Technische Hochschule Rosenheim

Deep Learning

Common Practices

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Overview

Common practices on how to
choose an architecture, **train** and **evaluate** a deep neural network:

- Training, Optimization, and Learning Rate
- Architecture Selection and Hyperparameter Optimization
- Class Imbalance
- Evaluation

Training, Optimization, and Learning Rate

Test Data

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- Overfitting is extremely easy with neural networks.
- True test set error/generalization error can be underestimated **substantially** when using the test set for model selection.
  - Attention: Choosing the architecture is the first element in model selection
    → should never be done on the test set.
- Do initial experimentation on a small subset of the dataset!

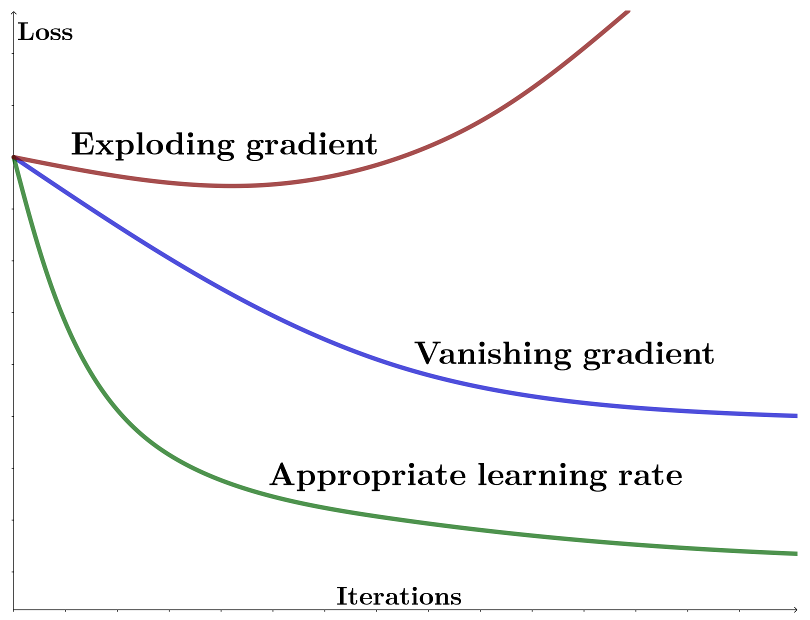
"Ideally, the test set should be kept in a vault, and be brought out only at the end of the data analysis."
T. Hastie, R. Tibshirani, J. Friedman: The Elements of Statistical Learning

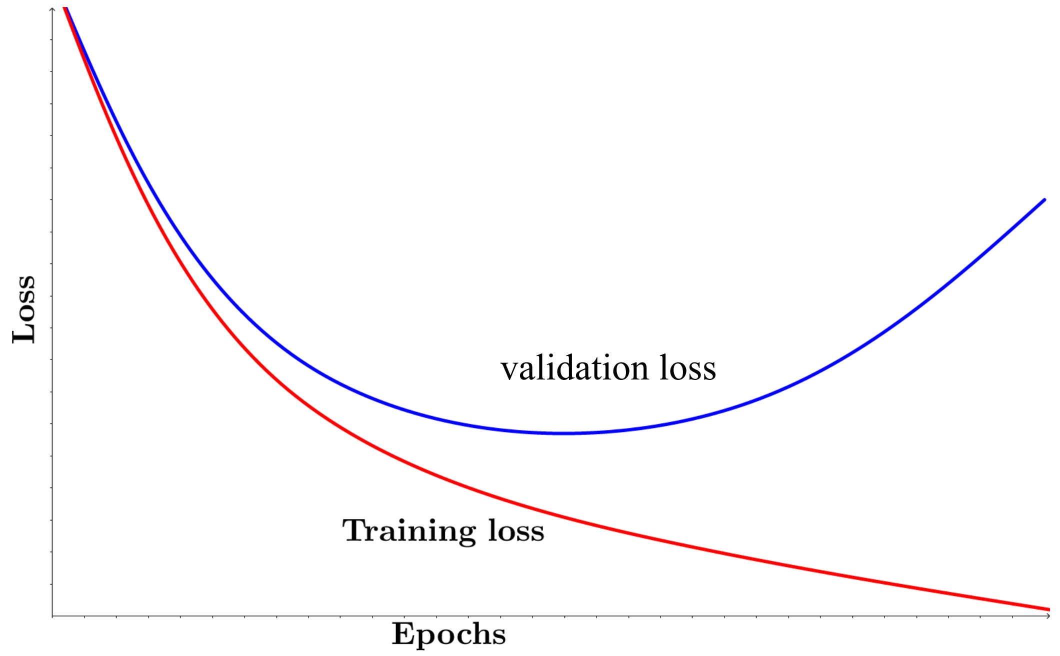
Before Training: Training!

