Machine Learning – Lecture 14

Tricks of the Trade

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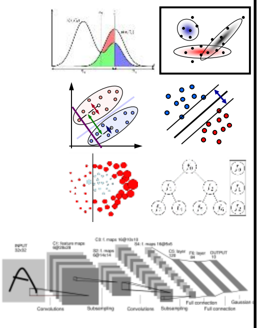
Course Outline

- 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

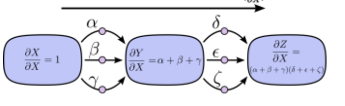


Topics of This Lecture

- Recap: Optimization
  - Effect of optimizers
- Tricks of the Trade
  - Shuffling
  - Data Augmentation
  - Normalization
- Nonlinearities
- Initialization
- Advanced techniques
  - Batch Normalization
  - Dropout

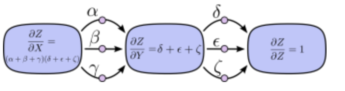
Recap: Computational Graphs

Forward-Mode Differentiation ($\frac{\partial}{\partial X}$)



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

Reverse-Mode Differentiation ($\frac{\partial Z}{\partial}$)



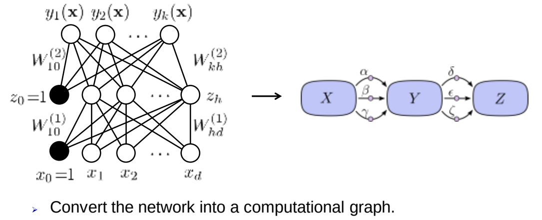
Apply operator $\frac{\partial Z}{\partial}$ to every node.

- 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!

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.

⇒ Very general algorithm, used in today's Deep Learning packages

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Correction: Implementing Softmax Correctly

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

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

- 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 nominator and log-sum-exp in the denominator.
  - Trick 2: Softmax has the property that for a fixed vector $\mathbf{b}$

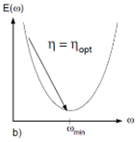
$$\text{softmax}(\mathbf{a}+\mathbf{b}) = \text{softmax}(\mathbf{a})$$

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

Recap: Choosing the Right Learning Rate

- Convergence of Gradient Descent
  - Simple 1D example

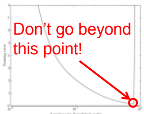
$$W^{(\tau-1)} = W^{(\tau)} - \eta \frac{\mathrm{d}E(W)}{\mathrm{d}W}$$



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

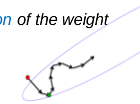
$$\eta_{\text{opt}} = \left(\frac{\mathrm{d}^2 E(W^{(\tau)})}{\mathrm{d}W^2} \right)^{-1}$$

  - Advanced optimization techniques try to approximate the Hessian by a simplified form.
  - *If we exceed the optimal learning rate, bad things happen!*



Recap: Advanced Optimization Techniques

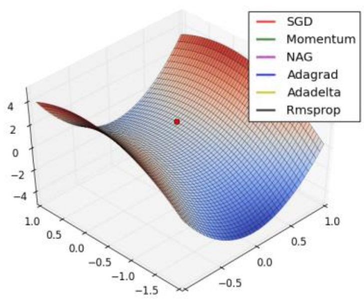
- Momentum
  - *Instead of using the gradient to change the position of the weight "particle", use it to change the velocity.*
  - Effect: dampen oscillations in directions of high curvature



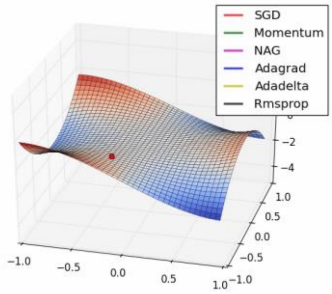
  - Nesterov-Momentum: Small variation in the implementation
- RMS-Prop
  - *Separate learning rate for each weight: Divide the gradient by a running average of its recent magnitude.*
- AdaGrad
- AdaDelta
- Adam

} Some more recent techniques, work better for some problems. Try them.

