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Short Introduction to Machine Learning 00 000000 Deep Neural Networks 0 000000 00 Convolutional Neural Networks

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Summary 00

Introduction to Feed-forward and Convolutional Neural Networks

Adrian Braemer

23.04.2019

Short Introduction to Machine Learning 00 000000 Deep Neural Networks 0 000000 00 Convolutional Neural Networks

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Summary 00

Outline

Short Introduction to Machine Learning

Basic concepts Example: Image Classification

Deep Neural Networks

General Network Architecture How to train a NN Example: MNIST

Convolutional Neural Networks

Convolutional Neural Networks

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Summary 00

What is Machine Learning?

• Goal: Make predictions based on given data

Convolutional Neural Networks

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Summary 00

- Goal: Make predictions based on given data
- Formalization:

Convolutional Neural Networks

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- Goal: Make predictions based on given data
- Formalization:
 - Independent quantities x, f. e. spring constant k, mass m

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- Goal: Make predictions based on given data
- Formalization:
 - Independent quantities x, f. e. spring constant k, mass m
 - Dependent quantity y, f. e. period of pendulum T

Convolutional Neural Networks

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Summary 00

- Goal: Make predictions based on given data
- Formalization:
 - Independent quantities x, f. e. spring constant k, mass m
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 - Dataset $\mathbf{X} = (\mathbf{x}_1, ...)$ and $\mathbf{Y} = (y_1, ...)$ f. e. experimental data

Convolutional Neural Networks

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- Goal: Make predictions based on given data
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 - Independent quantities x, f. e. spring constant k, mass m
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 - Dataset $\mathbf{X} = (\mathbf{x}_1, ...)$ and $\mathbf{Y} = (y_1, ...)$ f. e. experimental data
 - Model $f(\mathbf{x}; \mathbf{w}), f: \mathbf{x} \to y$ with parameters \mathbf{w} , f. e. $k^{w_1}m^{w_2}$

Convolutional Neural Networks

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 - Cost function $C(\mathbf{Y}, f(\mathbf{X}; \mathbf{w}))$, f.e. L_2 norm $\sum_i [y_i f(\mathbf{x}_i; \mathbf{w})]^2$

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- \rightarrow Best parameters $\hat{\mathbf{w}} = \operatorname{argmin}_{\mathbf{w}} \mathcal{C}(\mathbf{Y}, f(\mathbf{X}; \mathbf{w}))$

Convolutional Neural Networks

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- \rightarrow Best parameters $\hat{\mathbf{w}} = \operatorname{argmin}_{\mathbf{w}} \mathcal{C}(\mathbf{Y}, f(\mathbf{X}; \mathbf{w}))$
- \rightarrow "Training the model"

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Summary 00

Comparison to Fitting

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Summary 00

Comparison to Fitting

Fitting:

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Summary 00

Comparison to Fitting

Fitting:

Learning:

Goal: Best *estimation* of parameters w

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Summary 00

Comparison to Fitting

Fitting:

Learning:

- Goal: Best *estimation* of parameters w
- Use all data to fit

Convolutional Neural Networks

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Summary 00

Comparison to Fitting

Fitting:

Learning:

- Goal: Best *estimation* of parameters w
- Use all data to fit
- Minimize Cost function by all means

Convolutional Neural Networks

Summary 00

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- Goal: Best *estimation* of parameters w
- Use all data to fit
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Learning:

• Goal: Best *prediction* for unknown **x**

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Summary 00

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Fitting:

- Goal: Best *estimation* of parameters w
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Learning:

- Goal: Best prediction for unknown x
- Split data set in training and test sets

Convolutional Neural Networks

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 \rightarrow Cross validation

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Summary 00

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- \rightarrow Cross validation
 - Test set accuracy is important!

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- \rightarrow Cross validation
 - Test set accuracy is important!
- \rightarrow Regularization

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Convolutional Neural Networks

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- \rightarrow Cross validation
 - Test set accuracy is important!
- \rightarrow Regularization
- \rightarrow Subtle differences, very different algorithms!

