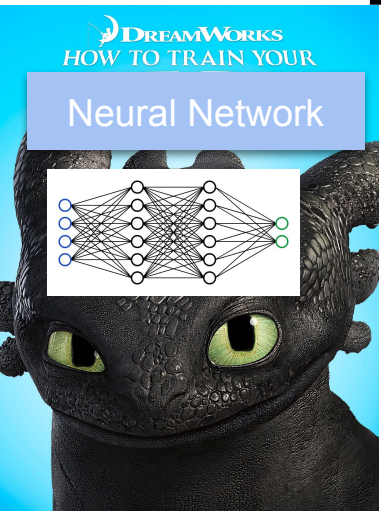
CSC413 Tutorial: Optimization for Machine Learning



"*How to train your neural network*"

Summer Tao

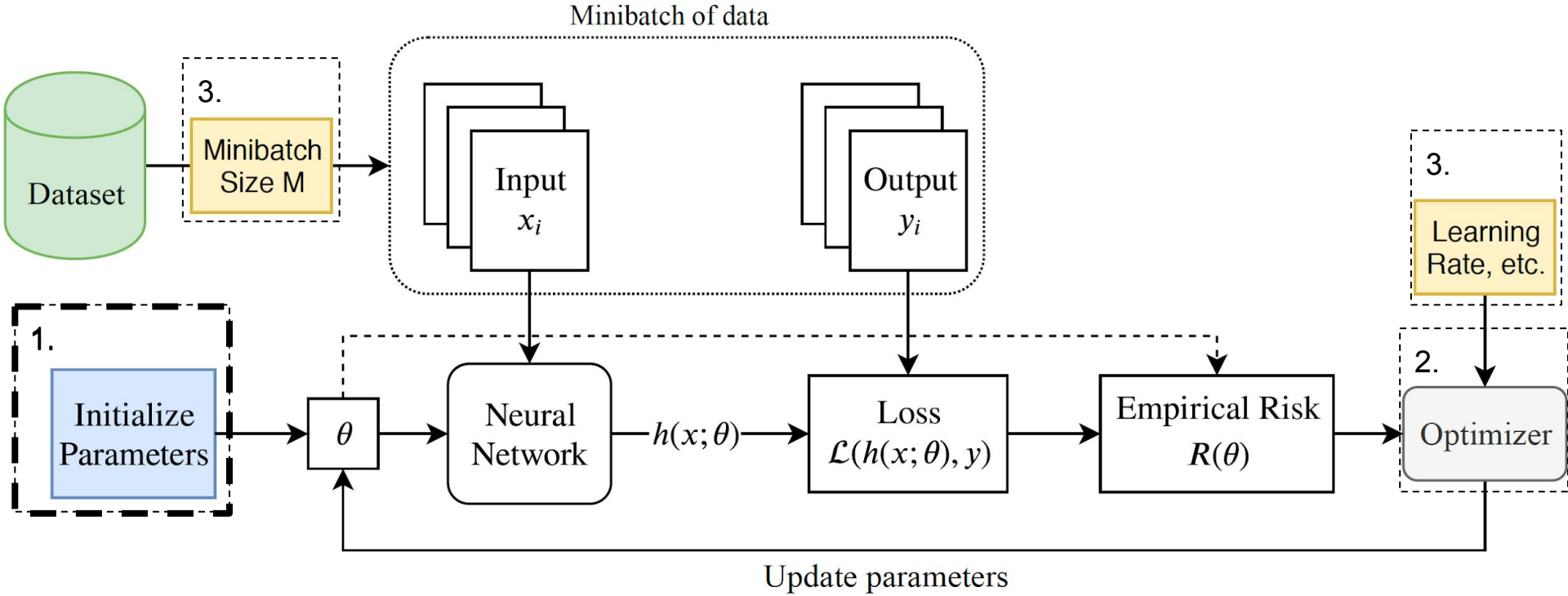
January 28, 2021

[1]Based on tutorials/slides by Harris Chan, Ladislav Rampasek, Jake Snell, Kevin Swersky, Shenlong Wang &

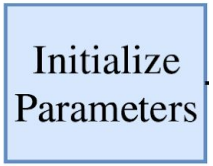
Overview

- Review: Overall Training Loop
- Initialization
- Optimization
    - Gradient Descent
    - Momentum, Nesterov Accelerated Momentum
    - Learning Rate Schedulers: Adagrad, RMSProp, Adam
- Hyperparameter tuning: learning rate, batch size, regularization
- Jupyter/Colab Demo in PyTorch

Neural Network Training Loop



Initialization of Parameters



Initial parameters of the neural network can affect the **gradients** and learning

Idea 1: Constant initialization

- *Result*: For fully connected layers: identical gradients, identical neurons. Bad!