Goal: Check whether the architecture is **in general** capable to learn the task.

- Before training the network on the full training data set, take a small subset (5-20 samples) and try to **overfit** the network to get zero loss.
  - Optionally: Turn off regularization that may hinder overfitting.
- If the network cannot overfit:
  - Bug in the implementation.
  - Model too small → increase number of parameters.
  - Model not suitable for the task.
- Also: Get a first idea about how the data, loss and network behave.

During Training: Monitor Loss Function



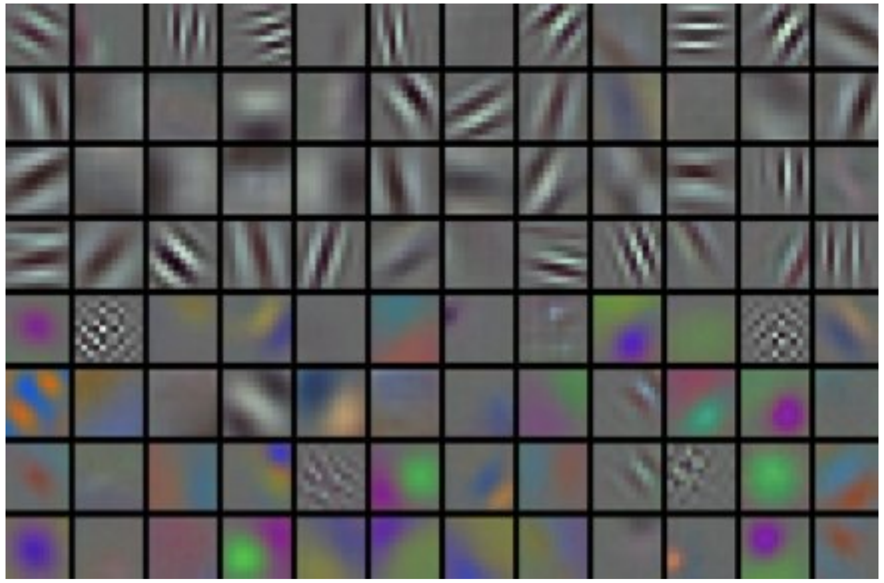


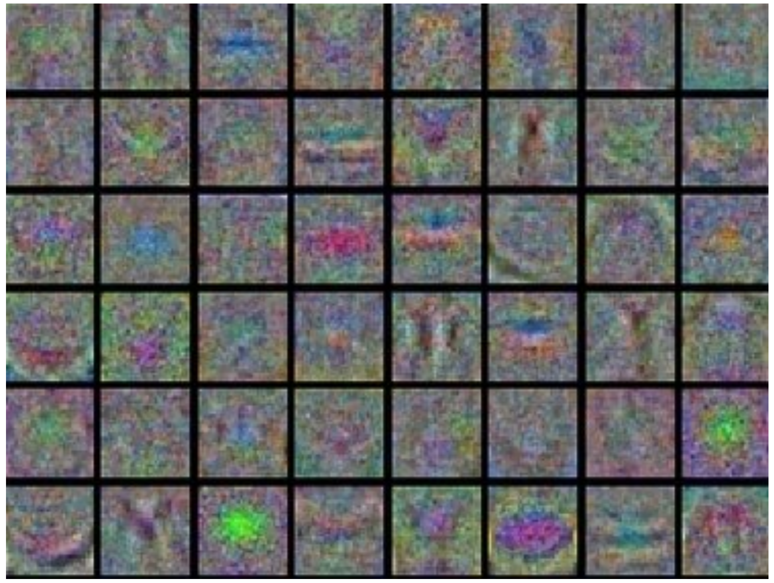
- Check learning rate (→ upcoming),
- Identify large jumps in the learning curve,
- Very noisy curves → increase batch size.

- Monitor amount of overfitting of the network.
- If training and validation loss diverge: overfitting → increase regularization/ early stopping
- If training and validation loss are close but high: underfitting → decrease regularization/ increase model size
- Save intermediate models if you want to use them for testing!

During Training: Monitor Weights and Activations

- Track relative magnitude of the weight update: Should be in a sensible range (approx. 10^{-3}).
- Check for very large or saturated activations ($\rightarrow$ dying ReLUs)
- Convolutional layers: check filters of the first few layers. Should develop towards smooth and regular filters.





Source: http://cs231n.github.io/neural-networks-3/

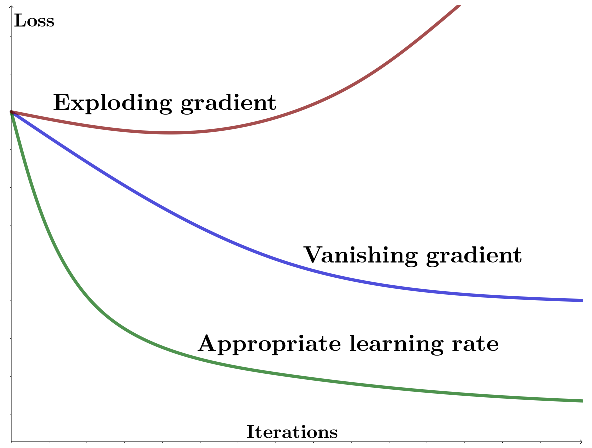
Choosing an Optimizer

- Batch gradient descent: Requires large memory, too slow, too few updates.
