# Biological Applications of Deep Learning Lecture 3 

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## Contents Today

- Gradient Descent: Reminder
- The Backpropagation Algorithm
- Regularization in detail:
- L1 / L2 Regularization
- Dropout / Early Stopping


## Reminder: Gradient Descent for Neural Networks

## Gradient Descent



- Let $C\left(v_{1}, \ldots, v_{n}\right)$ be a differentiable function in $n$ variables, here $n=2$. We look for the minimum of $C$.
- Idea: At point $v_{1}, v_{2}$ (green ball), move into direction of steepest decline (green arrow). Do this iteratively.
- The steepest decline is given by the gradient

$$
\nabla_{v_{1}, \ldots, v_{n}} C=\left(\frac{\partial C}{\partial v_{1}}, \ldots, \frac{\partial C}{\partial v_{n}}\right)
$$

## Gradient Descent for Neural Networks

## Practical Scheme

## Input

- A NN of depth $L$ where parameters $\mathbf{w}$ represent both
- weights $\mathbf{W}^{(j)} \in \mathbb{R}^{d(l) \times d(l-1)}, j=1, \ldots, L$
- biases $\mathbf{b}^{j}, j=1, \ldots, L$
- Let $\mathbf{w}_{0}$ be appropriately chosen initial parameters
- Let $\mathbf{X}^{(\text {train })} \in \mathbb{R}^{m \times n}, \mathbf{y}^{(\text {train })} \in \mathbb{R}^{m}$ be $m$ training data points $x \in \mathbb{R}^{n}$
- Let

$$
C=\frac{1}{m} \sum_{x} C_{x}=\frac{1}{m} \sum_{x} C\left(f_{\mathbf{w}}(x), y(x)\right)
$$

be a cost function.

- One can view $C=C(\mathbf{w})$ as a function in the parameters $\mathbf{w}$.


## Gradient Descent for Neural Networks

## Practical Scheme

- Let $\eta$ be an appropriately chosen learning rate.

Iteration $i$

1. Compute $\nabla_{\mathbf{w}} C\left(\mathbf{w}_{i-1}\right)$

- Need training data to update $C$, based on having updated $\mathbf{w}$

2. Update: $\mathbf{w}^{(\mathbf{i})} \leftarrow \mathbf{w}^{(\mathbf{i}-\mathbf{1})}+\eta \nabla_{\mathbf{w}} \mathrm{C}$

- $w_{k}^{(i)} \leftarrow w_{k}^{(i-1)}-\eta \frac{\partial C}{\partial w_{k}}$
- $b_{l}^{(i)} \leftarrow b_{l}^{(i-1)}-\eta \frac{\partial C}{\partial b_{l}}$

3. Stop, if appropriate

This minimizes the cost $C$, hence adjusts the NN to the training data.

## Deep Learning: Challenges

- The function $f$ representing a neural network with $L$ layers (with depth $L$ ) are written

$$
y=f\left(\mathbf{x}^{0}\right)=f^{(L)}\left(f^{(L-1)}\left(\ldots\left(f^{(1)}\left(\mathbf{x}^{(0)}\right)\right) \ldots\right)\right)
$$

where $\mathbf{x}^{l}=f^{(l)}\left(\mathbf{x}^{l-1}\right)=\mathbf{a}^{\mathbf{1}}\left(\mathbf{W}^{(\mathbf{1})} \mathbf{x}^{l-1}+\mathbf{b}^{\mathbf{l}}\right)$

- Functions $f_{\mathbf{w}}$ representing NN's cannot be described in closed form
- Hence the loss $C(\mathbf{w}):=C\left(f_{\mathbf{w}}\right):=C\left(f_{\mathbf{w}}, f^{*}\right)$ cannot be described in closed form either

How to compute gradients and perform gradient descent?

