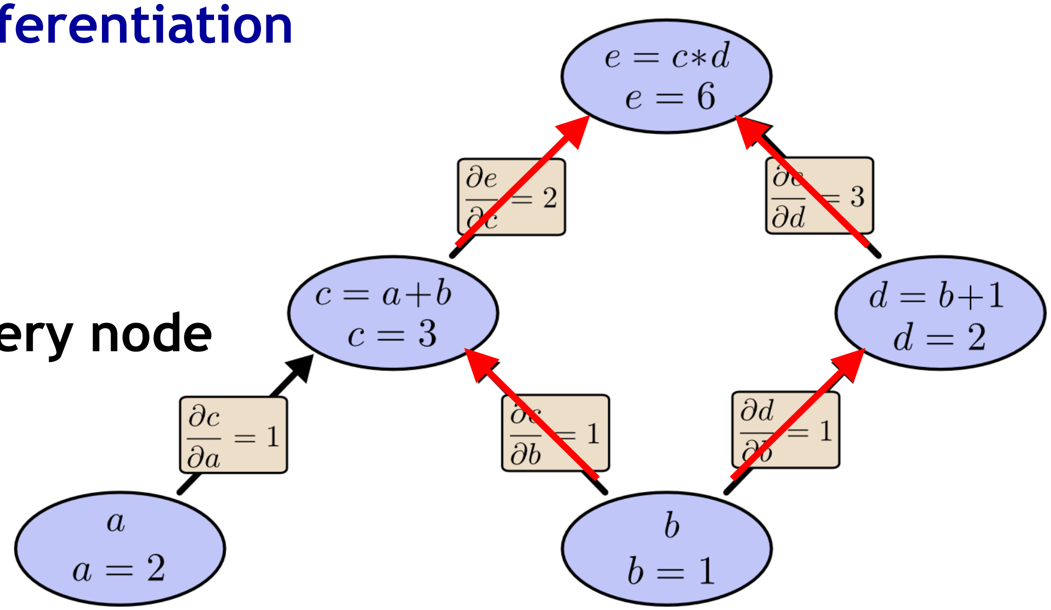
Apply operator $\frac{\partial}{\partial X}$ to every node.

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

- **Efficient algorithms for computing the sum**
  - **Instead of summing over all of the paths explicitly, compute the sum more efficiently by merging paths back together at every node.**

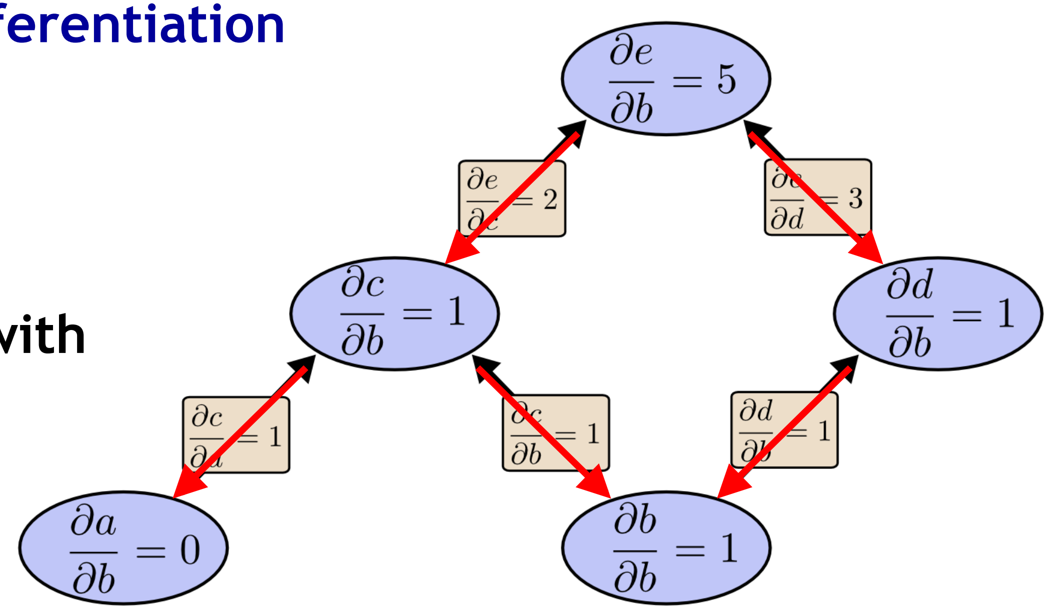
Why Do We Care?

- **Let's consider the example again**
  - **Using forward-mode differentiation from b up...**
  - **Runtime: $\mathcal{O}$(#edges)**
  - **Result: derivative of every node with respect to b.**



Why Do We Care?

- Let’s consider the example again
  - Using reverse-mode differentiation from e down...
  - Runtime: $\mathcal{O}(\text{\#edges})$
  - Result: derivative of e with respect to every node.



$\Rightarrow$ *This is what we want to compute in Backpropagation!*

- Forward differentiation needs one pass per node. With backward differentiation can compute all derivatives in one single pass.

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

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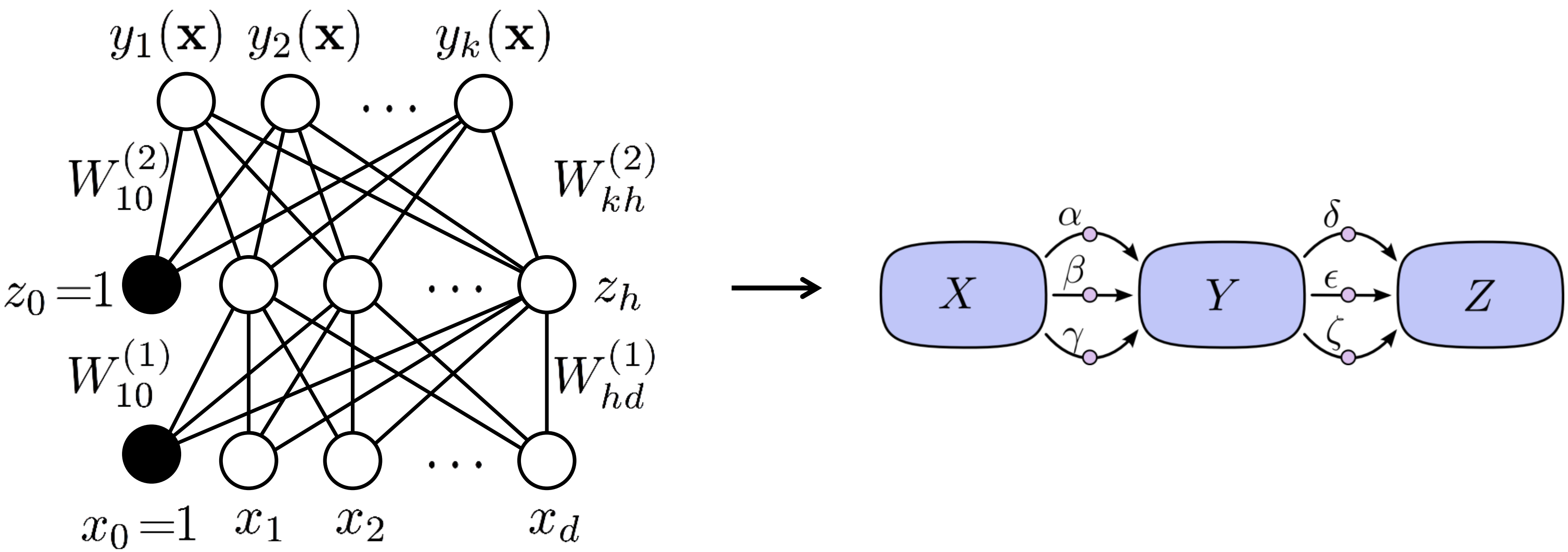
Obtaining the Gradients