- Stochastic gradient descent (SGD): loss function and gradient become very noisy if only one/few samples are used.
- SGD with mini-batches: “best of both worlds”
  - Frequent, more stable updates.
  - Gradient noisy enough to escape local minima.
  - Adapting mini-batch size yields smoother/noisier gradient.
  - Addition of momentum prevents oscillations and speeds up optimization.

- Recommendation: Start with Mini-Batch SGD + momentum.
- For faster convergence speed → ADAM.

Learning Rate: Observing the Loss Curve

- Learning α rate has a large impact on the successful training of a network.
- For almost all gradient based optimizers, α has to be set manually.
- Effect of learning rate is often directly observable in the loss curve.



- But this is a very simplified view!
- We want an adaptive learning rate: Progressively smaller steps to find the optimum
  $\rightarrow$ Annealing the learning rate

Annealing the Learning Rate

- In deep learning context often known as **learning rate decay**.
  - Decay means yet another hyper-parameter.
  - We need to avoid oscillation as well as a too fast cool down!
- Decay strategies:
  - **Stepwise decay**: Every n epochs, reduce learning rate by a certain factor, e.g., 0.5, or by a constant value, e.g., 0.01.
    Variant: Reduce learning rate when **validation error** stagnates.
  - **Exponential decay**: At epoch t: $\alpha \coloneqq \alpha_0 e^{-kt}$ with k controlling the decay.
  - **$^1/_t$ -decay**: At epoch t: $\alpha \coloneqq {}^{\alpha_0}/_{(1+kt)}$.
- Stepwise decay is most common: hyperparameters are easy to interpret.