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Explicit Example: Image Classification

• Independent quantities: Pixel data x (flattened to a vector)

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- Independent quantities: Pixel data x (flattened to a vector)
- Dependent quantity: Category $y \in 0, 1$

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- Independent quantities: Pixel data x (flattened to a vector)
- Dependent quantity: Category $y \in 0, 1$
- Linear model: $f(\mathbf{x}; \mathbf{w}, b) = \sigma(\mathbf{x}^T \mathbf{w} + b)$

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- Sigmoid function $\sigma(x) = \frac{1}{1+e^{-x}}$
- \rightarrow Model maps input to *probability*
- $\rightarrow f(\mathbf{x}; \mathbf{w}, b) = P(y = 1 | \mathbf{x}; \mathbf{w}, b)$

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Summary 00

Cost function for classification

• Idea: Maximize probability of correct classification

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Summary 00

Cost function for classification

- Idea: Maximize probability of correct classification
- Remember: $P(y = 1 | \mathbf{x}) = \sigma(\mathbf{x}^T \mathbf{w} + b) = 1 P(y = 0 | \mathbf{x})$

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Summary 00

Cost function for classification

- Idea: Maximize probability of correct classification
- Remember: $P(y = 1 | \mathbf{x}) = \sigma(\mathbf{x}^T \mathbf{w} + b) = 1 P(y = 0 | \mathbf{x})$
- Probability *P_{correct}* that classification is correct:

$$P_{correct}(\mathbf{x}, y) = \begin{cases} P(y = 1 | \mathbf{x}) & y = 1\\ 1 - P(y = 1 | \mathbf{x}) & y = 0\\ = P(y = 1 | \mathbf{x})^{y} [1 - P(y = 1 | \mathbf{x})]^{1-y} \end{cases}$$

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Summary 00

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• For multiple predictions: $P_{correct}(\mathbf{X}, \mathbf{Y}) = \prod_{i} P_{correct}(\mathbf{x}_{i}, y_{i})$

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Cost function for classification

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$$= P(y = 1 | \mathbf{x})^{y} [1 - P(y = 1 | \mathbf{x})]^{1-y}$$

- For multiple predictions: $P_{correct}(\mathbf{X}, \mathbf{Y}) = \prod_{i} P_{correct}(\mathbf{x}_{i}, y_{i})$
- Cross entropy:

$$-\sum_{i} y_{i} \log \left[\sigma(\mathbf{x}_{i}^{T}\mathbf{w}+b)\right] + (1-y_{i}) \log \left[1-\sigma(\mathbf{x}_{i}^{T}\mathbf{w}+b)\right]$$

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Summary 00

Practical Example: MNIST

• Dataset of 70.000 handwritten digits
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Summary 00

- Dataset of 70.000 handwritten digits
- Commonly used for machine learning experiments

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Summary 00

- Dataset of 70.000 handwritten digits
- Commonly used for machine learning experiments
- Lowest error rate 0,21% (CNN)

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Summary 00

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- Commonly used for machine learning experiments
- Lowest error rate 0,21% (CNN)



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Summary 00

MNIST classifier

• Cross entropy: only 2 output states



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Summary 00

- Cross entropy: only 2 output states
- $\rightarrow\,$ Take 1 classifier for every class

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Summary 00

- Cross entropy: only 2 output states
- ightarrow Take 1 classifier for every class
 - Probabilities don't add to 1

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Summary 00

- Cross entropy: only 2 output states
- ightarrow Take 1 classifier for every class
 - Probabilities don't add to 1
- \rightarrow Take SoftMax (= Boltzmann distribution) function

$$x_i \mapsto rac{e^{x_i}}{\sum_j e^{x_j}}$$

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Summary 00

Can we do better with a more complex model?

