Common Practices

A. Maier, V. Christlein, K. Breininger, S. Vesal, F. Meister, C. Liu, S. Gündel, S. Jaganathan, N. Maul, M. Vornehm, L. Reeb, F. Thamm, M. Hoffmann, C. Bergler, F. Denzinger, W. Fu, B. Geissler, Z. Yang
Pattern Recognition Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg
May 16, 2020

Outline


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Recap


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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.)

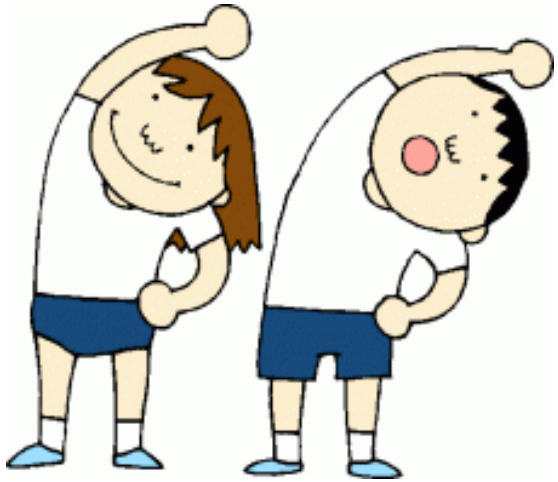
- Overfitting is extremely easy with neural networks (see e.g. ImageNet with random labels [5]).
- True test set error/generalization error can be underestimated **substantially** when using the test set for model selection!
- Attention: Choosing the architecture is the first element in model selection ➔ 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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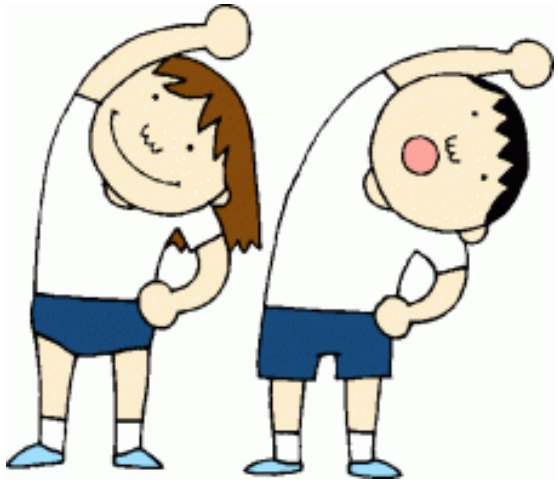

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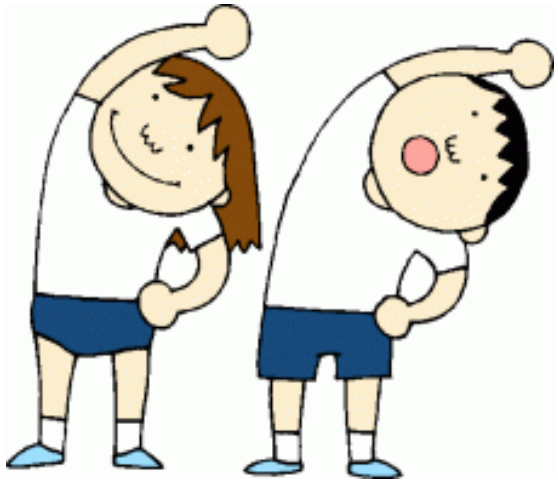
Before Training: Gradient Checks

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

- Use centered differences for numeric gradient.
- 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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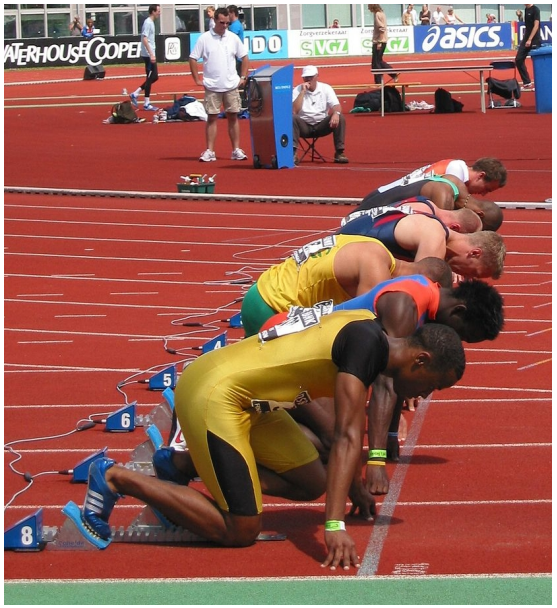
Before Training: Gradient Checks (cont.)

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.



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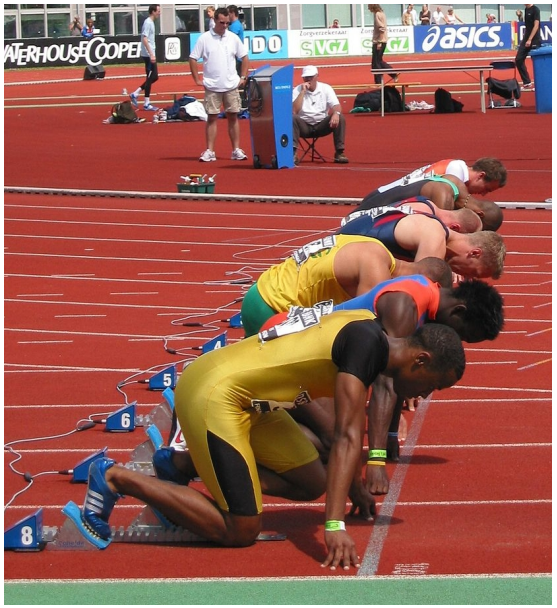

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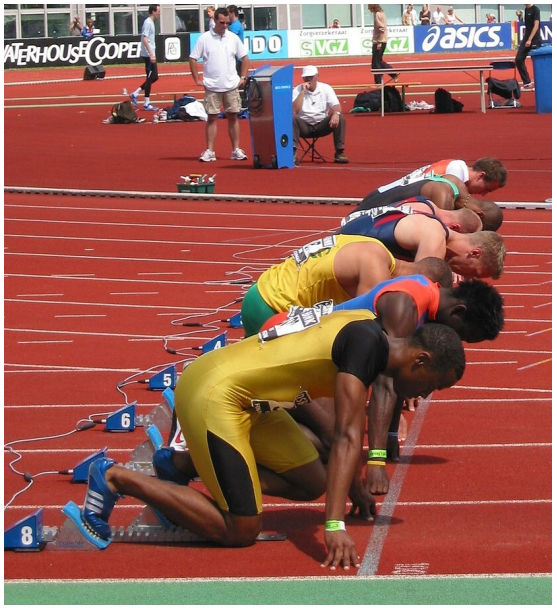
- Repeat with multiple random initializations.



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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 too small ➔increase number of parameters.
  - Model not suitable for the task.