- **Approach 4: Automatic Differentiation**



  - 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

Modular Implementation (e.g., Torch)

- Solution in many current Deep Learning libraries
  - Provide a limited form of automatic differentiation
  - Restricted to “programs” composed of “modules” with a predefined set of operations.

- Each module is defined by two main functions
  1. Computing the outputs $\mathbf{y}$ of the module given its inputs $\mathbf{x}$

$$\mathbf{y} = \text{module}.\mathbf{fprop}(\mathbf{x})$$

     where $\mathbf{x}$, $\mathbf{y}$, and intermediate results are stored in the module.

  2. Computing the gradient $\partial E / \partial \mathbf{x}$ of a scalar cost w.r.t. the inputs $\mathbf{x}$ given the gradient $\partial E / \partial \mathbf{y}$ w.r.t. the outputs $\mathbf{y}$

$$\frac{\partial E}{\partial \mathbf{x}} = \text{module}.\mathbf{bprop}\left(\frac{\partial E}{\partial \mathbf{y}}\right)$$

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- **Gradient Descent**
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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?

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

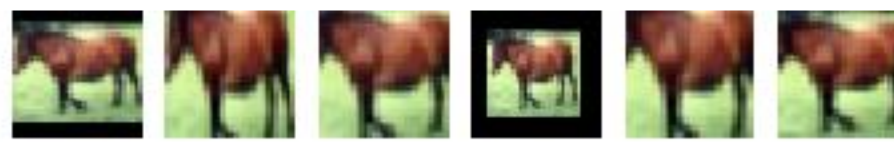
- **Idea**
  - Process only a small batch of training examples together
  - Start with a small batch size & increase it as training proceeds.
- **Advantages**
  - Gradients will more stable than for stochastic gradient descent, but still faster to compute than with batch learning.
  - Take advantage 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

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

Data Augmentation

- Idea
  - Augment original data with synthetic variations to reduce overfitting
- Example augmentations for images
  - Cropping

