Deep Learning: Lecture 6

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UU

November 13, 2019

Reminder: Dropout, Regularization

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.

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Regularization Revisited

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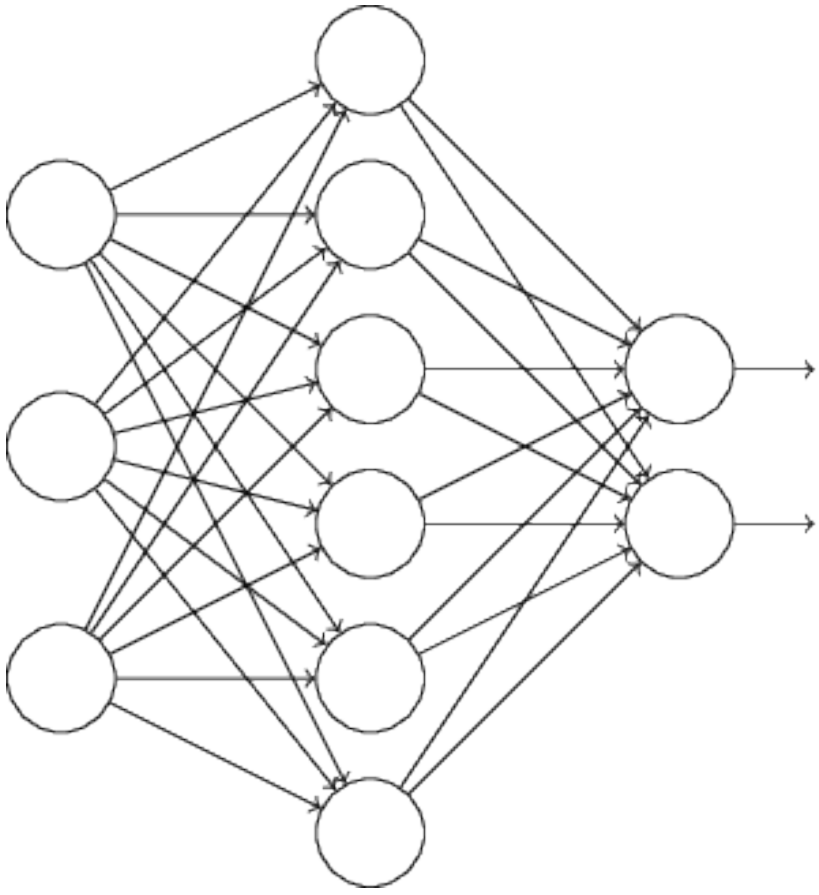
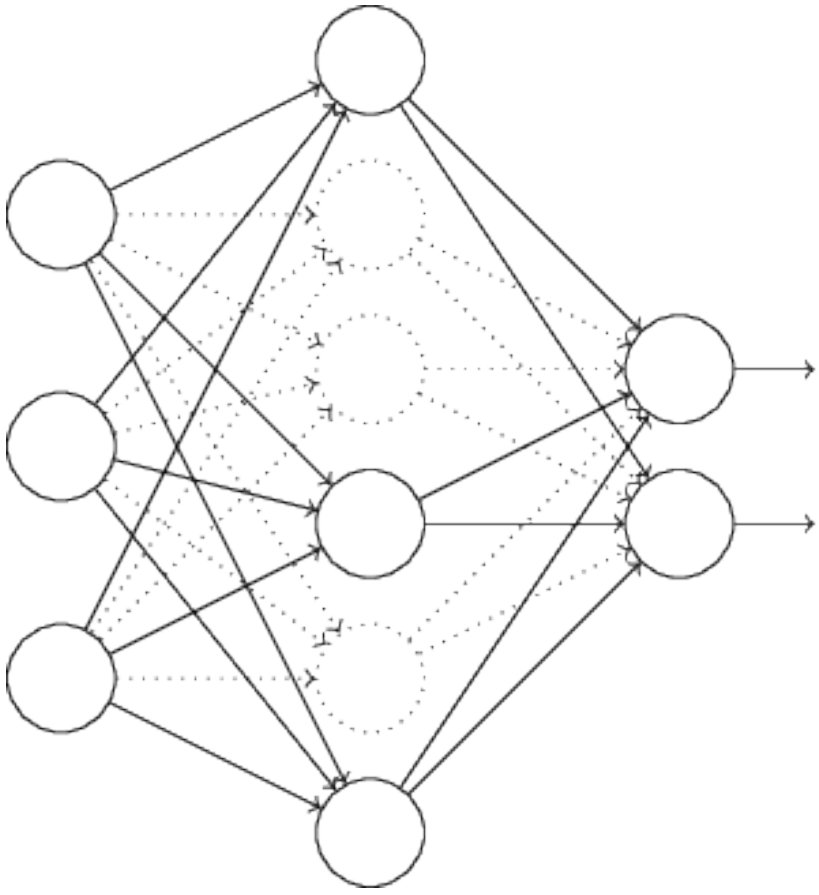


Full network, before dropout

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 $\frac{1}{2}$

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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”

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L1/2 Regularization, Dropout, Early Stopping

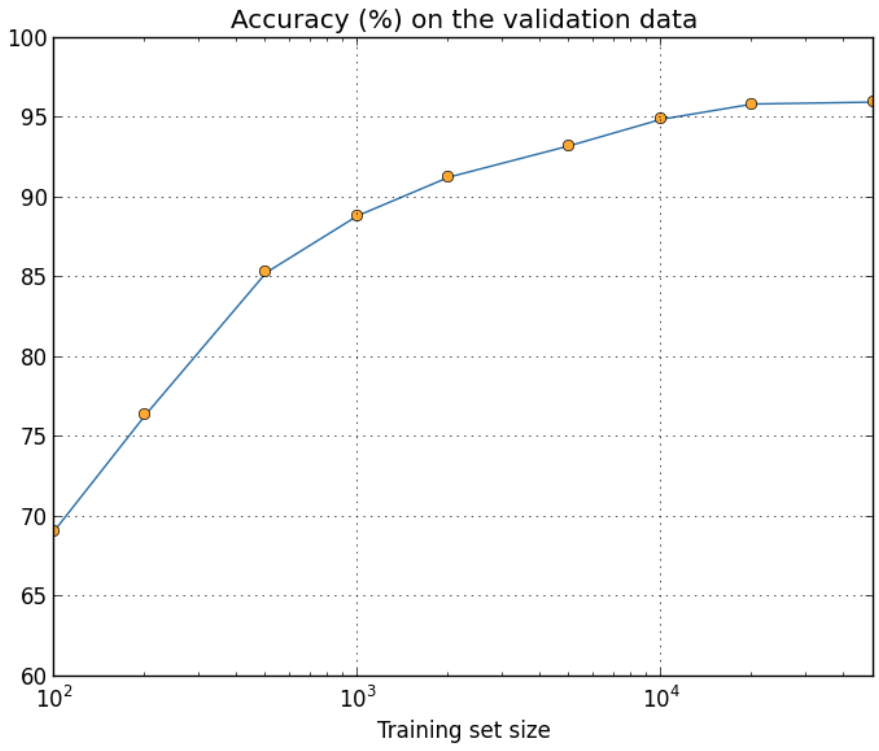
Take-Home Message

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

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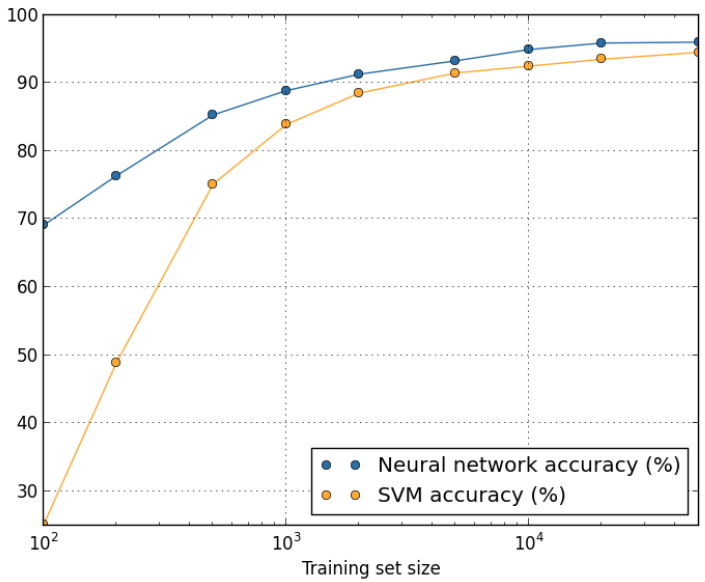