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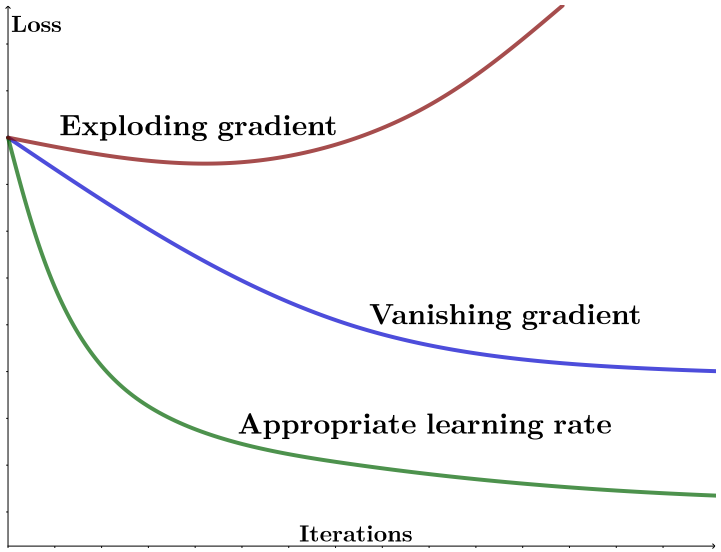
  - Model not suitable for the task.
- Also: Get a first idea about how the data, loss and network behave.

During Training: Monitor loss function

- Recap:



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- Identify large jumps in the learning curve.

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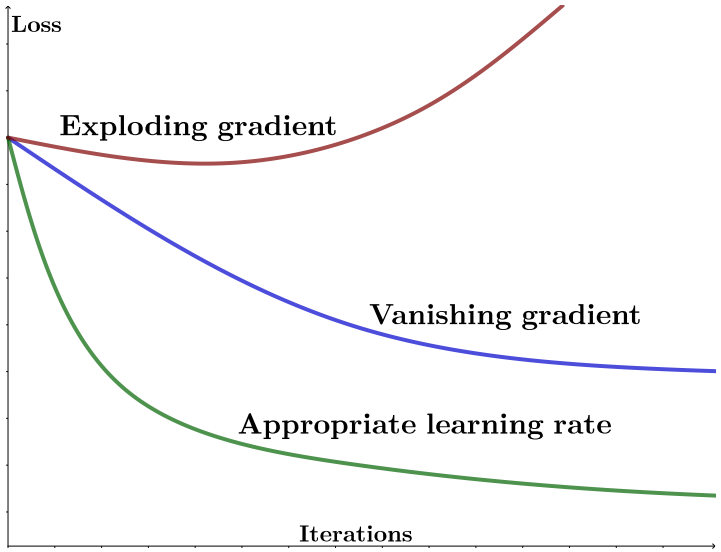
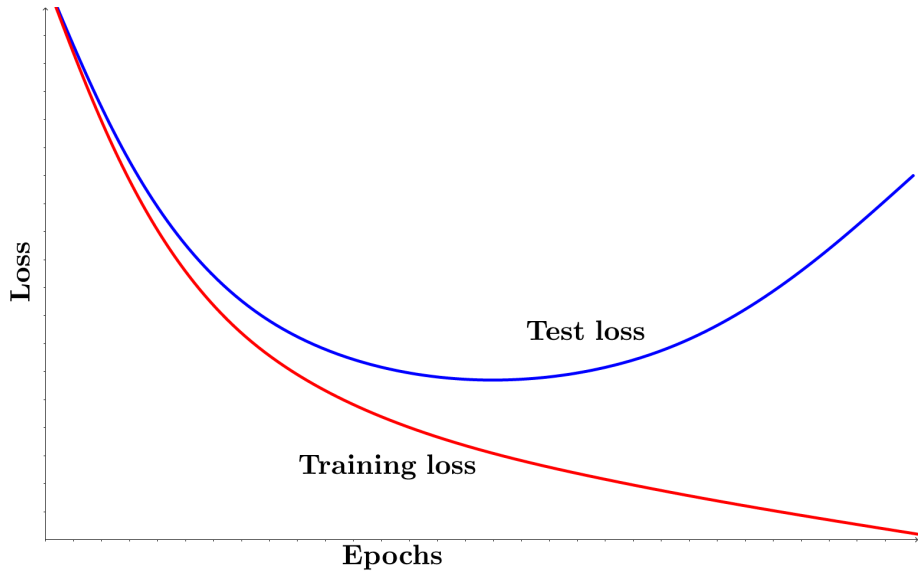


- Check learning rate (➔more in a bit).
- Identify large jumps in the learning curve.
- Very noisy curves ➔increase batch size.

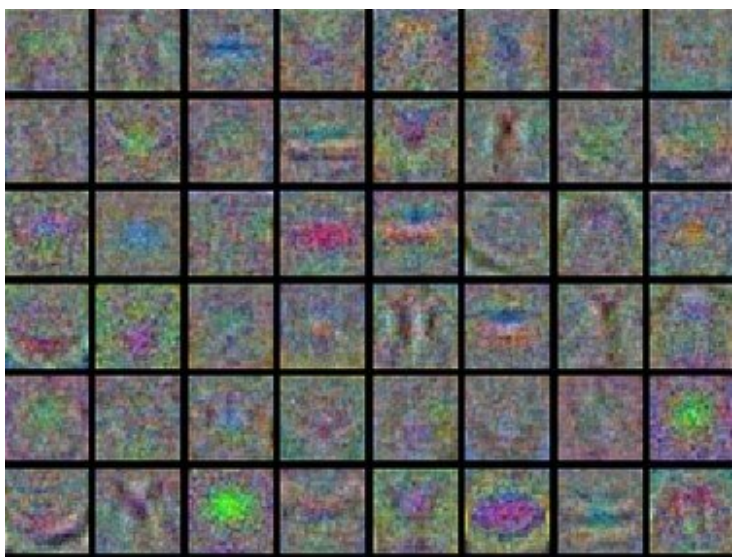
During Training: Monitor Validation Loss

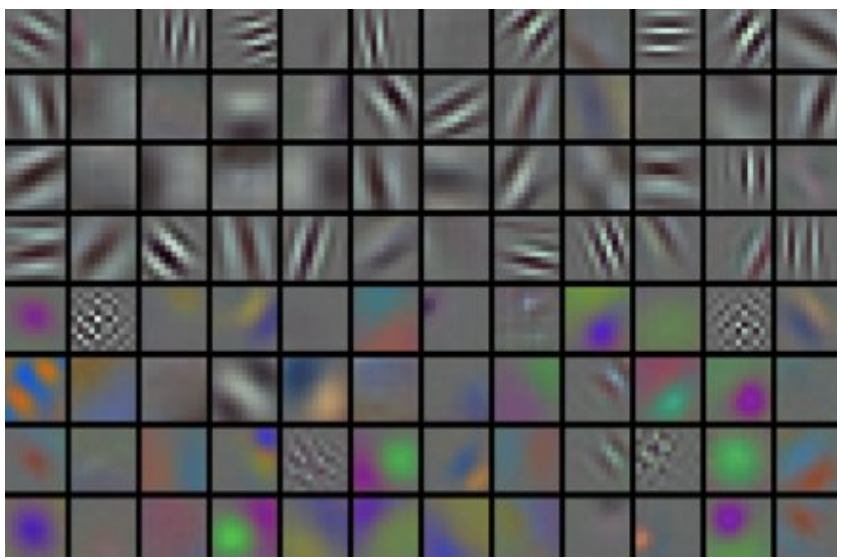


- Monitor amount of overfitting of the network.
- If training and validation loss diverge: overfitting ➔ increase regularization/ early stopping
- If training and validation loss are close but high: underfitting ➔ decrease regularization/ increase model size
- Save intermediate models if you want to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