  - Zooming



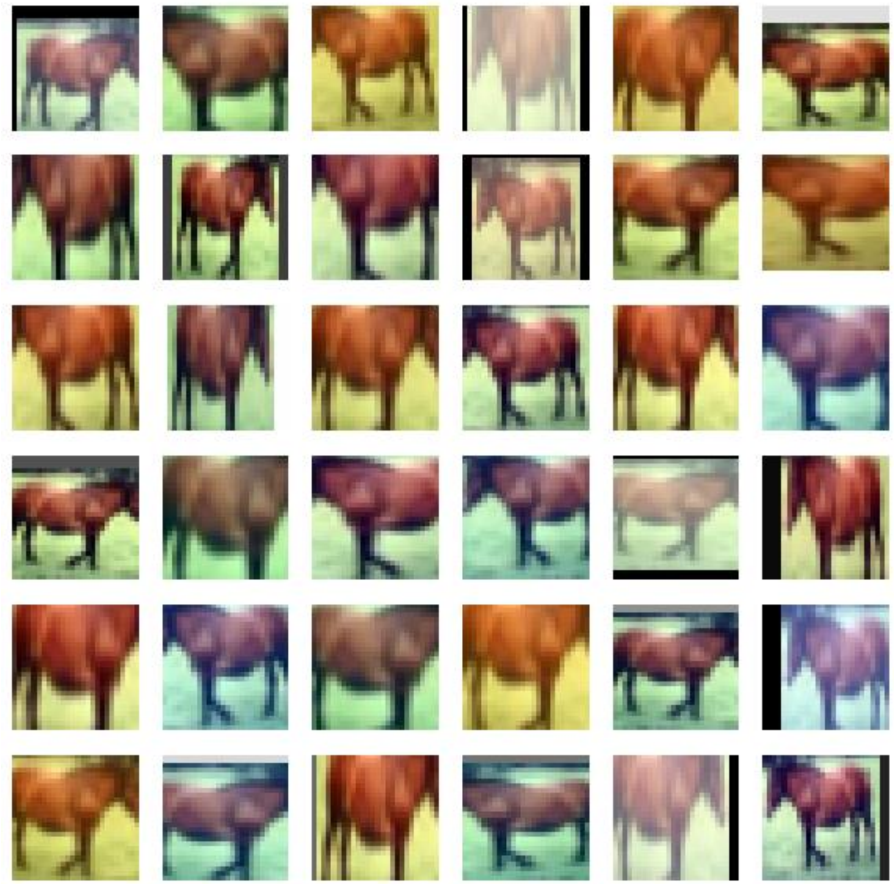
  - Flipping

  - Color PCA

Image source: Lucas Beyer

Data Augmentation

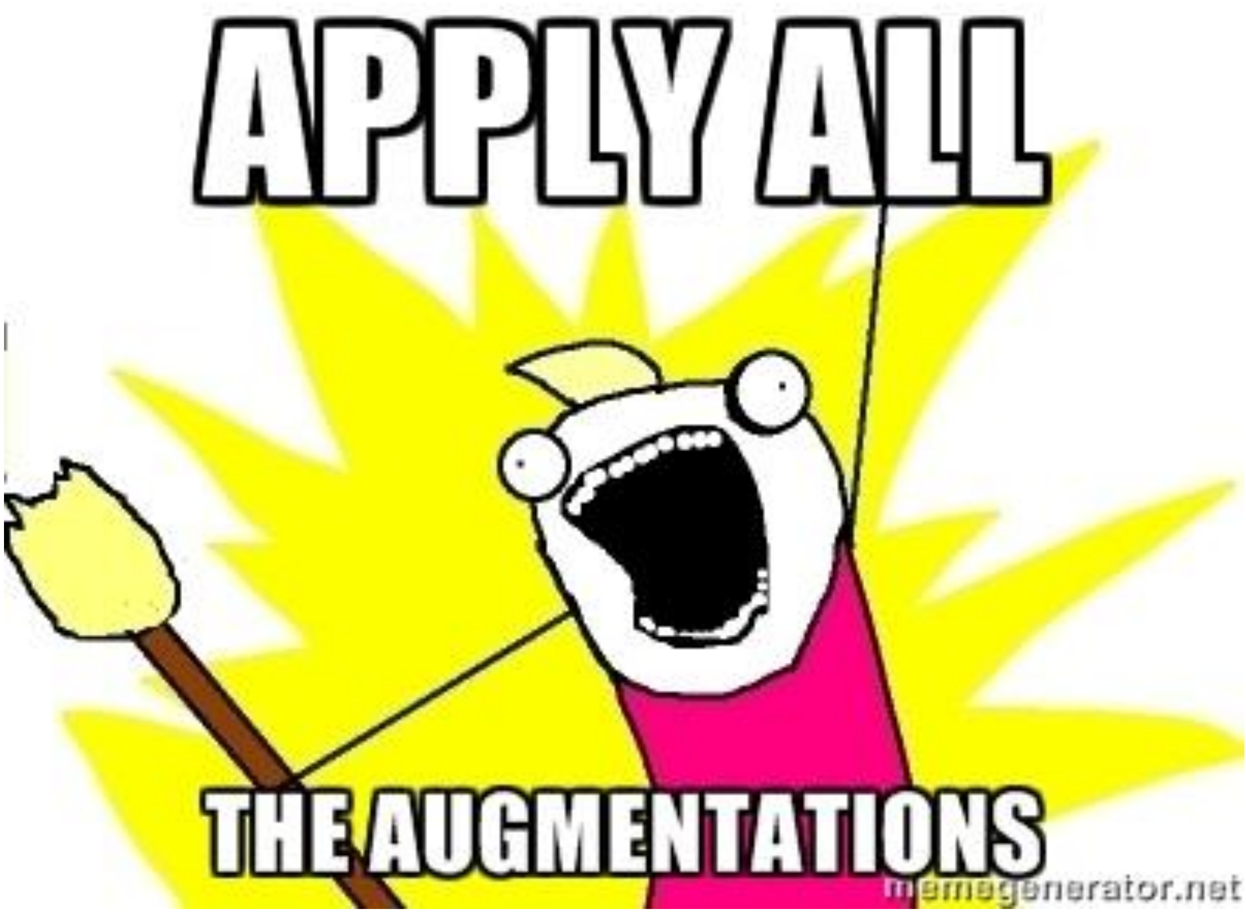
- **Effect**
  - Much larger training set
  - Robustness against expected variations
- **During testing**
  - When cropping was used during training, need to again apply crops to get same image size.
  - Beneficial to also apply flipping during test.
  - Applying several ColorPCA variations can bring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



Augmented training data (from one original image)

Image source: Lucas Beyer

General Guideline



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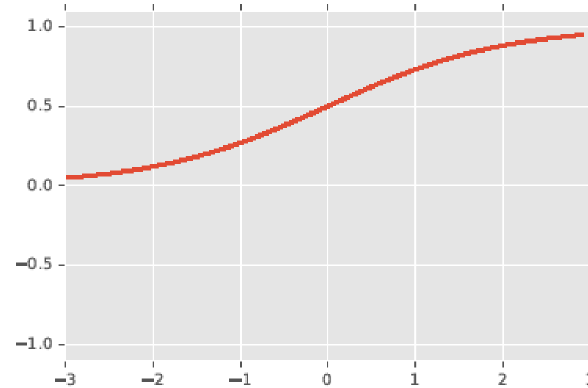
Commonly Used Nonlinearities

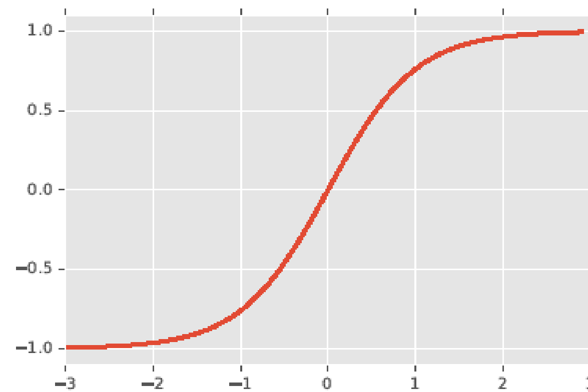
- **Sigmoid**

$$\begin{aligned} g(a) &= \sigma(a) \\ &= \frac{1}{1+\exp\{-a\}} \end{aligned}$$



- **Hyperbolic tangent**

$$\begin{aligned} g(a) &= tanh(a) \\ &= 2\sigma(2a) - 1 \end{aligned}$$



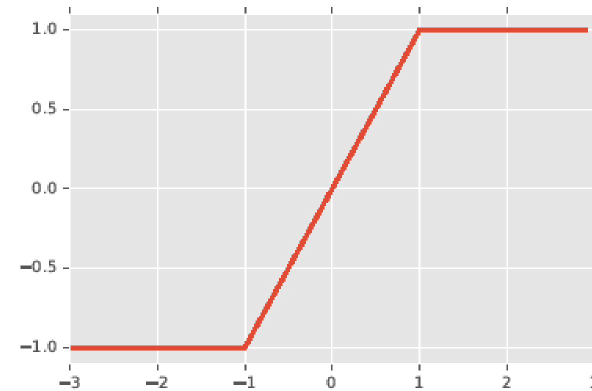
- **Softmax**

$$g(\mathbf{a}) = \frac{\exp\{-a_i\}}{\sum_j \exp\{-a_j\}}$$

Commonly Used Nonlinearities (2)

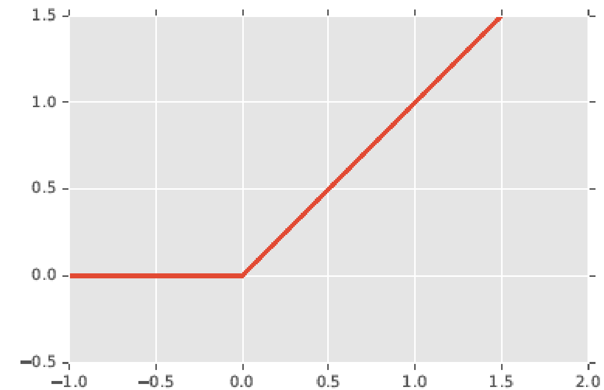
- **Hard tanh**

$$g(a) \;=\; \max\{-1, \min\{1, a\}\}$$



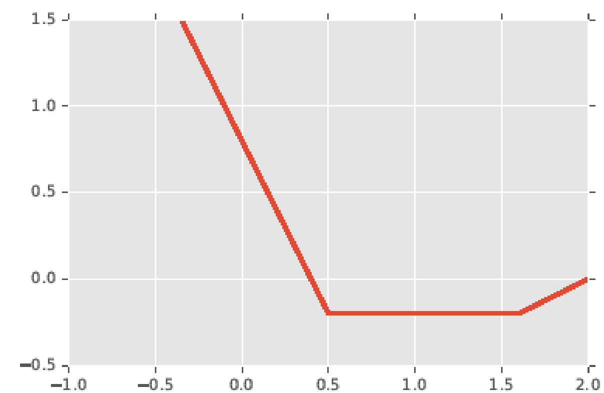
- **Rectified linear unit (ReLU)**

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



- **Maxout**

$$g(\mathbf{a}) \;=\; \max_i \left\{ \mathbf{w}_i^\top \mathbf{a} + b_i \right\}$$