Idea 2: Random weights, to break symmetry

- Too **large** of initialization: **exploding** gradients
- Too **small** of initialization: **vanishing** gradients

Initialization: Calibrate the variance

Initialize Parameters

Two popular initialization schemes:

1: **Xavier** Init: For **Tanh** activation

$$W^{[l]} \sim \mathcal{N}(\mu = 0, \sigma^2 = \frac{1}{n^{[l-1]}})$$

$$b^{[l]} = 0$$

or

$$W^{[l]} \sim \mathcal{N}(0, \frac{2}{n^{[l-1]} + n^{[l]}})$$

$$b^{[l]} = 0$$

2. **Kaiming He** Init: **ReLU** activation

$$W^{[l]} \sim \mathcal{N}(\mu = 0, \sigma^2 = \frac{2}{n^{[l-1]}})$$

$$b^{[l]} = 0$$

# of neurons in layer $l-1$

1: Glorot & Bengio: Understanding the difficulty of training deep feedforward neural networks

2: He et al.: Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification

Initialization: Xavier Initialization Intuition

Initialize Parameters

For networks with **Tanh** activation functions, Xavier Init aim for the following behaviour of the activations:

1. **Variance** of activation **~ constant** across every layer

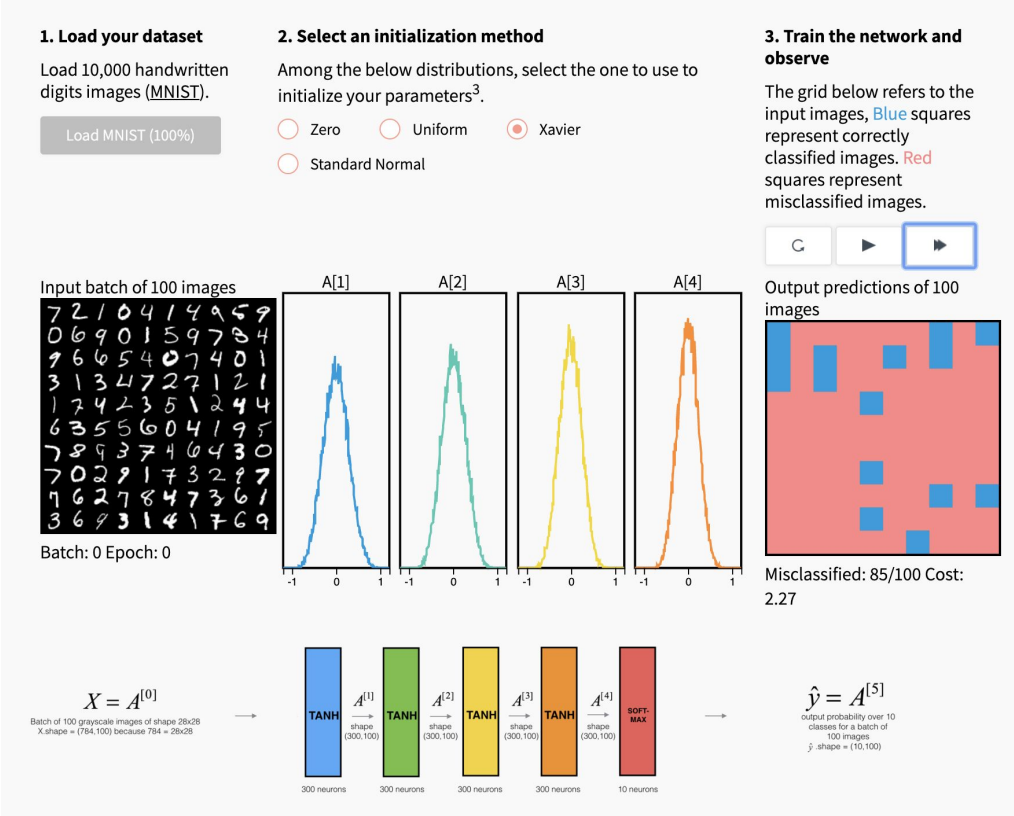
$$\mathrm{Var}(a^l) = \mathrm{Var}(a^{l-1})$$

2. **Mean** of the activation and weights = **zero**

$$\mathbb{E}[w^l] = 0 \qquad \mathbb{E}[a^l] = 0$$

Interactive Demo: Initialization Schemes

Initialize Parameters



Source: Initializing neural networks. https://www.deeplearning.ai/ai-notes/initialization/

Batch Normalization Layer

Initialize Parameters

Can we compensate for bad initializations in some other way?