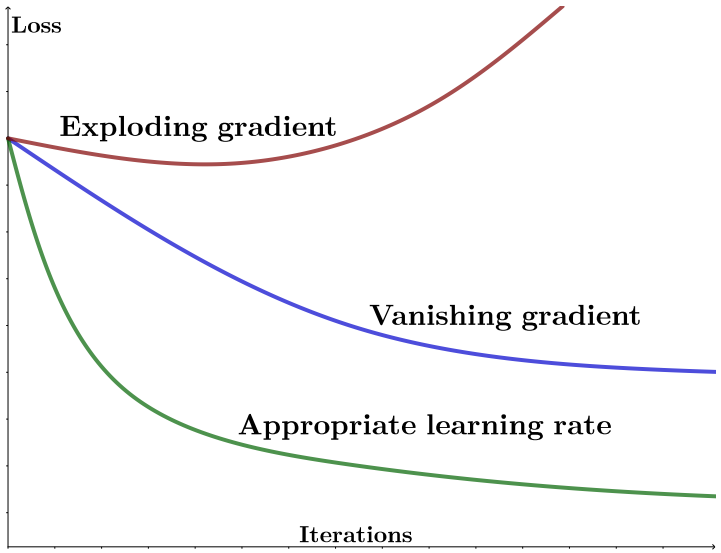
Optimization and Learning Rate

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 η has a large impact on the successful training of a network.
- For almost all gradient based optimizers, η 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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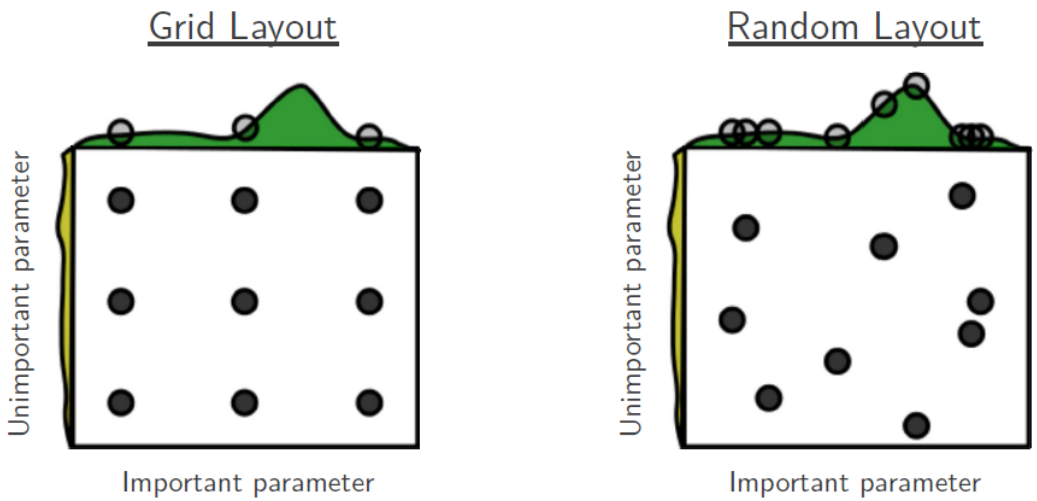
- Still, networks can take days/weeks to train!
- Search for hyperparameters using a log scale (e.g., $\eta \in \{0.1, 0.01, 0.001\}$).
- Options: Grid search or random search:
  - Use random search instead of grid search [2]:

➔ 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.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Ensembling


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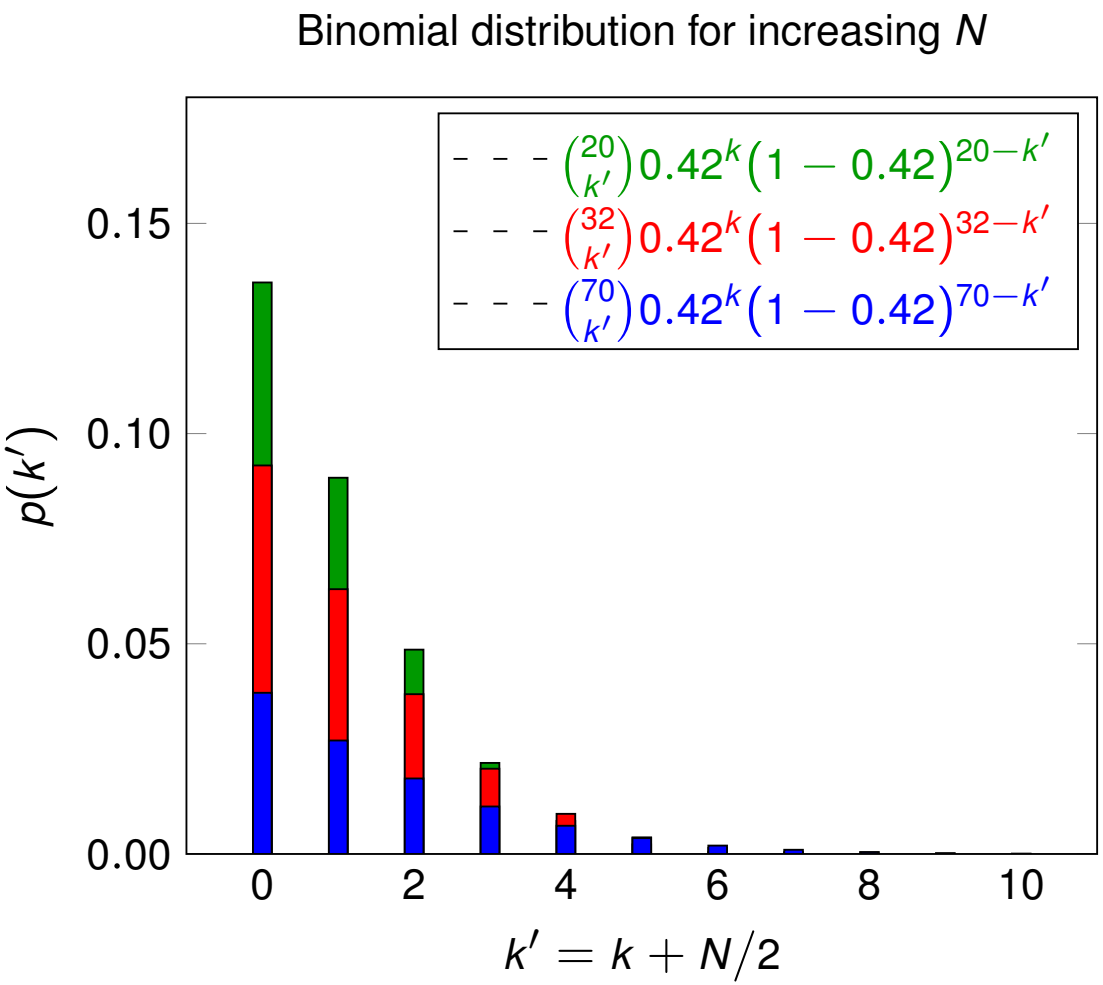
Concept