Usage

- **Output nodes**
  - **Typically, a** sigmoid **or** tanh **function is used here.**
    - **Sigmoid for nice probabilistic interpretation (range [0,1]).**
    - **tanh for regression tasks**

- **Internal nodes**
  - **Historically,** tanh **was most often used.**
  - tanh **is better than** sigmoid **for internal nodes, since it is already centered.**
  - **Internally,** tanh **is often implemented as piecewise linear function (similar to** hard tanh **and** maxout**).**
  - **More recently:** ReLU **often used for classification tasks.**

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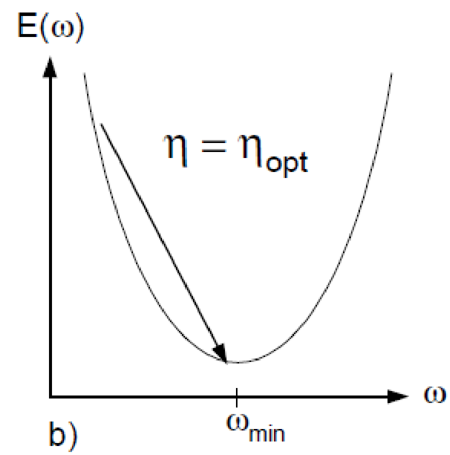
Choosing the Right Learning Rate

- **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

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

  - *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**

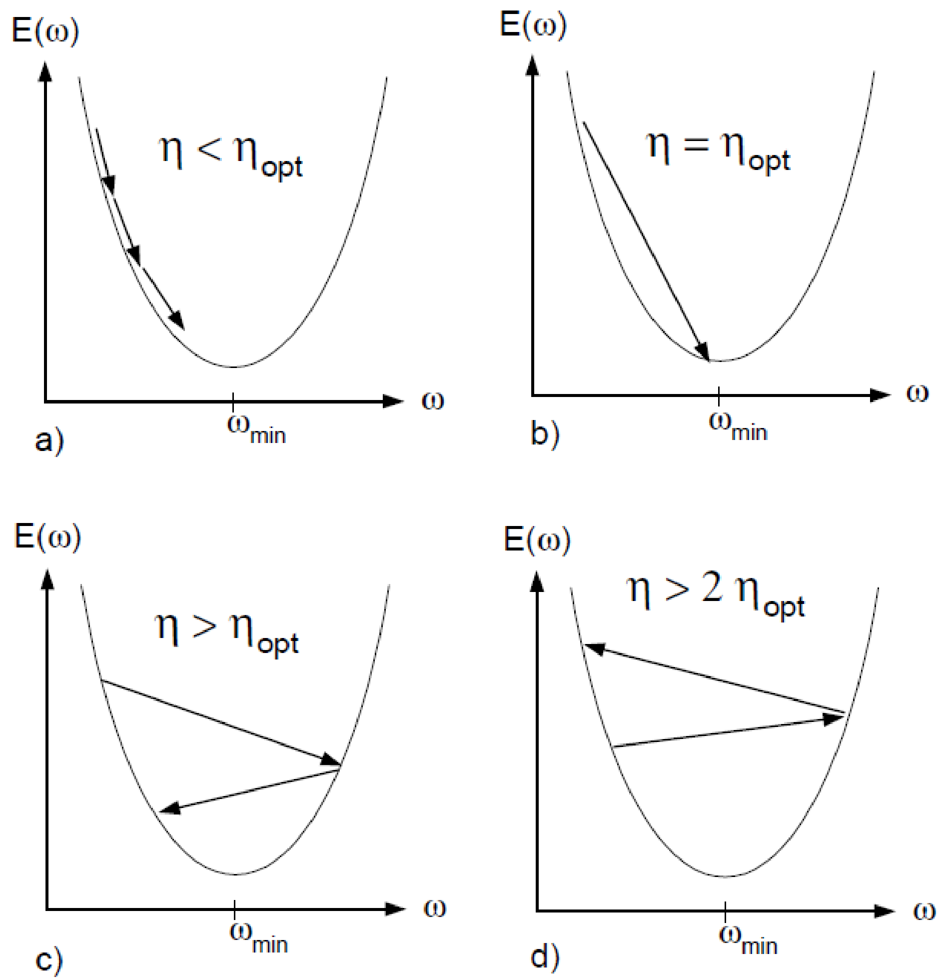


Image source: Yann LeCun et al., Efficient BackProp (1998)