- Second-order methods are currently uncommon in practice
  - computationally very expensive
  - and therefore they do not scale well.

Architecture Selection and Hyperparameter Optimization

Reminder

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Test data → vault

Hyperparameter Optimization

Neural networks have an enormous amount of hyperparameters

- Architecture:
  - Number of layers & number of nodes per layer
  - Activation function
  - …
- Optimization
  - Initialization
  - Loss function
  - Optimizer (SGD, Momentum, ADAM, …)
  - Learning rate, decay, batchsize
  - …
- Regularization
  - Regularizer, e.g., L_2 -, L_1 -loss
  - Batch normalization?
  - Dropout?
  - …
- …

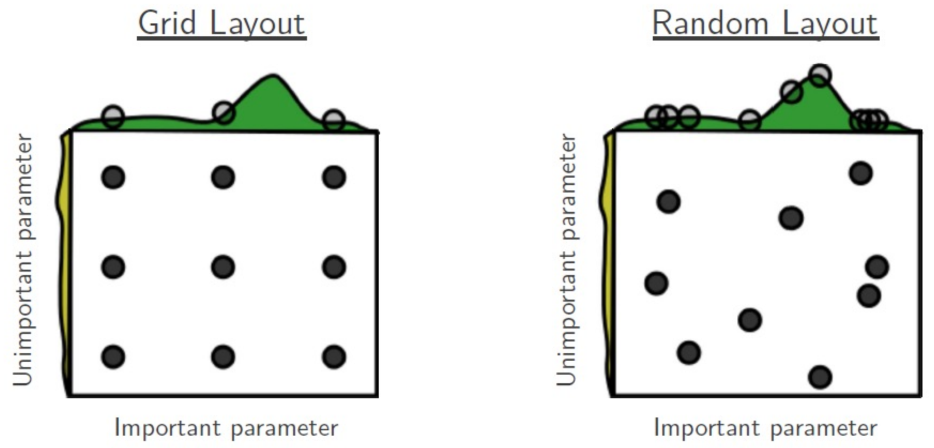
Choosing Architecture and Loss Function

- First step: Think about the problem and the data:
  - What could the features look like?
  - What kind of spatial correlation do you expect?
  - What data augmentation makes sense?
  - How will the classes be distributed?
  - What is important regarding the target application?

- Start with simple architectures and loss functions.
- Do your research: Try **well-known** models first and foremost!
- If you change/adapt the architecture: Find reasons why the network should perform better.

Hyperparameter Search

- Learning rate, decay, regularization/dropout etc. can be tuned more easily.
- Still, networks can take days/weeks to train.
- Search for hyperparameters using a log scale (e.g., $\alpha \in \{0.1, 0.01, 0.001\}$).
- Options: **Grid search** or **random search**:
  - Use random search instead of grid search [Ber12]:
    - Easier to implement.
    - Better exploration of parameters that have strong influence on the result.



Hyperparameter Search – Coarse to Fine Search

- Hyperparameters are highly interdependent.
- Optimize on a coarse to fine scale:
  - Training network only for a few epochs.
  - Bring all hyperparameters in sensible ranges.
  - Then refine using random/grid-search.

Class Imbalance

Motivation

- Often, different classes occur with very different frequencies in the data set.
  - This is a big challenge for machine learning algorithms.