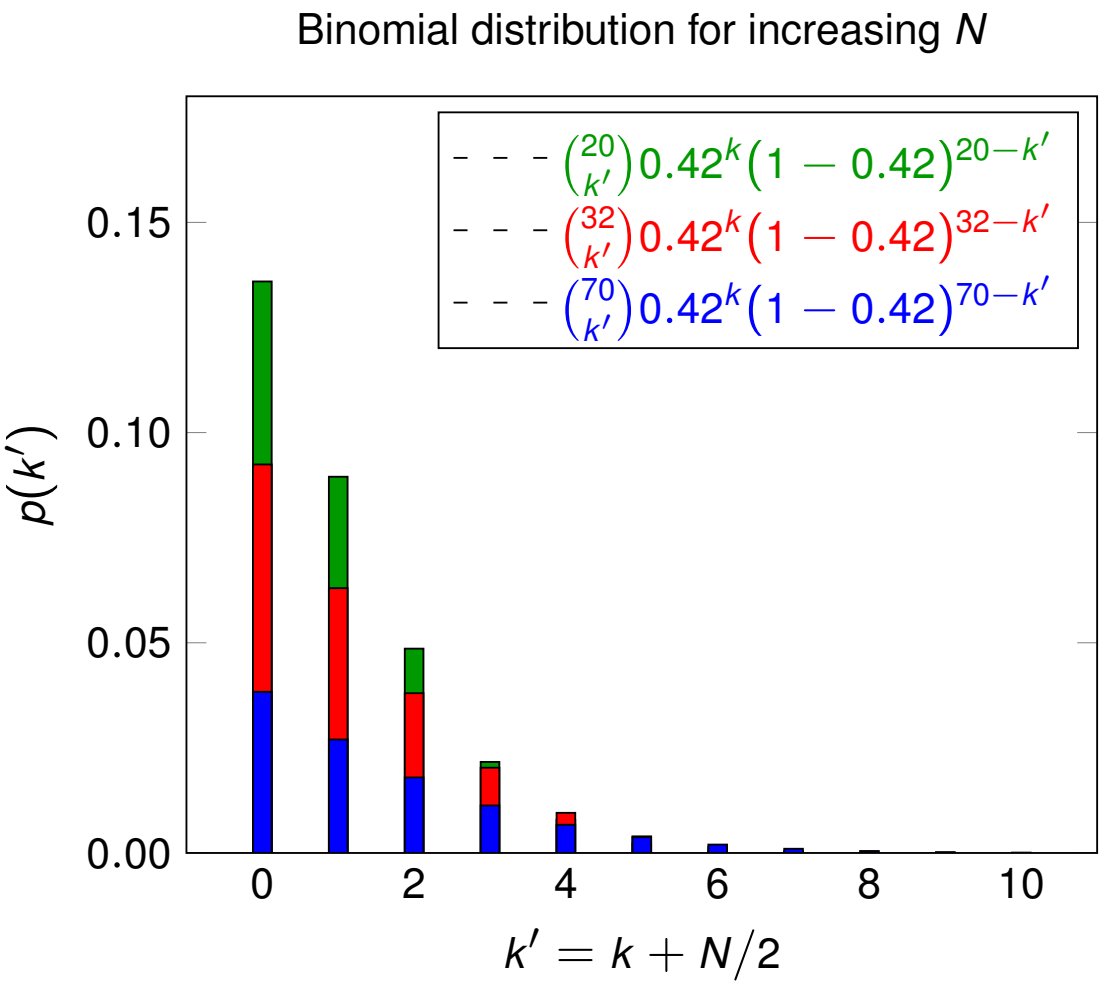
- So far we have always considered a **single** classifier. Can't we get better by using **many**?
- Assume N classifiers **independently** performing a correct prediction with probability $1 - p$
- The probability of seeing k errors is:

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

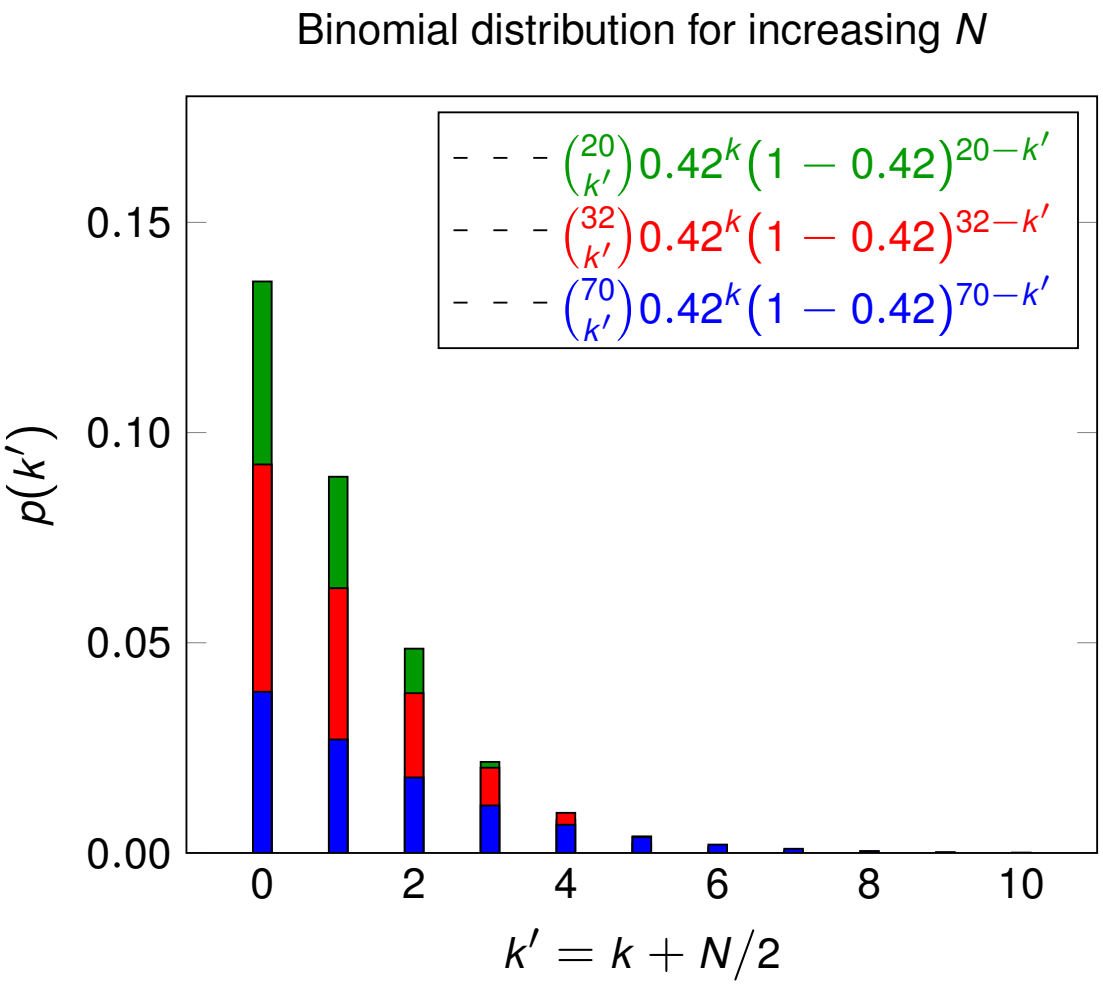
  known as binomial distribution
- So the probability of a majority $k > \frac{N}{2}$ to be wrong is:

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


Binomial distribution for increasing N
$\binom{20}{k'}0.42^k(1-0.42)^{20-k'}$
$\binom{32}{k'}0.42^k(1-0.42)^{32-k'}$
$\binom{70}{k'}0.42^k(1-0.42)^{70-k'}$
$p(k')$
0.15
0.10
0.05
0.00
0
2
4
6
8
10
$k' = k + N/2$



- $\sum_{k>\frac{N}{2}}^{N} \binom{N}{k} p^k (1-p)^{N-k}$ **monotonically decreasing** for $N \to \infty$



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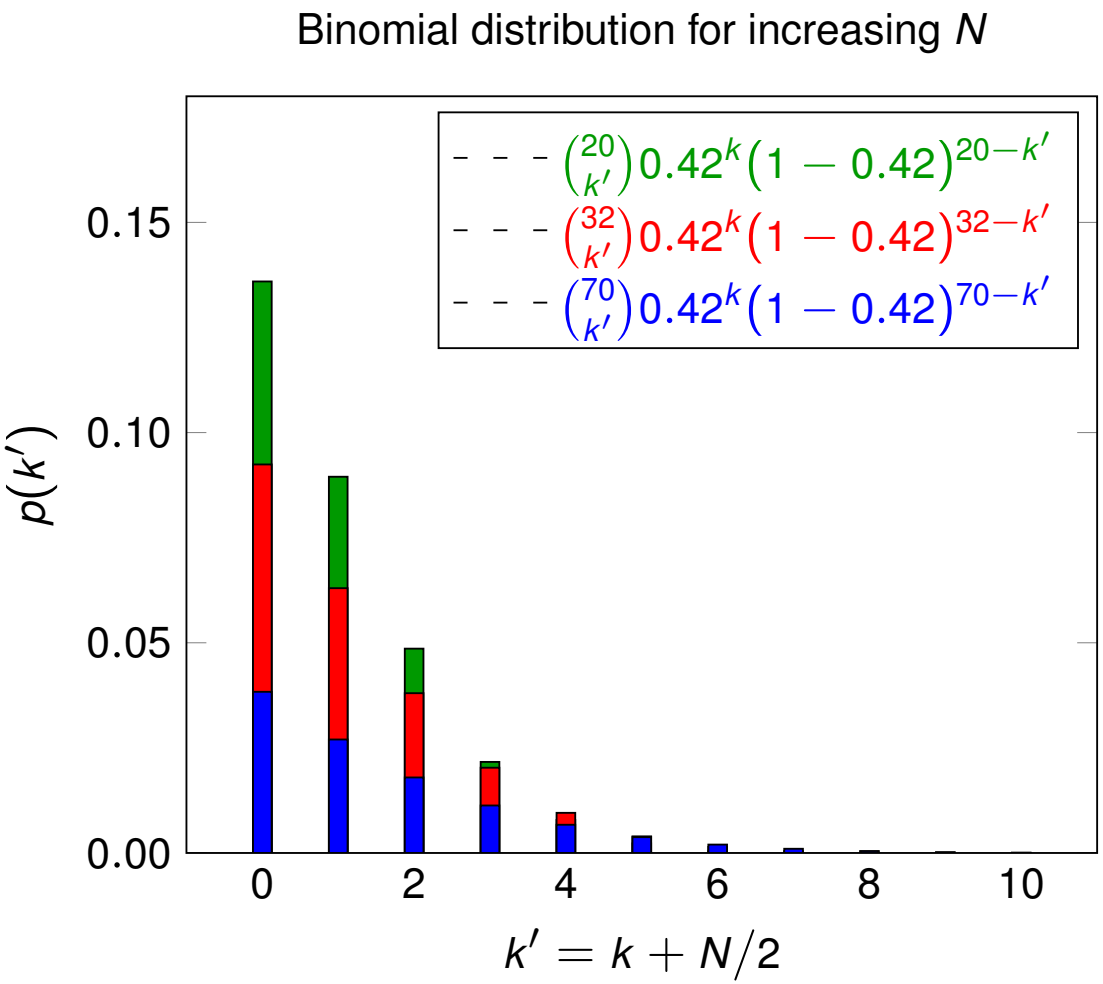

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- **Accuracy** $\to 1$!
- The big assumption here is **independence**

Concept (cont.)

Ensembling

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

How to produce the components?

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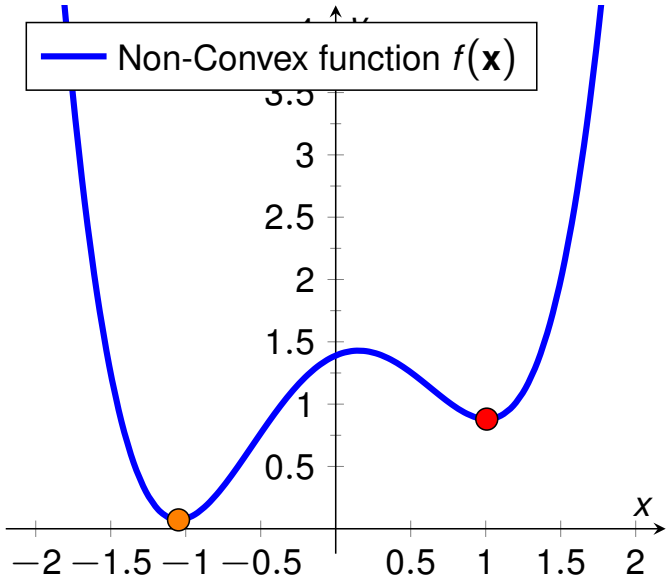
How to produce the components?

