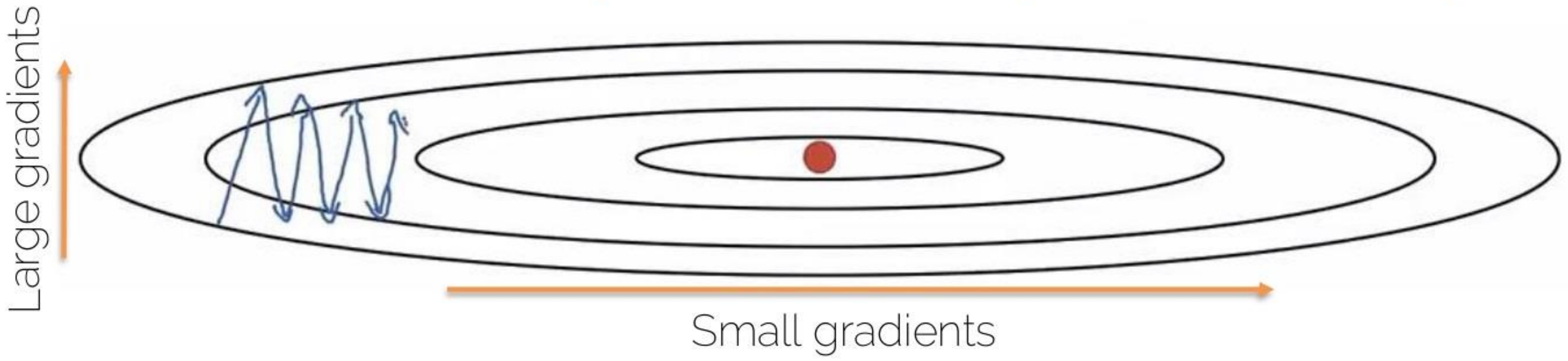
Lecture 7
Training Neural Nets

Root Mean Squared Prop (RMSProp)



Source: Andrew. Ng

- RMSProp divides the learning rate by an exponentially-decaying average of squared gradients.

Hinton et al. "Lecture 6.5-rmsprop: Divide the gradient by a running average of its recent magnitude." COURSERA: Neural networks for machine learning 4.2 (2012): 26-31.

RMSProp

$$\boldsymbol{s}^{k+1} = \beta \cdot \boldsymbol{s}^k + (1-\beta)\boxed{[\nabla_{\boldsymbol{\theta}} L \circ \nabla_{\boldsymbol{\theta}} L]}$$

Element-wise multiplication

$$\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^k - \alpha \cdot \frac{\nabla_{\boldsymbol{\theta}} L}{\sqrt{\boldsymbol{s}^{k+1}} + \epsilon}$$

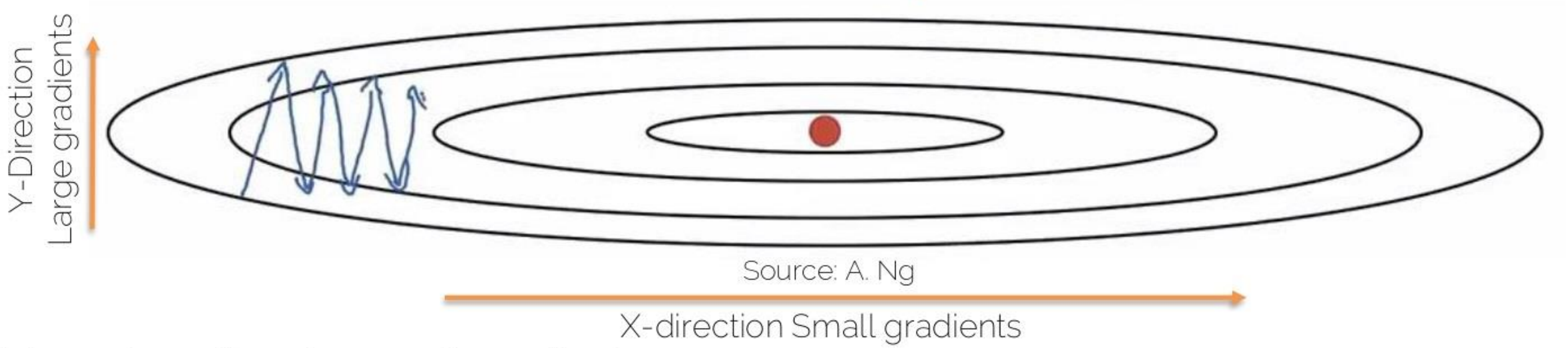
Hyperparameters: $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{\epsilon}$

Needs tuning!

Often $\mathbf{0.9}$

Typically $\mathbf{10^{-8}}$

RMSProp



(Uncentered) variance of gradients
→ second momentum

$$\boxed{\boldsymbol{s}^{k+1} = \beta \cdot \boldsymbol{s}^{k} + (1-\beta)[\nabla_{\boldsymbol{\theta}} L \circ \nabla_{\boldsymbol{\theta}} L]}$$

$$\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^{k} - \alpha \cdot \frac{\nabla_{\boldsymbol{\theta}} L}{\sqrt{\boldsymbol{s}^{k+1}} + \epsilon}$$

We're dividing by square gradients:
- Division in Y-Direction will be large
- Division in X-Direction will be small

Can increase learning rate!

RMSProp

- Dampening the oscillations for high-variance directions

- Can use faster learning rate because it is less likely to diverge
  → Speed up learning speed
  → Second moment

Adaptive Moment Estimation (Adam)

Idea : Combine Momentum and RMSProp

$$\boldsymbol{m}^{k+1} = \beta_1 \cdot \boldsymbol{m}^k + (1-\beta_1)\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^k)$$

First momentum: mean of gradients

$$\boldsymbol{v}^{k+1} = \beta_2 \cdot \boldsymbol{v}^k + (1-\beta_2)[\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^k) \circ \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^k)]$$

Second momentum: variance of gradients

$$\boxed{\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^k - \alpha \cdot \frac{\boldsymbol{m}^{k+1}}{\sqrt{\boldsymbol{v}^{k+1}} + \epsilon}}$$

Note : This is not the update rule of Adam

Q. What happens at $\boldsymbol{k} = 0$?
A. We need bias correction as $\boldsymbol{m}^0 = 0$ and $\boldsymbol{v}^0 = 0$

[Kingma et al., ICLR'15] Adam: A method for stochastic optimization

Adam : Bias Corrected

- Combines Momentum and RMSProp

$$\boldsymbol{m}^{k+1} = \beta_1 \cdot \boldsymbol{m}^k + (1-\beta_1)\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^k) \qquad \boldsymbol{v}^{k+1} = \beta_2 \cdot \boldsymbol{v}^k + (1-\beta_2)[\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^k) \circ \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^k)$$

- $\boldsymbol{m}^k$ and $\boldsymbol{v}^k$ are initialized with zero

  $\rightarrow$ bias towards zero

  $\rightarrow$ Need bias-corrected moment updates

Update rule of Adam

$$\boxed{\widehat{\boldsymbol{m}}^{k+1} = \frac{\boldsymbol{m}^{k+1}}{1-{\beta_1}^{k+1}} \qquad \widehat{\boldsymbol{v}}^{k+1} = \frac{\boldsymbol{v}^{k+1}}{1-{\beta_2}^{k+1}} \longrightarrow \boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^k - \alpha \cdot \frac{\widehat{\boldsymbol{m}}^{k+1}}{\sqrt{\widehat{\boldsymbol{v}}^{k+1}}+\epsilon}}$$

Adam

- Exponentially-decaying mean and variance of gradients (combines first and second order momentum)

- Hyperparameters: α, β_1, β_2, ϵ

Needs tuning!