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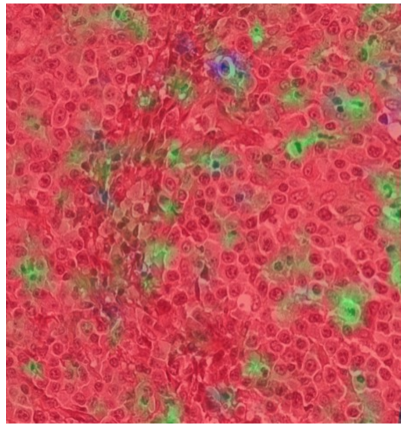
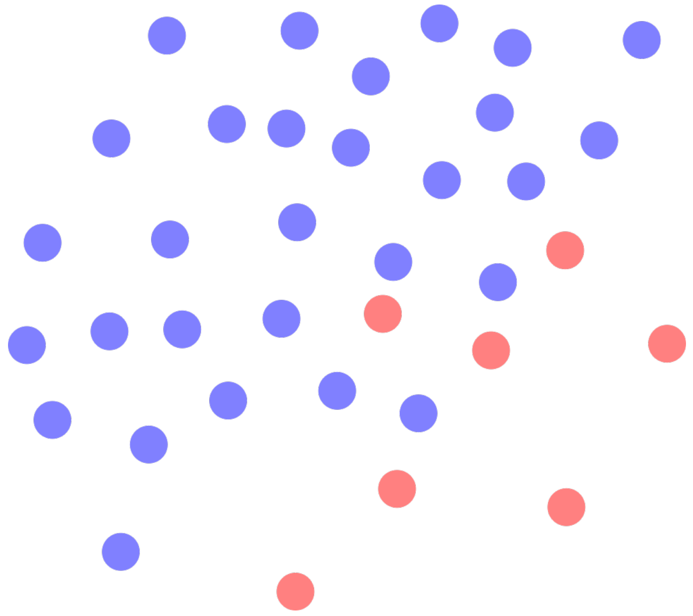
- Example 1: Fraud detection
  - Out of 10,000 transactions, 9,999 are genuine and 1 is fraudulent:
  - Classifying every transaction as genuine: 99.99% accuracy
  - Or, less extreme, using a method that misclassifies 1 out of 100 genuine transactions: 99% accuracy

- Example 2: Detect mitotic cells for tumor diagnostics [Aub17]
  - Problem: Mitotic cells only make up a very small portion of cells in tissues.
  - Data of a certain class is seen much less during training.



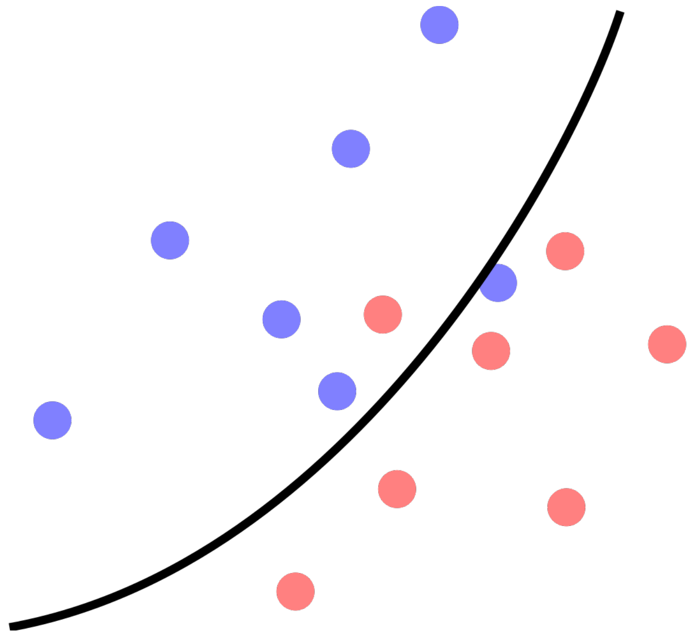
Resampling Strategies for Class Imbalance

Idea: Balance class frequencies by sampling classes differently.



