Advanced Machine Learning Lecture 11

Tricks of the Trade

08.12.2016

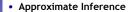
Bastian Leibe **RWTH Aachen** http://www.vision.rwth-aachen.de/

leibe@vision.rwth-aachen.de

This Lecture: Advanced Machine Learning

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

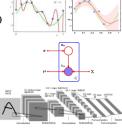
- Regression Approaches
 - Linear Regression
 - Regularization (Ridge, Lasso)
 - Kernels (Kernel Ridge Regression)
 - Gaussian Processes



- 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

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

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

E.g.,
$$L(t,y(\mathbf{x};\mathbf{W})) = \sum_n \left(y(\mathbf{x}_n;\mathbf{W}) - t_n\right)^2$$
 L₂ loss

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

L₂ regularizer ("weight decay")

RALLHAAC

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

Gradient Descent

- Two main steps
 - 1. Computing the gradients for each weight

2. Adjusting the weights in the direction of the gradient

last lecture

today

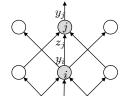
Recap: Backpropagation Algorithm

- 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

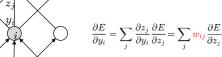
$$E = \frac{1}{2} \sum_{j \in output} (t_j - y_j)^2$$
$$\frac{\partial E}{\partial y_i} = -(t_j - y_j)$$



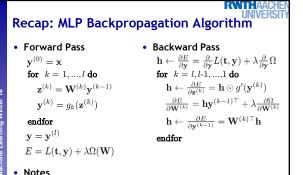
RWITHAACI Recap: Backpropagation Algorithm



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



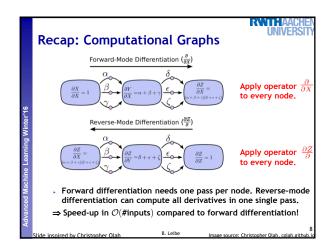
- $\frac{\partial E}{\partial w_{ij}} = \frac{\partial z_j}{\partial w_{ij}} \frac{\partial E}{\partial z_j} = \mathbf{y_i} \frac{\partial E}{\partial z_j}$
- Efficient propagation scheme
 - y_i is already known from forward pass! (Dynamic Programming)
 - \Rightarrow Propagate back the gradient from layer j and multiply with y_i .



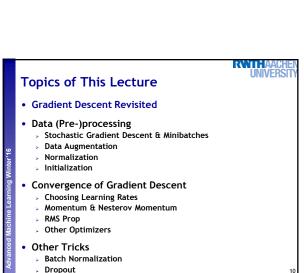
 \succ For efficiency, an entire batch of data ${\bf X}$ is processed at once.

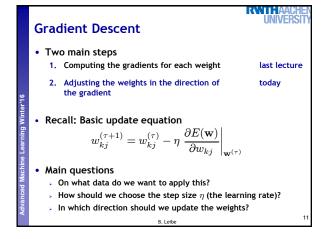
- > ① denotes the element-wise product

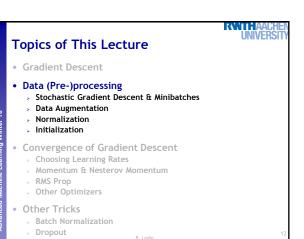
B. Leibe



Recap: Automatic Differentiation · Approach for obtaining the gradients $y_k(\mathbf{x})$ > 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 B. Leibe







Stochastic vs. Batch Learning

Batch learning

gradient.

Process the full dataset at once to compute the arguments
$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left. \frac{\partial E(\mathbf{w})}{\partial w_{kj}} \right|_{\mathbf{w}^{(\tau)}}$$

Stochastic learning

- > Choose a single example from the training set.
- $w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} \eta \left. \frac{\partial E_n(\mathbf{w})}{\partial w_{kj}} \right|_{\mathbf{w}}$ Compute the gradient only
- based on this example > This estimate will generally be noisy, which has some advantages.

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

- > 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.