BatchNorm's Idea:

- Explicitly normalize the activations of each layer to be unit Gaussian.
- Apply immediately *after* fully connected/conv layers and *before* non-linearities
- Learn an additional **scale** and **shift** and running statistics for test time

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β
Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

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

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

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

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

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

Ioffe & Szegedy: Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift

Batch Normalization Layer

Initialize Parameters

- BatchNorm significantly speeds up training in practice (Fig 1a)
- Distribution after connected layer is much more stable with BN, reducing the "**internal covariate shift**", **i.e.** *the change in the distribution of network activations due to the change in network parameters during training*

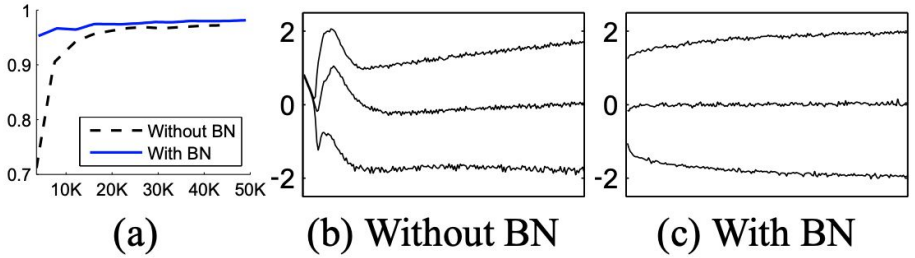
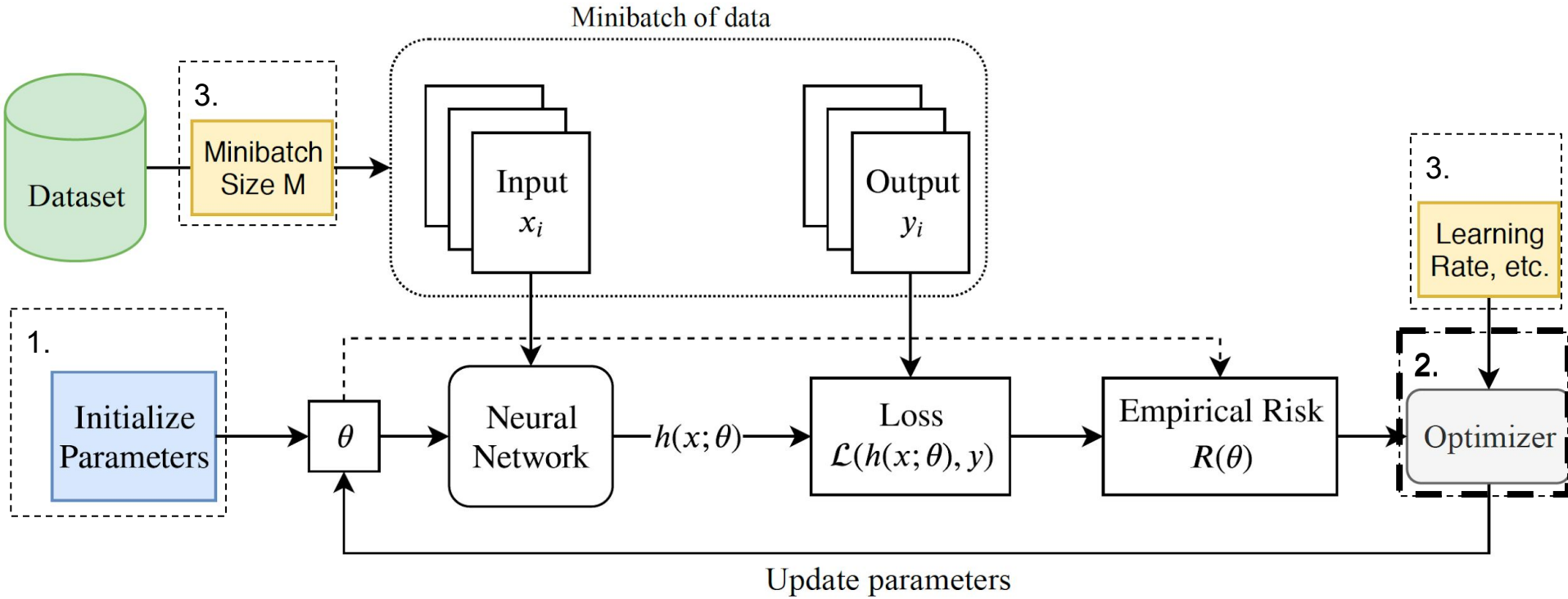


