# Common Practices

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April 24, 2023

# Outline

# Recap

# Training a Neural Network

- So far: all the nuts and bolts about how to train a network:
  - Fully connected and convolutional layers
  - Activation function
  - Loss function
  - Optimization
  - Regularization
- Today: Common practices on how to **choose an architecture**, **train** and **evaluate** a deep neural network.

## First Things First: Test Data


*"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

# First Things First: Test Data (cont.)

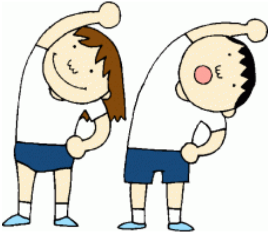
- Overfitting is extremely easy with neural networks (see e.g. ImageNet with random labels [5]).
- True test set error/generalization error can be underestimated **substantially** when using the test set for model selection!
- Attention: Choosing the architecture is the first element in model selection ➔ should never be done on the test set!
- Do initial experimentation on smaller subset of the dataset!

# Training Strategies

# Before Training: Gradient Checks

Own loss function, own layer implementation etc.: Check correct computation of gradient by comparing analytic and numerical gradient.

- Use centered differences for numeric gradient.



Source: https://fhsperformance.wordpress.com/2016/09/02/ramp-up-your-warm-ups/

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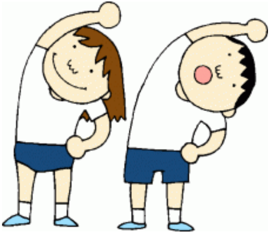

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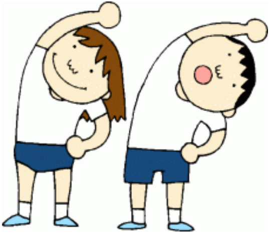
- Use centered differences for numeric gradient.
- Use relative error instead of absolute differences.
- Numerics:
  - Use double precision for checking.
  - Temporarily scale loss function if you observe very small values ($< 1e-9$).
  - Choose *h* appropriately.



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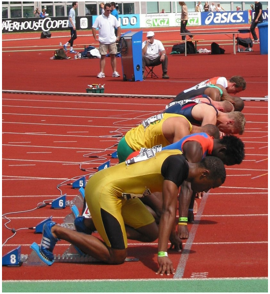
# Before Training: Gradient Checks (cont.)

Additional recommendations:

- Use only a few datapoints ➔less issues with non-differentiable parts of the loss function.
- Train the network for a short period of time before performing gradient checks.
- Check gradient first without, then with regularization terms.
- Turn off data augmentation and dropout.

# Before Training: Check Initalization and Loss

- Goal: Check correct random initialization of layers.
- Compute the loss for each class on the **untrained network**, with regularization turned off.




Source: https://commons.wikimedia.org/

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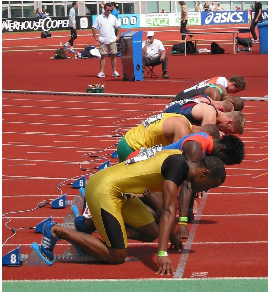


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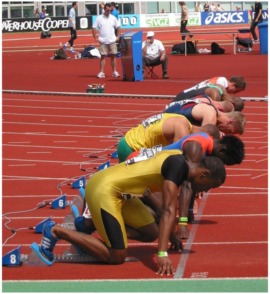
- Repeat with multiple random initializations.

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# 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.

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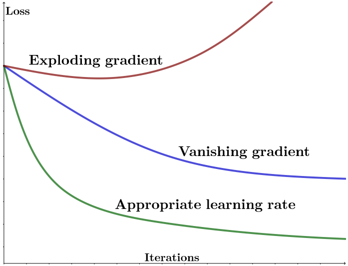
  - Model not suitable for the task.
- Also: Get a first idea about how the data, loss and network behave.

# During Training: Monitor loss function

- Recap:

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- Identify large jumps in the learning curve.

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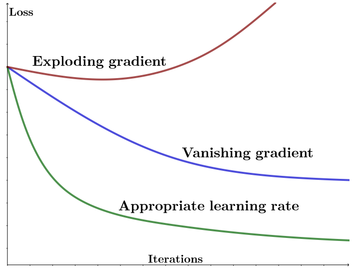
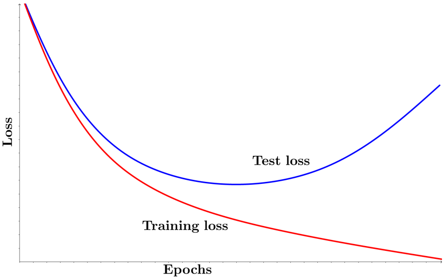



- Check learning rate (➔more in a bit).
- Identify large jumps in the learning curve.
- Very noisy curves ➔increase batch size.