- Different **models**

Local Minima



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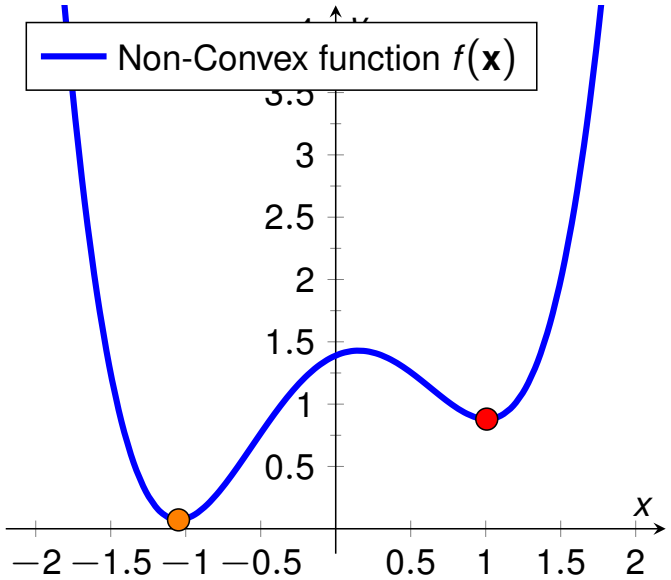

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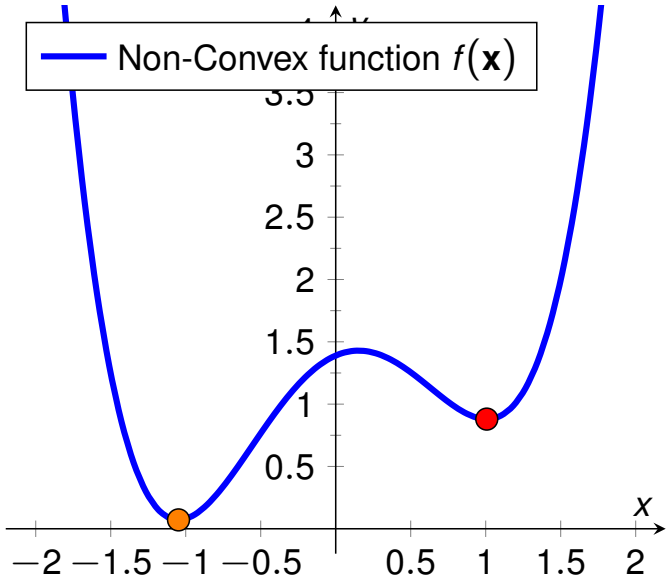

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- Combine models across optimization process
- Can be combined with a **cylic** learning rate

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

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Class Imbalance

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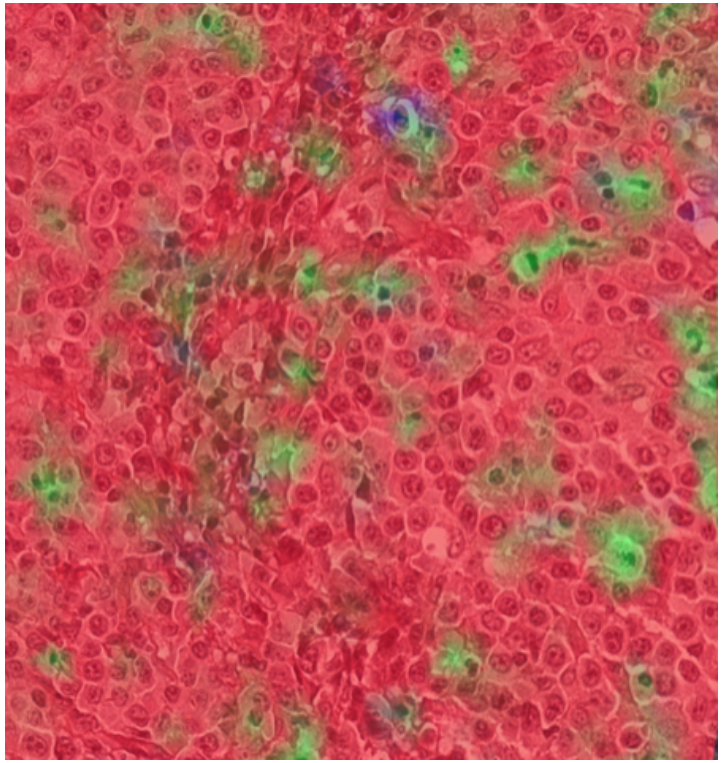
  - Out of 10000 transactions, 9999 are genuine and 1 is fraudulent:
  - ➔ Classifying every transaction as genuine: 99.99% accuracy
  - ➔ Misclassifying 1 out of 100 genuine transactions: 99% accuracy

Motivation (cont.)

- Task: Detect mitotic cells for tumor diagnostics [1].
- Problem: Mitotic cells only make up a very small portion of cells in tissues.



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- Task: Detect mitotic cells for tumor diagnostics [1].
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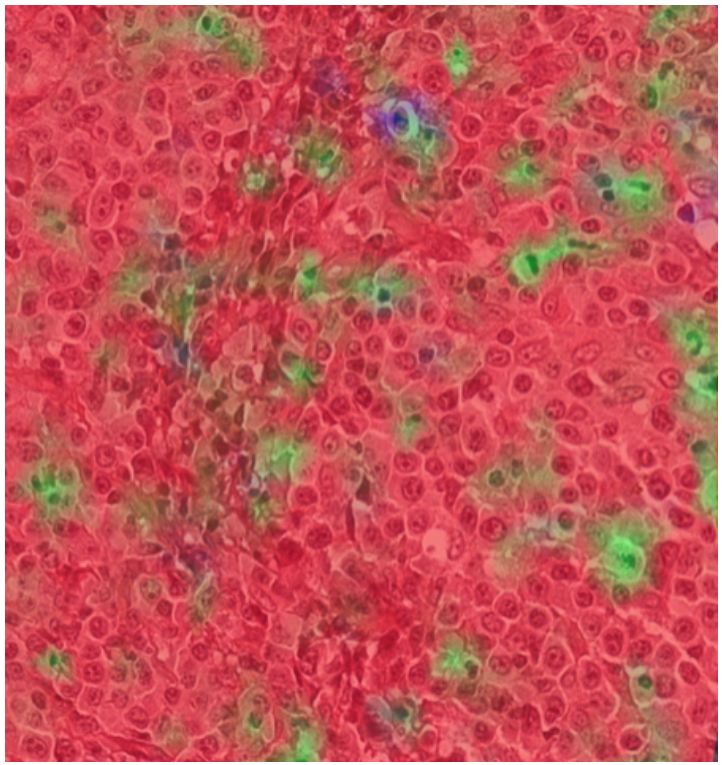

