Common Practices

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Outline

Recap

Training Strategies

Optimization and Learning Rate

Architecture Selection and Hyperparameter Optimization

Ensembling

Class Imbalance

Evaluation

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.)

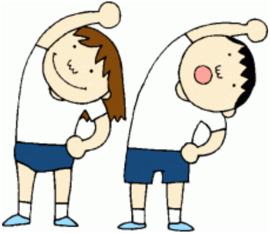
- Overfitting is extremely easy with neural networks (see e.g. ImageNet with random labels [5]).
- True test set error/generalization error can be underestimated **substantially** when using the test set for model selection!
- Attention: Choosing the architecture is the first element in model selection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



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

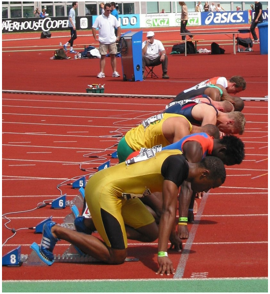
Before Training: Gradient Checks (cont.)

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.
- Compare loss with loss achieved when deciding for a class randomly (**chance**).
- Repeat with multiple random initializations.



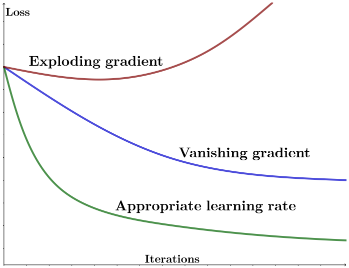
Source: https://commons.wikimedia.org/

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.

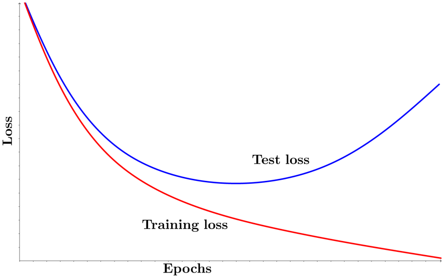
During Training: Monitor loss function

- Recap:



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

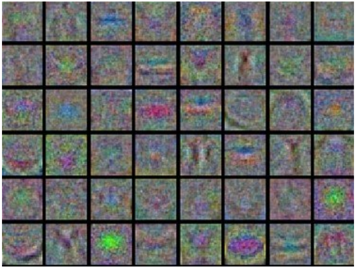
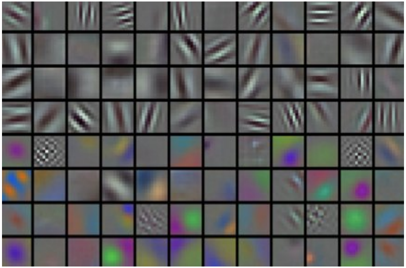
During Training: Monitor Validation Loss



- 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/

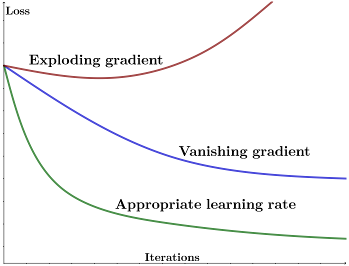
Optimization and Learning Rate

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.

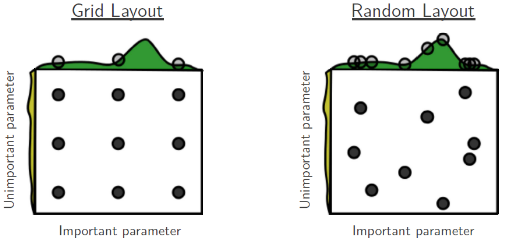
- Architecture:
  - Number of layers & number of nodes per layer
  - Activation function
  - ...
- Optimization
  - Initialization
  - Loss function
  - Optimizer (SGD, Momentum, ADAM, ...)
  - Learning rate, decay & batch size
  - ...
- Regularization
  - Regularizer, e.g., L_2-, L_1-loss
  - Batch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

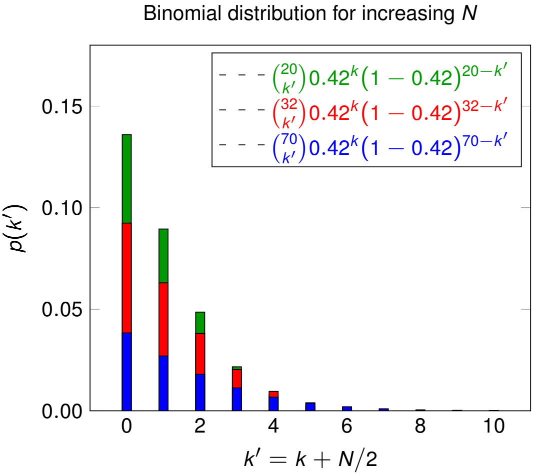
Concept

- 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:

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



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

Concept (cont.)

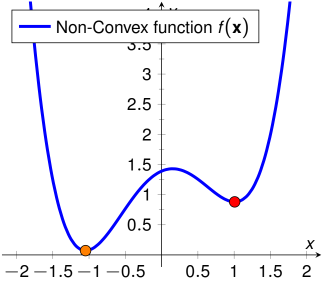
Ensembling

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

How to produce the components?

- Different **models**

Local Minima



- Can we use multiple local minima we get during training?
- Combine models across optimization process
- Can be combined with a **cylic** learning rate

Concept (cont.)

Ensembling

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

How to produce the components?

