Machine Learning – Lecture 13

Neural Networks II

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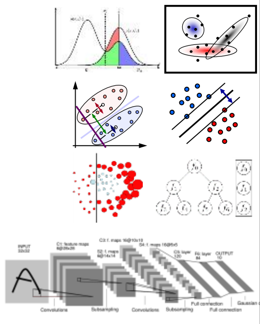
Course Outline

- Fundamentals
  - Bayes Decision Theory
  - Probability Density Estimation
- Classification Approaches
  - Linear Discriminants
  - Support Vector Machines
  - Ensemble Methods & Boosting
  - Random Forests
- Deep Learning
  - Foundations
  - Convolutional Neural Networks
  - Recurrent Neural Networks



Topics of This Lecture

- Learning Multi-layer Networks
  - Recap: Backpropagation
  - Computational graphs
  - Automatic differentiation
  - Practical issues
- Gradient Descent
  - Stochastic Gradient Descent & Minibatches
  - Choosing Learning Rates
  - Momentum
  - RMS Prop
  - Other Optimizers
- Tricks of the Trade
  - Shuffling
  - Data Augmentation
  - Normalization

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

$$\Omega(\mathbf{W}) = ||\mathbf{W}||_F^2$$ L_2 regularizer ("weight decay")

⇒ 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

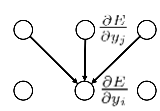
Recap: Backpropagation Algorithm

- 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.

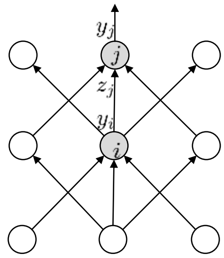


  3. Use error derivatives *w.r.t.* activities to get error derivatives *w.r.t.* the incoming weights

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

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.

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

Topics of This Lecture

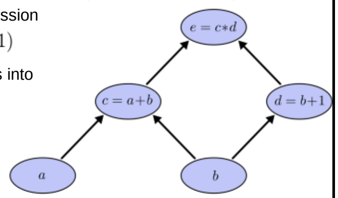
Computational Graphs

- 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

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

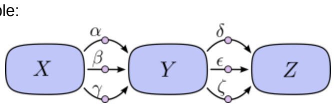


  and visualize this as a computational graph.

- 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:



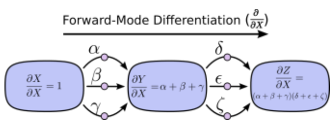
  - There are 3 paths from X to Y and 3 more from Y to Z.
  - If we want to compute $\frac{\partial Z}{\partial X}$, we need to sum over 3×3 paths:

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

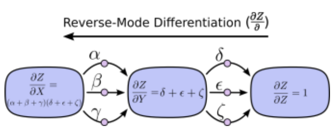
  - Instead of naively summing over paths, it's better to factor them

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

Efficient Factored Algorithms



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

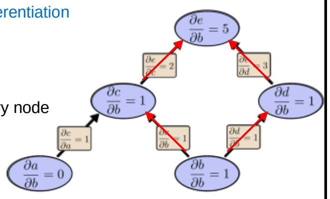


Apply operator $\frac{\partial Z}{\partial}$ to every node.

- 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.

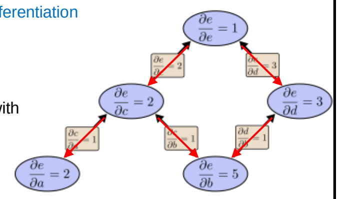
Why Do We Care?

- Let's consider the example again
  - Using forward-mode differentiation from b up...
  - Runtime: $\mathcal{O}(\#\text{edges})$
  - 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.



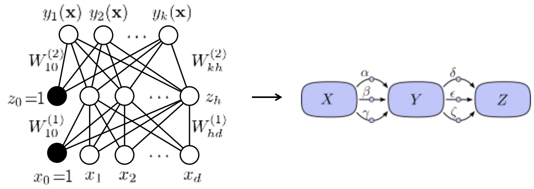
$\Rightarrow$ *This is what we want to compute in Backpropagation!*
  - Forward differentiation needs one pass per node. With backward differentiation can compute all derivatives in one single pass.