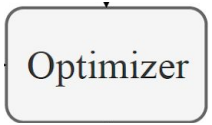
Figure 1: (a) *The test accuracy of the MNIST network trained with and without Batch Normalization, vs. the number of training steps. Batch Normalization helps the network train faster and achieve higher accuracy.* (b, c) *The evolution of input distributions to a typical sigmoid, over the course of training, shown as* $\{15, 50, 85\}$*th percentiles. Batch Normalization makes the distribution more stable and reduces the internal covariate shift.*

Ioffe & Szegedy: Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift

Neural Network Training Loop



Optimization: Formal definition



- Given a training set: $\{(x_1, y_1), \ldots, (x_n, y_n)\}$
- Prediction function: $h(x; \theta)$
- Define a loss function: $\mathcal{L}(h(x; \theta), y)$
- Find the parameters: $\theta = (\theta_1, \ldots, \theta_k)$
  which minimizes the **empirical risk** $R(\theta)$:

$$\min_\theta R(\theta) = \min_\theta \frac{1}{n} \sum_i^n \mathcal{L}(h(x_i; \theta), y_i)$$

Optimization: Formal definition

Optimizer

- **Empirical risk** $R(\theta)$:

$$\min_\theta R(\theta) = \min_\theta \frac{1}{n} \sum_i^n \mathcal{L}(h(x_i;\theta), y_i)$$

- The optimum satisfies: $\boxed{\nabla R(\theta^*) = 0}$
- Where $$\nabla R(\theta) = \left(\frac{\partial R}{\partial \theta_1}, \frac{\partial R}{\partial \theta_2}, \ldots, \frac{\partial R}{\partial \theta_k}\right)$$
- Sometimes the equation has closed-form solution (e.g. linear regression)

Optimization: Batch Gradient Descent

Optimizer

Batch Gradient Descent:

- Initialize the parameters randomly
- For each iteration, do until convergence:

$$\theta^{(k+1)} = \theta^{(k)} - \eta \nabla R(\theta^{(k)})$$

$\eta \in \mathbb{R}^+$ Learning rate (a small step)

Gradient Descent

Optimizer

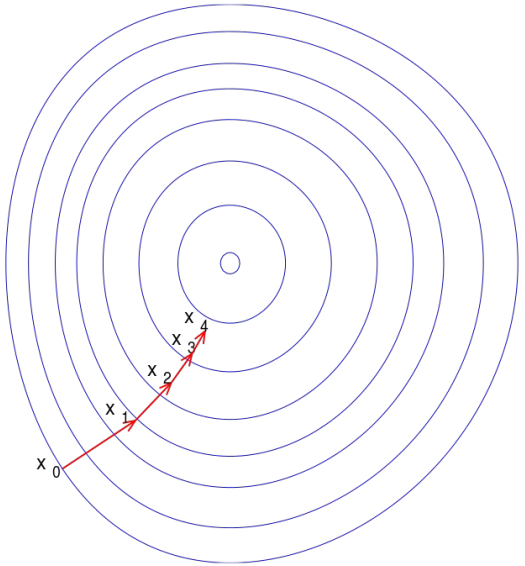
Geometric interpretation:

- Gradient is perpendicular to the tangent of the level set curve
- Given the current point, negative gradient direction decreases the function fastest

Alternative interpretation:

- Minimizing the first-order taylor approx of f keep the new point close to the current point

$$f(x^t) + \nabla f(x^t)^T (x - x^t) + \frac{1}{2\eta} ||x - x^t||_2^2$$



Source: Wikipedia

Stochastic Gradient Descent

Optimizer

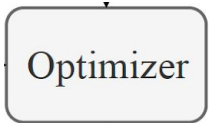
- Initialize the parameters randomly
- For each iteration, do until convergence:
  - Randomly select a training sample i (or a small subset of the training samples)
  - Conduct gradient descent:

$$\theta^{(k+1)} = \theta^{(k)} - \eta \nabla f_i(\theta^{(k)})$$

- **Intuition**: A noisy approximation of the gradient of the whole dataset
- **Pro**: each update requires a small amount of training data, good for training algorithms for a large-scale dataset

- **Tips**
  - Subsample *without* replacement so that you visit each point on each pass through the dataset ("epoch")
  - Divide the log-likelihood estimate by the size of mini-batches, making learning rate invariant to the mini-batch size.