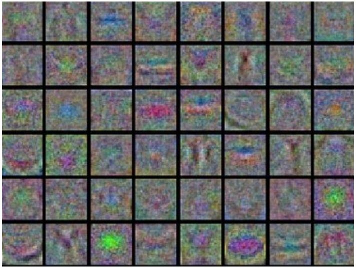
# During Training: Monitor Validation Loss

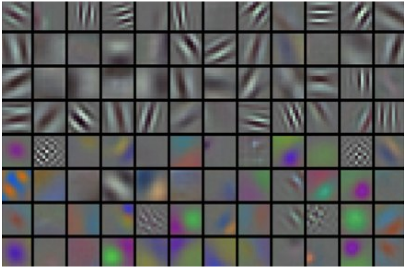



- Monitor amount of overfitting of the network.
- If training and validation loss diverge: overfitting ➔ increase regularization/ early stopping
- If training and validation loss are close but high: underfitting ➔ decrease regularization/ increase model size
- Save intermediate models if you want to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

# During Training: Monitor Weights and Activations

- Track relative magnitude of the weight update: Should be in a sensible range (approx. 1e-3).
- Convolutional layers: check filters of the first few layers. Should develop towards smooth and regular filters.
- Check for very large or saturated activations (➔dying ReLUs)





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

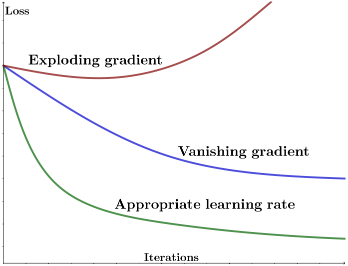
# Optimization and Learning Rate

# 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/more noisy gradient.
- Addition of momentum prevents oscillations and speeds up optimization.
- Effect of hyper-parameters relatively straight forward.
- Recommendation: Start with Mini-Batch SGD + momentum.
- For faster convergence speed ➔ADAM.

# Learning rate: Observing the loss curve

- Learning rate $\eta$ has a large impact on the successful training of a network.
- For almost all gradient based optimizers, $\eta$ has to be set.
- 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

➔ **Annealing** the learning rate.

# Annealing the Learning Rate

- In deep learning context often known as **learning rate decay**.
- Decay means yet another hyper-parameter.
- Need 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 $t$: $\eta = \eta_0 e^{-kt}$ with $k$ controlling the decay.
  - **$1/t$-decay**: At epoch $t$: $\eta = \eta_0/(1 + kt)$.
- Stepwise decay most common: hyper-parameters are easy to interpret.
- Second-order methods are currently uncommon in practice, as they do not scale as well.

# NEXT TIME

# ON DEEP LEARNING

# Common Practices - Part 2

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# Architecture Selection and Hyperparameter Optimization

# Reminder


**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 & batch size
  - ...
- 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:
  - How 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!

Source: [2]

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- Search for hyperparameters using a log scale (e.g., $\eta \in \{0.1, 0.01, 0.001\}$).

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- Options: Grid search or random search:

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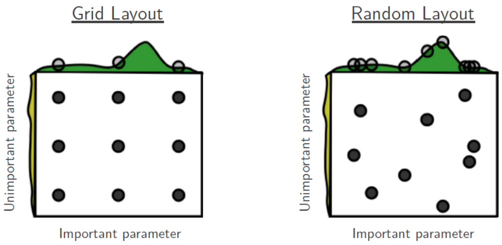
- Still, networks can take days/weeks to train!
- Search for hyperparameters using a log scale (e.g., $\eta \in \{0.1, 0.01, 0.001\}$).
- Options: Grid search or random search:
  - Use random search instead of grid search [2]:
  - ➔ Easier to implement.
  - ➔ Better exploration of parameters that have strong influence on the result.




Source: [2]

# Hyperparameter search: Coarse to fine search

- Hyperparameters 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.