RWITHAACH

Data Augmentation

Augment original data with synthetic variations to reduce overfitting



RWITHAAI

· Example augmentations for images

Cropping



Zooming



Flipping Color PCA



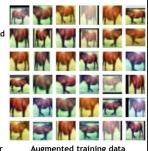
Data Augmentation

Effect

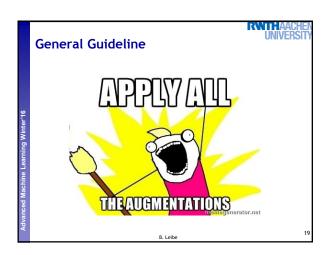
- Much larger training set
- Robustness against expected variations

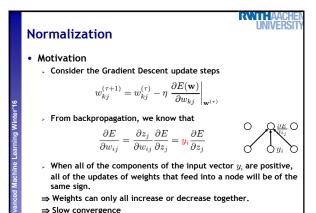
· During testing

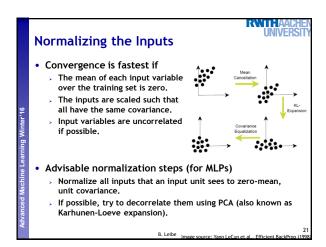
- When cropping was used during training, need to again apply crops to get same image size.
- Beneficial to also apply flipping during test.
- Applying several ColorPCA variations can bring another ~1% improvement, but at a significantly increased runtime.

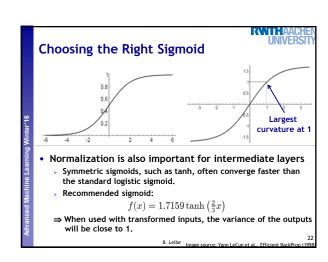


(from one original image)

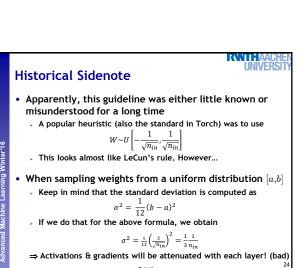








Initializing the Weights • Motivation • The starting values of the weights can have a significant effect on the training process. • Weights should be chosen randomly, but in a way that the sigmoid is primarily activated in its linear region. • Guideline (from [LeCun et al., 1998] book chapter) • Assuming 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).



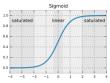
Glorot Initialization

automatic initialization.

- · Breakthrough results In 2010, Xavier Glorot published an analysis of what went wrong in the initialization and derived a more general method for
 - 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, <u>Understanding the Difficulty of Training Deep Feedforward Neural Networks</u>, 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

Analysis

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

$$Y = W_1 X_1 + W_2 X_2 + \dots + W_n X_n$$

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

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

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

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

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

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

RWITHAAI

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

$$\operatorname{Var}(W_i) = rac{1}{n} = rac{1}{n_{ ext{in}}}$$

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

$$\operatorname{Var}(W_i) = rac{1}{n_{\operatorname{out}}}$$

> As a compromise, Glorot & Bengio propose to use

$$\operatorname{Var}(W) = rac{2}{n_{ ext{in}} + n_{ ext{out}}}$$

⇒ 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 $\sigma^2 = \frac{1}{12}(b-a)^2$

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

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

Extension to ReLU

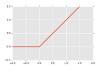
- · Another improvement for learning deep models
 - Use Rectified Linear Units (ReLU)