Gradient Descent with Momentum



- Initialize the parameters randomly
- For each iteration, do until convergence:
  - Update the momentum

$$\delta^{(k+1)} = -\eta \nabla R(\theta^{(k)}) + \alpha \delta^{(k)}$$

  - Conduct gradient descent:

$$\theta^{(k+1)} = \theta^{(k)} + \delta^{(k+1)}$$

- **Pro**: “accelerate” learning by accumulating some “velocity/momentum” using the past gradients

Nesterov Accelerated Gradient

Optimizer

- Initialize the parameters randomly
- For each iteration, do until convergence:
  - Update the momentum

$$\delta^{(k+1)} = -\eta \nabla R(\theta^{(k)} + \alpha\delta^{(k)}) + \alpha\delta^{(k)}$$

  - Conduct gradient descent:

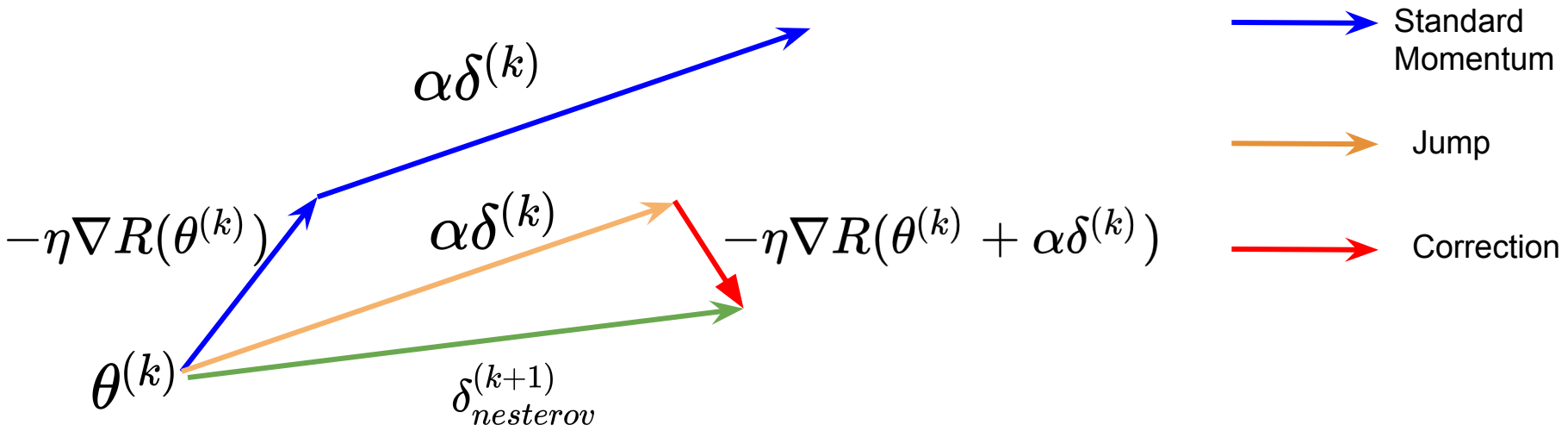
$$\theta^{(k+1)} = \theta^{(k)} + \delta^{(k+1)}$$

- **Pro**: Look into the future to see how much momentum is required

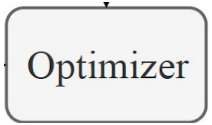
Nesterov Accelerated Gradient

Optimizer

- **First** make a big jump in the direction of the previous accumulated gradient
- **Then** measure the gradient where you end up and make a correction



Learning Rate Schedulers



What if we want to be able to have a **per-parameter learning rate**?

- Certain parameter may be more sensitive (i.e. have higher curvature)

Learning Rate Schedulers: Adagrad

Optimizer

- Initialize the parameters randomly
- For each iteration, do until convergence:
  - Conduct gradient descent on i-th parameter:

$$\theta_{k+1,i} = \theta_{k,i} - \frac{\eta}{\sqrt{G_{k,i} + \epsilon}} \cdot \nabla R(\theta_{k,i})$$

$$G_{k,i} = G_{k-1,i} + (\nabla R(\theta_{k,i}))^2$$

Intuition: It increases the learning rate for more sparse features and decreases the learning rate for less sparse ones, according to the history of the gradient

Learning Rate Schedulers: RMSprop/Adadelta

Optimizer

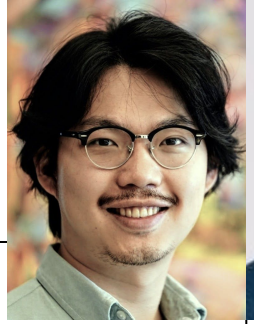
- Initialize the parameters randomly
- For each iteration, do until convergence:
  - Conduct gradient descent on i-th parameter:

$$\theta_{k+1,i} = \theta_{k,i} - \frac{\eta}{\sqrt{G_{k,i} + \epsilon}} \cdot \nabla R(\theta_{k,i})$$

$$G_{k,i} = \gamma\, G_{k-1,i} + (1-\gamma)\left(\nabla R(\theta_{k,i})\right)^2$$

Intuition: Unlike Adagrad, the denominator places a significant weight on the most recent gradient. This also helps avoid decreasing learning rate too much.