NN versus SVM on same training data

- 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

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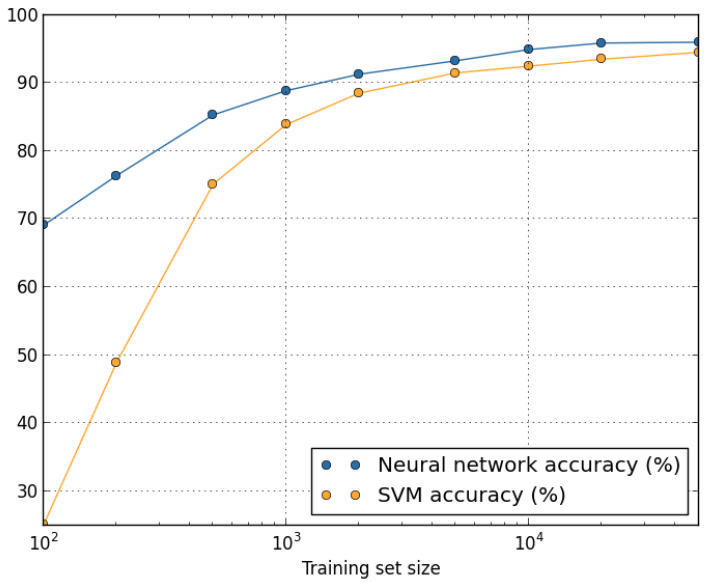

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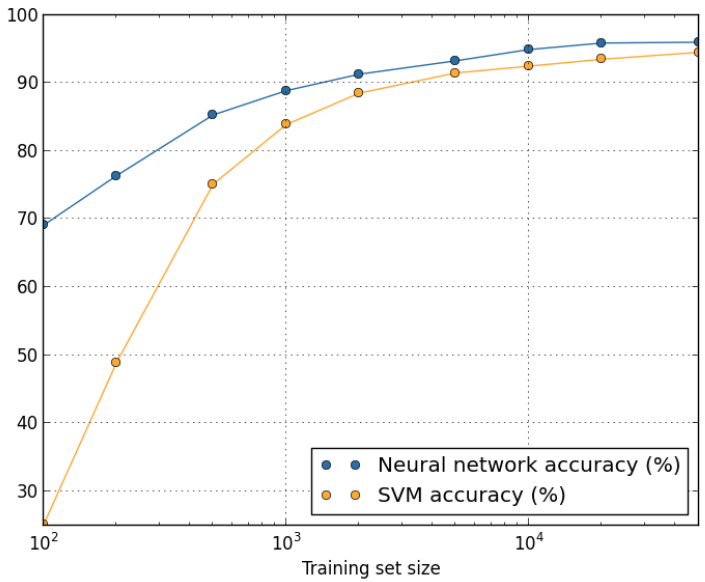

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Regularization Revisited

Generating Artificial Training Data

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

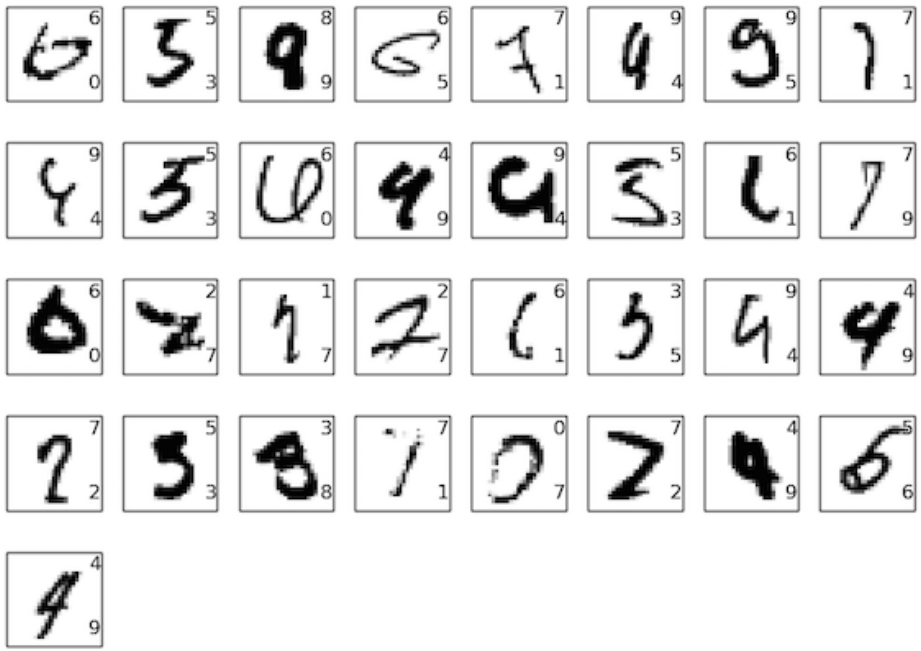
Other Techniques

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

Convolutional Neural Networks (CNNs)

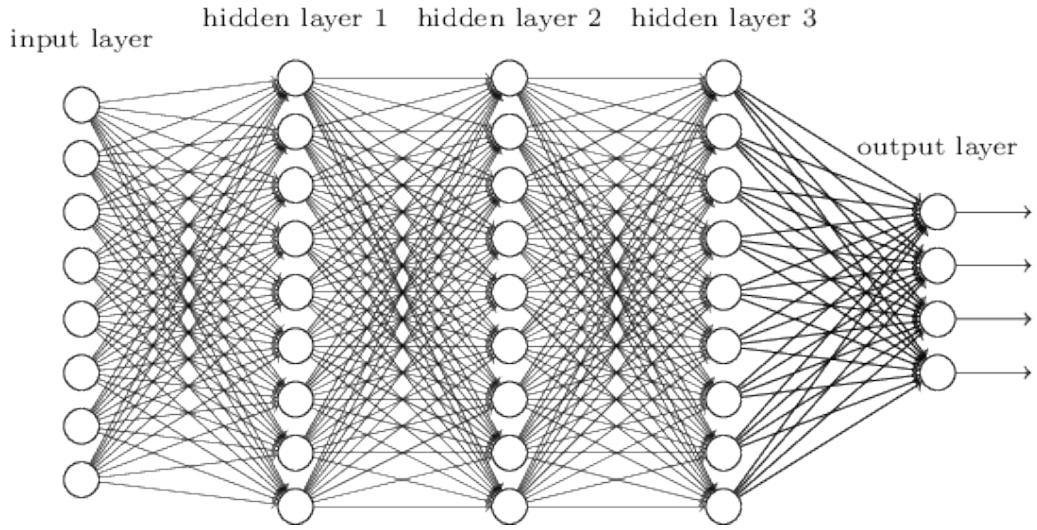
Goal

Setting up a neural network that correctly classifies 9967 out of 10 000 images; see below for the 33 misclassified ones.



33 misclassified images; correct/predicted classification upper/lower right corner

Fully Connected Networks



Fully connected neural network with 3 hidden layers

Issue: With fully connected NN's, we only reach about 98% accuracy in prediction.

Question: How to get to 99,67% accuracy?

Convolutional Neural Networks

Motivation

- Use that images have a spatial structure
  - ☞ Neighboring pixels are more likely to belong to the same structural elements
- Exploit this to speed up training, and reduce number of parameters (weights)

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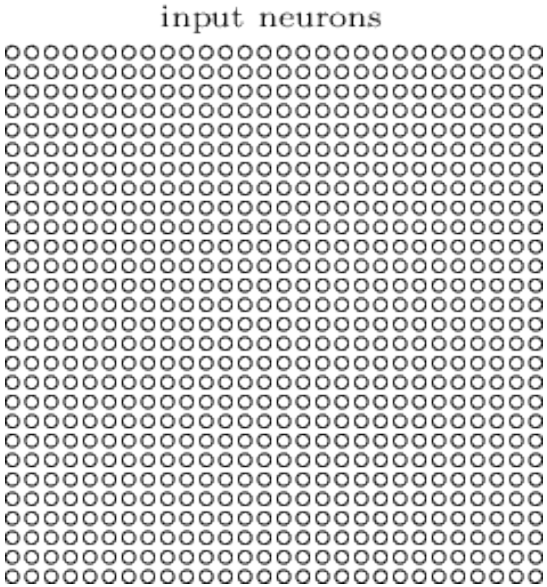
Basic Ideas

- Local receptive fields
- Shared weights
- Pooling

Convolutional Neural Networks

Local Receptive Fields



One image are 28 x 28 = 784 pixels

In a fully connected network

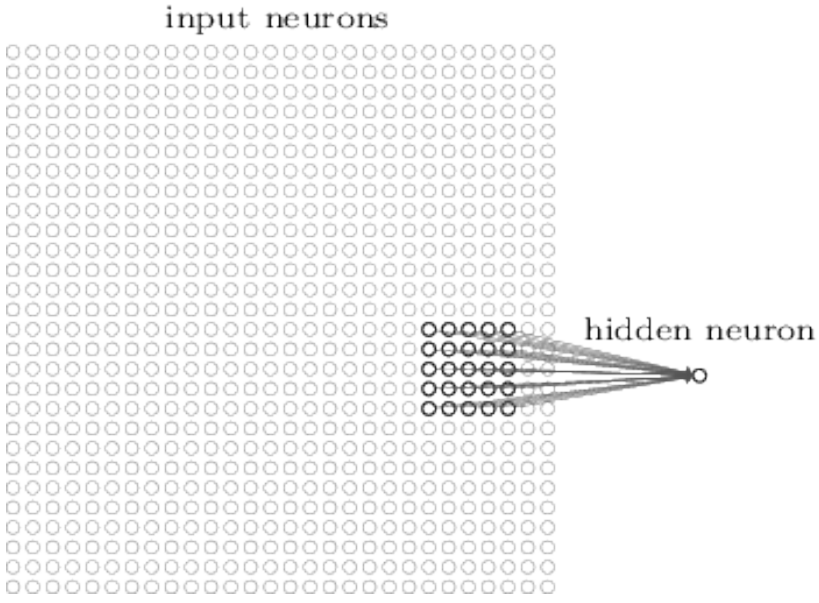
- Every node of the first hidden layer is connected to every input neuron (a.k.a pixel)
- Every node of the second layer is connected to every neuron in the first hidden layer