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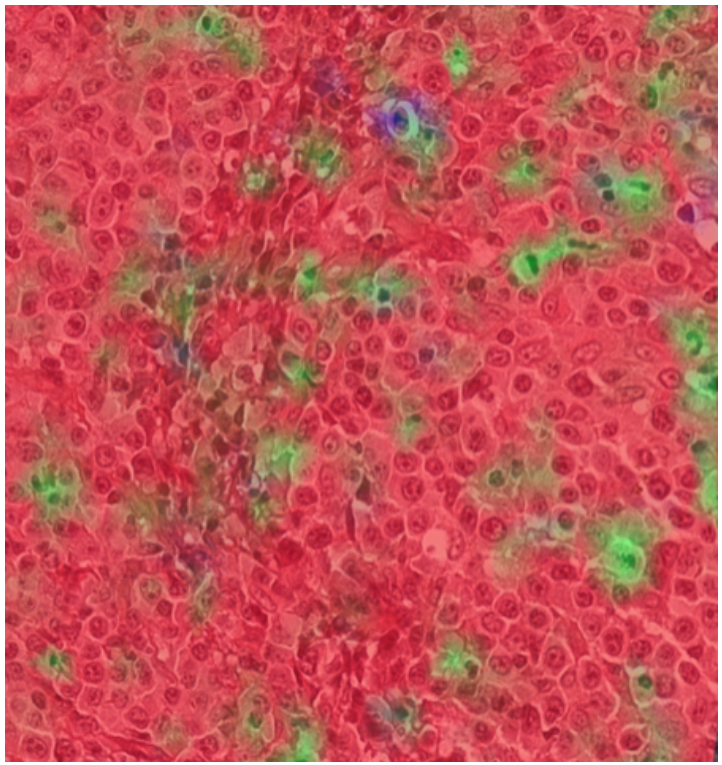
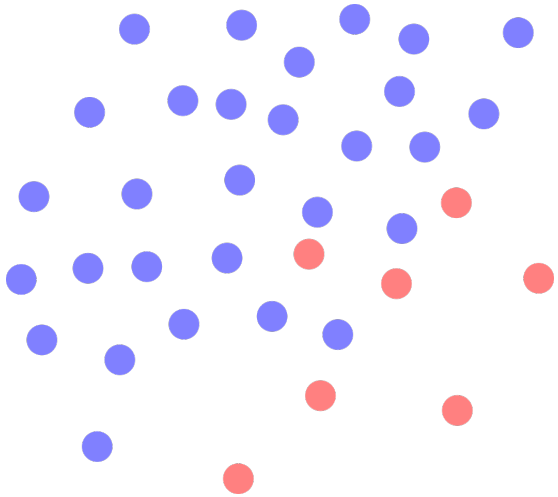
- Measures like accuracy, L_2 norm, cross-entropy do not show imbalance.



Resampling Strategies for Class Imbalance

- Idea: Balance class frequencies by sampling classes differently.



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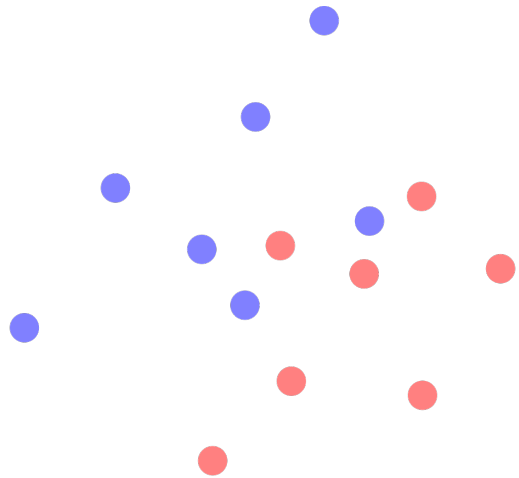

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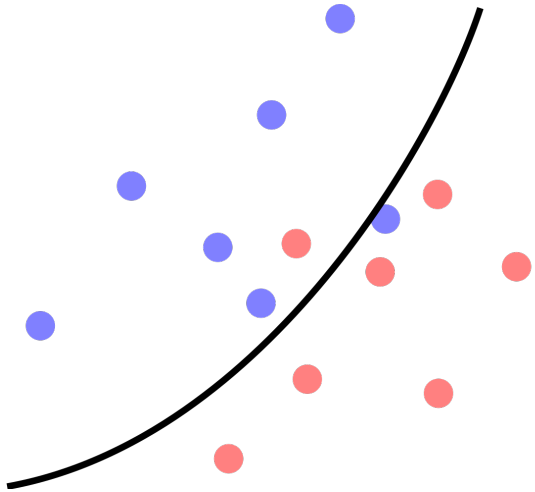

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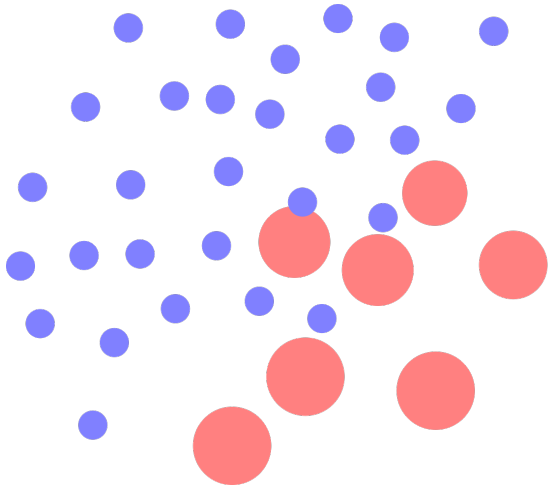

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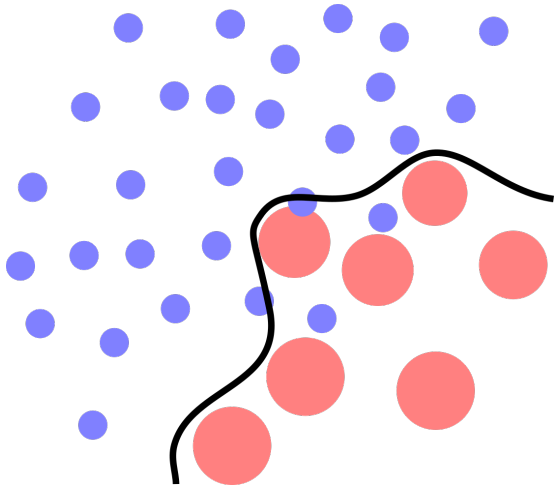

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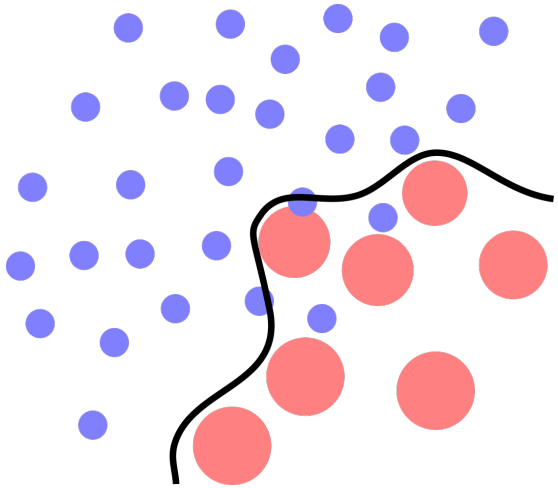
  - Disadvantage: Can lead to overfitting.
- Also possible: Combine Under- and Oversampling.