Learning Rate Schedulers: Adam



Optimizer

- Initialize the parameters randomly
- For each iteration, do until convergence:
  - Conduct gradient descent on i-th parameter:

$$\theta^{(k+1),i} = \theta^{(k,i)} + \frac{\eta \cdot \hat{m}^{(k,i)}}{\sqrt{\hat{G}^{(k,i)} + \epsilon}} \cdot \nabla R(\theta^{(k,i)})$$

$$G^{(k,i)} = \gamma G^{(k-1,i)} + (1-\gamma)(\nabla R(\theta^{(k,i)}))^2$$

$$m^{(k,i)} = \alpha m^{(k-1,i)} + (1-\alpha)\nabla R(\theta^{(k,i)})$$

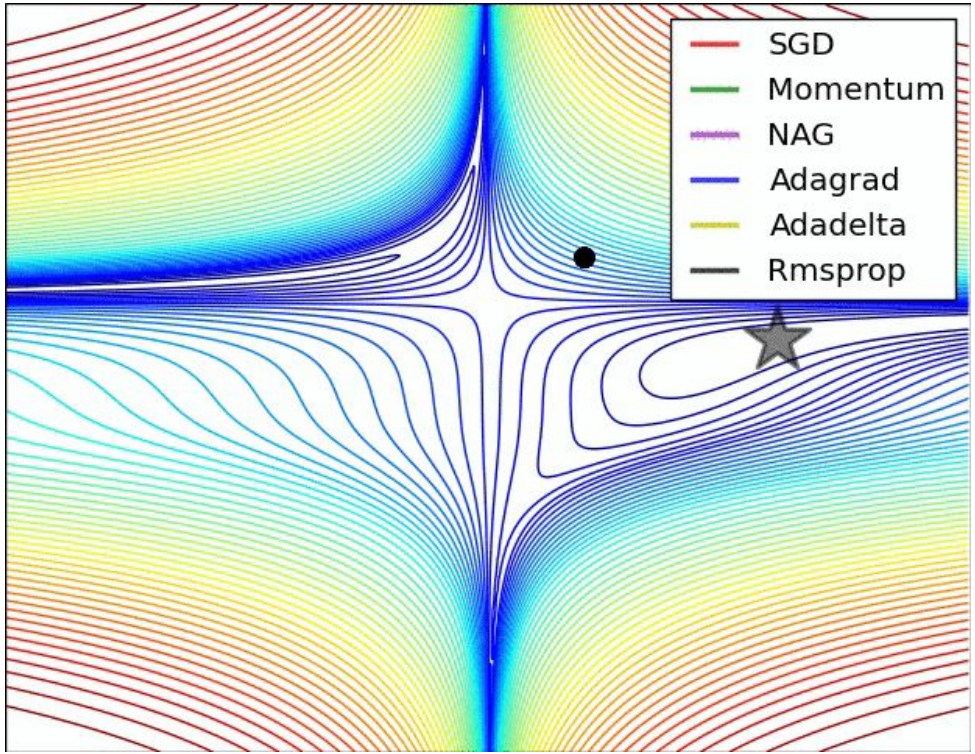
$$\hat{m}^{(k,i)} = \frac{m^{(k,i)}}{1-\alpha^t}$$