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

Effect: gradient is propagated with

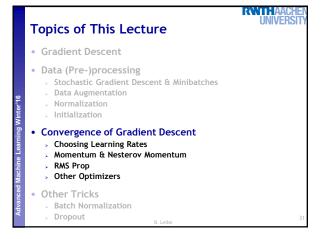
a constant factor

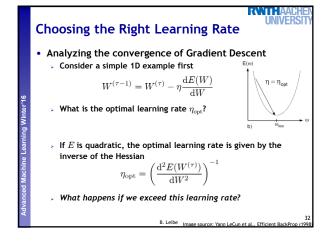


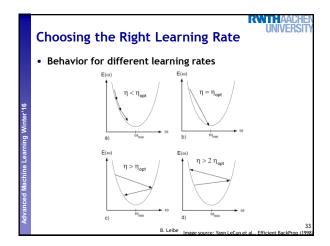


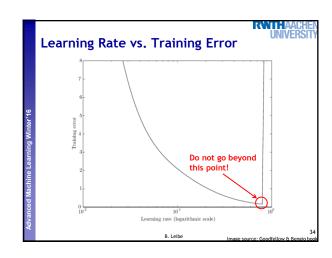
- · We can also improve them with proper initialization
 - However, the Glorot derivation was based on tanh units, linearity assumption around zero does not hold for ReLU.
 - He et al. made the derivations, proposed to use instead

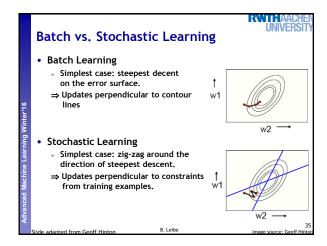
$$\mathrm{Var}(W) = \frac{2}{n_{\mathrm{in}}}$$

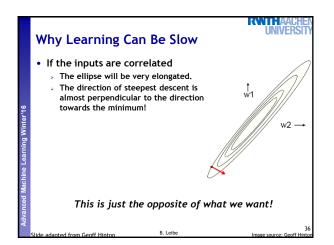






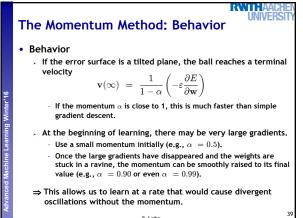


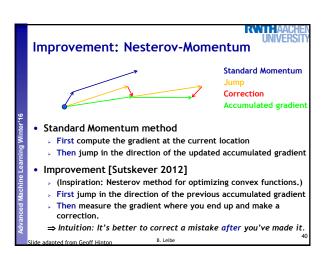


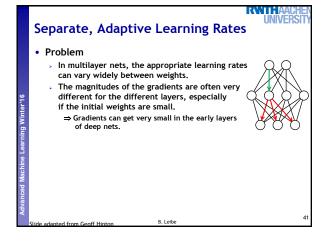


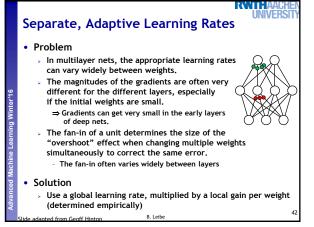
The Momentum Method • Idea • Instead of using the gradient to change the position of the weight "particle", use it to change the velocity. • Intuition • Example: Ball rolling on the error surface • It starts off by following the error surface, but once it has accumulated momentum, it no longer does steepest 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.

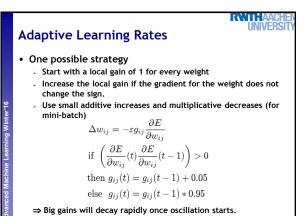
The Momentum Method: Implementation • Change in the update equations • Effect of the gradient: increment the previous velocity, subject to a decay by $\alpha < 1$. • $\mathbf{v}(t) = \alpha \mathbf{v}(t-1) - \varepsilon \frac{\partial E}{\partial \mathbf{w}}(t)$ • Set the weight change to the current velocity $\Delta \mathbf{w} = \mathbf{v}(t)$ $= \alpha \mathbf{v}(t-1) - \varepsilon \frac{\partial E}{\partial \mathbf{w}}(t)$ $= \alpha \Delta \mathbf{w}(t-1) - \varepsilon \frac{\partial E}{\partial \mathbf{w}}(t)$