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Summary 00

Neural Networks

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Summary 00



Figure: General architecture

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Summary 00

How to train a NN

• Want to minimize $\mathcal{C}(X; \mathbf{w})$ w. r. t. w

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Summary 00

- Want to minimize $C(X; \mathbf{w})$ w. r. t. w
- Gradient Descent:

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Summary 00

- Want to minimize $C(X; \mathbf{w})$ w. r. t. w
- Gradient Descent:
 - 1. Choose some initial \mathbf{w}_0

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Summary 00

- Want to minimize $C(X; \mathbf{w})$ w. r. t. w
- Gradient Descent:
 - 1. Choose some initial \mathbf{w}_0
 - 2. Compute gradient $\mathbf{v}_i = \nabla \mathcal{C}(X; \mathbf{w}_i)$

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Summary 00

- Want to minimize $C(X; \mathbf{w})$ w. r. t. w
- Gradient Descent:
 - 1. Choose some initial \mathbf{w}_0
 - 2. Compute gradient $\mathbf{v}_i = \nabla \mathcal{C}(X; \mathbf{w}_i)$
 - 3. Update weights $\mathbf{w}_{i+1} = \mathbf{w}_i \eta \mathbf{v}_i$ where η is the learning rate

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- Want to minimize $C(X; \mathbf{w})$ w. r. t. w
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 - 4. Repeat until converged to minimum

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- Want to minimize $C(X; \mathbf{w})$ w. r. t. w
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 - 1. Choose some initial \mathbf{w}_0
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 - 3. Update weights $\mathbf{w}_{i+1} = \mathbf{w}_i \eta \mathbf{v}_i$ where η is the learning rate
 - 4. Repeat until converged to minimum
- \rightarrow Problems at every step!

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Summary 00

Simple algorithm - many problems

• How to choose **w**₀?



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- How to choose **w**₀?
- $\rightarrow\,$ Zero-mean, normal-distributed values work well enough in most cases



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- How to choose **w**₀?
- $\rightarrow\,$ Zero-mean, normal-distributed values work well enough in most cases
 - How to compute $-\nabla C(X; \mathbf{w})$?



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- How to choose **w**₀?
- $\rightarrow\,$ Zero-mean, normal-distributed values work well enough in most cases
 - How to compute $-\nabla C(X; \mathbf{w})$?
- ightarrow Backpropagation



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- How to choose **w**₀?
- $\rightarrow\,$ Zero-mean, normal-distributed values work well enough in most cases
 - How to compute $-\nabla C(X; \mathbf{w})$?
- ightarrow Backpropagation
 - How to choose learning rate η ?



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- How to choose **w**₀?
- $\rightarrow\,$ Zero-mean, normal-distributed values work well enough in most cases
 - How to compute $-\nabla C(X; \mathbf{w})$?
- \rightarrow Backpropagation
 - How to choose learning rate η ?
- \rightarrow Need to tune



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- How to choose **w**₀?
- $\rightarrow\,$ Zero-mean, normal-distributed values work well enough in most cases
 - How to compute $-\nabla C(X; \mathbf{w})$?
- \rightarrow Backpropagation
 - How to choose learning rate η ?
- \rightarrow Need to tune
 - How do we know we have the correct minimum?



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- How to choose **w**₀?
- $\rightarrow\,$ Zero-mean, normal-distributed values work well enough in most cases
 - How to compute $-\nabla C(X; \mathbf{w})$?
- \rightarrow Backpropagation
 - How to choose learning rate η ?
- $\rightarrow\,$ Need to tune
 - How do we know we have the correct minimum?
- \rightarrow We don't

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- How to choose **w**₀?
- $\rightarrow\,$ Zero-mean, normal-distributed values work well enough in most cases
 - How to compute $-\nabla C(X; \mathbf{w})$?
- \rightarrow Backpropagation
 - How to choose learning rate η ?
- \rightarrow Need to tune
 - How do we know we have the correct minimum?
- \rightarrow We don't
 - Do we even converge?

