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# Advanced Machine Learning Lecture 13

## Backpropagation

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## This Lecture: Advanced Machine Learning

- Regression Approaches
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Gaussian Processes
- Learning with Latent Variables
  - Prob. Distributions & Approx. Inference
  - Mixture Models
  - EM and Generalizations
- Deep Learning
  - Linear Discriminants
  - Neural Networks
  - Backpropagation
  - CNNs, RNNs, RBMs, etc.

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## Recap: Perceptrons

- One output node per class

Output layer  
Weights  
Input layer

- Outputs
  - Linear outputs

$$y_k(\mathbf{x}) = \sum_{i=0}^d W_{ki} x_i$$

With output nonlinearity

$$y_k(\mathbf{x}) = g\left(\sum_{i=0}^d W_{ki} x_i\right)$$

⇒ Can be used to do multidimensional linear regression or multiclass classification.

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## Recap: Non-Linear Basis Functions

- Straightforward generalization

Output layer  
Weights  
Feature layer  
Mapping (fixed)  
Input layer

- Outputs
  - Linear outputs

$$y_k(\mathbf{x}) = \sum_{i=0}^d W_{ki} \phi(x_i)$$

with output nonlinearity

$$y_k(\mathbf{x}) = g\left(\sum_{i=0}^d W_{ki} \phi(x_i)\right)$$

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## Recap: Non-Linear Basis Functions

- Straightforward generalization

Output layer  
Weights  
Feature layer  
Mapping (fixed)  
Input layer

- Remarks
  - Perceptrons are generalized linear discriminants!
  - Everything we know about the latter can also be applied here.
  - Note: feature functions  $\phi(\mathbf{x})$  are kept fixed, not learned!

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## Recap: Perceptron Learning

- Process the training cases in some permutation
  - If the output unit is correct, leave the weights alone.
  - If the output unit incorrectly outputs a zero, add the input vector to the weight vector.
  - If the output unit incorrectly outputs a one, subtract the input vector from the weight vector.
- Translation
 
$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta (y_k(\mathbf{x}_n; \mathbf{w}) - t_{kn}) \phi_j(\mathbf{x}_n)$$
  - This is the Delta rule a.k.a. LMS rule!
  - ⇒ Perceptron Learning corresponds to 1<sup>st</sup>-order (stochastic) Gradient Descent of a quadratic error function!

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## Recap: Loss Functions

- We can now also apply other loss functions
  - $L_2$  loss  $\Rightarrow$  Least-squares regression  

$$L(t, y(\mathbf{x})) = \sum_n (y(\mathbf{x}_n) - t_n)^2$$
  - $L_1$  loss:  $\Rightarrow$  Median regression  

$$L(t, y(\mathbf{x})) = \sum_n |y(\mathbf{x}_n) - t_n|$$
  - Cross-entropy loss  $\Rightarrow$  Logistic regression  

$$L(t, y(\mathbf{x})) = -\sum_n \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$
  - Hinge loss  $\Rightarrow$  SVM classification  

$$L(t, y(\mathbf{x})) = \sum_n [1 - t_n y(\mathbf{x}_n)]_+$$
  - Softmax loss  $\Rightarrow$  Multi-class probabilistic classification  

$$L(t, y(\mathbf{x})) = -\sum_n \sum_k \mathbb{I}(t_n = k) \ln \frac{\exp(y_k(\mathbf{x}))}{\sum_j \exp(y_j(\mathbf{x}))}$$

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## Recap: Multi-Layer Perceptrons

- Adding more layers
- Output

$$y_k(\mathbf{x}) = g^{(2)} \left( \sum_{i=0}^h W_{ki}^{(2)} g^{(1)} \left( \sum_{j=0}^d W_{ij}^{(1)} x_j \right) \right)$$

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## Topics of This Lecture

- Learning with Hidden Units
- Obtaining the Gradients
  - Naive analytical differentiation
  - Numeric differentiation
  - Backpropagation
  - Computational graphs
  - Automatic differentiation
- Practical Issues
  - Nonlinearities
  - Sigmoid outputs and the  $L_2$  loss
  - Implementing Softmax correctly

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

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## Gradient Descent

- Two main steps
  - Computing the gradients for each weight today
  - Adjusting the weights in the direction of the gradient Thursday

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## Obtaining the Gradients

- Approach 1: Naive Analytical Differentiation

$$\frac{\partial E(\mathbf{W})}{\partial W_{10}^{(2)}} \cdots \frac{\partial E(\mathbf{W})}{\partial W_{kh}^{(2)}} \quad \frac{\partial E(\mathbf{W})}{\partial W_{10}^{(1)}} \cdots \frac{\partial E(\mathbf{W})}{\partial W_{hd}^{(1)}}$$

- Compute the gradients for each variable analytically.
- What is the problem when doing this?