# Computing Gradients: The Backpropagation Algorithm 

## Notation


$w_{j k}^{l}$ is the weight from the $k^{\text {th }}$ neuron in the $(l-1)^{\text {th }}$ layer to the $j^{\text {th }}$ neuron in the $l^{\text {th }}$ layer

- weight $w_{j k}^{l}$ links node $k$ in layer $l-1$ with node $j$ in layer $l$
- $w_{j k}^{l}=\mathbf{W}_{j k}^{(l)}$ in the earlier notation
- Reminder: width of layer $l: d(l)$, so $\mathbf{W}^{(l)} \in \mathbb{R}^{d(l) \times d(l-1)}$


## Notation



- $b_{j}^{l}$ is the bias of neuron $j$ in layer $l$
- $a_{j}^{l}$ is the activation value of neuron $j$ in layer $l$
- $b_{j}^{l}=\mathbf{b}_{j}^{(l)}, a_{j}^{l}=\mathbf{x}_{j}^{(l)}, \mathbf{a}^{l}=\mathbf{x}^{(l)}$ in earlier notation


## Notation

Using a sigmoid function $\sigma$ as activation function, we obtain

$$
\begin{equation*}
a_{j}^{l}=\sigma\left(\sum_{k} w_{j k}^{l} a_{k}^{l-1}+b_{j}^{l}\right) \tag{1}
\end{equation*}
$$

which can further be written

$$
\begin{equation*}
\mathbf{a}^{l}=\sigma\left(\mathbf{W}^{(l)} \mathbf{a}^{l-1}+\mathbf{b}^{l}\right) \tag{2}
\end{equation*}
$$

Remark: here and in the following, $\sigma$ can be replaced by an arbitrary activation function that is differentiable.

We further define

$$
\begin{equation*}
z_{j}^{l}=\sum_{k} w_{j k}^{l} a_{k}^{l-1}+b_{j}^{l} \quad \text { that is } \quad a_{j}^{l}=\sigma\left(z_{j}^{l}\right) \tag{3}
\end{equation*}
$$

such that

$$
\begin{equation*}
\mathbf{z}^{l}:=\left(z_{1}^{l}, \ldots, z_{d(l)}^{l}\right)^{T}=\mathbf{W}^{(l)} \mathbf{a}^{l-1}+\mathbf{b}^{l} \quad \text { that is } \quad \mathbf{a}^{l}=\sigma\left(\mathbf{z}^{l}\right) \tag{4}
\end{equation*}
$$

## Notation

We further write

- $y(x)$ for the label of a training data point $x$
- Note: $y(x)$ can be identified with $f^{*}(x)$ where $f^{*}$ is the true function
- $\mathbf{a}^{L}(x)$, the output of the last layer, represents the network function, so $\mathbf{a}^{L}(x)=f(x)$ in earlier notation.


## BACKPROPAGATION

## Goal

- We would like to compute gradient $\nabla_{\mathbf{W}, \mathbf{b}} C$
- Therefore, we need to compute all partial derivatives

$$
\begin{equation*}
\frac{\partial C}{\partial w_{j k}^{l}} \text { and } \frac{\partial C}{\partial b_{j}^{l}} \tag{5}
\end{equation*}
$$

- For further convenience, we define

$$
\begin{equation*}
\delta_{j}^{l}:=\frac{\partial C}{\partial z_{j}^{l}} \tag{6}
\end{equation*}
$$

## BACKPROPAGATION

- For further convenience, we define

$$
\delta_{j}^{l}:=\frac{\partial C}{\partial z_{j}^{l}}
$$

- For example, by the chain rule of differentiation ( $\dagger$ ):