Often 0.9

Often 0.999

Typically 10^{-8}

Defaults in PyTorch

$$\boldsymbol{m}^{k+1} = \beta_1 \cdot \boldsymbol{m}^k + (1 - \beta_1)\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^k)$$

$$\boldsymbol{v}^{k+1} = \beta_2 \cdot \boldsymbol{v}^k + (1 - \beta_2)[\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^k) \circ \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^k)]$$

$$\hat{\boldsymbol{m}}^{k+1} = \frac{\boldsymbol{m}^{k+1}}{1-{\beta_1}^{k+1}} \qquad \hat{\boldsymbol{v}}^{k+1} = \frac{\boldsymbol{v}^{k+1}}{1-{\beta_2}^{k+1}}$$

$$\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^k - \alpha \cdot \frac{\hat{\boldsymbol{m}}^{k+1}}{\sqrt{\hat{\boldsymbol{v}}^{k+1}} + \epsilon}$$

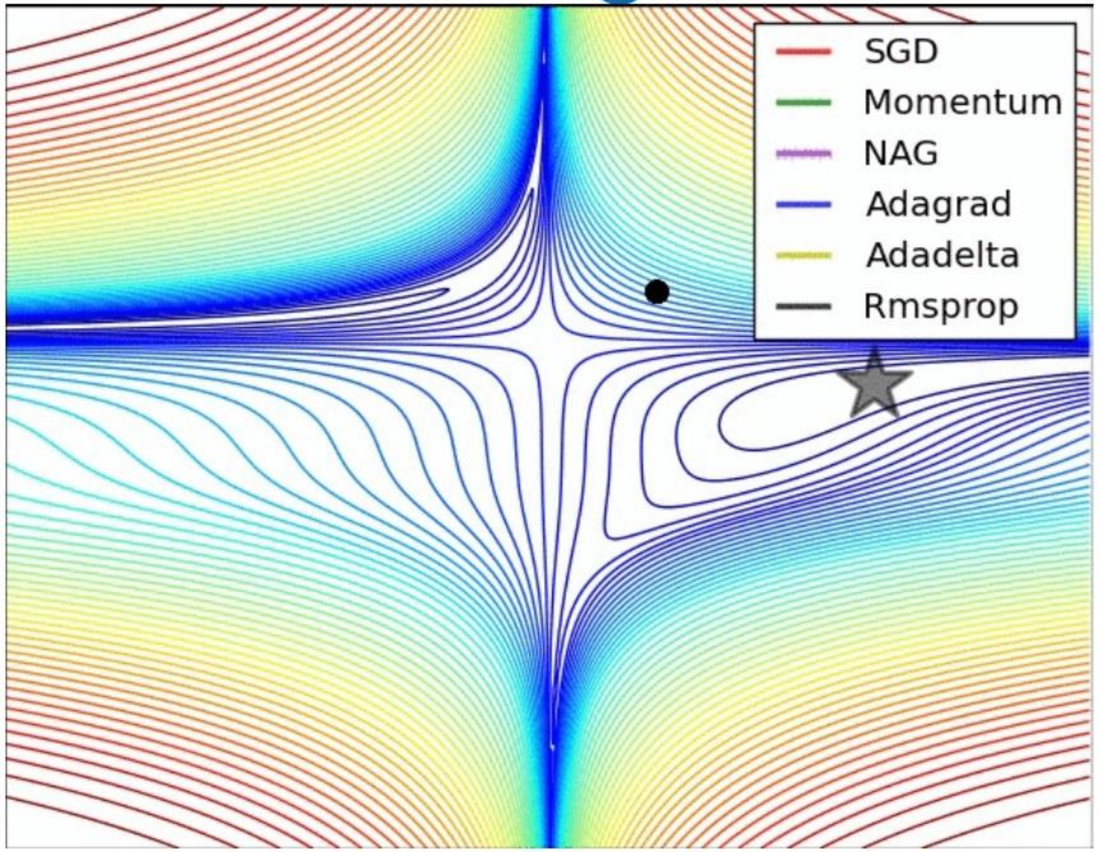
There are a few others…

- 'Vanilla' SGD
- Momentum
- RMSProp
- Adagrad
- Adadelta
- AdaMax
- Nada
- AMSGrad

Adam is mostly method of choice for neural networks!

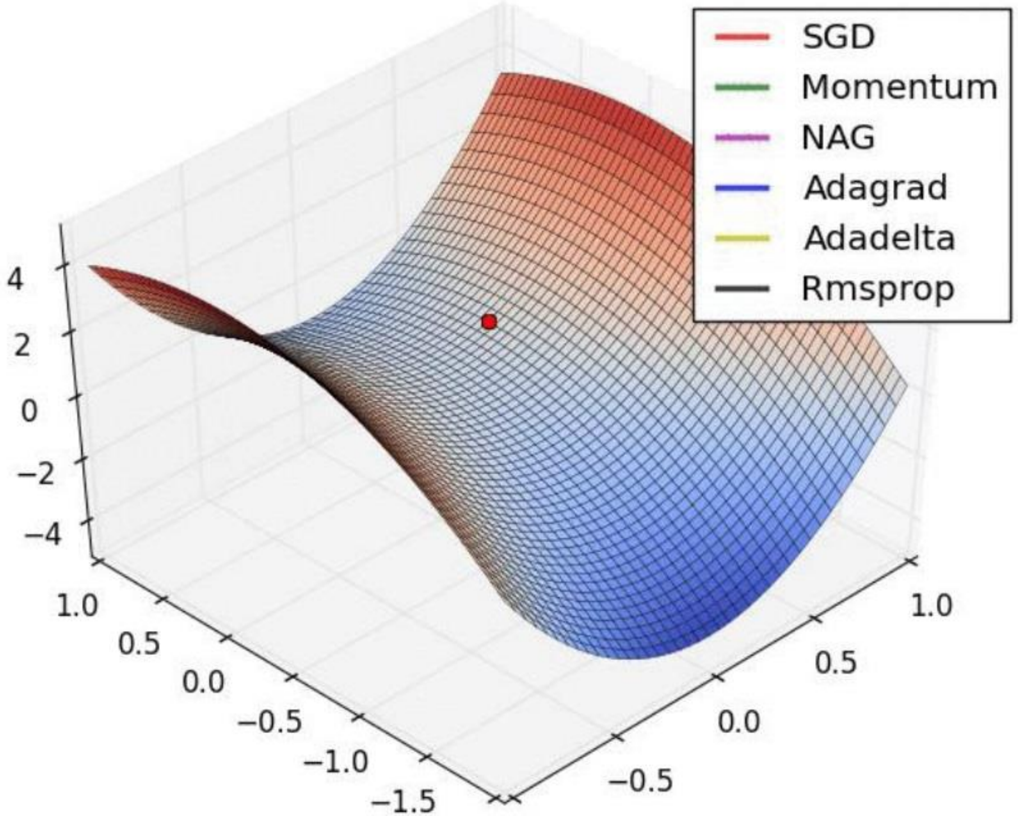
It's actually fun to play around with SGD updates. It's easy and you get pretty immediate feedback ☺