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

Topics of This Lecture

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

- 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 $\mathbf{y}$

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

Topics of This Lecture

Implementing Softmax Correctly

- Softmax output
  - De-facto standard for multi-class outputs

$$E(\mathbf{w}) = -\sum_{n=1}^{N}\sum_{k=1}^{K}\left\{\mathbb{I}\left(t_n = k\right)\ln\frac{\exp(\mathbf{w}_k^\top \mathbf{x})}{\sum_{j=1}^{K}\exp(\mathbf{w}_j^\top \mathbf{x})}\right\}$$

- Practical issue
  - Exponentials get very big and can have vastly different magnitudes.
  - Trick 1: Do not compute first softmax, then log, but instead directly evaluate log-exp in the denominator.
  - Trick 2: Softmax has the property that for a fixed vector $\mathbf{b}$

$$\mathrm{softmax}(\mathbf{a}+\mathbf{b}) = \mathrm{softmax}(\mathbf{a})$$

$\Rightarrow$ Subtract the largest weight vector $\mathbf{w}_j$ from the others.

Topics of This Lecture

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.

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

Stochastic 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

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

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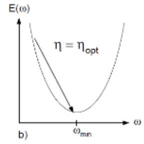
Choosing the Right Learning Rate

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

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



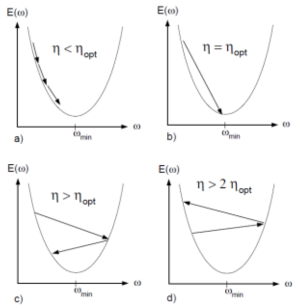
  - What is the optimal learning rate η_{opt}?
  - If E is quadratic, the optimal learning rate is given by the inverse of the Hessian

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

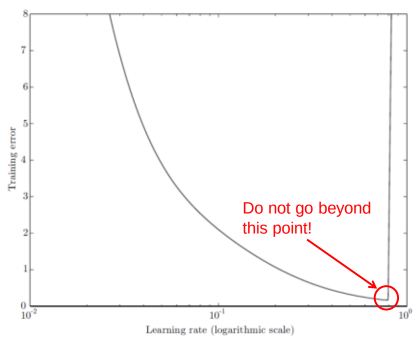
  - *What happens if we exceed this learning rate?*

Choosing the Right Learning Rate

- Behavior for different learning rates



Learning Rate vs. Training Error



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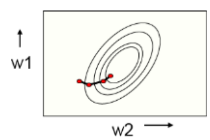
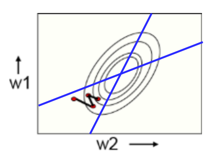
Batch vs. Stochastic Learning

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

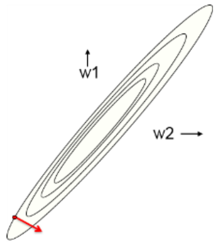


- Stochastic Learning
  - Simplest case: zig-zag around the direction of steepest descent.
  - ⇒ Updates perpendicular to constraints from training examples.



Why Learning Can Be Slow

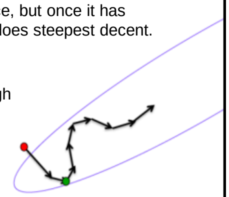
- If the inputs are correlated
  - The ellipse will be very elongated.
  - The direction of steepest descent is almost perpendicular to the direction towards the minimum!



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

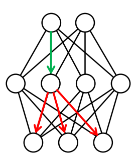
$$\mathbf{v}(\infty) = \frac{1}{1-\alpha}\left(-\varepsilon \frac{\partial E}{\partial \mathbf{w}}\right)$$

    - 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 $\alpha = 0.99$).

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

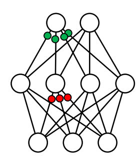
Separate, Adaptive Learning Rates

- 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.