$$
\begin{array}{cc}
\frac{\partial C}{\partial b_{j}^{l}} \quad \stackrel{(\dagger)}{=} \quad \delta_{j}^{l} \frac{\partial z_{j}^{l}}{\partial b_{j}^{l}}=\delta_{j}^{l} \frac{\partial\left(\sum_{k} w_{j k}^{l} l_{k}^{l-1}+b_{j}^{l}\right)}{\partial b_{j}^{l}}=\delta_{j}^{l} \\
\frac{\partial C}{\partial w_{j k^{*}}^{l}} \quad \stackrel{(\dagger)}{=} \delta_{j}^{l} \frac{\partial z_{j}^{l}}{\partial w_{j k^{*}}^{l}}=\delta_{j}^{l} \frac{\partial\left(\sum_{k} w_{j k_{k}^{l}}^{l-1}+b_{j}^{l}\right)}{\partial w_{j k^{*}}^{l}}=\delta_{j}^{l} a_{k^{*}}^{l-1} \tag{7}
\end{array}
$$

- Idea: Focus on computing $\delta_{j}^{l}$, derive $\frac{\partial C}{\partial b_{j}^{l}}$ and $\frac{\partial C}{\partial w_{j k}^{l}}$ by (7)


## Notation

- Let $m$ be the total number of training examples. Then we define C

$$
\begin{equation*}
C\left(f, f^{*}\right)=C\left(a^{L}\right):=\frac{1}{2 m} \sum_{x}\left\|y(x)-a^{L}(x)\right\|^{2} \tag{8}
\end{equation*}
$$

as quadratic cost function (only for easier presentation!)

- Note: $y$ resp. $f^{*}(x)$ are fixed, so $C$ varies in $a^{L}(=f)$ only.
- Important: $C=\frac{1}{m} \sum_{x} C_{x}$ where $C_{x}=\frac{1}{2}\left\|y(x)-a^{L}(x)\right\|^{2}$ is the cost on one individual training example
- Idea: Compute $\frac{\delta C_{x}}{\delta w}, \frac{\delta C_{x}}{\delta b}$ for all training data $x$ and recover $\frac{\delta C}{\delta w}, \frac{\delta C}{\delta b}$ by averaging over $x$


# DEFINITION 

The Hadamard Product

## Definition

Let $\mathbf{s}, \mathbf{t} \in \mathbb{R}^{n}$ be two vectors of equal length. Then the Hadamard product $\mathbf{s} \odot \mathbf{t}$ is defined by

$$
\begin{equation*}
(\mathbf{s} \odot \mathbf{t})_{j}=\mathbf{s}_{j} \cdot \mathbf{t}_{j} \quad \text { for } j=1, \ldots, n \tag{9}
\end{equation*}
$$

## BACKPROPAGATION

Start: Output Layer - Computing $\delta^{L}$

We have $a_{j}^{L}=\sigma\left(z_{j}^{L}\right)$, so

$$
\begin{equation*}
\delta_{j}^{L}=\frac{\partial C}{\partial z_{j}^{L}}=\sum_{k} \frac{\partial C}{\partial a_{k}^{L}} \frac{\partial a_{k}^{L}}{\partial z_{j}^{L}}{ }^{\frac{\partial a_{k}^{L}}{\partial z_{j}^{L}}=0, j \neq k}=\frac{\partial C}{\partial a_{j}^{L}} \cdot \sigma^{\prime}\left(z_{j}^{L}\right) \tag{10}
\end{equation*}
$$

In other words,

$$
\begin{equation*}
\delta^{L}=\nabla_{\mathbf{a}^{L}} C \odot \sigma^{\prime}\left(\mathbf{z}^{L}\right) \tag{11}
\end{equation*}
$$

## BACKPROPAGATION

Start: Output Layer - Computing $\delta^{L}$

Further

$$
\sigma^{\prime}(z)=\sigma(z)(1-\sigma(z))
$$

and

$$
\frac{\partial C}{\partial a_{j}^{L}}=\frac{\partial\left(\frac{1}{2} \sum_{j^{\prime}}\left(y_{j^{\prime}}-a_{j^{\prime}}^{L}\right)^{2}\right)}{\partial a_{j}^{L}}=\left(a_{j}^{L}-y_{j}\right),
$$

so overall

$$
\begin{equation*}
\delta_{j}^{L}=\left(a_{j}^{L}-y_{j}\right) \sigma\left(z_{j}^{L}\right)\left(1-\sigma\left(z_{j}^{L}\right)\right) \tag{12}
\end{equation*}
$$