Convergence



Source: http://ruder.io/optimizing-gradient-descent/

Convergence



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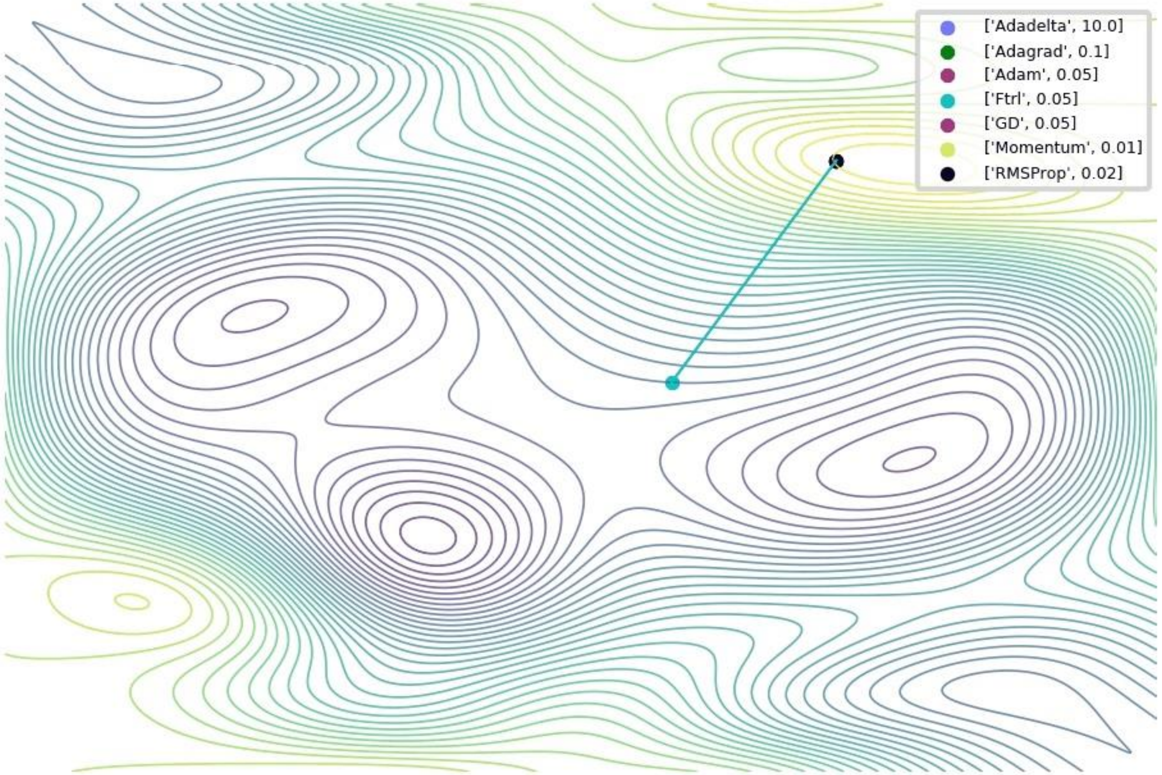
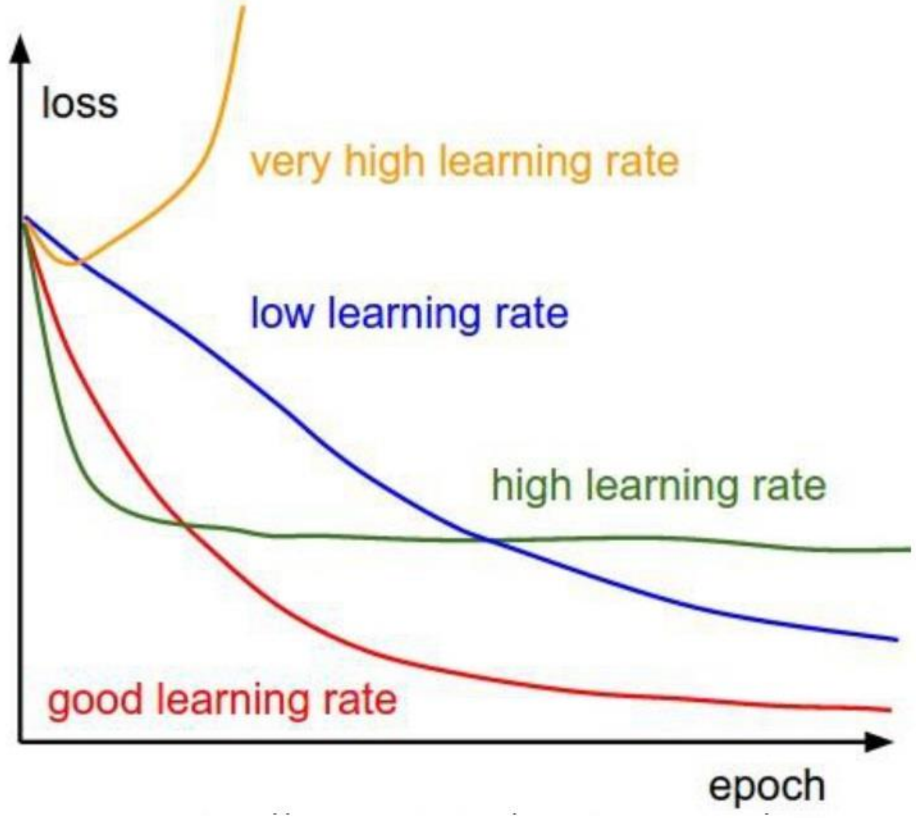
Convergence