# Ensembling

## Concept

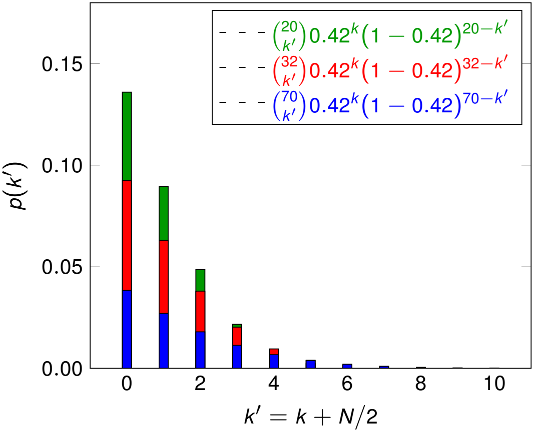
- So far we have always considered a **single** classifier. Can't we get better by using **many**?
- Assume $N$ classifiers **independently** performing a correct prediction with probability $1 - p$
- The probability of seeing $k$ errors is:

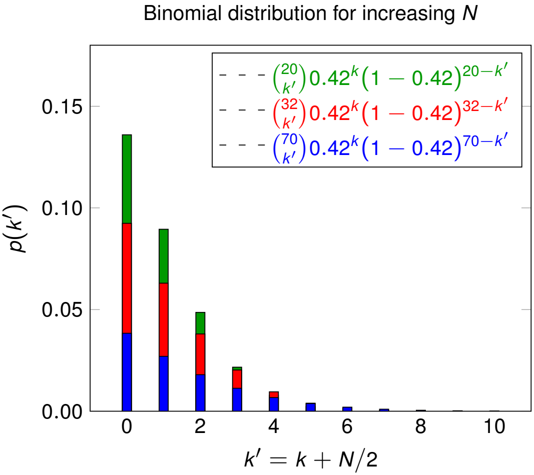
$$\binom{N}{k} p^k (1-p)^{N-k},$$

  known as binomial distribution
- So the probability of a majority $k > \frac{N}{2}$ to be wrong is:

$$\sum_{k>\frac{N}{2}}^{N} \binom{N}{k} p^k (1-p)^{N-k}$$

Binomial distribution for increasing $N$



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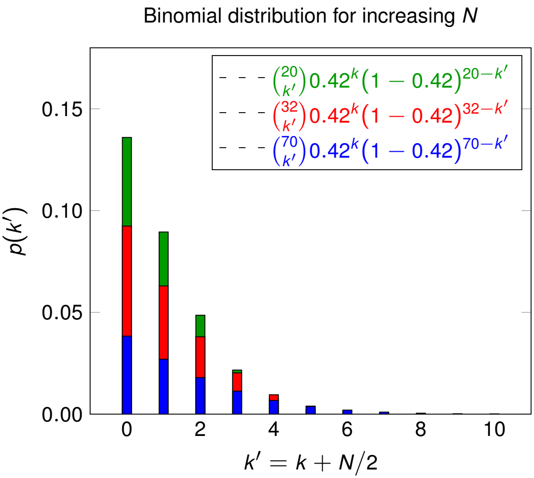


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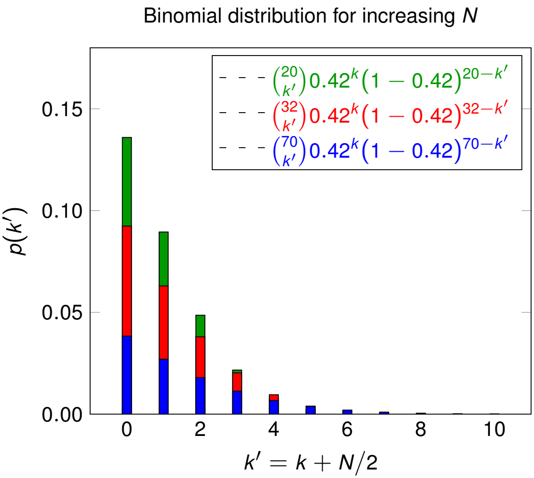


- $\sum_{k>\frac{N}{2}}^{N}\binom{N}{k}p^k(1-p)^{N-k}$ **monotonically decreasing** for $N \rightarrow \infty$
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- The big assumption here is **independence**

# Concept (cont.)

## Ensembling

- Produce $N$ **independent** classifiers/regressors
- **Combine** their **predictions** by majority/averaging

## How to produce the components?

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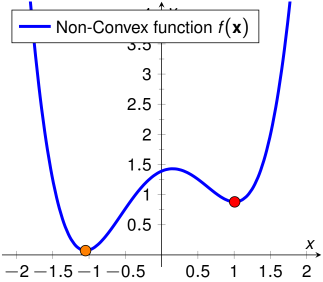
## How to produce the components?