Resampling Strategies – Undersampling

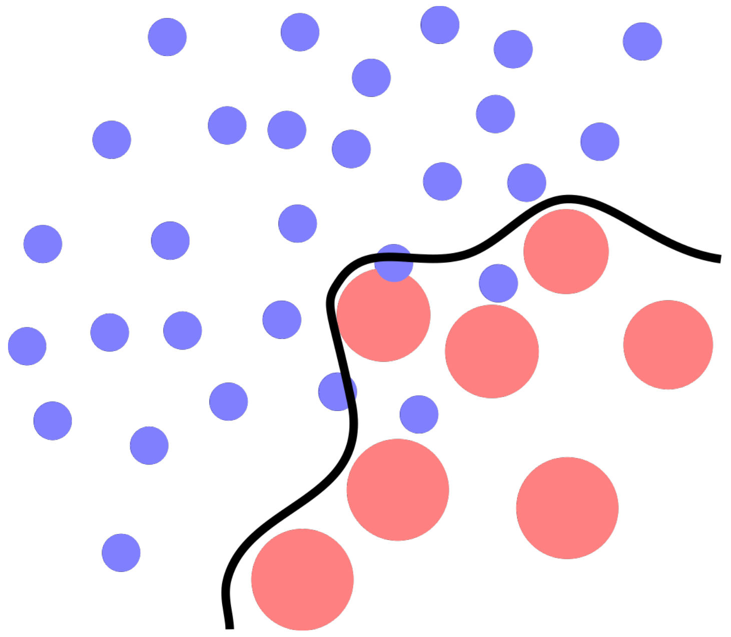
- In each iteration, take a subset of the overrepresented class.
- Samples of all classes are now presented to the network equally often.
- Disadvantage: Not all available data is used for training and can lead to underfitting.



Resampling Strategies – Oversampling

- Use sample from underrepresented class multiple times.
- All available data can be used.
- Disadvantage: Can lead to overfitting.

- Also possible: Combine Under- and Oversampling.



Resampling Strategies for Class Imbalance

- More advanced resampling strategies available that try to avoid the shortcomings of simple under-/oversampling, e.g., Synthetic Minority Over-Sampling Technique (SMOTE).
    - Rather uncommon in deep learning.
- Underfitting caused by undersampling can be reduced by taking a different subset after each epoch.
- Data augmentation can help to reduce overfitting for underrepresented class.

Class Imbalance – Adapt the Loss Function

- Instead of “fixing” the data, adapt the loss function to be stable with respect to class imbalance.
- Weigh loss with inverse class frequency w_k, e.g., weighted cross entropy:

$$-w_k y_k \ln \hat{y}_k$$

- Instead of class frequency, weights can be adapted with regards to other considerations.

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Evaluation

Performance Evaluation

- Network was trained on training set, hyper-parameters estimated on the validation set.

- Evaluate generalization performance on previously unseen data: the test set.
- We can now open the vault!

VAULT DOOR
WEIGHT: 22 1/2 Tons
THICKNESS: 22 Inches
STEEL: 11 Layers of Special Cutting and Drill Resistant
LOCKS: 4 Hamilton Watch Movements for Time Locks

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Of All Things the Measure is Man*

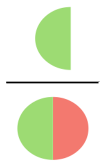
- Data is annotated and labeled by humans.
- During training, all labels are assumed to be correct ⚡ "to err is human"
- Additionally: Ambiguous data.
- Multiple human voters: Take mean (if possible) or majority vote.
- Steidl et al. [Ste05]: Entropy-based measure that takes "confusions" of human reference labelers into account:
  - Humans confuse certain classes more often than others (Angry vs. Happy/Angry vs. Annoyed)
  - Mistakes by the classifier are less severe if the same classes are confused by humans.