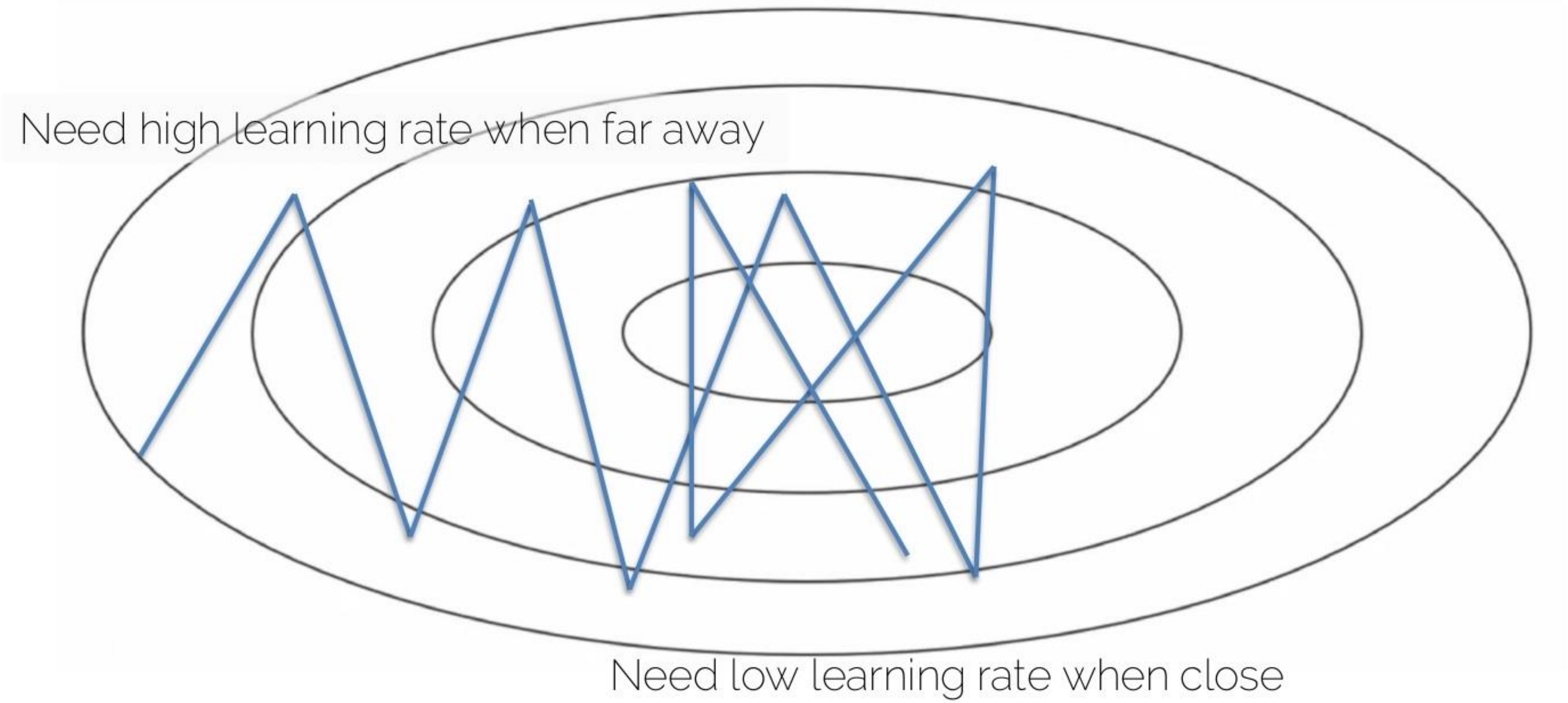
Source: https://github.com/Jaewan-Yun/optimizer-visualization

Learning Rate: Implications

- What if too high?
- What if too low?



Learning Rate

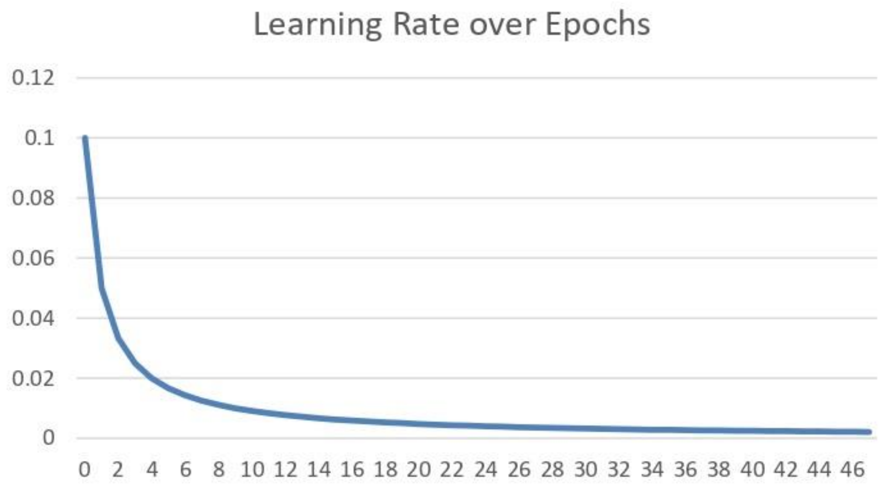


Learning Rate Decay

- $\alpha = \frac{1}{1+decay\_rate*epoch} \cdot \alpha_0$
  - E.g., $\alpha_0 = 0.1$, $decay\_rate = 1.0$

→ Epoch 0: 0.1
→ Epoch 1: 0.05
→ Epoch 2: 0.033
→ Epoch 3: 0.025

...



Learning Rate Decay

Many options:

- Step decay $\alpha = \alpha - t \cdot \alpha$ (only every n steps)
  - T is decay rate (often 0.5)
- Exponential decay $\alpha = t^{epoch} \cdot \alpha_0$
  - t is decay rate (t < 1.0)
- $\alpha = \frac{t}{\sqrt{epoch}} \cdot a_0$
  - t is decay rate
- Etc.

Training Schedule

Manually specify learning rate for entire training process

- Manually set learning rate every n-epochs
- How?
  - Trial and error (the hard way)
  - Some experience (only generalizes to some degree)

Consider: #epochs, training set size, network size, etc.

Basic Recipe for Training

- Given ground dataset with ground labels
  - $\{x_i, y_i\}$
    - x_i is the $\boldsymbol{i^{th}}$ training image, with label $\boldsymbol{y_i}$
    - Often $\mathbf{dim}(x) \gg \mathbf{dim}(y)$ (e.g., for classification)
    - $\boldsymbol{i}$ is often in the 100-thousands or millions
  - Take network $\boldsymbol{f}$ and its parameters $\boldsymbol{w, b}$
  - Use SGD (or variation) to find optimal parameters $\boldsymbol{w, b}$
    - Gradients from backpropagation

Gradient Descent on Train Set

- Given large train set with ($\boldsymbol{n}$) training samples $\{\boldsymbol{x}_i, \boldsymbol{y}_i\}$
  - Let's say 1 million labeled images
  - Let's say our network has 500k parameters

- Gradient has 500k dimensions
- $n = 1\ million$
- Extremely expensive to compute

Learning

- Learning means generalization to unknown dataset
  - (So far no 'real' learning)
  - I.e., train on known dataset → test with optimized parameters on unknown dataset

- Basically, we hope that based on the train set, the optimized parameters will give similar results on different data (i.e., test data)

Learning

- Training set ('*train*'):
  - Use for training your neural network
- Validation set ('*val*'):
  - Hyperparameter optimization
  - Check generalization progress
- Test set ('*test*'):
  - Only for the very end
  - NEVER TOUCH DURING DEVELOPMENT OR TRAINING