$$\hat{G}^{(k,i)} = \frac{G^{(k,i)}}{1-\gamma^t}$$

Bias-corrected forms of $m^{(k,i)}$, $G^{(k,i)}$

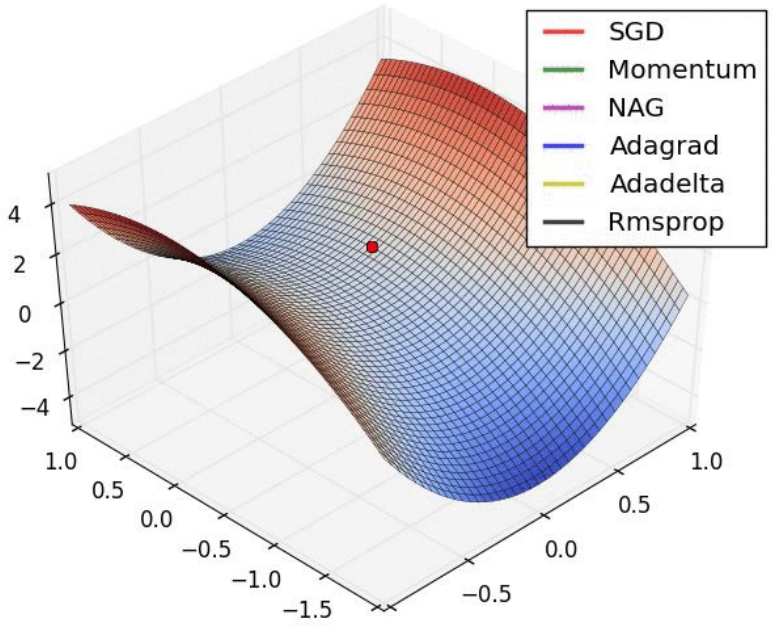
TITLE		CITED BY	YEAR
Adam: A method for stochastic optimization D Kingma, J Ba International Conference on Learning Representation	Paper Link	36831	2015

Optimizers Comparison (excluding Adam)



SGD optimization on loss surface contours

Optimizer



SGD optimization on loss surface contours

Source: Sebastian Ruder, https://ruder.io/optimizing-gradient-descent/, Image: Alec Radford

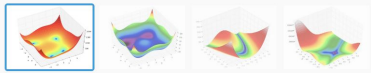
Interactive Demo: Optimizers

Optimizer

In this visualization, you can compare optimizers applied to different cost functions and initialization. For a given cost landscape (**1**) and initialization (**2**), you can choose optimizers, their learning rate and decay (**3**). Then, press the play button to see the optimization process (**4**). There's no explicit model, but you can assume that finding the cost function's minimum is equivalent to finding the best model for your task.

1. Choose a cost landscape

Select an artificial landscape $\mathcal{J}(w_1, w_2)$.



2. Choose initial parameters

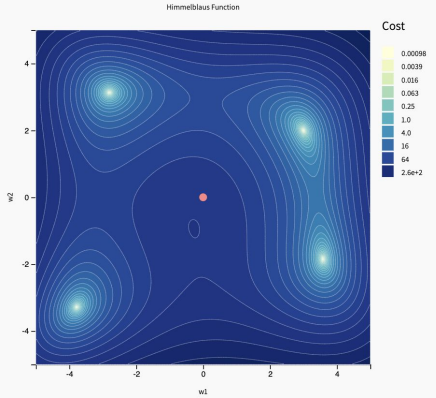
On the cost landscape graph, drag the red dot to choose initial parameter values and thus the initial value of the cost.

3. Choose an optimizer

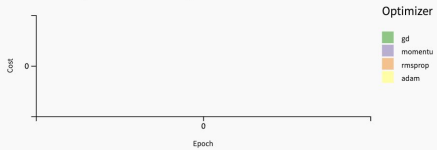
Select the optimizer(s) and hyperparameters.

Optimizer	Learning Rate	Learning Rate Decay
☑ Gradient Descent	0.001	0
☑ Momentum	0.001	0
☑ RMSprop	0.001	0
☑ Adam	0.001	0

This 2D plot describes the cost function's value for different values of the two parameters (w_1, w_2). The lighter the color, the smaller the cost value.