Convolutional Neural Networks

Local Receptive Fields

In a convolutional NN,

- Every node in the first hidden layer is connected to a rectangular subregion
- Here: subregion = square of 5x5=25 input neurons



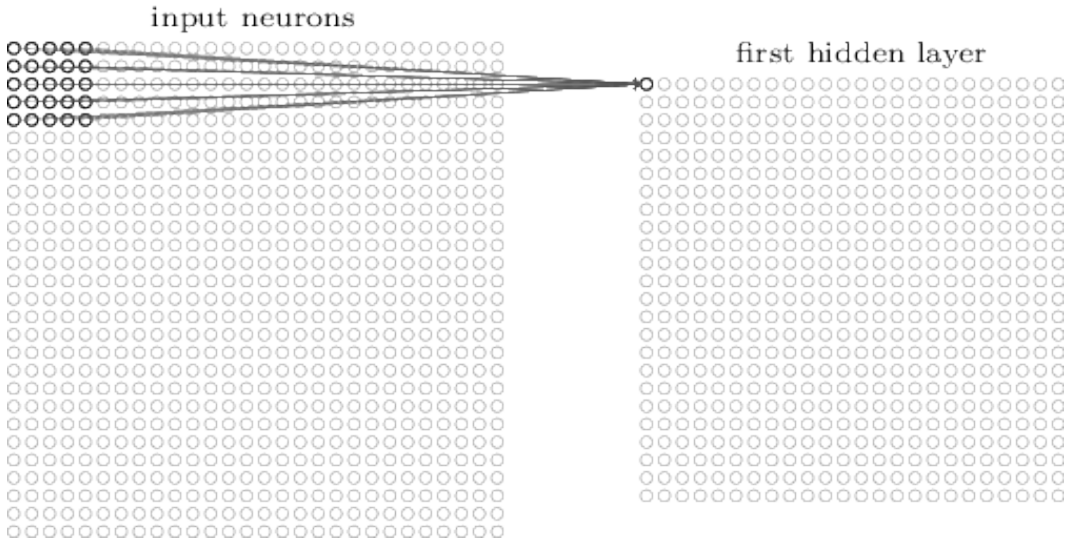
Convolutional filter of size 5 x 5

Definition

The region in the input images to which a hidden neuron is connected is called the *local receptive field (LRF)* of the hidden neuron.

Convolutional Neural Networks

Local Receptive Fields



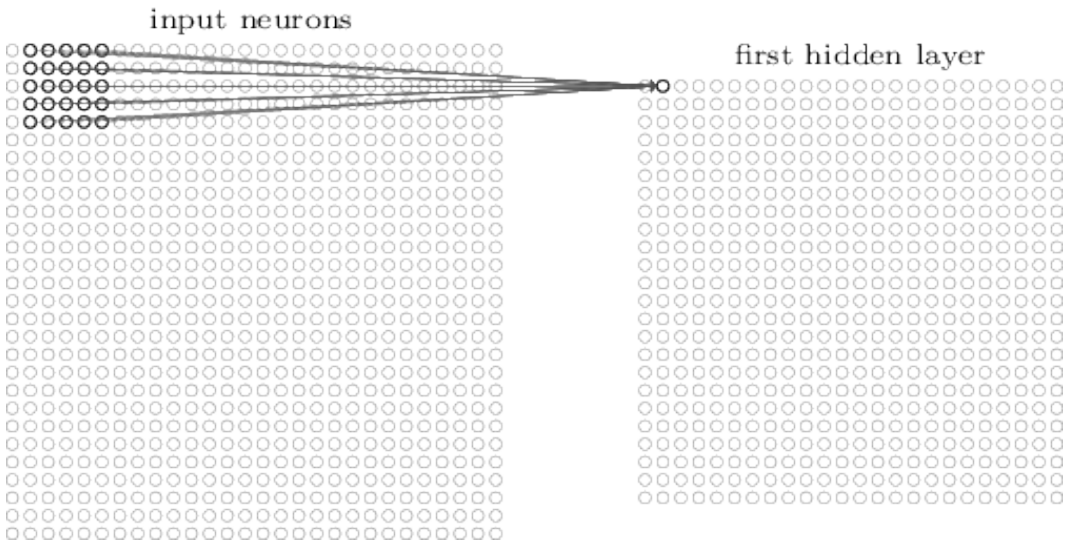
One receptive field is responsible for one hidden layer

Procedure

- Slide the local receptive field across the entire image
- *Stride length*: Step size in sliding field (example here: stride = 1)

Convolutional Neural Networks

Local Receptive Fields



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Convolutional Neural Networks

Computing Hidden Layers

- One *hidden layer* is generated by one pass of the LRF
- Several hidden layers will be generated by several passes of the LRF
- The activation a_{jk}^{l+1} of the j,k-th hidden neuron within the layer, using a $M \times M$ LRF, is computed as (σ may represent activation function of choice)

$$a_{jk}^{(l+1)} = \sigma(b + \sum_{l=0}^{M} \sum_{m=0}^{M} w_{l,m} a_{j+l,k+m}^{l}) \tag{1}$$

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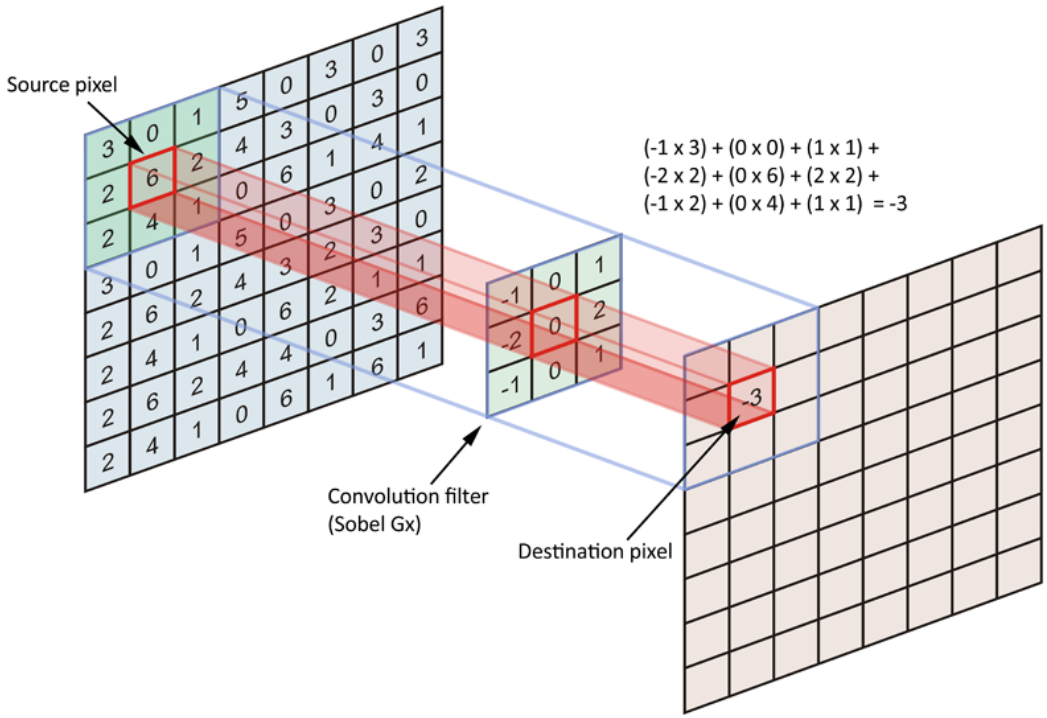

For generating one hidden layer, identical parameters, together defining one convolutional filter, are used

Convolutional Neural Networks

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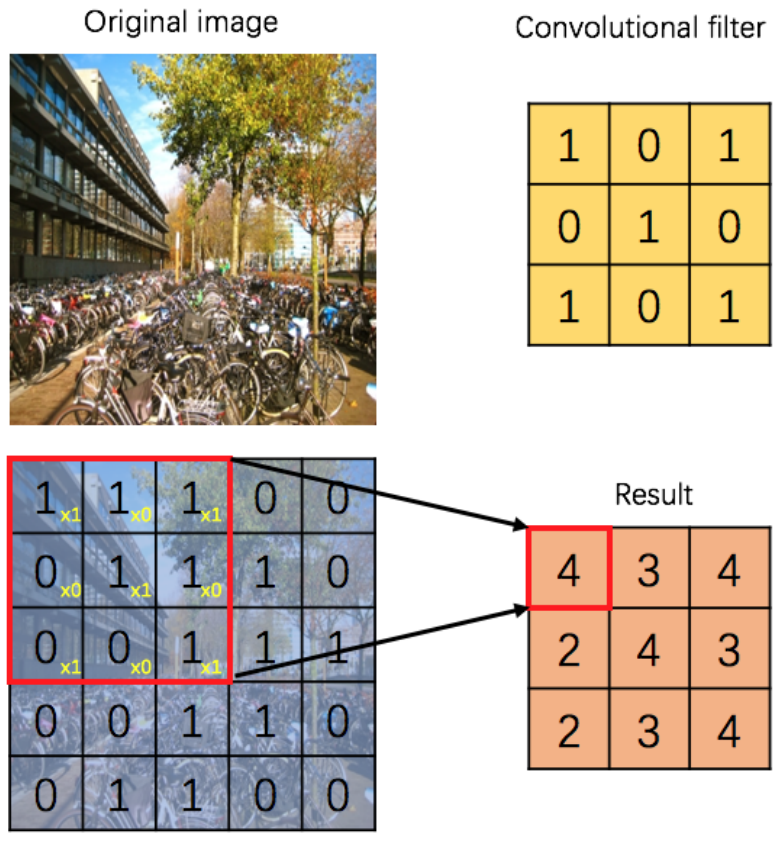