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)



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

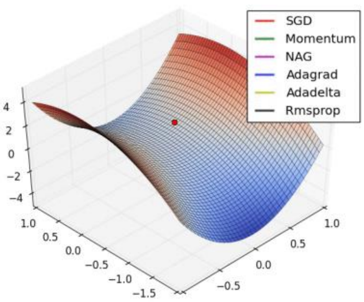
$$MeanSq(w_{ij},t) = 0.9 MeanSq(w_{ij},t-1) + 0.1 \left(\frac{\partial E}{\partial w_{ij}}(t)\right)^2$$

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

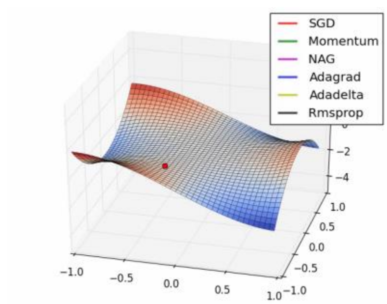
Other Optimizers

- 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

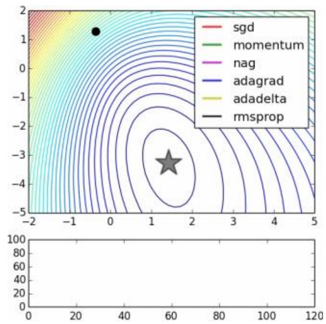
Behavior in a Long Valley



Behavior around a Saddle Point

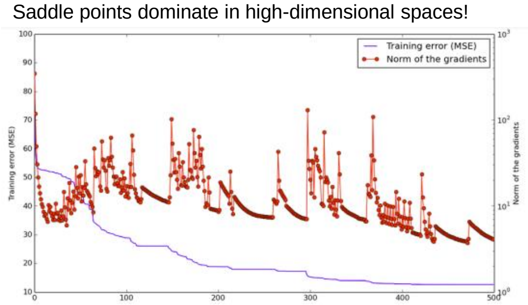


Visualization of Convergence Behavior



Trick: Patience

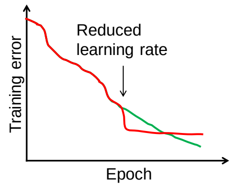
- Saddle points dominate in high-dimensional spaces!



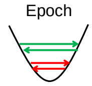
$\Rightarrow$ Learning often doesn't get stuck, you just may have to wait...

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/impossible 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 the following, we will take a look at the most important factors (to be continued in the next lecture…)*

Topics of This Lecture

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.

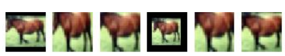
  ⇒ It can make sense to present such inputs more frequently.
    - But: be careful, this can be disastrous when the data are outliers.
- Practical advice
  - When working with stochastic gradient descent or minibatches, make use of shuffling.

Data Augmentation

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

- Example augmentations for images
  - Cropping

  - Zooming

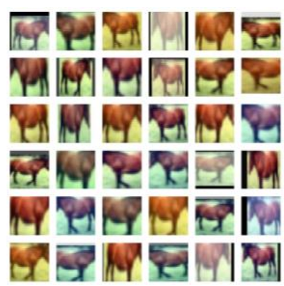


  - Flipping

  - Color PCA

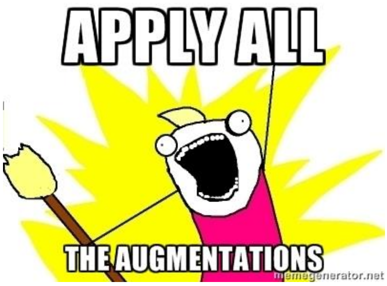
Data Augmentation

- 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)

Practical Advice



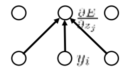
Normalization

- 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

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



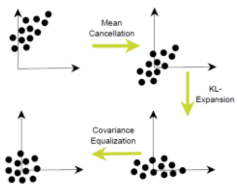
  - When all of the components of the input vector y_i are positive, all of the updates of weights that feed into a node will be of the same sign.

⇒ 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.



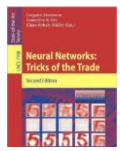
- Advisable normalization steps (for MLPs only, not for CNNs)
  - Normalize all inputs that an input unit sees to zero-mean, unit covariance.
  - If possible, try to decorrelate them using PCA (also known as Karhunen-Loeve expansion).

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

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.