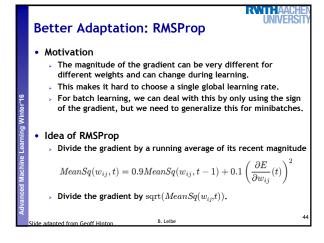


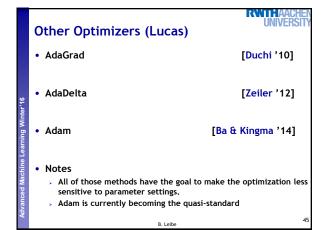


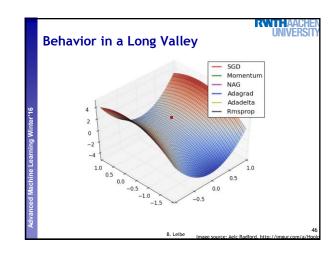


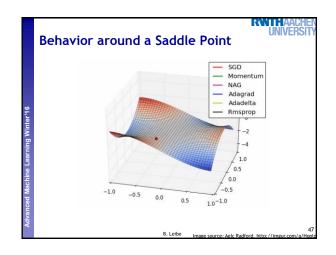


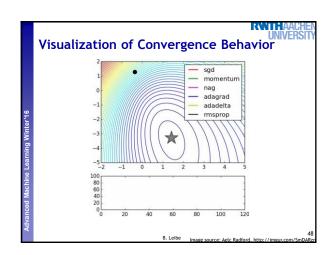


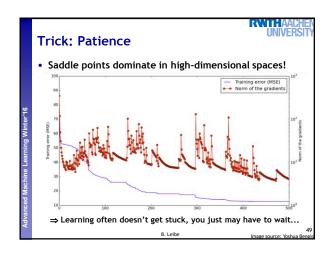


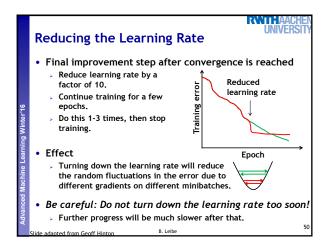


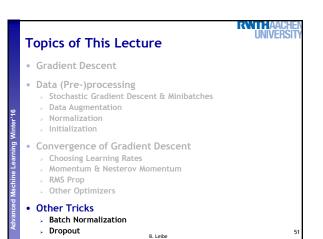


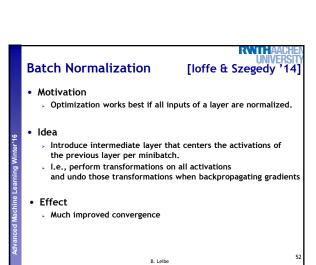


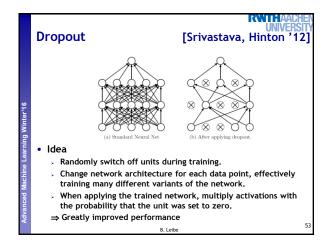


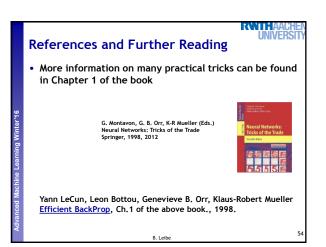












RWTHAACHEI UNIVERSIT

References

ReLu

X. Glorot, A. Bordes, Y. Bengio, <u>Deep sparse rectifier neural networks</u>, AISTATS 2011.

Initialization

- X. Glorot, Y. Bengio, <u>Understanding the difficulty of training</u> deep feedforward neural networks, AISTATS 2010.
- K. He, X.Y. Zhang, S.Q. Ren, J. Sun, <u>Delving Deep into</u> <u>Rectifiers: Surpassing Human-Level Performance on ImageNet</u> <u>Classification</u>, 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.

B. Leibe

References and Further Reading

RWTHAACHEN UNIVERSITY

- Batch Normalization
 - S. loffe, C. Szegedy, <u>Batch Normalization</u>; <u>Accelerating Deep Network Training by Reducing Internal Covariate Shift</u>, ArXiV 1502.03167, 2015.
- Dropout

N. Srivastava, G. Hinton, A. Krizhevsky, I. Sutskever, R. Salakhutdinov, <u>Dropout: A Simple Way to Prevent Neural Networks from Overfitting</u>, JMLR, Vol. 15:1929-1958, 2014.

10