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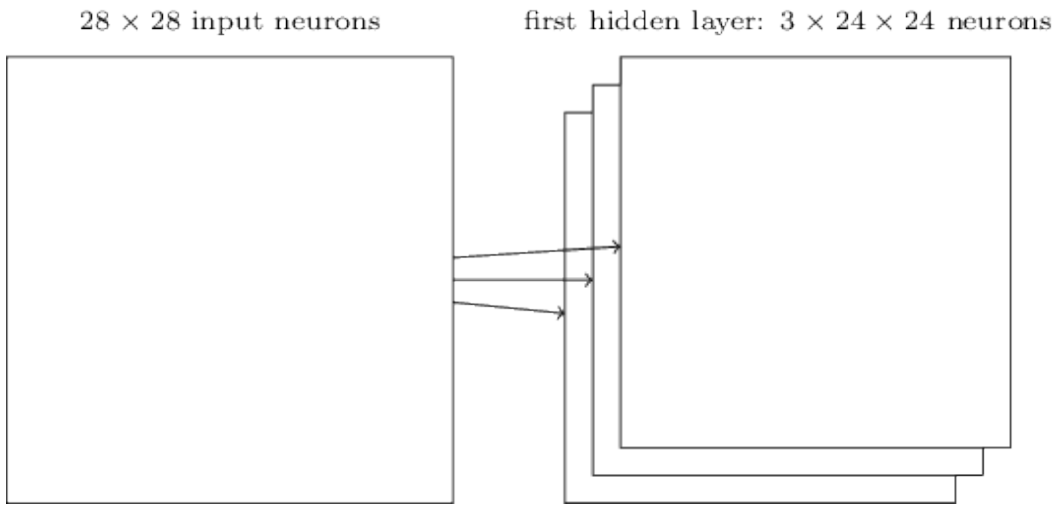
Convolutional Neural Networks

Convolutional Filters

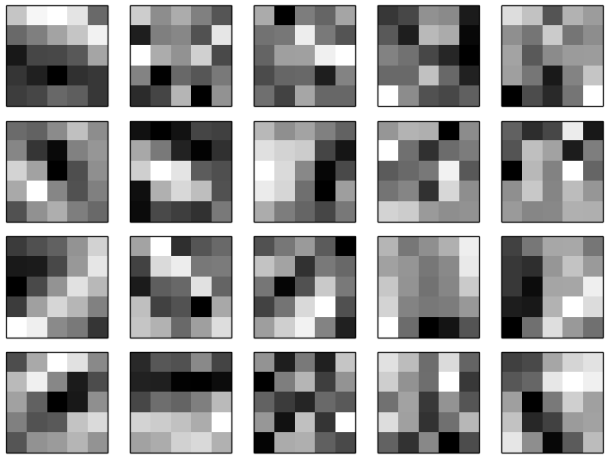
Definition
A *feature map* is a mapping associated with one convolutional filter.



- A complete convolutional layer consists of several hidden sublayers
- Each sublayer is defined by one feature map

Convolutional Neural Networks

Convolutional Filters Real World Example



MNIST example, 20 different filters

- The darker the more positive, the whiter the more negative
- In reality, convolutional filters are hard to interpret
- Literature: M.D. Zeiler, R. Fergus, "Visualizing and Understanding Convolutional Networks", https://arxiv.org/abs/1311.2901

Convolutional Neural Networks

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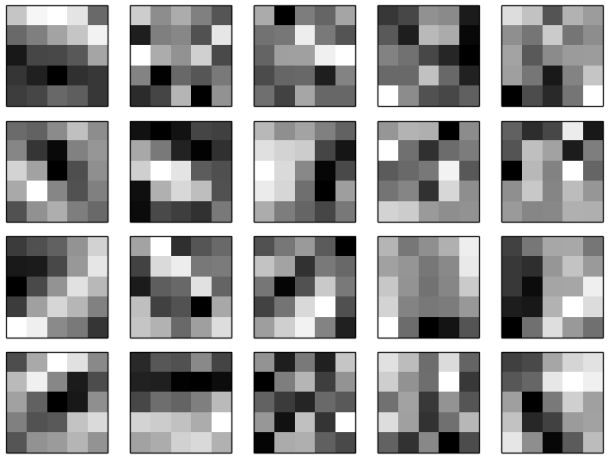

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Convolutional Neural Networks

Shared Weights and Biases

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$$a_{jk}^{l+1} = \sigma(b + \sum_{l=0}^{M} \sum_{m=0}^{M} w_{l,m} a_{j+l,k+m}^{l}) \tag{2}$$

- *Observation:* For each node in the same hidden layer, the same parameters $w_{l,m}, 1 \leq l, m \leq M$ are used
- That is, we only need $M \times M$ parameters to generate the entire hidden layer

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Convolutional Neural Networks

Shared Weights and Biases

MNIST example

:

- Convolutional layer, 20 feature maps, each of size 5×5, roughly requires $20 \times 5 \times 5 = 500$ weights
- Fully connected network, connecting 784 input neurons with 30 hidden neurons requires $784 \times 30 = 23\,520$ weights
- **CNN requires roughly 40 times less parameters**

Convolutional Neural Networks

Convolutional Layer

- *Remark*: Sometimes it helps to think of a convolutional layer, as a new type of image, where each sublayer refers to a different color.
- Note that colored pictures of size $N \times N$ come in 3 input layers of size $N \times N$, each of which refers to one of the 3 base colors red, green and blue.
- So, when using $M \times M$-filters, one applies a $3 \times M \times M$ sized *tensor* (and not an $M \times M$-sized matrix) to the input layer
- This principle can later be repeated: hence the name *tensor flow*.

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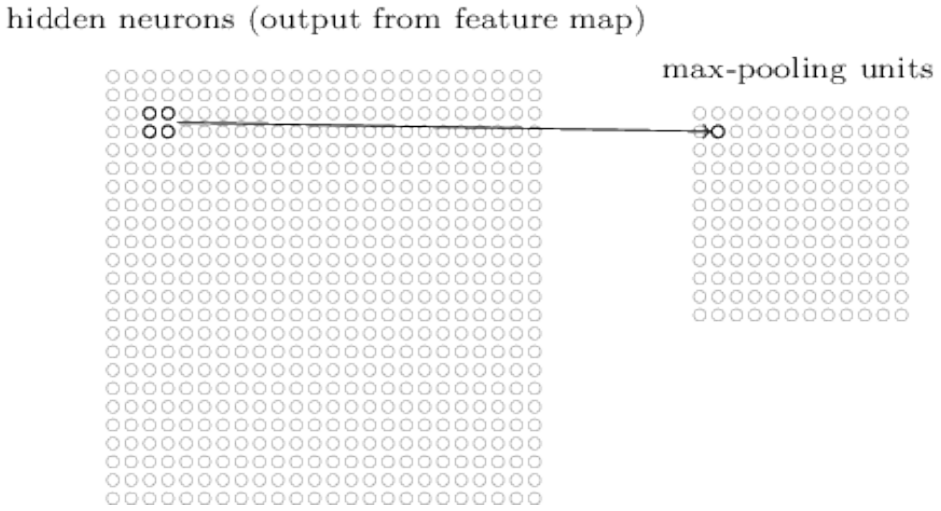
Convolutional Neural Networks

Pooling Layers

- In addition to convolutional layers, CNN's make use of *pooling layers*.
- Pooling layers generate *condensed feature maps*: it takes a rectangle of neurons, and summarizes their values into one value
- This generates a considerably smaller layer

Convolutional Neural Networks

Pooling Layers

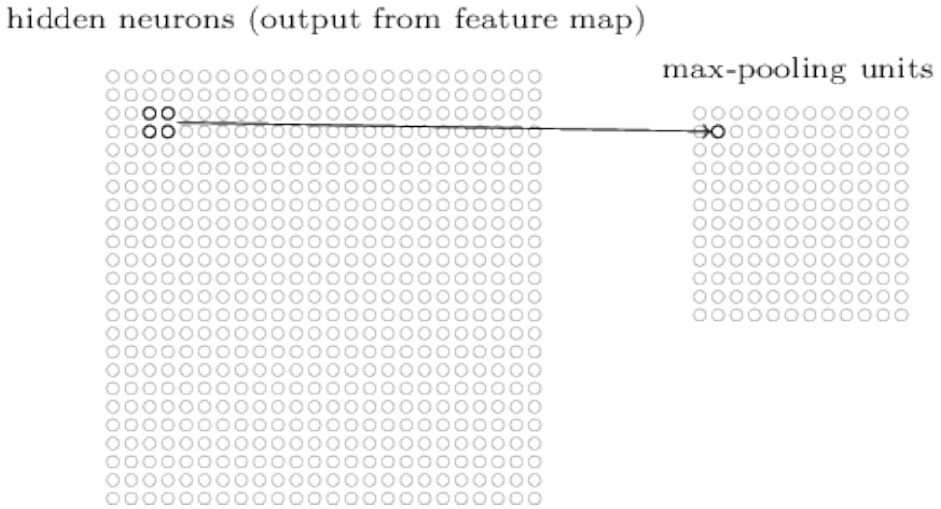


2×2 pooling

- *Max pooling*: Each $L \times L$ rectangle is mapped onto the maximum of its values
- *L2 pooling*: Each $L \times L$ rectangle is mapped to the rooted average of the squares of the values
- This overall yields a layer that is $L \times L$ times smaller
- Usually $L = 2$ is used