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Summary 00



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Summary 00

Backpropagation Algorithm

• Weigths w'_{jk} between *j*-th neuron in layer l-1 and *k*-th neuron in layer l



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Summary 00

- Weigths w'_{jk} between *j*-th neuron in layer l-1 and *k*-th neuron in layer l
- Biases b_i^l



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Summary 00

- Weigths w'_{jk} between *j*-th neuron in layer l-1 and *k*-th neuron in layer l
- Biases b_i^l
- Weighted inputs to neuron $z'_k = \sum_j w'_{jk} a'^{-1}_j + b'_k$



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- Biases b_j^l
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- Activation levels a_k^l :



Summary 00

- Weigths w'_{jk} between *j*-th neuron in layer l-1 and *k*-th neuron in layer l
- Biases b_i^l
- Weighted inputs to neuron $z_k^{\prime} = \sum_j w_{jk}^{\prime} a_j^{\prime-1} + b_k^{\prime}$
- Activation levels a_k^l :
 - a_k^1 are the inputs


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- Weigths w'_{jk} between *j*-th neuron in layer l-1 and *k*-th neuron in layer l
- Biases b_j^l
- Weighted inputs to neuron $z_k^{\prime} = \sum_j w_{jk}^{\prime} a_j^{\prime-1} + b_k^{\prime}$
- Activation levels a_k^l :
 - a_k^1 are the inputs

•
$$a'_k = \sigma(z'_k) = \sigma\left(\sum_j w'_{jk}a'^{-1}_j + b'_k\right)$$



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- Weighted inputs to neuron $z'_k = \sum_j w'_{jk} a'^{-1}_j + b'_k$
- Activation levels a^l_k:
 - a_k^1 are the inputs

•
$$a'_k = \sigma(z'_k) = \sigma\left(\sum_j w'_{jk}a'^{-1}_j + b'_k\right)$$

• Error
$$\Delta_k^l = \frac{\partial C}{\partial z_k^l}$$



Summary 00

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- Weighted inputs to neuron $z_k^{\prime} = \sum_j w_{jk}^{\prime} a_j^{\prime-1} + b_k^{\prime}$
- Activation levels a^l_k:
 - a_k^1 are the inputs

•
$$a'_k = \sigma(z'_k) = \sigma\left(\sum_j w'_{jk}a'^{-1}_j + b'_k\right)$$

• Error
$$\Delta_k^l = \frac{\partial C}{\partial z_k^l} = \frac{\partial C}{\partial a_k^l} \frac{\partial a_k^l}{\partial z_k^l}$$



Summary 00

Backpropagation Algorithm

- Weigths w'_{jk} between *j*-th neuron in layer l-1 and *k*-th neuron in layer l
- Biases b_i^I
- Weighted inputs to neuron $z'_k = \sum_j w'_{jk} a'^{-1}_j + b'_k$
- Activation levels a^l_k:
 - a_k^1 are the inputs

•
$$a_k^l = \sigma(z_k^l) = \sigma\left(\sum_j w_{jk}^l a_j^{l-1} + b_k^l\right)$$

• Error $\Delta_k^l = \frac{\partial \mathcal{C}}{\partial z_k^l} = \frac{\partial \mathcal{C}}{\partial a_k^l} \frac{\partial a_k^l}{\partial z_k^l} = \frac{\partial \mathcal{C}}{\partial a_k^l} \sigma'(z_k^l)$



Summary 00

- Weigths w'_{jk} between *j*-th neuron in layer l-1 and *k*-th neuron in layer l
- Biases b_i^l
- Weighted inputs to neuron $z_k^{\prime} = \sum_j w_{jk}^{\prime} a_j^{\prime-1} + b_k^{\prime}$
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• $\Delta_k^l = \sum_k \frac{\partial C}{\partial z_k^{l+1}} \frac{\partial z_k^{l+1}}{\partial z_k^l}$



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Summary 00

Backpropagation Algorithm

- Weigths w'_{jk} between *j*-th neuron in layer l-1 and *k*-th neuron in layer l
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Summary 00