*Protagoras of Abdera (c.490 - c.411 BC)

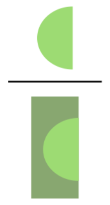
Performance Measures – Binary Classification

- We have
  - Total number of Positives/Negatives: P/N
  - True/False Positives: TP/FP
  - True/False Negatives: TN/FN

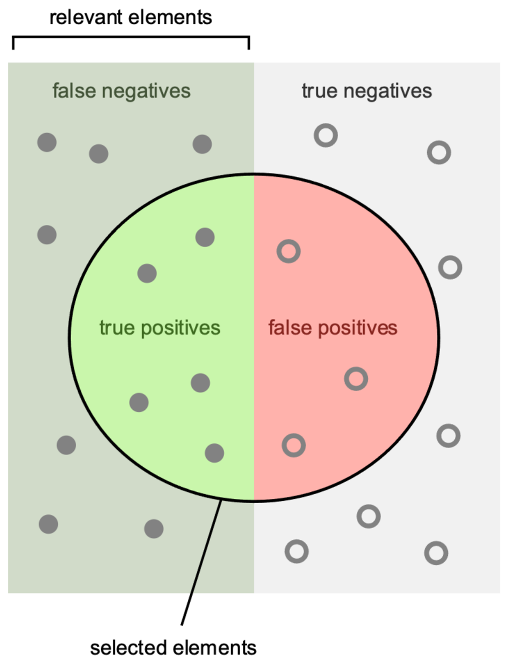
- Accuracy: $ACC = \frac{TP+TN}{P+N}$
- Precision/positive predictive value: $precision = \frac{TP}{TP+FP}$ =



- Recall/true positive value: $recall = \frac{TP}{TP+FN}$ =



- Specificity/true negative value: $specificity = \frac{TN}{TN+FP}$
- F1-score: $F_1 = 2 \cdot \frac{precision \cdot recall}{precision + recall}$
- Receiver operating characteristic (ROC) curve
  - Area Under Curve (AUC)



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Performance Measures – Multiple Classes

- Adapted versions of measures mentioned above.
- Top-K error: True class label is not in the K classes with the highest prediction score.
  - Common: Top-1 and Top-5 error.
  - Example: ImageNet performance usually measured with Top-5 error.
- Confusion matrix

Cross Validation

- k-fold cross validation:
  - Split data in k folds.
  - Use k−1 folds as training data, test on fold k.
  - Repeat k times.
- Rather uncommon in deep learning due to long training times.
- Can be used for hyperparameter estimation (nested!), or to evaluate stability of (hyper-)parameters.
  - Attention: almost always additional bias (when using it for architecture selection, hyperparameters).
  - Underestimates variance of results: Training runs are not independent.
- Even without cross-validation: Training is a highly stochastic process.

→ Retrain network multiple times and report average performance and standard deviation.

Comparing Classifiers

Example: Is my new method with 91.5% accuracy better than the state-of-the-art with 90.9%?

- Training a neural network is a stochastic process.
- Simply comparing two (or more) numbers yields biased results!

Actual question: Is there a **significant** difference between classifiers?

- Run training for each method/network multiple times.
- Determine whether performance is significantly different, e.g., **Student's t-test**!
  - Compares two normally distributed data sets with equal variance.
  - Determines whether the means are significantly different with respect to a **significance level** α (e.g., 5% or 1%).

Comparing Classifiers – Bonferroni Correction

- Significance level means: The probability that this difference is caused by **chance** $< \alpha$.
- If we compare several classifiers trained **on the same data**, this chance can rise significantly!
- Correct for multiple tests using Bonferroni correction:
  - For n tests with significance level α the total risk is $n\alpha$.
  - To reach a total significance level of α, we have to choose an adjusted $\alpha' = {}^{\alpha}/_{n}$ for each individual test.
- Assumes independence between tests: Pessimistic estimation of significance.
- More accurate, but incredibly time-consuming: Permutation tests [Dic11]

Summary

- Check your implementation before training: Gradient, initialization, …
- Monitor training process continuously: training/validation loss, weights, activations.
- Stick to established architectures before reinventing the wheel.
- Experiment with few data sets, keep your test data safe until evaluation.
- Decay the learning rate over time.
- Do random search (not grid search) for hyperparameters.
- Check for significance when comparing classifiers.

References

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