Convolutional Neural Networks

Pooling Layers



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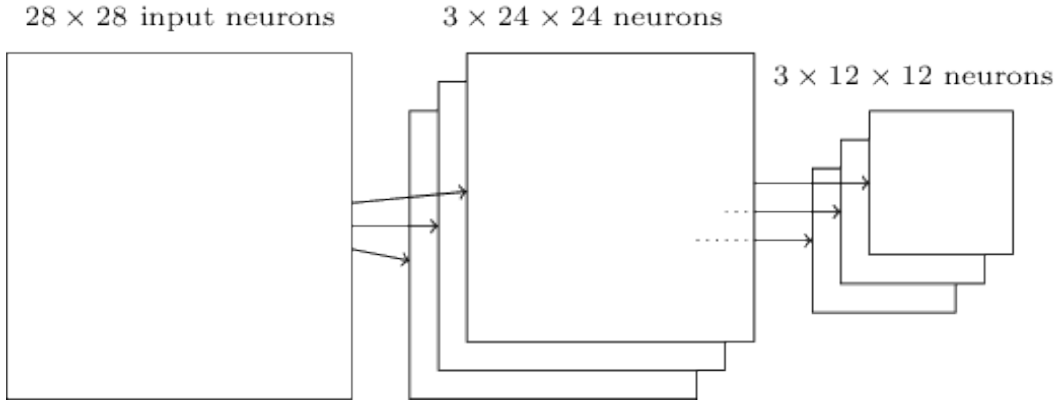
Convolutional Neural Networks

Combining Convolutional and Pooling Layers

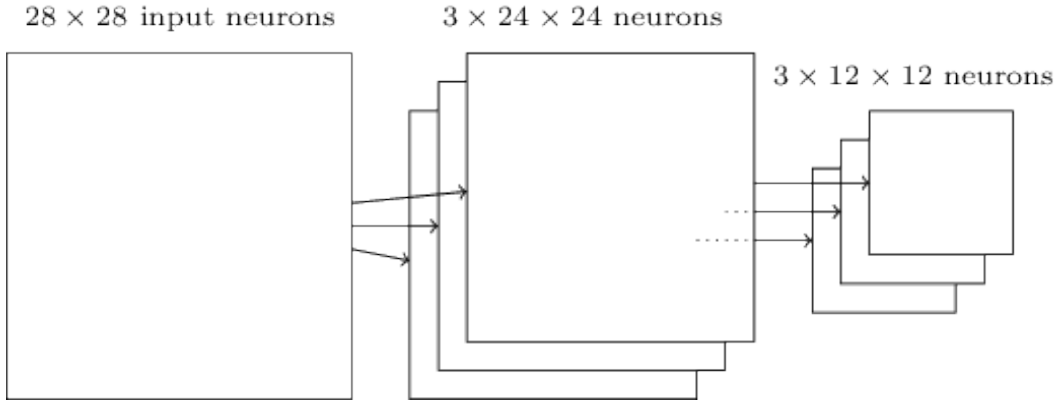


Convolutional layer followed by pooling layer

- Convolutional and pooling layers are used in combination
- Pooling layers usually follow convolutional layers
- *Intuition*:
  - The exact location of the occurrence of a feature is not important
  - Pooling helps to handle distortions and rotations

Convolutional Neural Networks

Combining Convolutional and Pooling Layers



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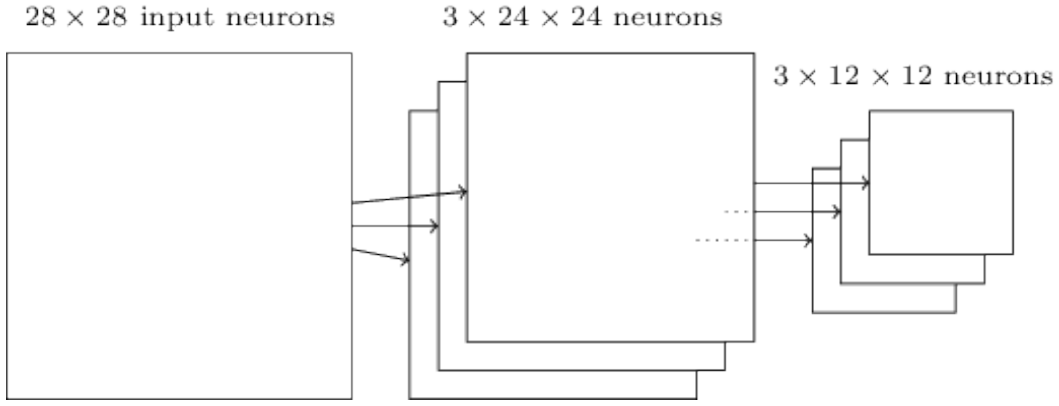

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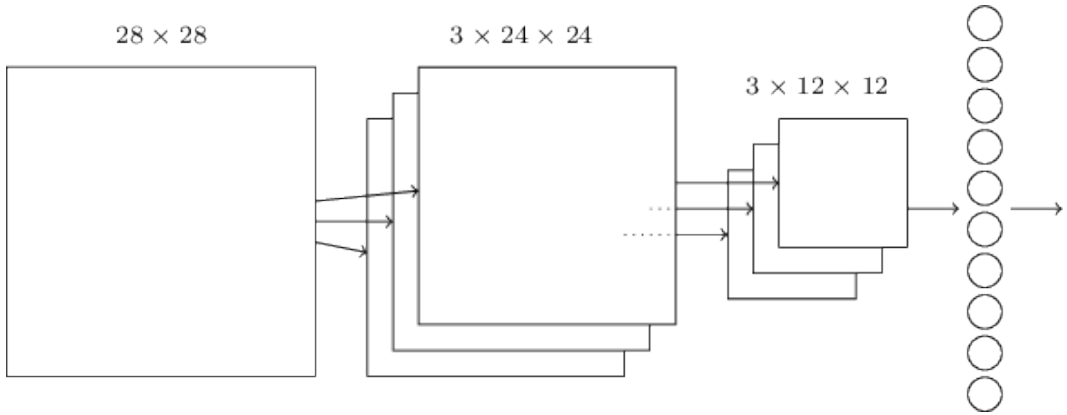
Convolutional Neural Networks

A Complete CNN



Convolution followed by pooling followed by fully connected output layer

- 10 output nodes, one for each digit
- Each output node is connected to *every* node of the pooling layer
- *Training*: Stochastic gradient descent plus backpropagation

Convolutional Neural Networks in Practice

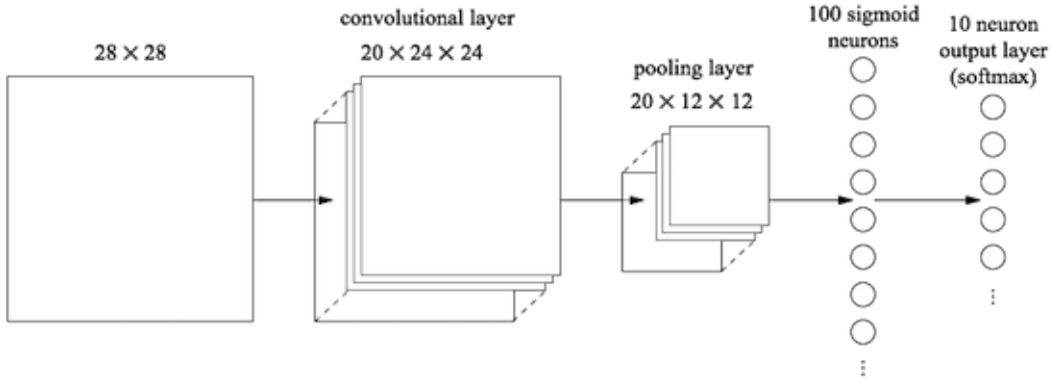
CNNs in Practice

Baseline: Simple Fully Connected Network

- *Baseline*:
  - One hidden layer, 100 neurons
  - Output layer, cost function: softmax + log-likelihood
- *Training*:
  - 60 epochs
  - Learning rate $\eta = 0.1$
  - Mini-batch size 10
- *Test accuracy*: 97.80%

CNNs in Practice

First CNN: one covolution-pooling layer



Inserting a convolution and max-pooling layer

- *Convolutional layer*:
  - 5×5 LRFs, stride length 1
  - 20 feature maps
- *Pooling layer*:
  - 2×2 max-pooling
- *Accuracy*: 98.78% test accuracy