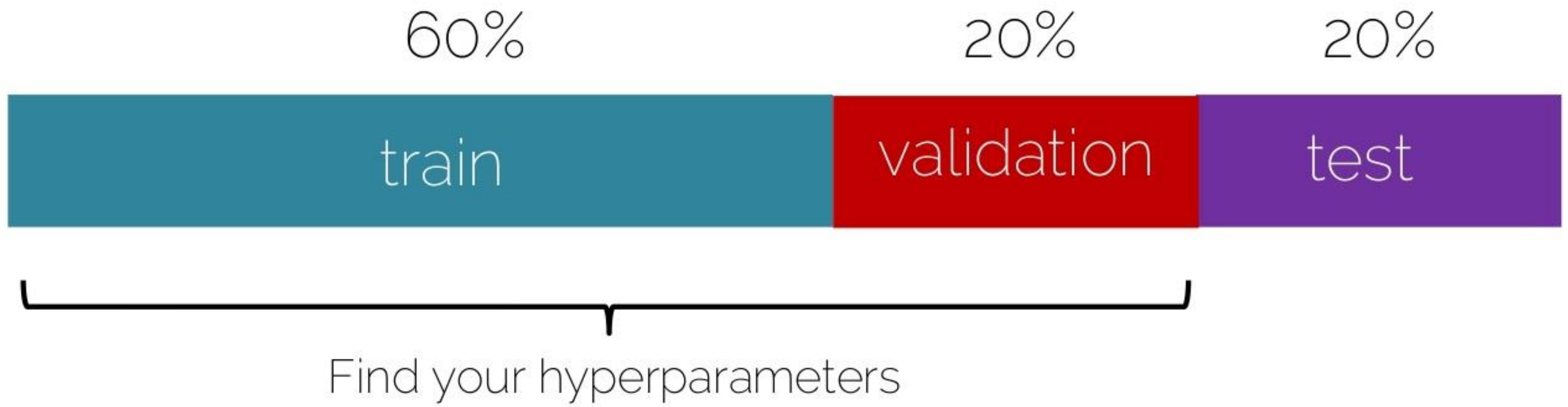
Learning

- Typical splits
  - Train (60%), Val (20%), Test (20%)
  - Train (80%), Val (10%), Test (10%)

- During training:
  - Train error comes from average minibatch error
  - Typically take subset of validation every n iterations

Basic Recipe for Machine Learning

- Split your data



Basic Recipe for Machine Learning

- Split your data

Example scenario

Ground truth error 1%

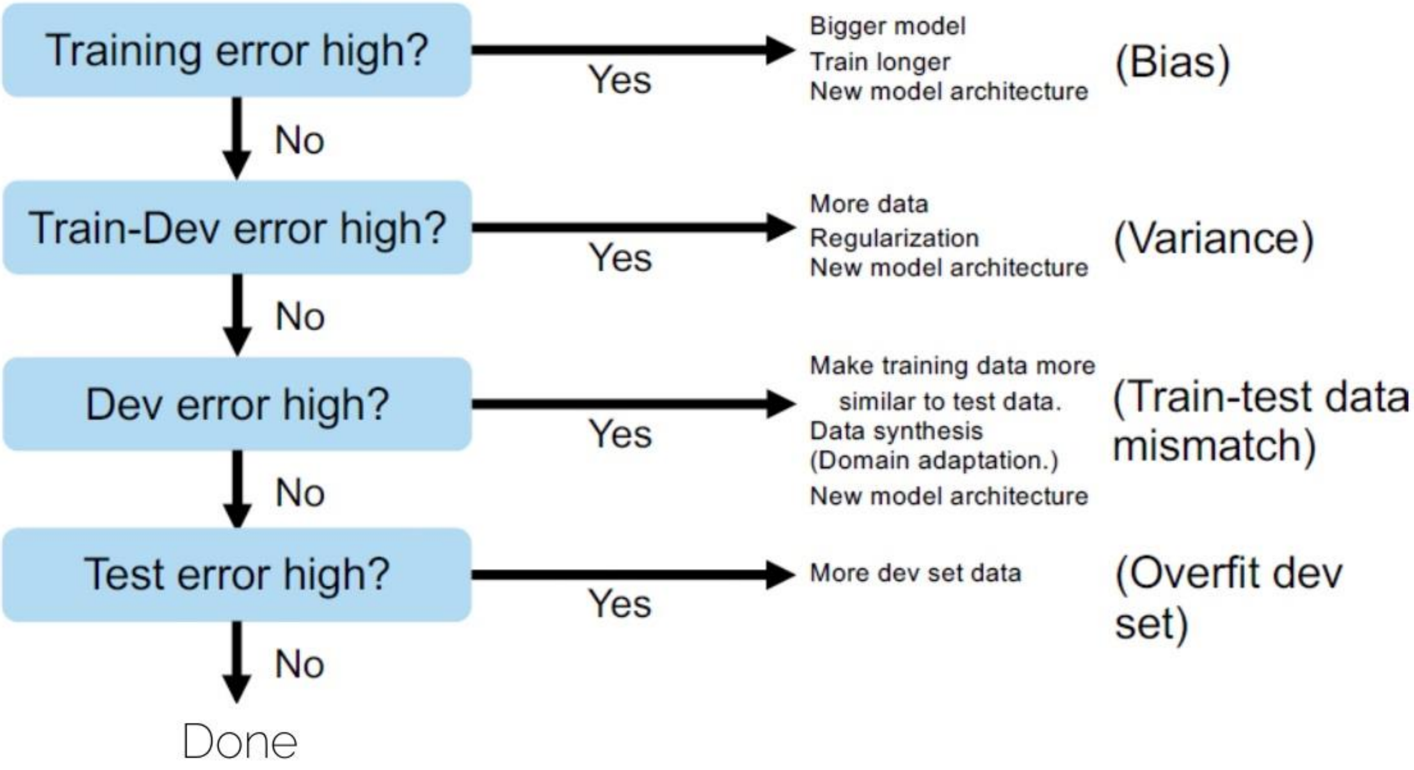
Training set error 5%

Val/test set error 8%

Bias
(underfitting)

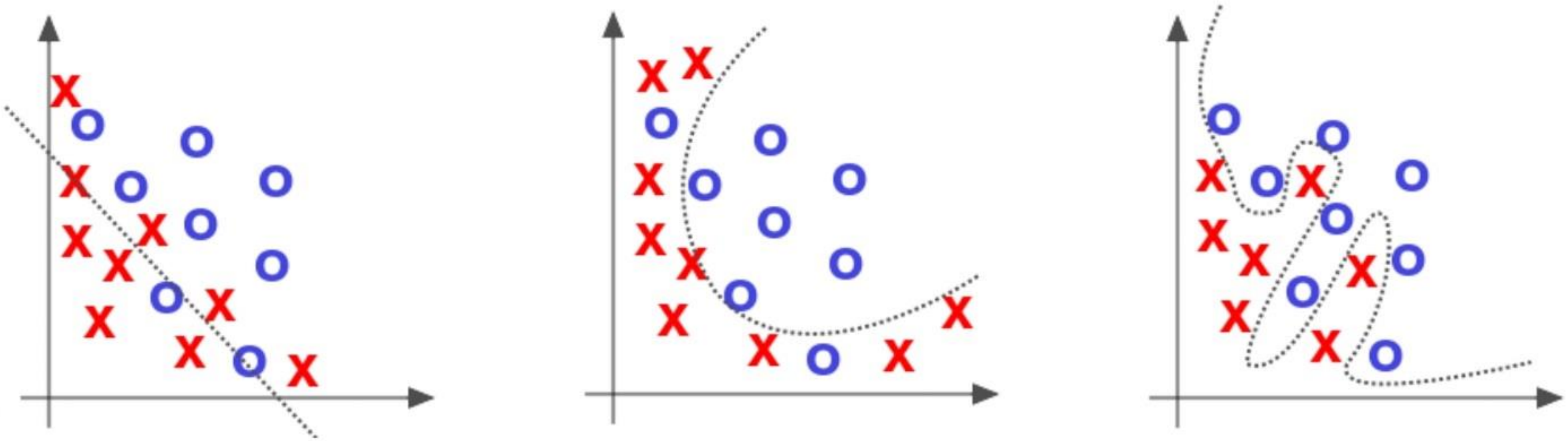
Variance
(overfitting)