Backpropagation Algorithm

- Weigths w'_{jk} between *j*-th neuron in layer l-1 and *k*-th neuron in layer l
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•
$$\Delta'_k = \sum_k \frac{\partial \mathcal{C}}{\partial z_k^{l+1}} \frac{\partial z_k^{l+1}}{\partial z_j^l} = \sigma'(z_j^l) \left(\sum_k w_{jk}^{l+1} \Delta_k^{l+1} \right)$$

• Gradient: $\frac{\partial C}{\partial w_{jk}^{l}}$



Summary 00

- Weigths w'_{jk} between *j*-th neuron in layer l-1 and *k*-th neuron in layer l
- Biases b_i^I
- Weighted inputs to neuron $z_k^{\prime} = \sum_j w_{jk}^{\prime} a_j^{\prime-1} + b_k^{\prime}$
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$$a'_k = \sigma(z'_k) = \sigma\left(\sum_j w'_{jk}a'^{-1}_j + b'_k\right)$$

- Error $\Delta_k^l = \frac{\partial \mathcal{C}}{\partial z_k^l} = \frac{\partial \mathcal{C}}{\partial a_k^l} \frac{\partial a_k^l}{\partial z_k^l} = \frac{\partial \mathcal{C}}{\partial a_k^l} \sigma'(z_k^l)$
- $\Delta_k^l = \sum_k \frac{\partial \mathcal{C}}{\partial z_k^{l+1}} \frac{\partial z_k^{l+1}}{\partial z_j^l} = \sigma'(z_j^l) \left(\sum_k w_{jk}^{l+1} \Delta_k^{l+1} \right)$

• Gradient:
$$\frac{\partial C}{\partial w_{jk}^{l}} = \frac{\partial C}{\partial z_{j}^{l}} \frac{\partial z_{j}^{l}}{\partial w_{jk}^{l}}$$



Summary 00

Backpropagation Algorithm

- Weigths w'_{jk} between *j*-th neuron in layer l-1 and *k*-th neuron in layer l
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- Activation levels a^l_k:
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•
$$\Delta'_k = \sum_k \frac{\partial \mathcal{C}}{\partial z_k^{l+1}} \frac{\partial z_k^{l+1}}{\partial z_j^l} = \sigma'(z_j^l) \left(\sum_k w_{jk}^{l+1} \Delta_k^{l+1} \right)$$

• Gradient:
$$\frac{\partial C}{\partial w'_{jk}} = \frac{\partial C}{\partial z'_j} \frac{\partial z'_j}{\partial w'_{jk}} = \Delta'_j a'^{-1}_k$$

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Backpropagation Algorithm

1. Calculate the activation levels z'_k and a'_k iteratively from front to back



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Summary 00

- 1. Calculate the activation levels z'_k and a'_k iteratively from front to back
- 2. Find the error at top level $\Delta_k^L = \frac{\partial C}{\partial a_k^L} \sigma'(z_k^L)$



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Summary 00

- 1. Calculate the activation levels z'_k and a'_k iteratively from front to back
- 2. Find the error at top level $\Delta_k^L = \frac{\partial C}{\partial a_L^L} \sigma'(z_k^L)$
- 3. Propagate errors backwards $\Delta_k^l = \sigma'(z_j^l) \left(\sum_k w_{jk}^{l+1} \Delta_k^{l+1} \right)$

Deep Neural Networks

Convolutional Neural Networks

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Summary 00

- 1. Calculate the activation levels z'_k and a'_k iteratively from front to back
- 2. Find the error at top level $\Delta_k^L = \frac{\partial C}{\partial a_L^L} \sigma'(z_k^L)$
- 3. Propagate errors backwards $\Delta'_k = \sigma'(z'_j) \left(\sum_k w'^{l+1}_{jk} \Delta'^{l+1}_k \right)$
- 4. Put everything together to find the gradient $\frac{\partial \mathcal{C}}{\partial w'_{jk}} = \Delta'_j a_k^{l-1}$