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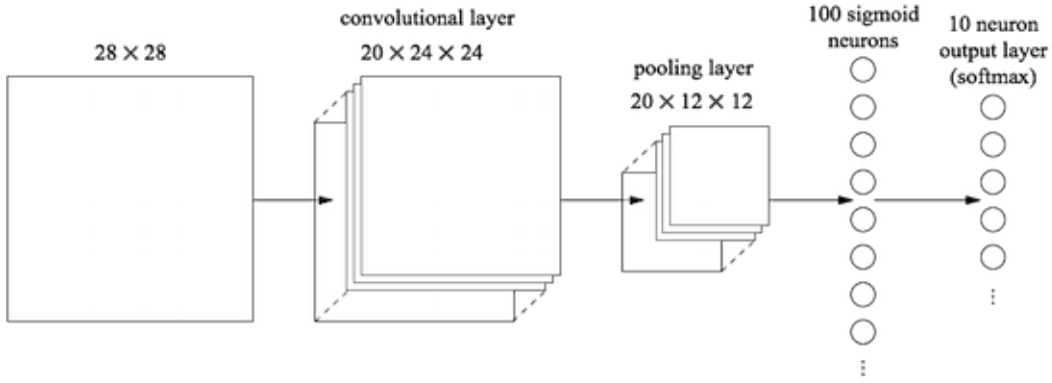

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CNNs in Practice

Two Convolution-Pooling Layers

- *2 Convolutional layers*:
  - *First convolution*: 20 feature maps, each associated with 5×5 LRFs, stride length 1
  - *Second convolution*: 40 feature maps, each associated with $20 \times 5 \times 5$ filter, stride length 1
- *Pooling layer*:
  - 2×2 max-pooling
- *Intuition*: after the first layer, each image consists of 12×12 pixels, where each pixel has 20 channels, each of which codes for a different "color"
- So, each LRF is a $20 \times 12 \times 12$ tensor
- Spatial strucure is still preserved in second conv-pooling layer, so employing conv-pooling makes sense
- *Accuracy*: 99.06% test accuracy

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CNNs in Practice

Trying alternative activation functions

- *Tanh activation function*:
  - Training is (a bit) faster
  - Results are near-identical
  - *Explanation*:

$$\sigma(z) = \frac{1 + \tanh(z/2)}{2} \tag{3}$$

- *Rectified linear units (ReLUs)*:
  - Activation:

$$f(z) = \max(0, z)$$

  - Learning rate: $\eta = 0.03$ (earlier: 0.1)
  - L2 regularization at $\lambda = 0.1$
  - *Test accuracy*: 99.23%
  - Modest gain, but also in other experiments ReLUs have shown to consistently outperform sigmoid neurons

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CNNs in Practice

Expanding the Training Data

- *Experiment*:
  - Displace each image by one pixel to above, the right, below, or to the left
  - Each image has 4 extra copies
  - ☞ 250 000 images instead of 50 000
- Run the same network with ReLU's (99.23%)
- Expanding training data yields 99.37%
- P. Simard, D. Steinkraus, J. Platt, "Best Practices for Convolutional Neural Networks Applied to Visual Document Analysis", 2003:
  - Very similar architecture
  - Training data expansion: rotations, translations, skewing
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Extra/Larger Fully Connected Layer

- *Larger fully connected layer*:
  - 300 neurons ☞ accuracy: 99.46%
  - 1000 neurons ☞ accuracy: 99.43%
  - Not really convincing
- *Extra fully connected layer*:
  - 2 fully connected layers, each of 100 neurons ☞ accuracy 99.43%
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CNNs in Practice

Dropout

- 2 fully connected layers each of 1000 neurons
- *Dropout* (probability = 0.5) applied to neurons in fully connected layers
- Accuracy: 99.6% (which is substantial improvement)
- *Remarks*:
  - Less epochs (40 instead of 60), because of faster training
  - More hidden neurons (1000 instead of 300 or 100) slightly preferable when using dropout
  - No dropout on convolutional layers: those have in-built resistance to overfitting because of parameter sharing

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CNNs in Practice

Ensemble of Networks

Ensemble of networks: Idea

- Train several different networks
- For example, employ repeated random initialization while always using the same architecture
- For classification, take the majority vote of the different networks
- While each network performs similarly, the majority vote may yield improvements
- Here: 5 randomly initialized network of the architecture o described in the slides before
- Accuracy: 99.67%
- That has been our goal!

CNNs in Practice

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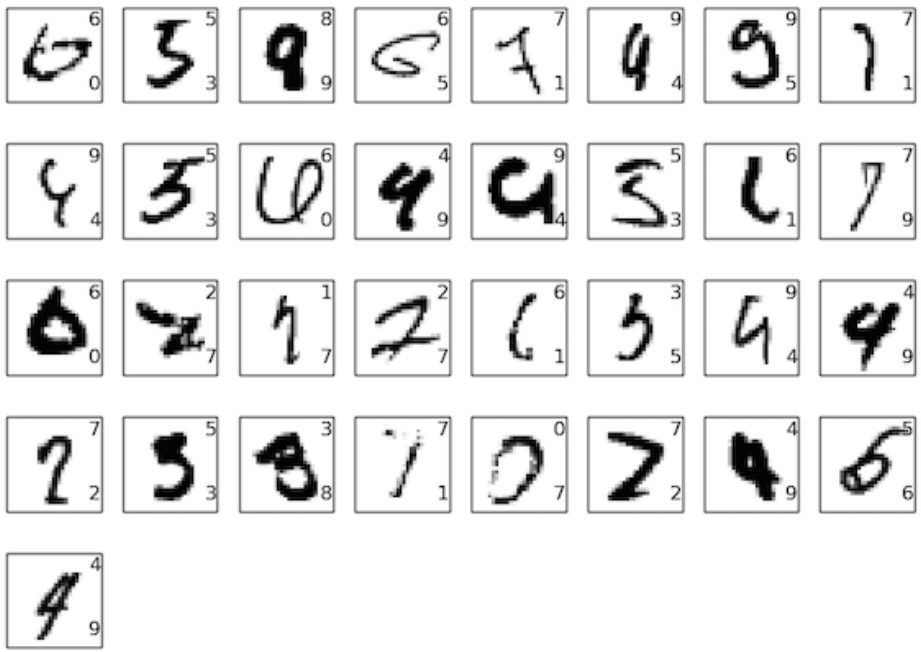


33 misclassified images; correct/predicted classification upper/lower right corner

CNNs in Practice

References

- Y. LeCun, L. Bottou, Y. Bengio, P. Haffner, "Gradient-based learning applied to document recognition", `http://yann.lecun.com/exdb/publis/pdf/lecun-98.pdf` [Architecture: "LeNet-5"]

CNNs on MNIST

Further Improvements

- For further improvements on MNIST (and on famous datasets in general see `http://rodrigob.github.io/are_we_there_yet/build/classification_datasets_results.html`
- *Noteworthy*:
  - See D.C. Ciresan, U. Meier, L.M. Gambardella, J. Schmidhuber, "Deep Big Simple Neural Nets Excel on Handwritten Digit Recognition", `https://arxiv.org/abs/1003.0358`
  - Fully connected network, without convolutional layers that achieves 99.65% accuracy.
  - Training for that non-convolutional network proceeds very slow, however.

Initializing Weights

Weight Initialization

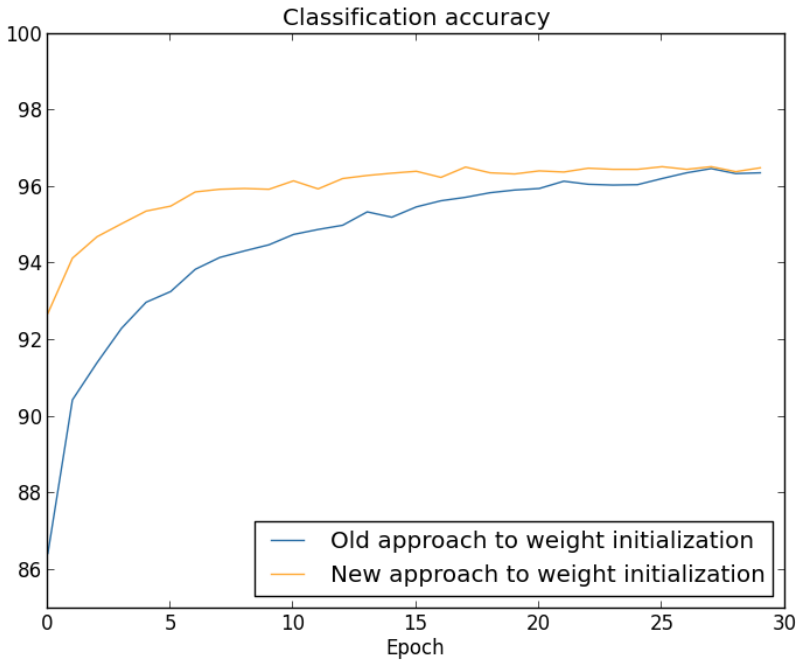
- Draw weights from normal distribution $\mathcal{N}_{0,\sigma}$ with mean 0 and standard deviation σ
- Let n_{in} be the number of inputs to the next node:

$$z = \sum_{j=1}^{n_{\text{in}}} x_j w_j + b \tag{4}$$

- Then $\sigma := \sqrt{n_{\text{in}}}$, so sample weights from $\mathcal{N}_{0,\sqrt{n_{\text{in}}}}$
- *Explanation*: So, input z to next node will (roughly) be sampled from $\mathcal{N}_{0,1}$

Weight Initialization

Consequence



- Improved initialization leads to faster learning
- See further ["Practical Recommendations for Gradient-Based Training of Deep Architectures", Bengio, 2012] (`https://arxiv.org/pdf/1206.5533v2.pdf`) for more details.