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## Excursion: Chain Rule of Differentiation

- One-dimensional case: Scalar functions

$$\Delta z = \frac{dz}{dy} \Delta y$$

$$\Delta y = \frac{dy}{dx} \Delta x$$

$$\Delta z = \frac{dz}{dy} \frac{dy}{dx} \Delta x$$

$$\frac{dz}{dx} = \frac{dz}{dy} \frac{dy}{dx}$$

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## Excursion: Chain Rule of Differentiation

- Multi-dimensional case: Total derivative

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y_1} \frac{\partial y_1}{\partial x} + \frac{\partial z}{\partial y_2} \frac{\partial y_2}{\partial x} + \dots$$

$$= \sum_{i=1}^k \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x}$$

⇒ Need to sum over all paths that lead to the target variable  $x$ .

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## Obtaining the Gradients

- Approach 1: Naive Analytical Differentiation

$$\frac{\partial E(\mathbf{W})}{\partial W_{10}^{(2)}} \cdots \frac{\partial E(\mathbf{W})}{\partial W_{kh}^{(2)}} \quad \frac{\partial E(\mathbf{W})}{\partial W_{10}^{(1)}} \cdots \frac{\partial E(\mathbf{W})}{\partial W_{hd}^{(1)}}$$

- Compute the gradients for each variable analytically.
- What is the problem when doing this?

⇒ With increasing depth, there will be exponentially many paths!

⇒ Infeasible to compute this way.

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## Obtaining the Gradients

- Approach 2: Numerical Differentiation

- Given the current state  $\mathbf{W}^{(v)}$ , we can evaluate  $E(\mathbf{W}^{(v)})$ .
- Idea: Make small changes to  $\mathbf{W}^{(v)}$  and accept those that improve  $E(\mathbf{W}^{(v)})$ .

⇒ Horribly inefficient! Need several forward passes for each weight. Each forward pass is one run over the entire dataset!

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## Obtaining the Gradients

- Approach 3: Incremental Analytical Differentiation

$$\frac{\partial E(\mathbf{W})}{\partial y_j} \rightarrow \frac{\partial E(\mathbf{W})}{\partial W_{ij}^{(2)}}$$

$$\frac{\partial E(\mathbf{W})}{\partial z_i} \rightarrow \frac{\partial E(\mathbf{W})}{\partial W_{ij}^{(1)}}$$

$$\frac{\partial E(\mathbf{W})}{\partial x_i}$$

- Idea: Compute the gradients layer by layer.
- Each layer below builds upon the results of the layer above.
- ⇒ The gradient is propagated backwards through the layers.
- ⇒ **Backpropagation** algorithm

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## Backpropagation Algorithm

- Core steps

1. Convert the discrepancy between each output and its target value into an error derivative.
 
$$E = \frac{1}{2} \sum_{j \in \text{output}} (t_j - y_j)^2$$

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

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## Backpropagation Algorithm

E.g. with sigmoid output nonlinearity

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

- Notation
  - $y_j$  Output of layer  $j$
  - $z_j$  Input of layer  $j$

Connections:  $z_j = \sum_i w_{ij} y_i$   
 $y_j = g(z_j)$

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## Backpropagation Algorithm

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

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

- Notation
  - $y_j$  Output of layer  $j$
  - $z_j$  Input of layer  $j$

Connections:  $z_j = \sum_i w_{ij} y_i$   
 $\frac{\partial z_j}{\partial y_i} = w_{ij}$

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## Backpropagation Algorithm

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

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

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

- Notation
  - $y_j$  Output of layer  $j$
  - $z_j$  Input of layer  $j$

Connections:  $z_j = \sum_i w_{ij} y_i$   
 $\frac{\partial z_j}{\partial w_{ij}} = y_i$

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## Backpropagation Algorithm

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

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

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

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

Slide adapted from Geoff Hinton. B. Leibe. 25

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## Summary: MLP Backpropagation