Learning Rate vs. Training Error

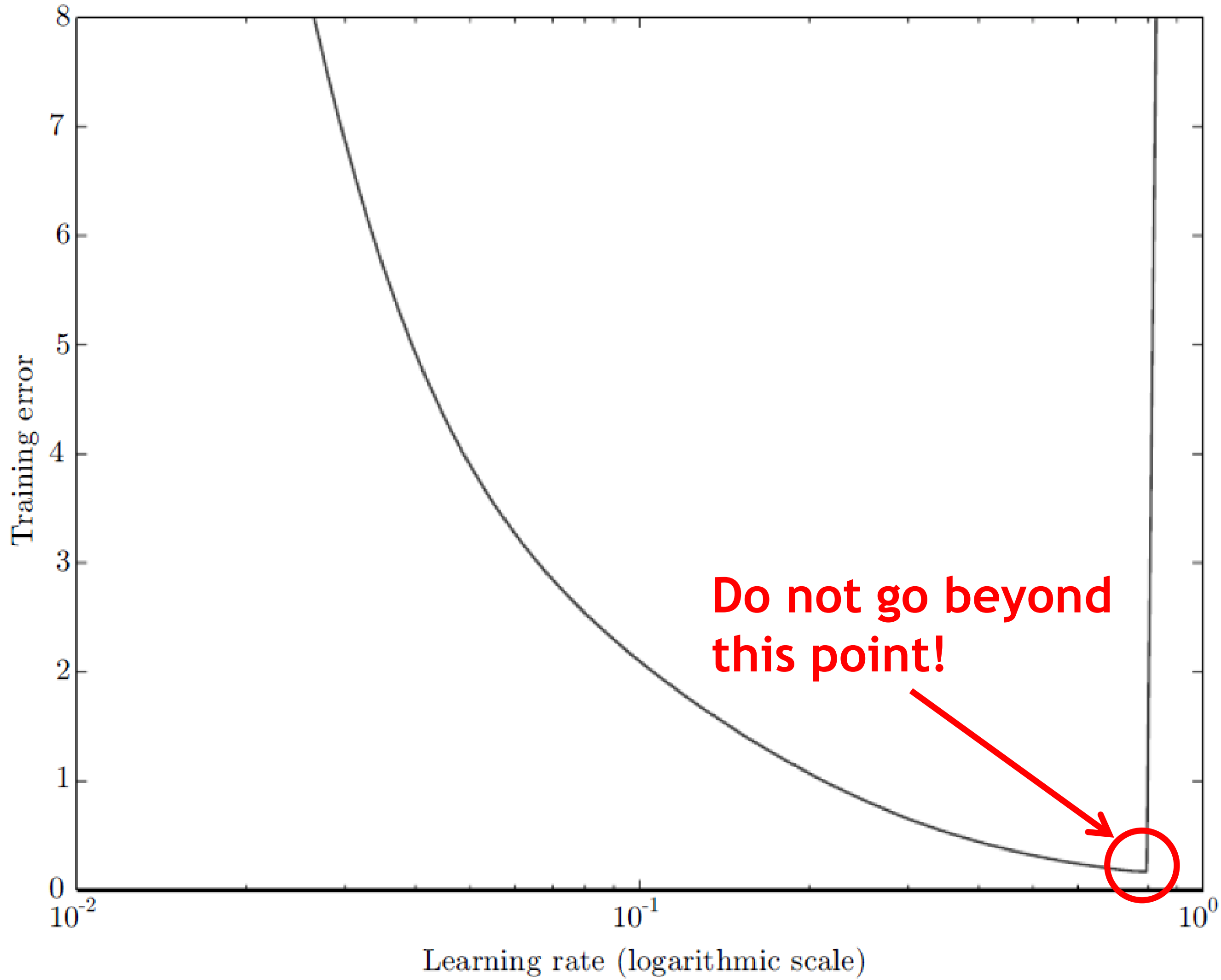
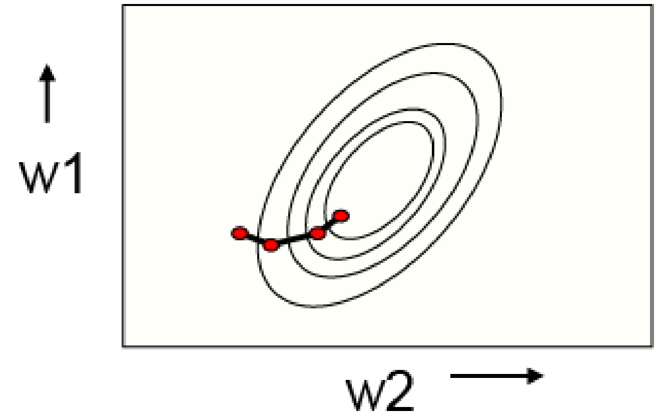


Image source: Goodfellow & Bengio book

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.

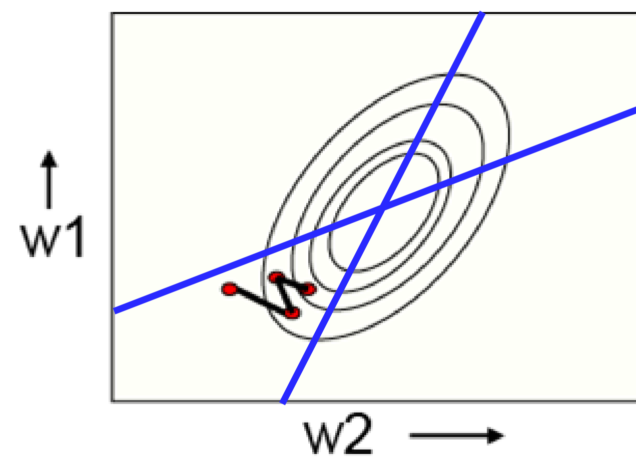
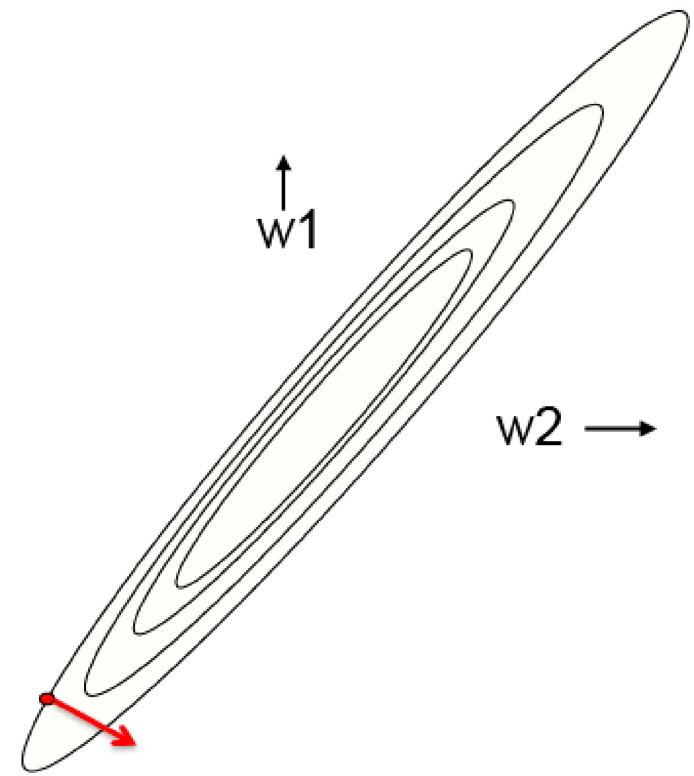


Image source: Geoff Hinton

Why Learning Can Be Slow

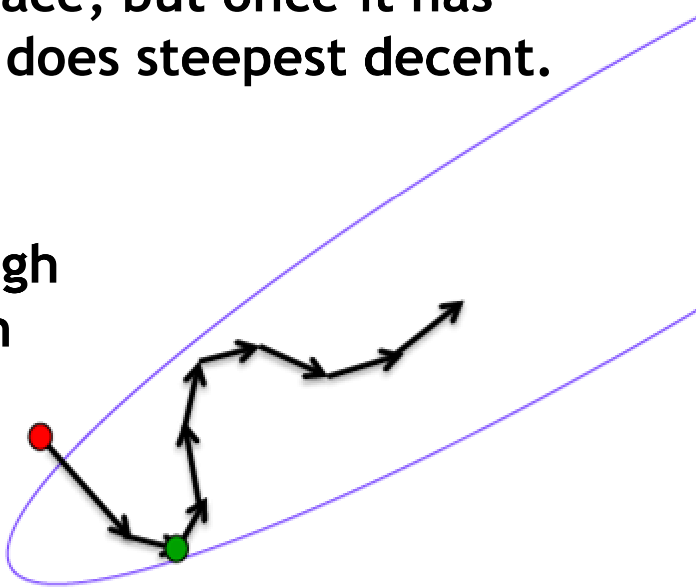
- **If the inputs are correlated**
  - **The ellipse will be very elongated.**
  - **The direction of steepest descent is almost perpendicular to the direction towards the minimum!**



This is just the opposite of what we want!