Choosing Hyperparameters

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Hyperparameters to be determined:

- Number (and composition) of hidden neurons
- In stochastic gradient descent: mini-batch size
- Number of epochs in training
- Learning rate η
- Regularization parameter λ
- If chosen inappropriately
  ☞ random exploration of search space
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General Strategy

First Challenge

Establish *any* non-trivial learning, that is, train a network that classifies better than chance

Strategies

- Turn multi-class problem into binary problem
- Start experimenting with the simplest possible architecture
- Small batch size: monitor changes in classification accuracy after each batch
- Check that *weight decay* (see (26), Lecture 5) is constant with respect to number of training data ☞ affects both η and λ

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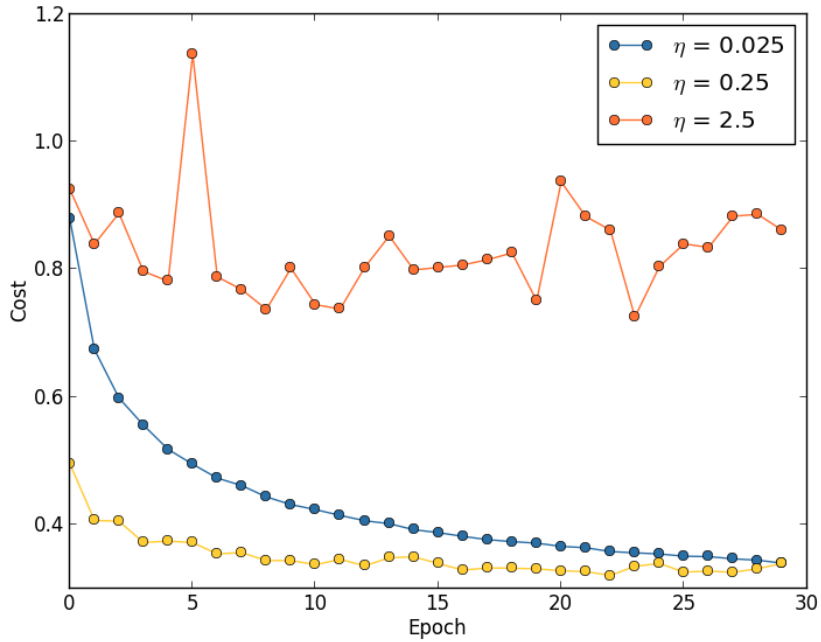

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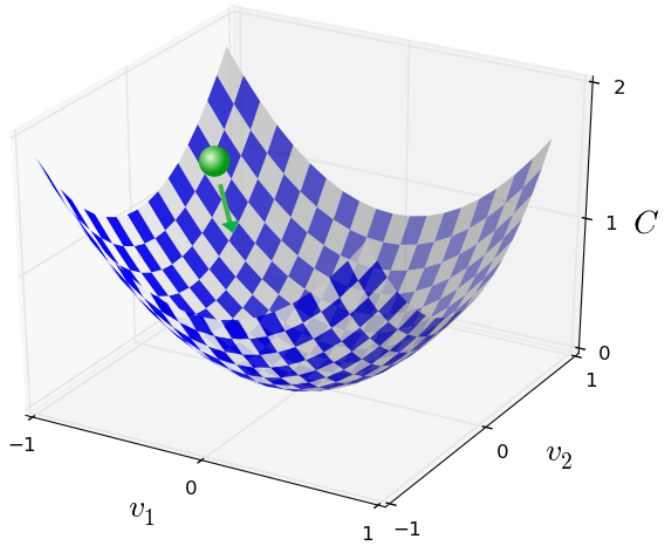

- Learning rate η too large: random oscillations ☞ parameters "jump across" optimum, back and forth
- Learning rate η too small: training too slow
- *Strategy*: Pick η as large as possible, while avoiding random oscillation
- To refine training, decrease η along epochs

Choosing Regularization Parameter

Suggestions

- Start with no regularization ($\lambda = 0$)
- Determine the learning rate η, as described above
- Then do $\lambda = 1.0$, and compare accuracy with $\lambda = 0$
- Depending on the outcome, multiply or divide by ten ($\lambda = 10.0$ or $\lambda = 0.1$)
- Once reached the right order of magnitude, finetune

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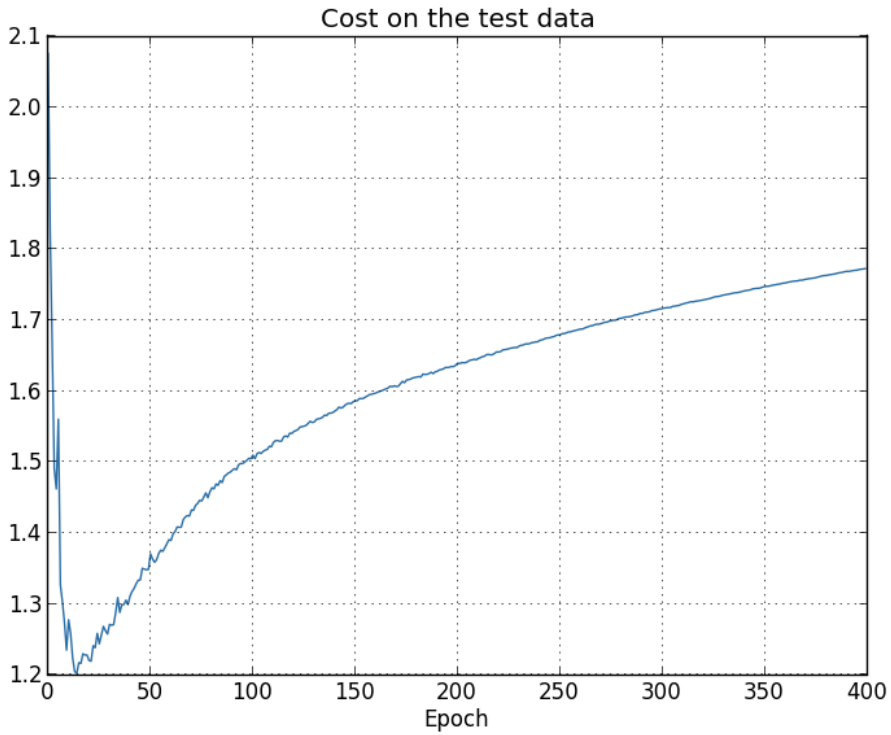
Choosing Number of Epochs

- Use validation data; see earlier lectures for training, validation and test data. Validation is to be used for determining hyperparameters.
- Stop as soon as validation accuracy, the ratio of correctly classified validation data samples over the total number of validation data samples, no longer improves
- "No improvement-in-ten rule": stop 10 epochs after classification accuracy starts to stall