Basic Recipe for Machine Learning



Credits: A. Ng

Over- and Underfitting

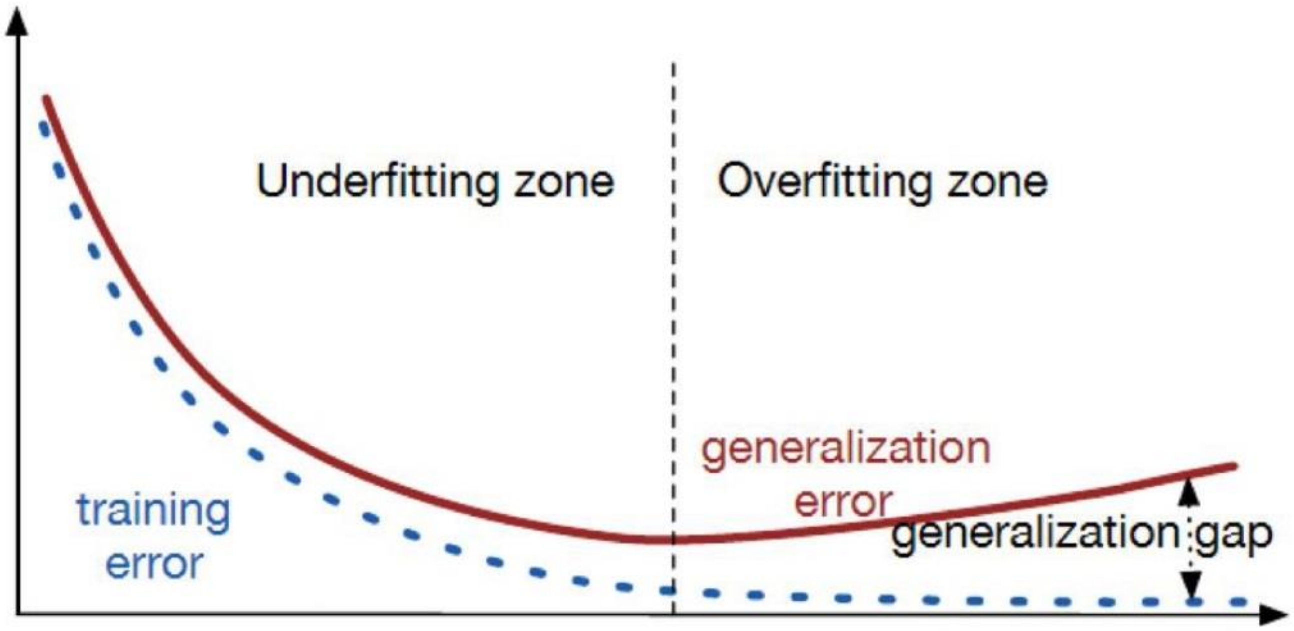


Underfitted
Overfitted

Appropriate

Source: Deep Learning by Adam Gibson, Josh Patterson, O'Reily Media Inc., 2017

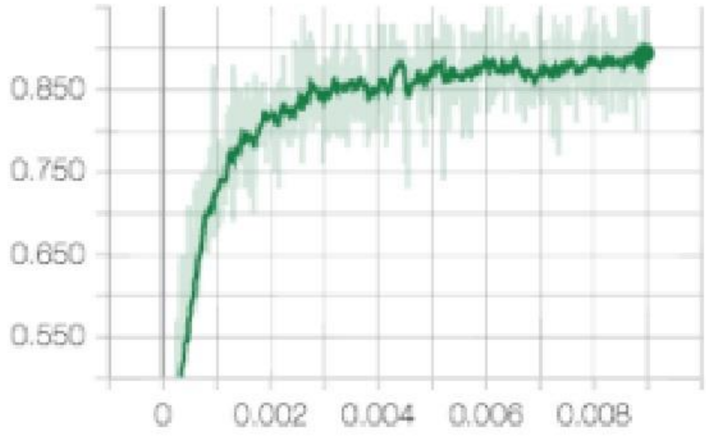
Over- and Underfitting



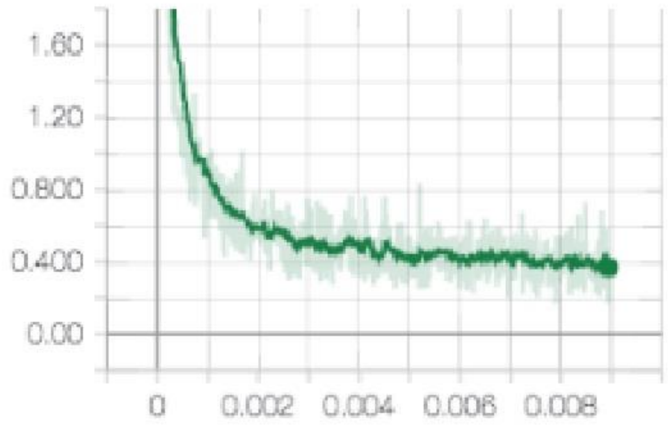
Source: https://srdas.github.io/DLBook/ImprovingModelGeneralization.html