## BACKPROPAGATION

Start: Output Layer - Computing $\delta^{L}$

$$
\begin{equation*}
\delta_{j}^{L}=\left(a_{j}^{L}-y_{j}\right) \sigma^{\prime}\left(z_{j}^{L}\right) \quad \text { that is } \quad \delta^{L}=\left(\mathbf{a}^{L}-\mathbf{y}\right) \odot \sigma^{\prime}\left(\mathbf{z}^{L}\right) \tag{13}
\end{equation*}
$$

Interpretation

- $a_{j}^{L}-y_{j}$ determines how far off $a_{j}^{L}$ from $y_{j}$ is
- The further off, the steeper the gradient, the greater the adjustment
- $\sigma^{\prime}\left(z_{j}^{L}\right)$ is close to zero if $\sigma\left(z_{j}^{L}\right)$ is either close to zero or close to one
- This can make sense, but can cause problems, because updates get very small (note remarks on alternative
$\square$ unvesiriactivation functions)


## EXAMPLE

## MNIST Network



- Truth: One $y_{j}$ is one, all others are zero
- If $a_{j}^{L}$ is not one, updates are large: we need to make changes
- If $a_{j}^{L}$ is close to one, and all others are close to zero, updates are Unlvesiräsmall: no further adjustments necessary


## Propagation - Computing $\delta^{l}$ FROM $\delta^{l+1}$

We compute

$$
\begin{equation*}
\delta_{j}^{l}=\frac{\partial C}{\partial z_{j}^{l}}=\sum_{k} \frac{\partial C}{\partial z_{k}^{l+1}} \frac{\partial z_{k}^{l+1}}{\partial z_{j}^{l}}=\sum_{k} \frac{\partial z_{k}^{l+1}}{\partial z_{j}^{l}} \delta_{k}^{l+1} \tag{14}
\end{equation*}
$$

We further observe

$$
\begin{equation*}
z_{k}^{l+1}=\sum_{j} w_{k j}^{l+1} a_{j}^{l}+b_{k}^{l+1}=\sum_{j} w_{k j}^{l+1} \sigma\left(z_{j}^{l}\right)+b_{k}^{l+1} \tag{15}
\end{equation*}
$$

which, by differentiation, leads to

$$
\begin{equation*}
\frac{\partial z_{k}^{l+1}}{\partial z_{j}^{l}}=w_{k j}^{l+1} \sigma^{\prime}\left(z_{j}^{l}\right) \tag{16}
\end{equation*}
$$

## BACKPROPAGATION

Propagation - COMPUTiNG $\delta^{l}$ From $\delta^{l+1}$
Substituting (16) into (14), we obtain

$$
\begin{equation*}
\delta_{j}^{l}=\sum_{k} w_{k j}^{l+1} \delta_{k}^{l+1} \sigma^{\prime}\left(z_{j}^{l}\right) \tag{17}
\end{equation*}
$$

which can be overall expressed as

$$
\begin{equation*}
\delta^{l}=\left(\left(\mathbf{W}^{(l+1)}\right)^{T} \delta^{l+1}\right) \odot \sigma^{\prime}\left(z^{l}\right) \tag{18}
\end{equation*}
$$

- (18) "moves the error one layer backward" backpropagation
- Applying $\mathbf{W}^{(l+1)}$ to $\delta^{l+1}$ moves the error from the input of neurons in layer $l+1$ to the outputs of neurons in layer $l$
- $\sigma^{\prime}\left(z^{l}\right)$ moves the error from the output of neurons in layer $l$ to the inputs of neurons in layer $l$