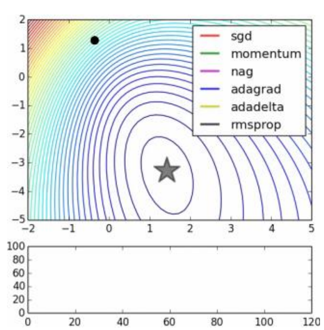
Example: Behavior in a Long Valley



Example: Behavior around a Saddle Point

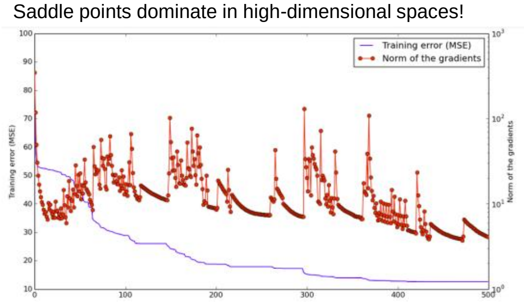


Visualization of Convergence Behavior



Trick: Patience

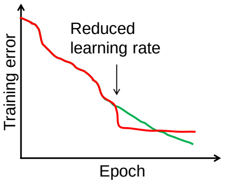
- Saddle points dominate in high-dimensional spaces!



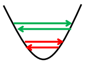
⇒ Learning often doesn't get stuck, you just may have to wait...

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*

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.

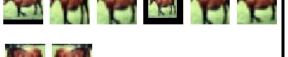
  ⇒ It can make sense to present such inputs more frequently.
    - But: be careful, this can be disastrous when the data are outliers.
- Practical advice
  - When working with stochastic gradient descent or minibatches, make use of shuffling.

Data Augmentation

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

- Example augmentations for images
  - Cropping

  - Zooming



  - Flipping

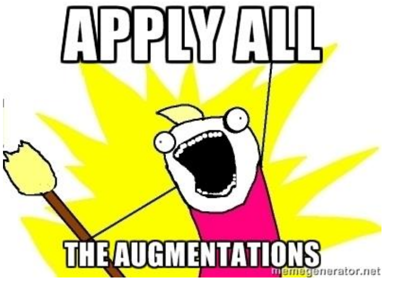
  - Color PCA

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



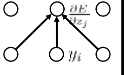
Normalization

- 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

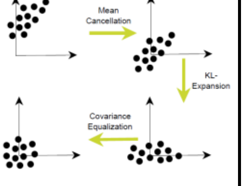
$$\frac{\partial E}{\partial w_{ij}} = \frac{\partial z_j}{\partial w_{ij}}\frac{\partial E}{\partial z_j} = y_i \frac{\partial E}{\partial z_j}$$



  - 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.

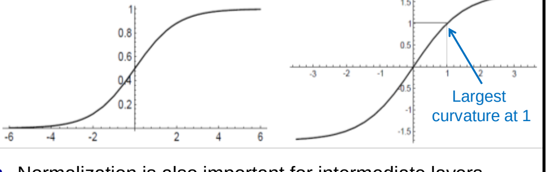


- Advisable normalization steps (for MLPs only, not for CNNs)
  - Normalize all inputs that an input unit sees to zero-mean, unit covariance.
  - If possible, try to decorrelate them using PCA (also known as Karhunen-Loeve expansion).

Topics of This Lecture

Choosing the Right Sigmoid

$\tanh(a) = 2\sigma(2a) - 1$



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

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

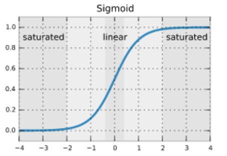
  - ⇒ When used with transformed inputs, the variance of the outputs will be close to 1.

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.