- Different **models**
- Different model **checkpoints**
- **Moving average** of $\mathbf{w}$ [6]
- Different **methods**

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

NEXT TIME

ON DEEP LEARNING

Common Practices - Part 3

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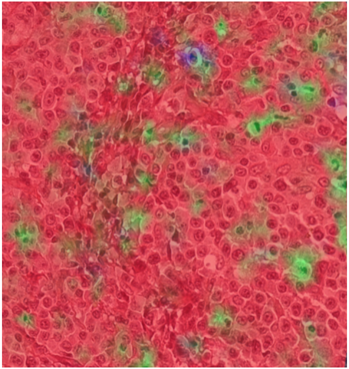
Class Imbalance

Motivation

- Often, different classes are available with very different frequencies in the data set.
- Big challenge for machine learning algorithms.
- Example 1: Fraud detection
  - 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

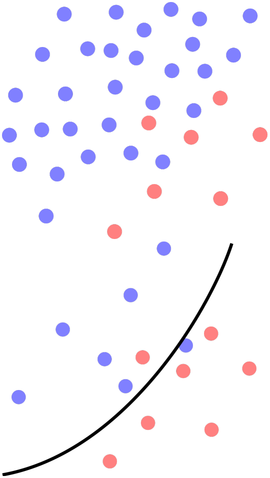
Motivation (cont.)

- Task: Detect mitotic cells for tumor diagnostics [1].
- Problem: Mitotic cells only make up a very small portion of cells in tissues.
- Data of a certain class is seen much less during training.
- Measures like accuracy, L_2 norm, cross-entropy do not show imbalance.



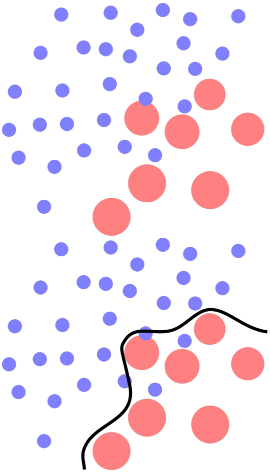
Resampling Strategies for Class Imbalance

- Idea: Balance class frequencies by sampling classes differently.
- **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 for Class Imbalance (cont.)

- **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 (cont.)

- 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 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.
- Weight loss with inverse class frequency, e.g., weighted cross entropy:

$$L(\mathbf{y}, \hat{\mathbf{y}}) = -w_k \log(\hat{y}_k)\big|_{y_k=1} \tag{1}$$

- More common in segmentation problems: Dice-loss based on Dice coefficient.
- Instead of class frequency, weights can be adapted with regards to other considerations.

NEXT TIME

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Common Practices - Part 4

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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!

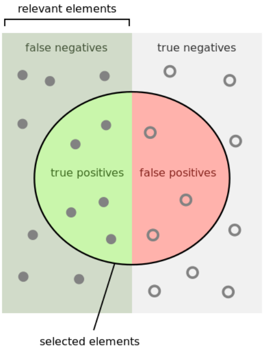
Source: de.disney.wikia.com/wiki/Dagobert_Duck

Of All Things the Measure is Man [8]

- Protagoras of Abdera (c.490 - c.420 BCE)
- Data is annotated and labeled by humans.
- During training, all labels are assumed to be correct $\lightning$ "to err is human"
- Additionally: Ambiguous data.
- 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:
- Binary classification problem:
  - True/False Positives: TP/FP
  - True/False Negatives: TN/FN
- Accuracy: $\mathrm{ACC} = \frac{\mathrm{TP}+\mathrm{TN}}{\mathrm{P}+\mathrm{N}}$
- Precision/pos. predictive value: $\mathrm{precision} = \frac{\mathrm{TP}}{\mathrm{TP}+\mathrm{FP}}$
- Recall/true positive value: $\mathrm{recall} = \frac{\mathrm{TP}}{\mathrm{TP}+\mathrm{FN}}$
- Specificity/true negative value: $\mathrm{specificity} = \frac{\mathrm{TN}}{\mathrm{TN}+\mathrm{FP}}$
- F1-score: $\mathrm{F1} = 2 \cdot \frac{\mathrm{TPV} \cdot \mathrm{TNV}}{\mathrm{TPV}+\mathrm{TNV}}$
- Receiver operating characteristic (ROC) curve.



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.
- Rather uncommon in deep learning due to long training times.
- Can be used for hyperparameter estimation (nested!), or to evaluate stability of (hyper-)parameters.
- 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%?
- 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. 0.05 or 0.01).

Comparing Classifiers: Bonferroni Correction

- Interpretation: The probability that this difference is caused by **chance** $< \alpha$.
- If we compare multiple classifiers, this chance can rise significantly due to **multiple comparisons**!
- Correct for multiple tests using Bonferroni correction:
  - For *n* tests with significance level α, the total risk is $n \cdot \alpha$.
  - → 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

[1] M. Aubreville, M. Krappmann, C. Bertram, et al. "A Guided Spatial Transformer Network for Histology Cell Differentiation". In: ArXiv e-prints (July 2017). arXiv: 1707.08525 [cs.CV].

[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.

[4] Yoshua Bengio. "Practical recommendations for gradient-based training of deep architectures". In: Neural networks: Tricks of the trade. Springer, 2012, pp. 437–478.

References II

[5] Chiyuan Zhang, Samy Bengio, Moritz Hardt, et al. "Understanding deep learning requires rethinking generalization". In: arXiv preprint arXiv:1611.03530 (2016).

[6] Boris T Polyak and Anatoli B Juditsky. "Acceleration of stochastic approximation by averaging". In: SIAM Journal on Control and Optimization 30.4 (1992), pp. 838–855.

[7] Prajit Ramachandran, Barret Zoph, and Quoc V. Le. "Searching for Activation Functions". In: CoRR abs/1710.05941 (2017). arXiv: 1710.05941.

[8] Stefan Steidl, Michael Levit, Anton Batliner, et al. "Of All Things the Measure is Man: Automatic Classification of Emotions and Inter-labeler Consistency". In: Proc. of ICASSP. IEEE â€“ Institute of Electrical and Electronics Engineers, Mar. 2005.