## BACKPROPAGATION

Computing $\frac{\partial C}{\partial b_{j}^{l}}$ AND $\frac{\partial C}{\partial w_{j k}^{l}}$
We further see that

$$
\begin{equation*}
\frac{\partial C}{\partial b_{j}^{l}}=\delta_{j}^{l} \tag{19}
\end{equation*}
$$

and

$$
\begin{equation*}
\frac{\partial C}{\partial w_{j k}^{l}}=a_{k}^{l-1} \delta_{j}^{l} \tag{20}
\end{equation*}
$$

(20) explains that changes in weights are small if the input is small, or the error in the output is small:

$$
\frac{\partial C}{\partial w}=
$$



## BACKPROPAGATION

The Equations

Summary: the equations of backpropagation
$\delta^{L}=\nabla_{a} C \odot \sigma^{\prime}\left(z^{L}\right)$
(BP1)
$\delta^{l}=\left(\left(w^{l+1}\right)^{T} \delta^{l+1}\right) \odot \sigma^{\prime}\left(z^{l}\right)$
$\frac{\partial C}{\partial b_{j}^{L}}=\delta_{j}^{l}$
$\frac{\partial C}{\partial w_{j k}^{l}}=a_{k}^{l-1} \delta_{j}^{l}$
(BP3)
(BP4)

## BACKPROPAGATION

The Algorithm

1. Input $x$ : Set the corresponding activation $a^{1}$ for the input layer.
2. Feedforward: For each $l=2,3, \ldots, L$ compute

$$
z^{l}=w^{l} a^{l-1}+b^{l} \text { and } a^{l}=\sigma\left(z^{l}\right)
$$

3. Output error $\delta^{L}$ : Compute the vector $\delta^{L}=\nabla_{a} C \odot \sigma^{\prime}\left(z^{L}\right)$.
4. Backpropagate the error: For each $l=L-1, L-2, \ldots, 2$ compute $\delta^{l}=\left(\left(w^{l+1}\right)^{T} \delta^{l+1}\right) \odot \sigma^{\prime}\left(z^{l}\right)$.
5. Output: The gradient of the cost function is given by

$$
\frac{\partial C}{\partial w_{j k}^{l}}=a_{k}^{l-1} \delta_{j}^{l} \text { and } \frac{\partial C}{\partial b_{j}^{l}}=\delta_{j}^{l}
$$

## BACKPROPAGATION

## Stochastic Gradient Descent

1. Input a set of training examples
2. For each training example $x$ : Set the corresponding input activation $\alpha^{x, 1}$, and perform the following steps:

- Feedforward: For each $l=2,3, \ldots, L$ compute

$$
z^{x, l}=w^{l} a^{x, l-1}+b^{l} \text { and } a^{x, l}=\sigma\left(z^{x, l}\right)
$$

- Output error $\delta^{r, L}$ : Compute the vector

$$
\delta^{x, L}=\nabla_{a} C_{x} \odot \sigma^{\prime}\left(z^{x, L}\right) .
$$

- Backpropagate the error: For each
$l=L-1, L-2, \ldots, 2$ compute
$\delta^{x, l}=\left(\left(w^{l+1}\right)^{T} \delta^{x, l+1}\right) \odot \sigma^{\prime}\left(z^{r^{x, l}}\right)$.

3. Gradient descent: For each $l=L, L-1, \ldots, 2$ update the weights according to the rule $w^{l} \rightarrow w^{l}-\frac{\eta}{m} \sum_{x} \delta^{x, l}\left(a^{x, l-1}\right)^{T}$, and the biases according to the rule $b^{l} \rightarrow b^{l}-\frac{\eta}{m} \sum_{x} \delta^{x, l}$.