Effect of Sigmoid Nonlinearities

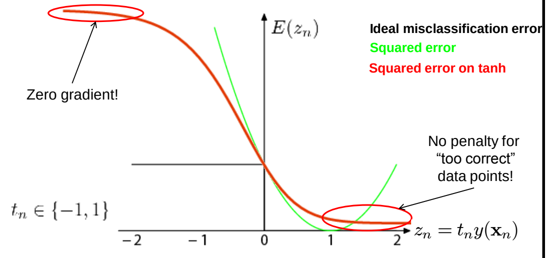
- Effects of sigmoid/tanh function
  - Linear behavior around 0
  - Saturation for large inputs



- 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
  - $\Rightarrow$ 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

Another Note on Error Functions



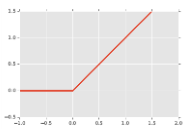
- Squared error on sigmoid/tanh output function
  - Avoids penalizing "too correct" data points.
  - But: zero gradient for confidently incorrect classifications!
  - $\Rightarrow$ Do not use L_2 loss with sigmoid outputs (instead: cross-entropy)!

Image source: Bishop, 2006

Extension: 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

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

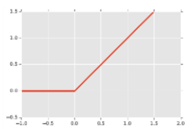
- Advantages
  - Much easier to propagate gradients through deep networks.
  - We do not need to store the ReLU output separately
    - Reduction of the required memory by half compared to tanh!

$\Rightarrow$ *ReLU has become the de-facto standard for deep networks.*

Extension: 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

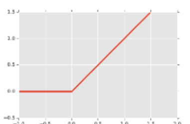
$$\frac{\partial g(a)}{\partial a} = \begin{cases} 1, & a > 0 \\ 0, & \text{else} \end{cases}$$

- Disadvantages / Limitations
  - A certain fraction of units will remain "stuck at zero".
    - If the initial weights are chosen such that the ReLU output is 0 for the entire training set, the unit will never pass through a gradient to change those weights.
  - ReLU has an offset bias, since its outputs will always be positive

Further Extensions

- Rectified linear unit (ReLU)

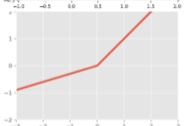
$$g(a) = \max\{0, a\}$$



- Leaky ReLU

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

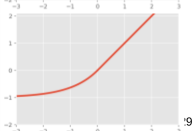
  - Avoids stuck-at-zero units
  - Weaker offset bias



- ELU

$$g(a) = \begin{cases} a, & x < 0 \\ e^a - 1, & x \geq 0 \end{cases}$$

  - No offset bias anymore
  - BUT: need to store activations



Topics of This Lecture

- Recap: Optimization
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- Tricks of the Trade
  - Shuffling
  - Data Augmentation
  - Normalization
- Nonlinearities
- Initialization
- Advanced techniques
  - Batch Normalization
  - Dropout

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

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

  $\Rightarrow$ 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.

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 $n\ \text{Var}(W_i)$ should be 1. This means

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

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

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

  - As a compromise, Glorot & Bengio proposed to use

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

  $\Rightarrow$ 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

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

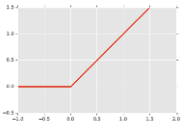
  - Glorot initialization with uniform distribution

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

Extension to ReLU

- Important for learning deep models
  - 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, derived to use instead

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

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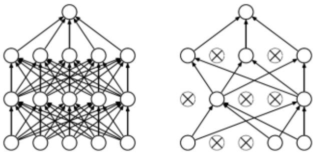
Batch Normalization [Ioffe & Szegedy '14]

- 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
  - Complication: centering + normalization also needs to be done at test time, but minibatches are no longer available at that point.
    - Learn the normalization parameters to compensate for the expected bias of the previous layer (usually a simple moving average)
- Effect
  - Much improved convergence (but parameter values are important!)
  - Widely used in practice

Dropout [Srivastava, Hinton '12]



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

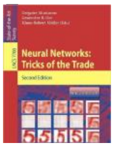
- Idea
  - Randomly switch off units during training.
  - Change network architecture for each data point, effectively training many different variants of the network.
  - When applying the trained network, multiply activations with the probability that the unit was set to zero.

  $\Rightarrow$ 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
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