- Different **models**

# Local Minima

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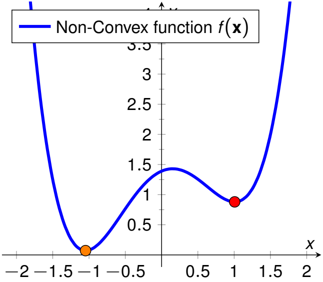


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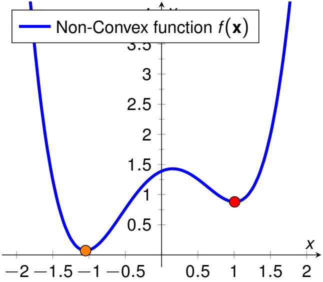


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- Can be combined with a **cylic** learning rate

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➔ **Easy performance boost if you need just a bit more**

# NEXT TIME

# ON DEEP LEARNING

# Common Practices - Part 3

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  ➔ Misclassifying 1 out of 100 genuine transactions: 99% accuracy

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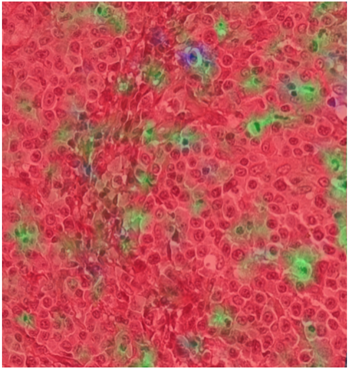
- Problem: Mitotic cells only make up a very small portion of cells in tissues.



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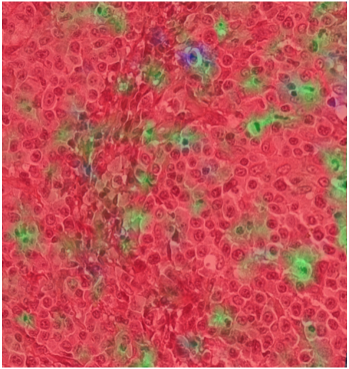

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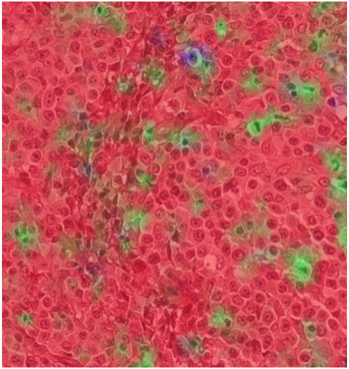
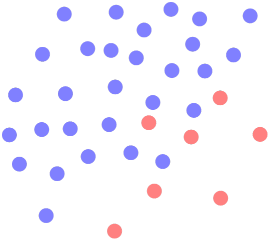
- Measures like accuracy, $L_2$ norm, cross-entropy do not show imbalance.



# Resampling Strategies for Class Imbalance

- Idea: Balance class frequencies by sampling classes differently.



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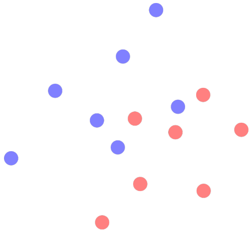

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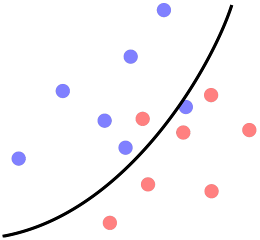

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- **Oversampling**:
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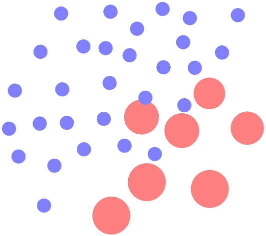

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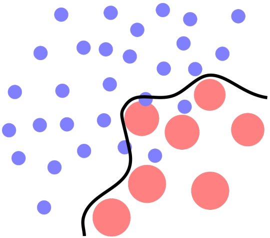

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- **Oversampling**:
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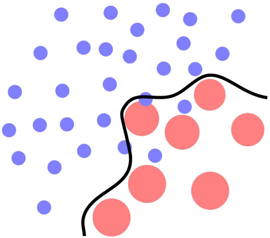
  - Disadvantage: Can lead to overfitting.
- Also possible: Combine Under- and Oversampling.