## Employing Regularization

## Regularization Revisited

## Motivation



No regularization leads to overfitting

## L2-REGULARIZED CROSS Entropy

We add a L2 regularization term to the cost (here:
cross-entropy). Thereby $\lambda$ is the regularization parameter.

$$
\begin{equation*}
C=-\frac{1}{m} \sum_{x} \sum_{j}\left[y_{j} \log a_{j}^{L}+\left(1-y_{j}\right) \log \left(1-a_{j}^{L}\right)\right]+\frac{\lambda}{2 m} \sum_{w} w^{2} \tag{21}
\end{equation*}
$$

Writing $C_{0}=-\frac{1}{m} \sum_{x} \sum_{j}\left[y_{j} \log a_{j}^{L}+\left(1-y_{j}\right) \log \left(1-a_{j}^{L}\right)\right]$ then makes

$$
\begin{equation*}
C=C_{0}+\frac{\lambda}{m} \sum_{w} w^{2} \tag{22}
\end{equation*}
$$

Remark: This can be done with any cost function $C_{0}$.

## L2-REGULARIZED Cross Entropy

This further yields the partial derivatives

$$
\begin{align*}
& \frac{\partial C}{\partial w}=\frac{\partial C_{0}}{\partial w}+\frac{\lambda}{m} w  \tag{23}\\
& \frac{\partial C}{\partial b}=\frac{\partial C_{0}}{\partial b} \tag{24}
\end{align*}
$$

with update rules (rescaling weights with $\left(1-\frac{\eta \lambda}{m}\right)$ is called weight decay)

$$
\begin{align*}
b & \leftarrow b-\eta \frac{\partial C_{0}}{\partial b}  \tag{25}\\
w & \leftarrow w-\eta \frac{\partial C_{0}}{\partial w}-\eta \frac{\lambda}{m} w=\left(1-\frac{\eta \lambda}{m}\right) w-\eta \frac{\partial C_{0}}{\partial w} \tag{26}
\end{align*}
$$

Update rules for stochastic gradient descent, for overall $m$ training data, batch size $\hat{m}$ :

$$
\begin{align*}
& b \leftarrow b-\frac{\eta}{\hat{m}} \sum_{x} \frac{\partial C_{x}}{\partial b}  \tag{27}\\
& w \leftarrow\left(1-\frac{\eta \lambda}{m}\right) w-\frac{\eta}{\hat{m}} \sum_{x} \frac{\partial C_{x}}{\partial w} \tag{28}
\end{align*}
$$

## L2 REGULARIZATION

EXPLANATIONS

- For sake of better illustration, consider
- $C_{0}$ to be a quadratic cost function, like mean squared loss
- In general, one can consider the quadratic (second order term) approximation of $C_{0}$
- only one training example, that is $m=1$ in the following
- Let

$$
\begin{equation*}
\mathbf{w}^{*}:=\underset{\mathbf{w}}{\arg \min } C_{0}(\mathbf{w}) \tag{29}
\end{equation*}
$$

be the true minimum (which we don't know).

- Let $k$ be the length of $\mathbf{w}$ (so $k$ the number of weights to be trained)


## L2 REGULARIZATION

## EXPLANATIONS

- Let the Hessian matrix $\mathbf{H} \in \mathbb{R}^{k \times k}$ be defined by

$$
\begin{equation*}
\mathbf{H}_{w w w^{\prime}}=\frac{\partial C_{0}}{\partial w \partial w^{\prime}} \tag{30}
\end{equation*}
$$

- The gradient of $C_{0}$ vanishes at $\mathbf{w}^{*}$, because $\mathbf{w}^{*}$ is the minimum.
- By Taylor's approximation, because $C_{0}$ is quadratic, we know that

$$
\begin{equation*}
C_{0}(\mathbf{w})=C_{0}\left(\mathbf{w}^{*}\right)+\frac{1}{2}\left(\mathbf{w}-\mathbf{w}^{*}\right)^{T} \mathbf{H}\left(\mathbf{w}-\mathbf{w}^{*}\right) \tag{31}
\end{equation*}
$$