Choosing Number of Epochs

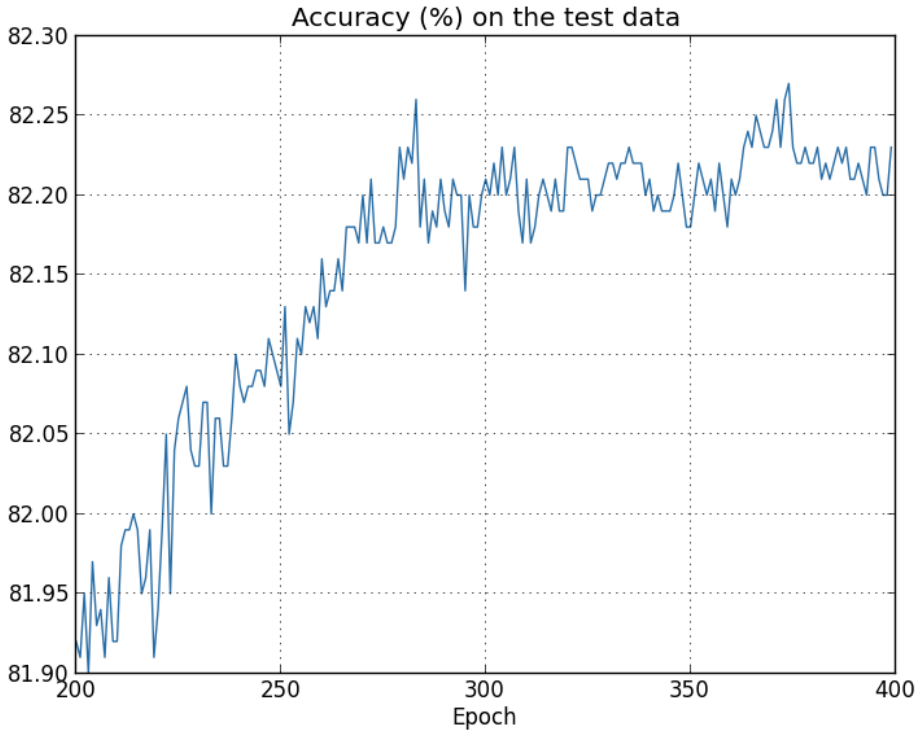
Cost versus Validation Accuracy



Validation accuracy (here: test accuracy) suggests to do ≈ 280 epochs

Choosing Number of Epochs

Cost versus Validation Accuracy

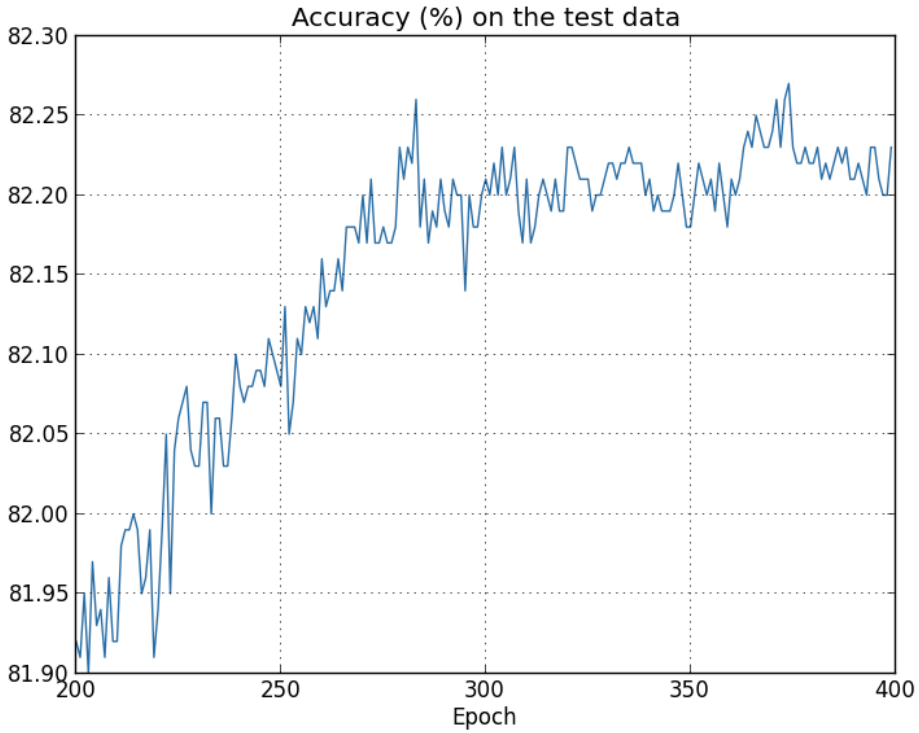


Validation cost (here: test cost) suggests to do ≈ 15 epochs

- What to do, use cost or validation accuracy to determine number of epochs?
- Cost has no meaning, while accuracy does: use accuracy!

Choosing Number of Epochs

Cost versus Validation Accuracy



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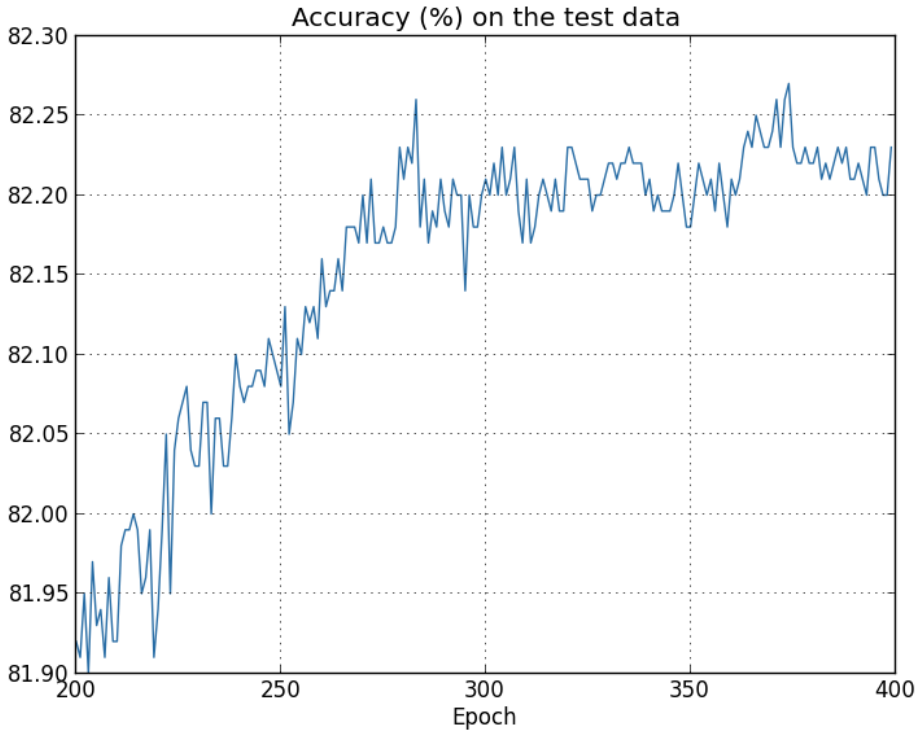

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Choosing Mini-Batch Size

Prelude

See Problem "Fully matrix-based approach to backpropagation over a mini-batch" in chapter 2 of Nielsen's book, see `http://neuralnetworksanddeeplearning.com/chap2.html`:

- Instead of looping over each training example, computing the gradient for each of them, and averaging eventually, one can apply matrix-based techniques to do this computation in about half of the time.
- Consider updates for one training example versus averaging over one mini-batch of examples of size m:

$$w \leftarrow w - \eta \nabla_w C_x \quad \text{versus} \quad w \leftarrow w - \eta \frac{1}{m} \sum_x \nabla_w C_x \tag{5}$$

  That advocates against mini-batches however, because updates will be very small ☞ slow learning!

- Anything to do about this trade-off?

Choosing Mini-Batch Size

Solution

- *Observation*: Multiplying η by m yields

$$w \leftarrow w - \eta \sum_x \nabla_w C_x \tag{6}$$

  which looks like summing over all individual examples, so issue of too little, and too small updates when using mini-batches mended.

Summary

- *Mini-batch size too small*: One does not exploit the advantages of matrix computation libraries.
- *Mini-batch size too large*: Too little updates.
- *Overall solution*: Find a good trade-off!
- Mini-batch size is fairly independent of other parameters.
- So, first optimize other hyperparameters. Then tune mini-batch size scaling η according to (6).

Choosing Hyperparameters

Search Techniques

- *Grid Search*: Try combinations of hyperparameters, viewing them as points of a grid, where each dimension refers to one of the hyperparameters
  - See `http://www.deeplearningbook.org/` 11.4.3 for details
- *Random Search*: Randomly pick combinations of hyperparameters, selected according to reasonable probability distributions
  - See `http://www.deeplearningbook.org/` 11.4.4 for details
- *Model-Based Hyperparameter Optimization*: Cast selection of hyperparameters as optimization problem, and try to pick hyperparameters that yield minimal error on validation data
  - See `http://www.deeplearningbook.org/` 11.4.5 for details
  - And the following slides for further information on automated optimization strategies

Choosing Hyperparameters

Guidelines for Automated Techniques

Automated Techniques

- ["Random search for hyper-parameter optimization", Bergstra & Bengio, 2012; https://dl.acm.org/citation.cfm?id=2188395]
- ["Practical Bayesian optimization of machine learning algorithms", Snoek, Larochelle & Adams, 2012; http://papers.nips.cc/paper/4522-practical-bayesian-optimization-of-machine-learning-algorithms.pdf]

Choosing Hyperparameters

Guidelines for Automated Techniques

Automated Techniques

- Currently hot topic: "Auto Machine Learning (AutoML)", methods to pick optimal selections of hyperparameters, in particular to pick optimal network architectures.
- See
  - `https://hackernoon.com/a-brief-overview-of-automatic-machine-learning-solutions-automl-2826c7807a2a`
  - `https://ai.googleblog.com/2017/05/using-machine-learning-to-explore.html`

  if interested
- *However*: usually very expensive in terms of compute resources

Practical Recommendations

Further Reading

- "Practical Recommendations for gradient-based training of deep architectures", Y. Bengio, 2012, see `https://arxiv.org/abs/1206.5533`
- "Efficient BackProp", Y. LeCun, L. Bottou, G. Orr, K.-R. Müller, 1998, see `http://yann.lecun.com/exdb/publis/pdf/lecun-98b.pdf`
- "Neural Networks: Tricks of the Trade", edited by G. Montavon, G. Orr, K.-R. Müller, see `https://www.springer.com/de/book/9783642352881` This book contains the above articles, is expensive, but many of the articles that appear in the book are freely available

Summary

- Convolutional Neural Networks
  - `http://www.deeplearningbook.org/`, Chapter 9
  - `http://neuralnetworksanddeeplearning.com/`, "Deep Learning"
- Choosing hyperparameters
  - `http://www.deeplearningbook.org/`, Chapter 11 (selected parts)
  - `http://neuralnetworksanddeeplearning.com/`, "Weight initialization" and "How to choose a network's hyperparameters?"

Thanks for your attention