- Forward Pass**

```

y(0) = x
for k = 1, ..., l do
  z(k) = W(k)y(k-1)
  y(k) = gk(z(k))
endfor
y = y(l)
E = L(t, y) + λΩ(W)

```

- Backward Pass**

```

h ← ∂E/∂y = ∂/∂y L(t, y) + λ ∂/∂y Ω
for k = l, l-1, ..., 1 do
  h ← ∂E/∂z(k) = h ⊙ g'(k)(y(k))
  ∂E/∂W(k) = hy(k-1)T + λ ∂Ω/∂W(k)
  h ← ∂E/∂y(k-1)} = W(k)Th
endfor

```

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

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## Analysis: Backpropagation

- Backpropagation is the key to make deep NNs tractable
  - However...
- The Backprop algorithm given here is specific to MLPs
  - It does not work with more complex architectures, e.g. skip connections or recurrent networks!
  - Whenever a new connection function induces a different functional form of the chain rule, you have to derive a new Backprop algorithm for it. ⇒ Tedious...
- Let's analyze Backprop in more detail
  - This will lead us to a more flexible algorithm formulation

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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.

Slide inspired by Christopher Olah. B. Leibe. Image source: Christopher Olah, colah.github.io. 28

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## 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  $3 \times 3$  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
 
$$\frac{\partial Z}{\partial X} = (\alpha + \beta + \gamma) * (\delta + \epsilon + \zeta)$$

Slide inspired by Christopher Olah. B. Leibe. Image source: Christopher Olah, colah.github.io. 29

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## Efficient Factored Algorithms

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

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

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

Apply operator  $\frac{\partial Z}{\partial Y}$  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.

Slide inspired by Christopher Olah. B. Leibe. Image source: Christopher Olah, colah.github.io. 30

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## 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  $b$ .

Slide inspired by Christopher Olah. B. Leibe. Image source: Christopher Olah, colah.github.io

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## 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.

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

Slide inspired by Christopher Olah. B. Leibe. Image source: Christopher Olah, colah.github.io

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

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## 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
  - Computing the outputs  $y$  of the module given its inputs  $x$ 

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

where  $x$ ,  $y$ , and intermediate results are stored in the module.
  - Computing the gradient  $\partial E / \partial x$  of a scalar cost w.r.t. the inputs  $x$  given the gradient  $\partial E / \partial y$  w.r.t. the outputs  $y$ 

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

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  - Implementing Softmax correctly
  - Efficient batch processing

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## Commonly Used Nonlinearities

- Sigmoid
 
$$g(a) = \sigma(a) = \frac{1}{1 + \exp\{-a\}}$$
- Hyperbolic tangent
 
$$g(a) = \tanh(a) = 2\sigma(2a) - 1$$
- Softmax
 
$$g(\mathbf{a}) = \frac{\exp\{-a_i\}}{\sum_j \exp\{-a_j\}}$$

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## Commonly Used Nonlinearities (2)

- Hard tanh
 
$$g(a) = \max\{-1, \min\{1, a\}\}$$
- Rectified linear unit (ReLU)
 
$$g(a) = \max\{0, a\}$$
- Maxout
 
$$g(\mathbf{a}) = \max_i \{\mathbf{w}_i^\top \mathbf{a} + b_i\}$$

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## 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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## Another Note on Error Functions

$t_n \in \{1, -1\}$   
 $z_n = t_n y(x_n)$

- Squared error on sigmoid/tanh output function
  - Avoids penalizing “too correct” data points.
  - But: zero gradient for confidently incorrect classifications!

⇒ Do not use  $L_2$  loss with sigmoid outputs (instead: cross-entropy)!

Image source: Bishop, 2006

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## Implementing Softmax Correctly

- Softmax output

- De-facto standard for multi-class outputs

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

- 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  $\mathbf{b}$ 

$$\text{softmax}(\mathbf{a} + \mathbf{b}) = \text{softmax}(\mathbf{a})$$
- ⇒ Subtract the largest weight vector  $\mathbf{w}_j$  from the others.

## References and Further Reading

- More information on Backpropagation can be found in Chapter 6 of the Goodfellow & Bengio book

Ian Goodfellow, Aaron Courville, Yoshua Bengio  
Deep Learning  
MIT Press, in preparation



<https://goodfeli.github.io/dlbook/>