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- Data augmentation can help to reduce overfitting for underrepresented class.

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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, S. Vesal, F. Meister, C. Liu, S. Gündel, S. Jaganathan, N. Maul, M. Vornehm, L. Reeb, F. Thamm, M. Hoffmann, C. Bergler, F. Denzinger, W. Fu, B. Geissler, Z. Yang
Pattern Recognition Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg
May 16, 2020


FRIEDRICH-ALEXANDER-
UNIVERSITÄT
ERLANGEN-NÜRNBERG
SCHOOL OF ENGINEERING

Evaluation


SIGILLVM ACADEMIAE FRIDERICO ALEXANDRINAE

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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]

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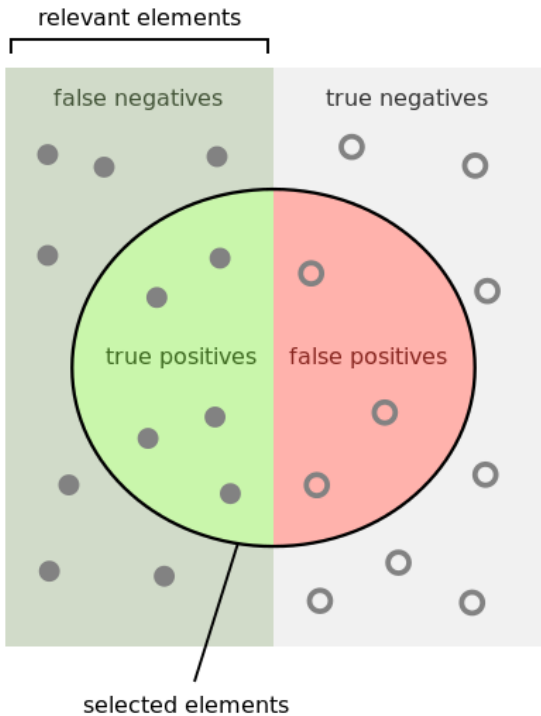
- Multiple human voters: Take mean (if possible) or majority vote.
- Steidl et al. 2005: Entropy-based measure that takes "confusions" of human reference labelers into account.
  - Humans confuse certain classes with each other more (Angry vs. Happy/Angry vs. Annoyed)
  - Mistakes by the classifier are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

Performance measures

- Classification problem ➔classification measures:



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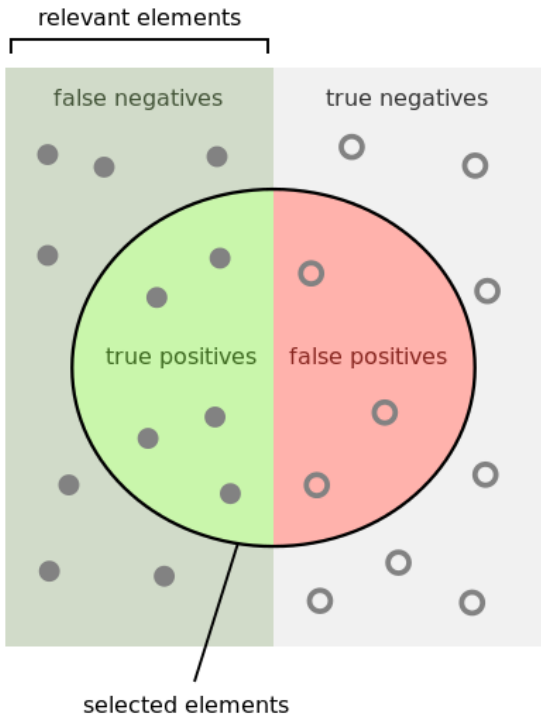

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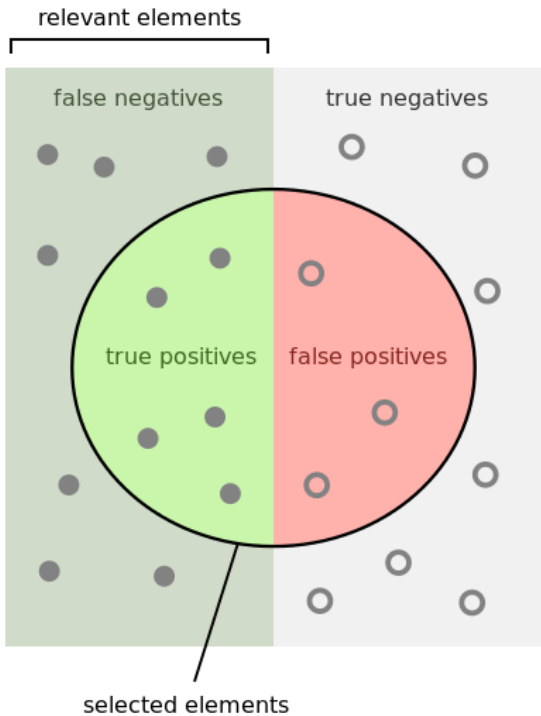

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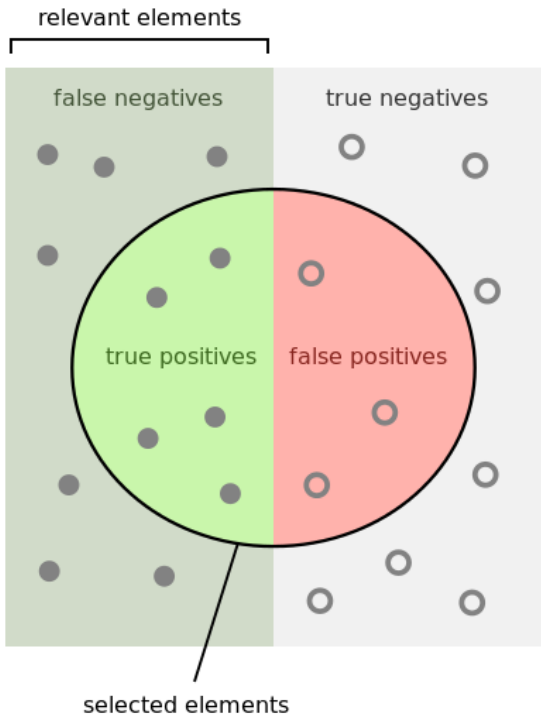
- Receiver operating characteristic (ROC) curve.



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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
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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** α (e.g. 0.05 or 0.01).

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  - ➔ To reach a total significance level of α, 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

References I

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