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.



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**

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

The Momentum Method: Behavior

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

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

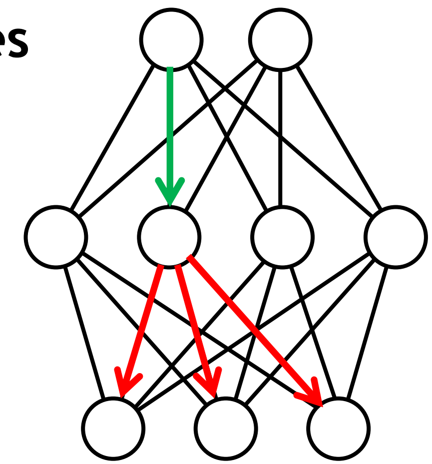
    - If the momentum α is close to 1, this is much faster than simple gradient descent.
  - At the beginning of learning, there may be very large gradients.
    - Use a small momentum initially (e.g., $\alpha = 0.5$).
    - Once the large gradients have disappeared and the weights are stuck in a ravine,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

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.



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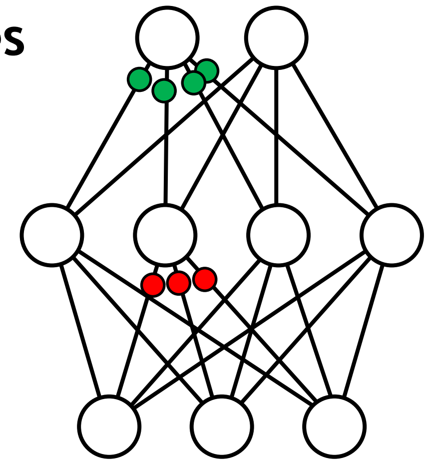
- Problem
  - In multilayer nets, the appropriate learning rates can vary widely between weights.
  - The magnitudes of the gradients are often very different for the different layers, especially if the initial weights are small.

    $\Rightarrow$ 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)

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 $\mathrm{sqrt}(MeanSq(w_{ij}, t))$.