Deep Neural Networks

Convolutional Neural Networks

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Summary 00

- 1. Calculate the activation levels z'_k and a'_k iteratively from front to back
- 2. Find the error at top level $\Delta_k^L = \frac{\partial C}{\partial a_L^L} \sigma'(z_k^L)$
- 3. Propagate errors backwards $\Delta'_k = \sigma'(z'_j) \left(\sum_k w'^{l+1}_{jk} \Delta'^{l+1}_k \right)$
- 4. Put everything together to find the gradient $\frac{\partial C}{\partial w_{l_k}^l} = \Delta_j^l a_k^{l-1}$
- $\rightarrow\,$ problem of vanishing or exploding gradients

Deep Neural Networks

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Summary 00

Repairing the gradient

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Convolutional Neural Networks

Summary 00

Repairing the gradient







Summary 00

Repairing the gradient

- Truncate too high values
- Use non-saturating activation functions, f. e. ReLU (rectified linear unit)

$$\sigma(x) = \max(0, x)$$





Summary 00

Repairing the gradient

- Truncate too high values
- Use non-saturating activation functions, f. e. ReLU (rectified linear unit)

$$\sigma(x) = \max(0, x)$$

Regularization also helps



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Summary 00

Regularization

• Stochastic Gradient Descent

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Summary 00

- Stochastic Gradient Descent
 - Randomly divide training data into *m* minibatches

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Summary 00

- Stochastic Gradient Descent
 - Randomly divide training data into *m* minibatches
 - Train on each minibatch (= epoch)

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Summary 00

- Stochastic Gradient Descent
 - Randomly divide training data into *m* minibatches
 - Train on each minibatch (= epoch)
- Dropout

Deep Neural Networks

Convolutional Neural Networks

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Summary 00

- Stochastic Gradient Descent
 - Randomly divide training data into *m* minibatches
 - Train on each minibatch (= epoch)
- Dropout
 - Randomly neglect neurons during training steps

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Summary 00

- Stochastic Gradient Descent
 - Randomly divide training data into *m* minibatches
 - Train on each minibatch (= epoch)
- Dropout
 - Randomly neglect neurons during training steps
- Batch normalization

Deep Neural Networks

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Summary 00

- Stochastic Gradient Descent
 - Randomly divide training data into *m* minibatches
 - Train on each minibatch (= epoch)
- Dropout
 - Randomly neglect neurons during training steps
- Batch normalization
 - Add 'Batch Normalization' layers

Deep Neural Networks

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Summary 00

- Stochastic Gradient Descent
 - Randomly divide training data into *m* minibatches
 - Train on each minibatch (= epoch)
- Dropout
 - Randomly neglect neurons during training steps
- Batch normalization
 - Add 'Batch Normalization' layers
 - Standardize mean and variance between layers

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Summary 00

- Stochastic Gradient Descent
 - Randomly divide training data into *m* minibatches
 - Train on each minibatch (= epoch)
- Dropout
 - Randomly neglect neurons during training steps
- Batch normalization
 - Add 'Batch Normalization' layers
 - Standardize mean and variance between layers
- \rightarrow Prevent overfitting



Summary 00

MNIST example revisited



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Summary 00

MNIST example revisited



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Summary 00

Weakpoints of DNNs

• No spatial structure



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Summary 00

Weakpoints of DNNs

- No spatial structure
- Do not scale well with input size

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Summary 00

Weakpoints of DNNs

- No spatial structure
- Do not scale well with input size
- $\rightarrow\,$ Can we reduce the network size?

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Summary 00

Basic Idea



Figure: General Structure of CNNs

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Summary 00

Example: Edge detection



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Summary 00

Example: Edge detection



$$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$$

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Summary 00

Example: Edge detection



$$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$$



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Summary 00

Low level convolutions



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Summary 00

High level convolutions



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Summary •0

Summary

• Basic Concepts of ML

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Summary •0



- Basic Concepts of ML
- Motivation and Structure of DNNs

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Summary •0



- Basic Concepts of ML
- Motivation and Structure of DNNs
- How to train a neural network

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Summary •0



- Basic Concepts of ML
- Motivation and Structure of DNNs
- How to train a neural network
- Short outlook to CNNs

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Summary

Discussion/Question