- That means that the minimum of $C_{0}$ appears where

$$
\begin{equation*}
\nabla_{\mathbf{w}} C_{0}(\mathbf{w})=\mathbf{H}\left(\mathbf{w}-\mathbf{w}^{*}\right)=\mathbf{0} \tag{32}
\end{equation*}
$$

## L2 REGULARIZATION

EXPLANATIONS

- Let $\tilde{\mathbf{w}}$ be the minimum of $C=C_{0}+\frac{1}{2}\|\mathbf{w}\|^{2}$
- Recalling $\frac{\partial C}{\partial w}=\frac{\partial C_{0}}{\partial w}+\lambda w$ (see (23) with $m=1$ ), we know that

$$
\begin{equation*}
\mathbf{H}\left(\tilde{\mathbf{w}}-\mathbf{w}^{*}\right)+\lambda \tilde{\mathbf{w}}=0 \tag{33}
\end{equation*}
$$

- This further leads to (I is the identity)

$$
\begin{equation*}
\tilde{\mathbf{w}}=(\mathbf{H}+\lambda \mathbf{I})^{-1} \mathbf{H} \mathbf{w}^{*} \tag{34}
\end{equation*}
$$

- For $\lambda \rightarrow 0$, we get $\tilde{\mathbf{w}} \rightarrow \mathbf{w}^{*}$


## L2 REGULARIZATION

## EXPLANATIONS

- Let $\mathbf{D}$ be diagonal where entries $\mathbf{D}_{i i}$ are the eigenvalues of $\mathbf{H}$
- Let $\mathbf{Q}$ collect the eigenvectors of $\mathbf{H}$
- Since $\mathbf{H}$ is real and symmetric, $\mathbf{Q}$ is orthogonal, and $\mathbf{H}$ can be written

$$
\begin{equation*}
\mathbf{H}=\mathbf{Q D Q}^{T} \tag{35}
\end{equation*}
$$

- Substituting (35) in (34), we obtain

$$
\begin{equation*}
\tilde{\mathbf{w}}=\left(\mathbf{Q D Q}^{T}+\lambda \mathbf{I}\right)^{-1} \mathbf{Q D Q} \mathbf{Q}^{T} \mathbf{w}^{*} \tag{36}
\end{equation*}
$$

- further yielding

$$
\begin{equation*}
\tilde{\mathbf{w}}=\mathbf{Q}(\mathbf{D}+\lambda \mathbf{I})^{-1} \mathbf{D} \mathbf{Q}^{T} \mathbf{w}^{*} \tag{37}
\end{equation*}
$$

## L2 REGULARIZATION

## EXPLANATIONS

- Interpretation:
- $\tilde{\mathbf{w}}$ is a rescaled version of $\mathbf{w}^{*}$
- The component of $\mathbf{w}^{*}$ that aligns with the $i$-th eigenvector of $\mathbf{H}$ is rescaled by a factor of

$$
\frac{\mathbf{D}_{i i}}{\mathbf{D}_{i i}+\lambda}
$$

- Eigenvectors of $\mathbf{H}$ referring to large eigenvalues indicate directions where the gradient rapidly changes (increases when going away from $\mathbf{w}^{*}$, where it is zero)
- Eigenvectors of $\mathbf{H}$ referring to small eigenvalues indicate directions where the gradient hardly changes
- The latter directions can be neglected
- In other words, components of weights referring to such Universitädirections can be decayed away by regularization
BiELLEFLD


## Regularization Revisited

Motivation


L2 regularization shrinks weights along eigenvectors of the Hessian

## Regularization Revisited

## Motivation



Regularization prevents overfitting

## Regularization Revisited

L1 Regularization

For L1 regularization, we modify the cost function

$$
\begin{equation*}
C=C_{0}+\frac{\lambda}{m} \sum_{w}|w| \tag{39}
\end{equation*}
$$

by adding the sum of the absolute values of the weights.
Gradient:

$$
\begin{equation*}
\frac{\partial C}{\partial w}=\frac{\partial C_{0}}{\partial w}+\frac{\lambda}{m} \operatorname{sgn}(w) \tag{40}
\end{equation*}
$$