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- Underfitting caused 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.

# Class imbalance: Adapt the Loss Function

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

# NEXT TIME

# ON DEEP LEARNING

# Common Practices - Part 4

**A. Maier**, V. Christlein, K. Breininger, Z. Yang, L. Rist, M. Nau, S. Jaganathan, C. Liu, N. Maul, L. Folle, K. Packhäuser, M. Zinnen
Pattern Recognition Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg
April 24, 2023

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→ We can now open the vault!

Source: de.disney.wikia.com/wiki/Dagobert_Duck

# Of All Things the Measure is Man [8]

- Protagoras of Abdera (c.490 - c.420 BCE)
- Data is annotated and labeled by humans.
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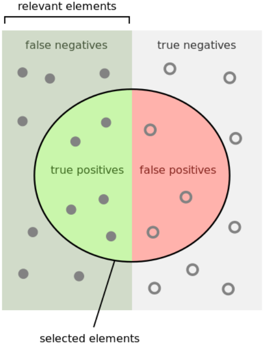
- Multiple human voters: Take mean (if possible) or majority vote.
- Steidl et al. 2005: Entropy-based measure that takes "confusions" of human reference labelers into account.
  - Humans confuse certain classes with each other more (Angry vs. Happy/Angry vs. Annoyed)
  - Mistakes by the classifier are less severe if the same classes are confused by humans.

# Performance measures

- Classification problem ➔classification measures:




Source: https://commons.wikimedia.org/

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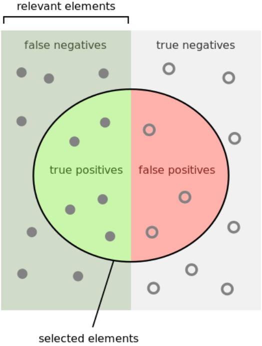


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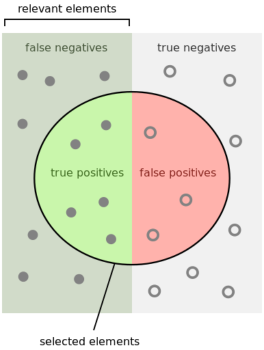


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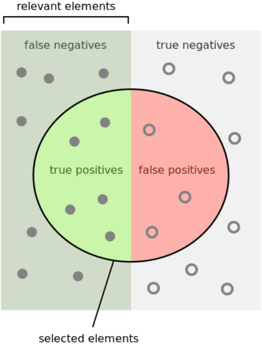


Source: https://commons.wikimedia.org/

# Performance measures: Multiclass classification

- 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.

# 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.
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- Underestimates variance of results: Training runs are not independent.
- Attention: almost always additional bias (architecture selection, hyperparameters).
- 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%?
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➔ 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** $\alpha$ (e.g. 0.05 or 0.01).

## Comparing Classifiers: Bonferroni Correction

- Interpretation: The probability that this difference is caused by **chance** $< \alpha$.
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  → To reach a total significance level of $\alpha$, choose adjusted $\alpha' = \alpha/n$ for each individual test.
- Assumes independence between tests: Pessimistic estimation of significance.
- More accurate, but incredibly time-consuming: Permutation tests [3].

# 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 evaluation data safe until evaluation.
- Decay the learning rate over time.
- Do random search (not grid search) for hyperparameters.
- Perform model ensembling for better performance.
- Check for significance when comparing classifiers.

# NEXT TIME

# ON DEEP LEARNING

# Coming Up

Evolution of neural network architectures:

- From deep networks to deeper networks.
- From “sparse” to dense connections.
- LeNet, GoogLeNet, ResNet, . . .

# Further Reading

- Link SGD Tricks by Leon Bottou.
- Link: Interesting loss functions.
- Link: Practical recommendations by Yoshua Bengio (from 2012).

# References

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[2] James Bergstra and Yoshua Bengio. “Random Search for Hyper-parameter Optimization”. In: J. Mach. Learn. Res. 13 (Feb. 2012), pp. 281–305.

[3] Jean Dickinson Gibbons and Subhabrata Chakraborti. “Nonparametric statistical inference”. In: International encyclopedia of statistical science. Springer, 2011, pp. 977–979.

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