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

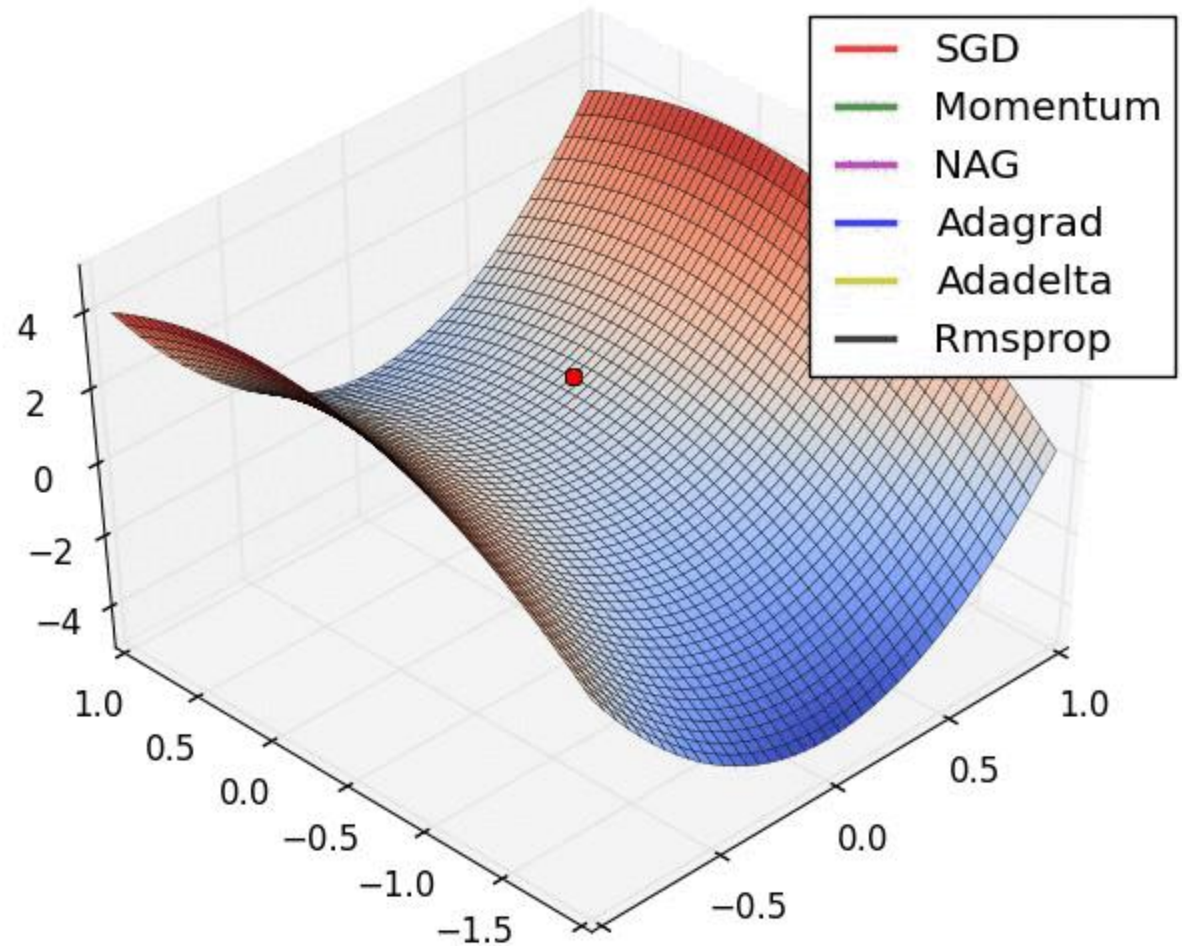


Image source: Aelc Radford, http://imgur.com/a/Hqolp

Behavior around a Saddle Point

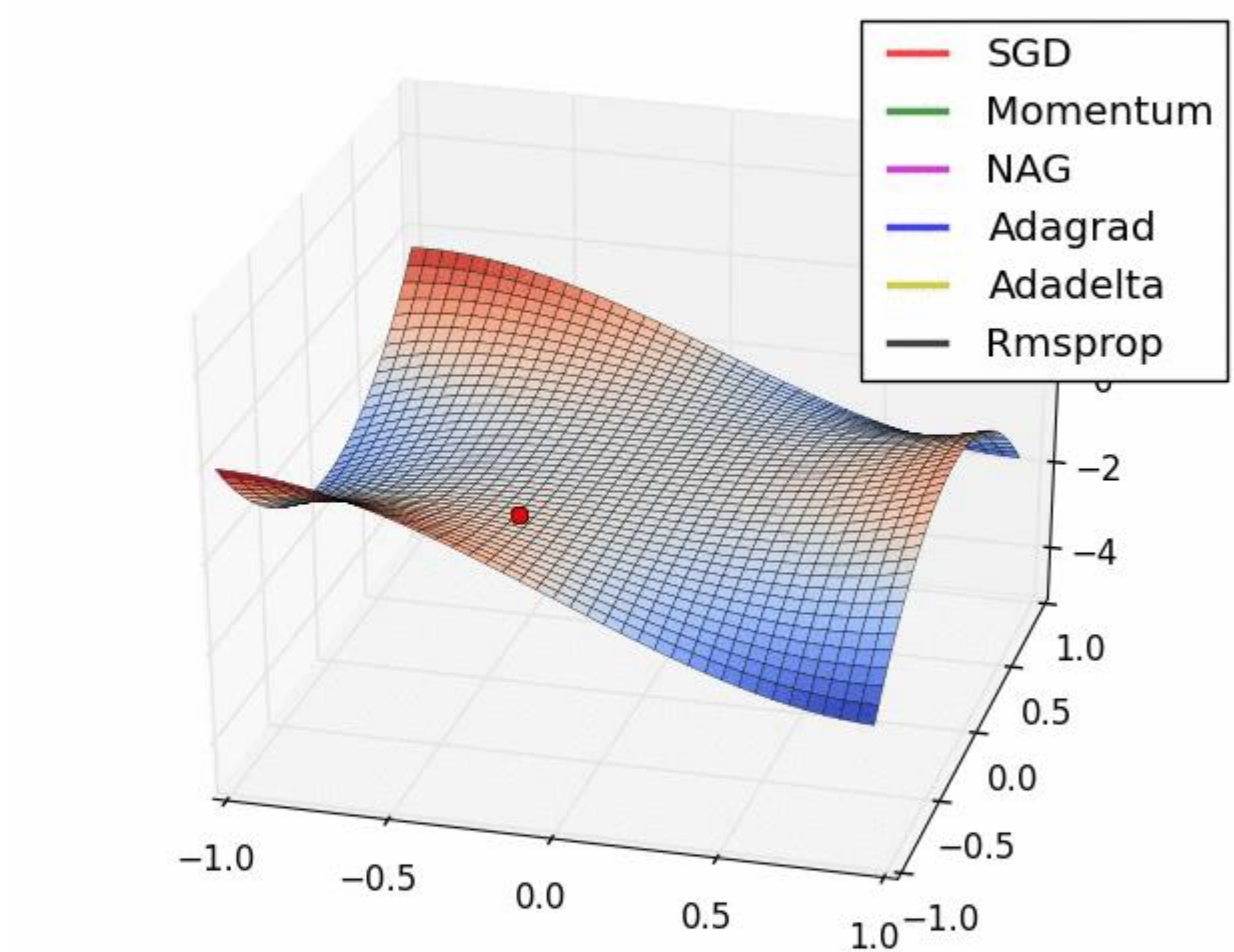


Image source: Aelc Radford, http://imgur.com/a/Hqolp

Visualization of Convergence Behavior

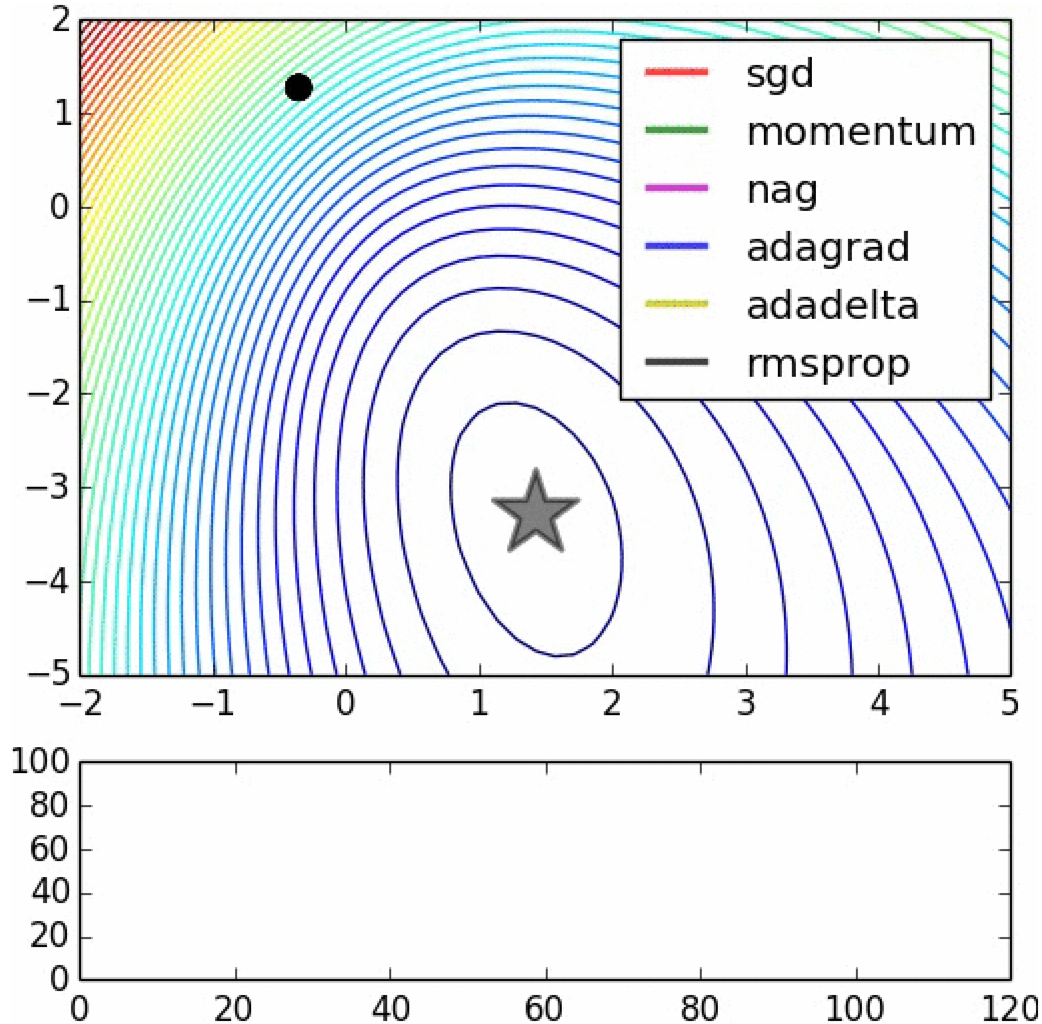
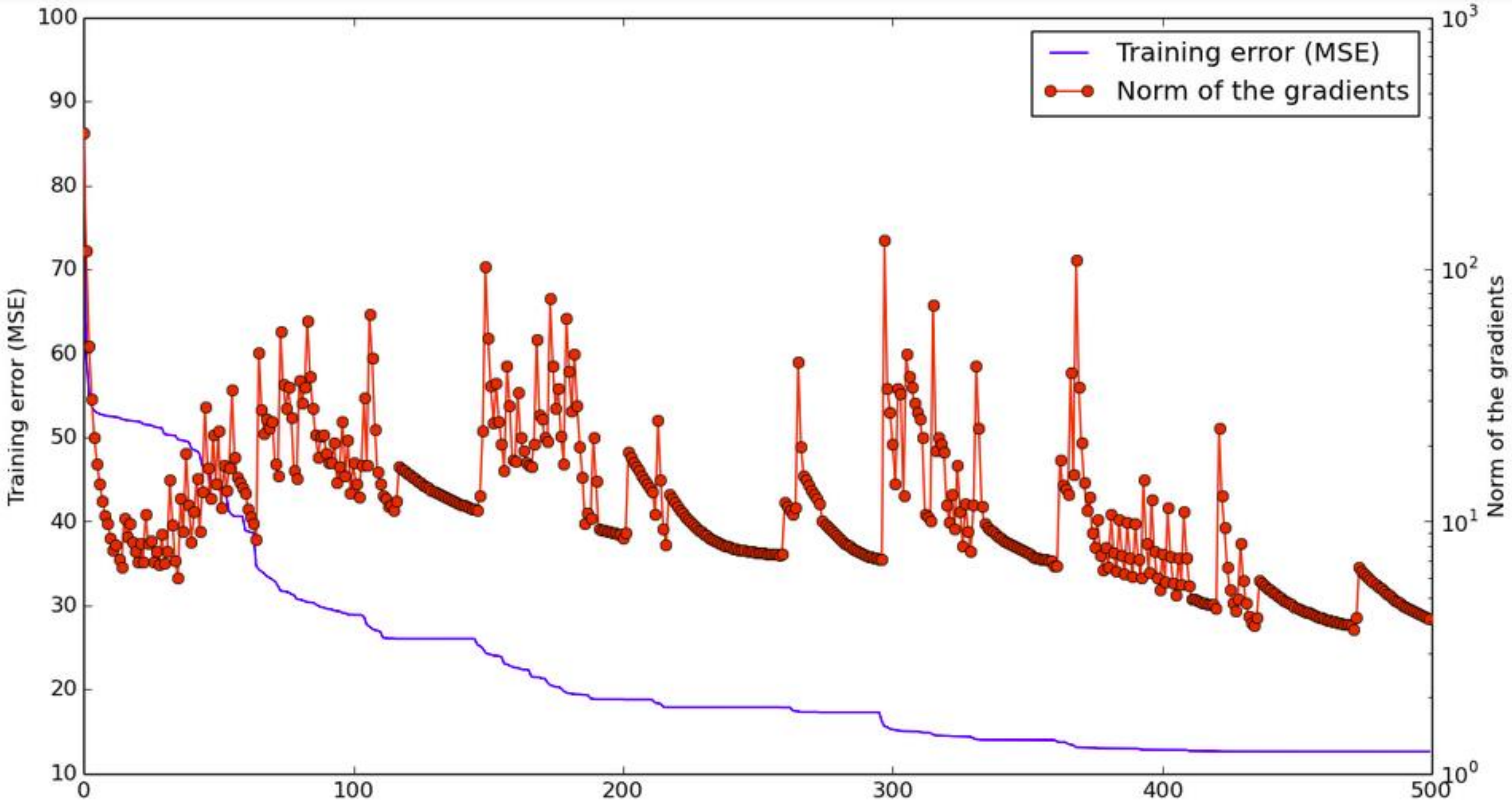


Image source: Aelc Radford, http://imgur.com/SmDARzn

Trick: Patience

- **Saddle points dominate in high-dimensional spaces!**

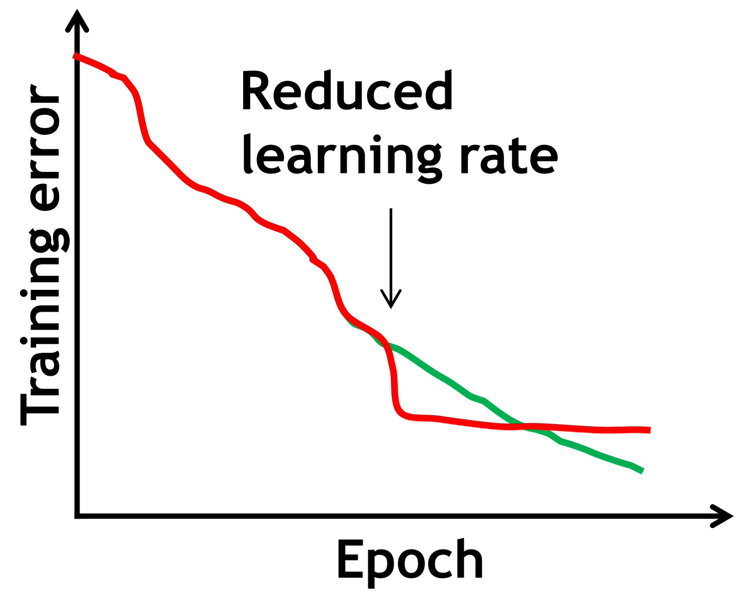


⇒ Learning often doesn't get stuck, you just may have to wait...

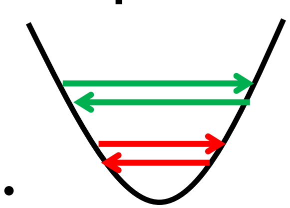
Image source: Yoshua Bengio

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.

Summary

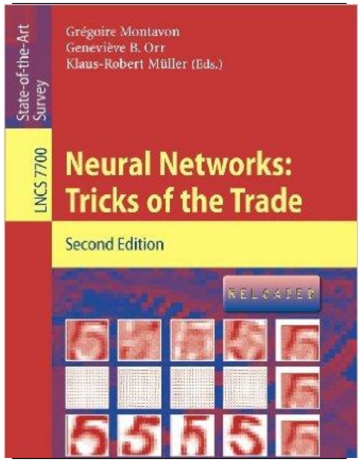
- Deep multi-layer networks are very powerful.
- But training them is hard!
  - Complex, non-convex learning problem
  - Local optimization with stochastic gradient descent
- Main issue: getting good gradient updates for the lower layers of the network
  - Many seemingly small details matter!
  - Weight initialization, normalization, data augmentation, choice of nonlinearities, choice of learning rate, choice of optimizer,…

  - *In this lecture, we could only skim the surface. If you are interested in using Deep Learning yourself, please check out the Advanced ML lecture from last winter!*

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.