Update:

$$
\begin{equation*}
w \leftarrow w^{\prime}=w-\frac{\eta \lambda}{m} \operatorname{sgn}(w)-\eta \frac{\partial C_{0}}{\partial w} \tag{41}
\end{equation*}
$$

## L1 REGULARIZATION

EXPLANATIONS

- L1 regularization does not have a similarly neat algebraic explanation like L2 regularization
- An approximate explanation is that components referring to small eigenvalues of the Hessian are set to zero, rather than smoothly shrunken
- Overall, a sparse set of weights is achieved


## Regularization Revisited

L1 versus L2 Regularization

- In L1 regularization, weights shrink by a constant amount.
- In L2 regularization, weights shrink by an amount proportionally to $w$.
- L1 regularization tends to bring forward a small number of high-importance connections.
- L2 regularization tends to keep all weights small.


## Regularization Revisited

Dropout


Full network, before dropout

## Regularization Revisited

Dropout


Network after having dropped half of the hidden nodes

## Regularization Revisited

Dropout

## Procedure

1. Choose a mini batch of training data of size $\hat{m}$
2. Randomly delete half of the hidden nodes, while keeping all input and output nodes
3. Train the resulting network using the mini batch; update all weights and biases
4. If validation accuracy not yet satisfying, return to 1 .
5. After each epoch, decrease each weight by a factor of $\frac{1}{2}$

## Dropout

EXPLANATIONS

- Dropout can be perceived as averaging over several smaller networks, where averaging over several models is generally helpful to prevent overfitting
- Dropout can be perceived as projecting points in parameter space onto the linear subspace defined by only half of the elementary basis vectors.
- Combining optima in subspaces yields a selection of parameters that are not optimal, but nearby an optimum experience shows that this prevents overfitting
- Dropout prevents "co-adaptation of neurons"


## L1/2 Regularization, Dropout, Early Stopping take-Home Message

Try to find a reasonable point near the very optimum

- L1/2 regularization: shrink or eliminate weights that don't change much
- Dropout: Randomly project points to linear subspaces, and optimize there, and then average out
- Early stopping: Stop before reaching the optimum


## Regularization Revisited

Artificial Expansion of Training Data



More training data improves test accuracy

## Regularization Revisited

## Artificial Expansion of Training Data



NN versus SVM on same training data

- Sometimes better training data delivers substantial improvements
- Always good to aim for methodical improvements, but:
- Don't miss "easy wins" by generating more and/or better training data


## Regularization Revisited

Generating Artificial Training Data


Rotating 5 by 15 degrees to the left yields new training datum
Other Techniques

- Translating, skewing
- "Elastic distortions"
- For more details, see [Simard, Steinkraus \& Platt, 2003] https://ieeexplore.ieee.org/document/1227801


## LECTURE3: SUMMARY

- Backpropagation: See http://www.deeplearningbook.org/ 6.5 and http://neuralnetworksanddeeplearning.com/, Chapter 2, until and including "The Backpropagation Algorithm"
- Regularization: See http://www.deeplearningbook.org/ Chapter 7, (for example 7.1, 7.8, 7.12) and http://neuralnetworksanddeeplearning.com/, Chapter 3
- For further reading, also consider:
- Read "In what sense is backpropagation a fast algorithm?" in Nielsen's book, chapter 2
(http://neuralnetworksanddeeplearning.com/chap2.html),
- Read "Backpropagation: the big picture" in Nielsen's book, chapter 2
- and try to make sense of what you have read.


## Outlook

- Convolutional Neural Networks
- http://www. deeplearningbook.org/, Chapter 9
- http://neuralnetworksanddeeplearning.com/, "Deep Learning"


## Thanks for your attention