Learning Curves

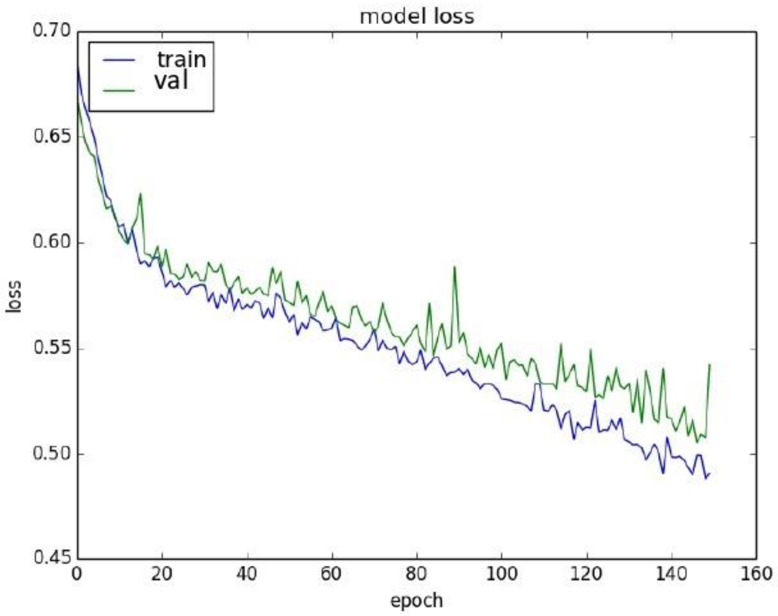
- Training graphs
  - Accuracy

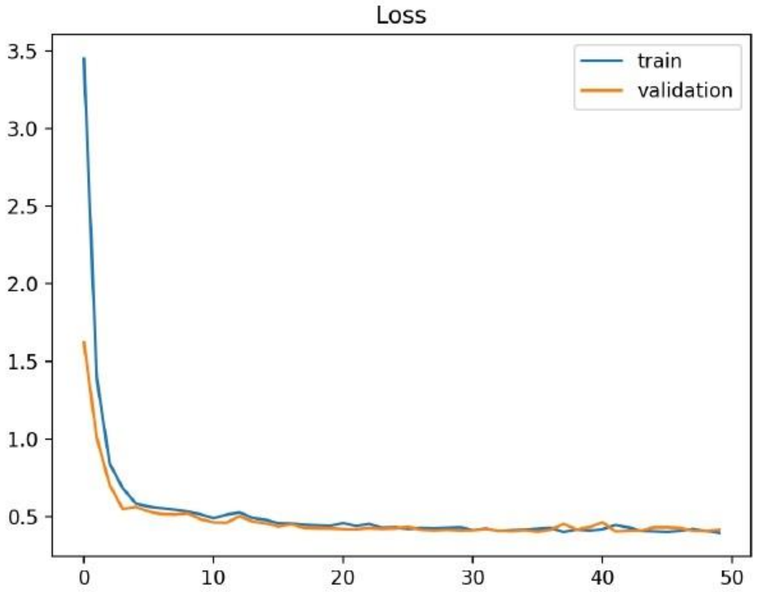


  - Loss



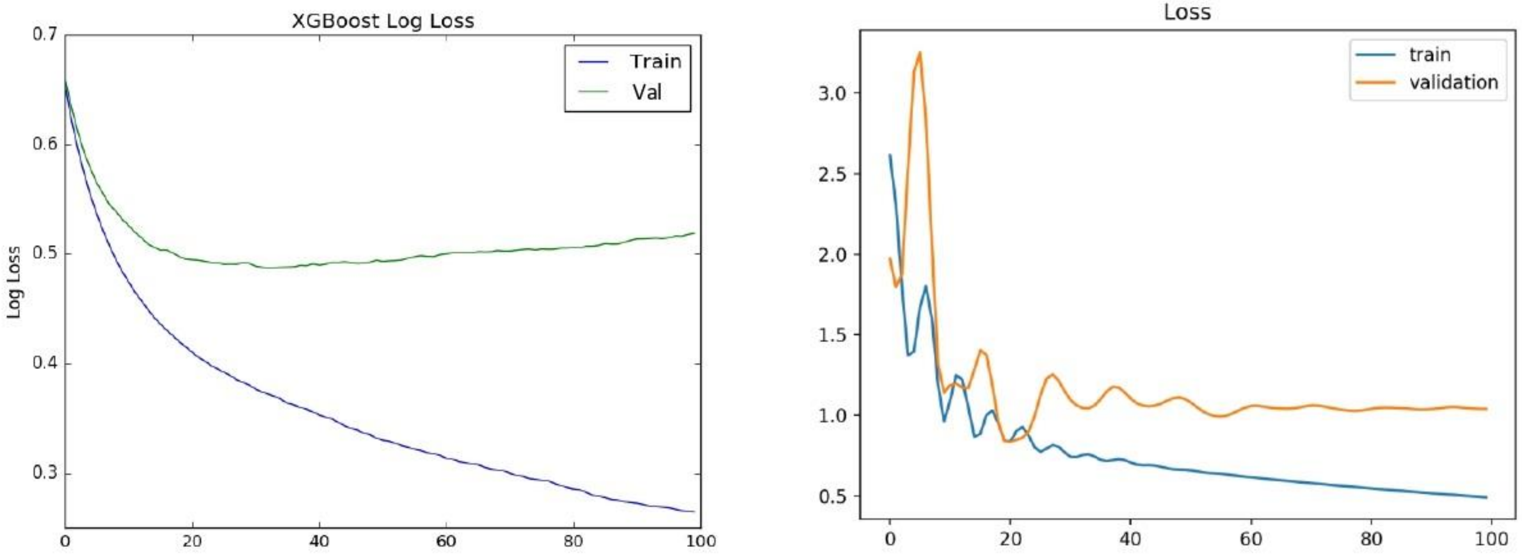
Learning Curves





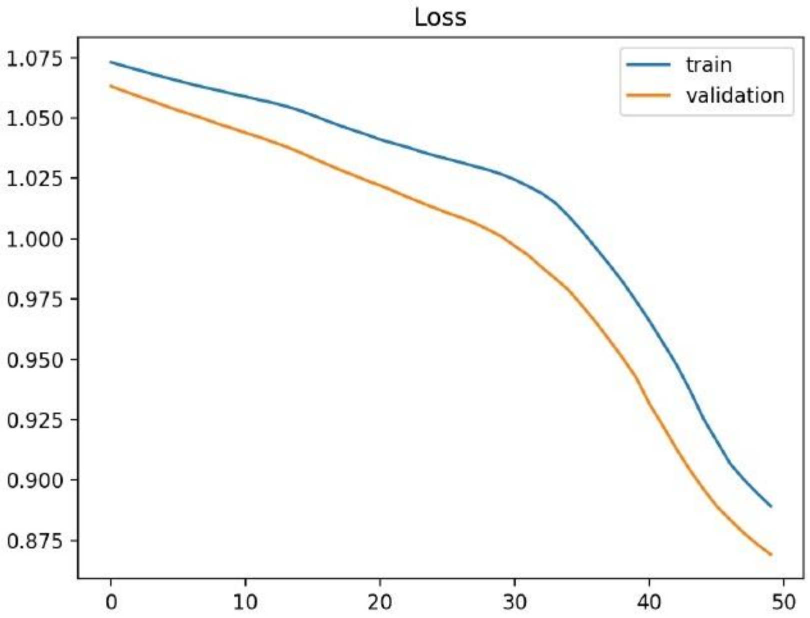
Source: https://machinelearningmastery.com/learning-curves-for-diagnosing-machine-learning-model-performance/

Overfitting Curves

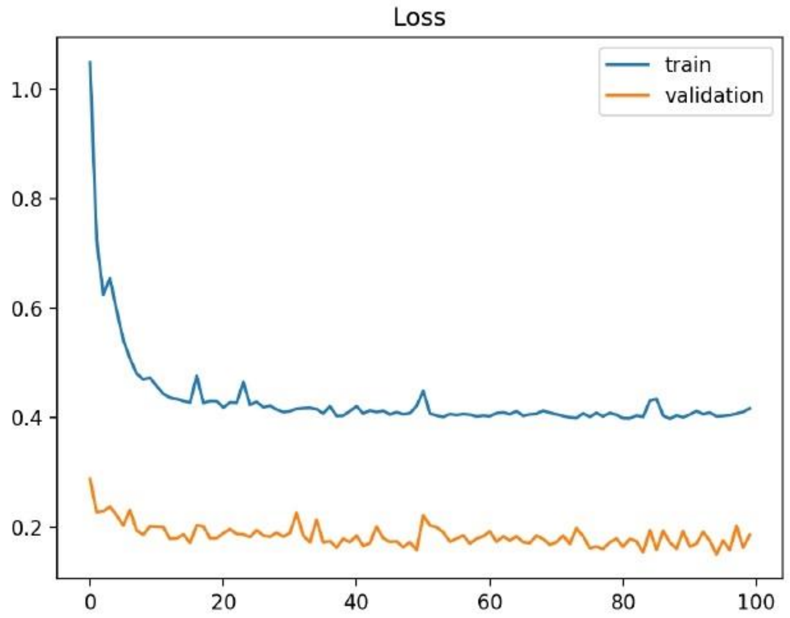


Source: https://machinelearningmastery.com/learning-curves-for-diagnosing-machine-learning-model-performance/

Other Curves



Underfitting (loss still decreasing)



Validation Set is easier than Training set

Source: https://machinelearningmastery.com/learning-curves-for-diagnosing-machine-learning-model-performance/

To Summarize

- Underfitting
  - Training and validation losses decrease even at the end of training
- Overfitting
  - Training loss decreases and validation loss increases
- Ideal Training
  - Small gap between training and validation loss, and both go down at same rate (stable without fluctuations).

