Neural Network Tricks

Technische Universität Berlin - Machine Learning Group

Agenda

Hyperparameters and Optimization

Controlling Overfitting

Tips, Tricks and Misc

Summary

Motivation

- Large number of parameters $\rightarrow$ overfitting
- Non-convex, high-dimensional optimization with SGD $\rightarrow$ local optima
- Learning from small datasets
- **Important:** Generalization error

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Training Curve

- Visualize evolution of learning
- Performance metrics: loss, accuracy, precision, recall etc.
- Training and **validation** performance

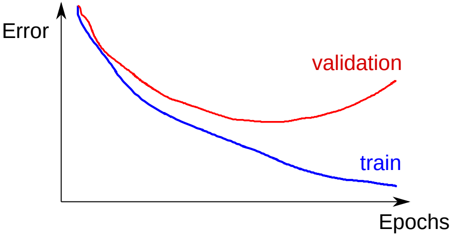

Figure: Typical SGD training curve for neural networks.

Learning Rate

- Far too high: divergence
- Too high: Fast initial improvement but convergence to bad optimum
- Appropriate: typically exponentially shaped
- Too low: Linear improvement
- Search in logarithmic space
- Typical value: 10^{-2}

Learning Rate Scheduling

- High initial learning rate
- Decrease to find minimum more accurately
- Variants:
  - Step
  - Exponential
  - $^{1}/_{t}$
  - Reduction on plateau

Batch Size

- Control “stochasticity” of SGD $\rightarrow$ “noise” in training curve
- Influence mainly on training speed, not test performance
- Typical value: 64

Parameter Initialization

- Break symmetry by random initialization
- Size of weights should depend on number of input connections
- Method by Glorot and Bengio 2010 (“Xavier initialization”)

Momentum

- “Smooth out” oscillations in training curve
- Moving average of past gradient values
- Typical value: $\mu = 0.9$ (can be lower in the beginning)

$$\Lambda_{\text{mom}}^{t+1} = \mu \Lambda_{\text{mom}}^{t} - \lambda \cdot \nabla E\left(\Theta^{t}\right) \quad , \tag{1}$$

where μ is the momentum parameter, Λ is the parameter update, Θ is the parameter vector and λ is the learning rate.

Advanced Update Functions

Automatic adaptation of learning rate

- AdaGrad: Duchi, Hazan, and Singer 2011
- AdaDelta: Zeiler 2012
- Adam: Kingma and Ba 2014
- RMSprop: Tieleman and Hinton 2012
- Nesterov's Accelerated Gradient (NAG): Nesterov 1983

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Hyperparameter Search

- Grid search
- Random search (Bergstra and Bengio 2012)
- Bayesian hyperparameter optimization

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Early Stopping

- Select model with best validation performance
- Stop training if validation performance has not improved for some epochs ("patience")

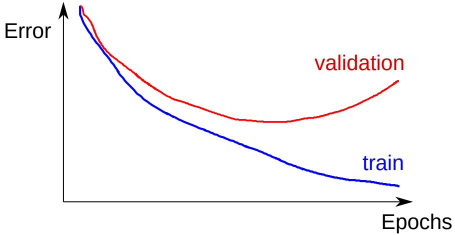

Figure: Early stopping.

Early Stopping

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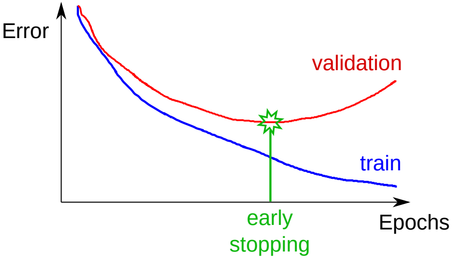
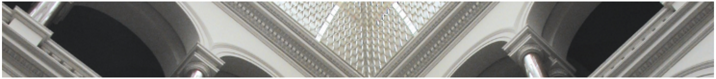


Figure: Early stopping.

Dropout

– Co-adapting neurons: “errors” of certain neurons may be compensated by others
– Dropout neurons randomly during training (Srivastava et al. 2014)
– Ensemble of pruned networks
– Averaging in test phase
– Takes longer to train (2-3 times)
– Dropout ratio ρ: probability that neuron is kept in SGD iteration
– Typical value: $\rho = 0.5$

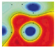


Weight Regularization

- Regularize length of parameter vector
- L_1 and L_2
- “Weight decay”: regularization strength
- Typical value: 10^{-3}

$$J = E(\Theta) + \omega \left\|\Theta\right\|_2^2 \rightarrow \text{min} \quad , \tag{2}$$

where J is the objective function, E is the cost function, ω is the weight decay and Θ are the parameters of the model.



Data Augmentation

– More data always reduces overfitting

– Generate synthetic data by applying transformations, e. g. for images:

- random crops
- mirroring
- rotation
- elastic deformations
- color augmentation

Transfer Learning

- Extract knowledge from *source task* and apply to *target task*
- Pretraining and finetuning $\rightarrow$ pretrained parameters as initialization
- Unsupervised and supervised
- Narrow down exploration space
- Acts as regularizer

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Standardization

- Features should all be in same scale and centered around zero
- Express features in terms of standard deviations from the mean

$$x' = \frac{x - \mu}{\sigma} \tag{3}$$

- Images: μ and σ can be computed per:
  - feature $\rightarrow$ "mean image"
  - channel
  - sample
- Standardize validation and test set with training statistics

Batch Normalization

- Standardize input features in each layer by mini-batch statistics
- Enables higher learning rates
- Proposed by Ioffe and Szegedy 2015

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1\ldots m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m} (x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

Algorithm 1: Batch Normalizing Transform, applied to activation x over a mini-batch.

Ensembles

- Boost performance by averaging predictions of several models
- Average predictor's variance (bias-variance trade-off)
- Models should be as diverse as possible, e. g. :
  - Different architectures
  - Different initializations ($\rightarrow$ pretraining)
  - Different optimization
  - Best models of cross validation
  - Models that are not neural networks, e. g. SVMs, Random Forests

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Recommendations

- Most important hyperparameters:
  - Initial learning rate
  - Learning rate schedule (step?)
  - Regularization strength (dropout and weight decay)
  - Batch size
- Random search better than grid search
- Overfit subset of data
- SGD + momentum or Adam
- Standardization is crucial!
- One validation fold better than k-fold cross validation for big data
- Get more data
- Get more GPUs

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Thank you!