To Summarize

- Bad Signs
  - Training error not going down
  - Validation error not going down
  - Performance on validation better than on training set
  - Tests on train set different than during training
- Bad Practice
  - Training set contains test data
  - Debug algorithm on test data

Never touch during development or training

Hyperparameters

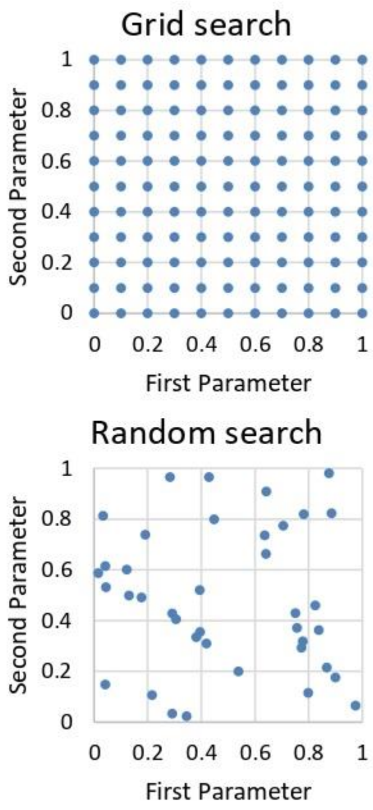
- Network architecture (e.g., num layers, #weights)
- Number of iterations
- Learning rate(s) (i.e., solver parameters, decay, etc.)
- Regularization (more later next lecture)
- Batch size
- …
- Overall:
  learning setup + optimization = hyperparameters

Hyperparameter Tuning

- Methods:
  - **Manual** search:
    - most common ☺
  - **Grid** search (structured, for ‘real’ applications)
    - Define ranges for all parameters spaces and select points
    - Usually pseudo-uniformly distributed

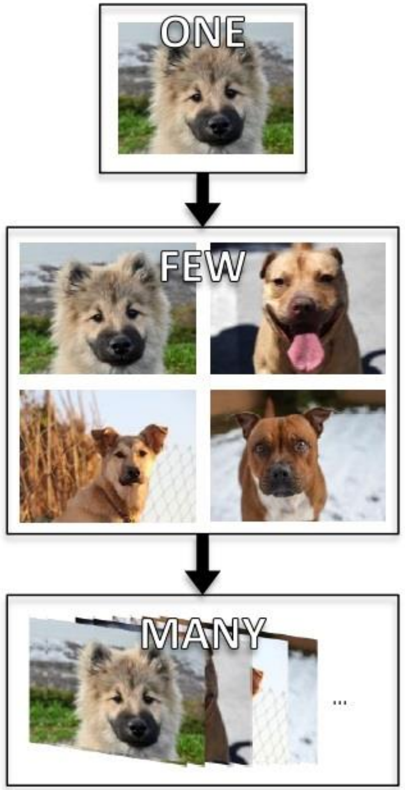
    → Iterate over all possible configurations
  - **Random** search:

    Like grid search but one picks points at random in the predefined ranges



How to Start

- Start with single training sample
  - Check if output correct
  - Overfit → train accuracy should be 100% because input just memorized
- Increase to handful of samples (e.g., 4)
  - Check if input is handled correctly
- Move from overfitting to more samples
  - 5, 10, 100, 1000, …
  - At some point, you should see generalization

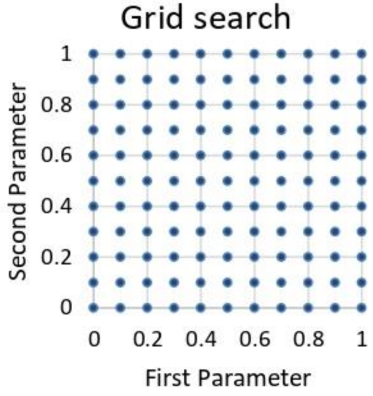


Find a Good Learning Rate

- Use all training data with small weight decay
- Perform initial loss sanity check e.g., $\log(C)$ for softmax with C classes
- Find a learning rate that makes the loss drop significantly (exponentially) within 100 iterations
- Good learning rates to try: 1e-1, 1e-2, 1e-3, 1e-4

Coarse Grid Search

- Choose a few values of learning rate and weight decay around what worked from
- Train a few models for a few epochs.
- Good weight decay to try: 1e-4, 1e-5, 0

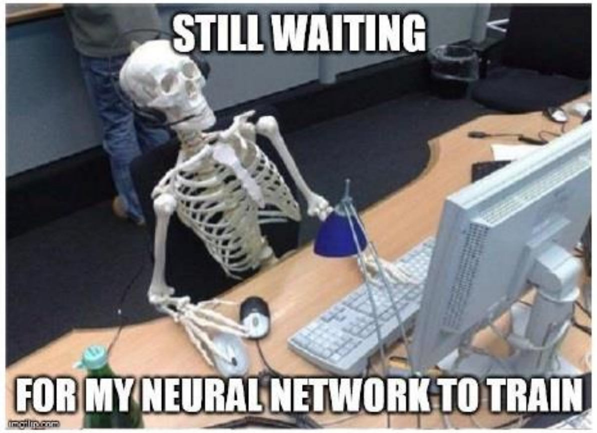


Refine Grid

- Pick best models found with coarse grid.
- Refine grid search around these models.
- Train them for longer (10-20 epochs) without learning rate decay
- Study loss curves <- most important debugging tool!

Timings

- How long does each iteration take?
  - Get **precise** timings!
  - If an iteration exceeds **500**ms, things get dicey
- Look for bottlenecks
  - Dataloading: smaller resolution, compression, train from SSD
  - Backprop
- Estimate total time
  - How long until you see some pattern?
  - How long till convergence?



Network Architecture

- Frequent mistake: "*Let's use this super big network, train for two weeks and we see where we stand.*"

- Instead: start with simplest network possible
  - Rule of thumb divide #layers you started with by 5
- Get debug cycles down
  - Ideally, minutes

Debugging

- Use train/validation/test curves
  - Evaluation needs to be consistent
  - Numbers need to be comparable

- Only make **one change at a time**
  - "I've added 5 more layers and double the training size, and now I also trained 5 days longer. Now it's better, but why?"

Common Mistakes in Practice

- Did not overfit to single batch first
- Forgot to toggle train/eval mode for network
  - Check later when we talk about dropout…
- Forgot to call **.zero_grad()** (*in PyTorch*) before calling **.backward()**
- Passed softmaxed outputs to a loss function that expects raw logits