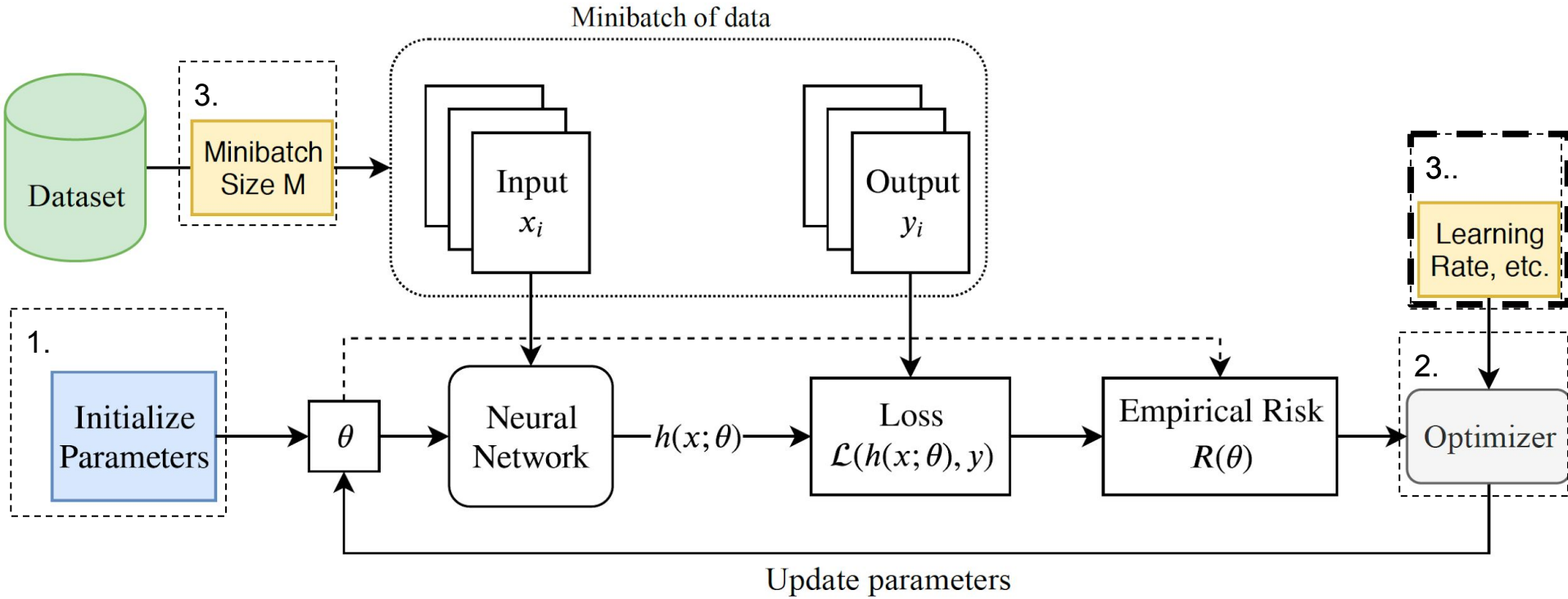


The graph below shows how the value of the cost changes through successive epochs for each optimizer.



Source: Parameter optimization in neural networks: https://www.deeplearning.ai/ai-notes/optimization/

Neural Network Training Loop



Learning Rate

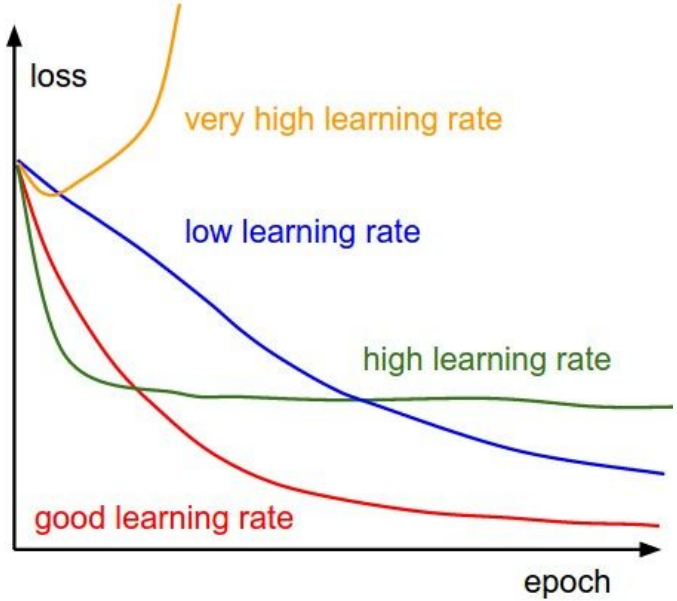
Learning Rate, etc.

Ideal Learning Rate should be:

- Should not be too big (objective will blow up)
- Should not be too small (takes longer to converge)

Convergence criteria:

- Change in objective function is close to zero
- Gradient norm is close to zero
- Validation error starts to increase (early-stopping)



Idealized cartoon depiction of different learning rates.

Image Credit: Andrej Karpathy

Learning Rate: Decay Schedule

Learning Rate, etc.

Anneal (decay) learning rate over time so the parameters can settle into a local minimum. Typical decay strategies:

1. **Step Decay**: reduce by factor every few epochs (e.g. a half every 5 epochs, or by 0.1 every 20 epochs), or when validation error stops improving
2. **Exponential Decay:** Set learning rate according to the equation

$$\eta(t) = \eta_0 e^{-kt}$$

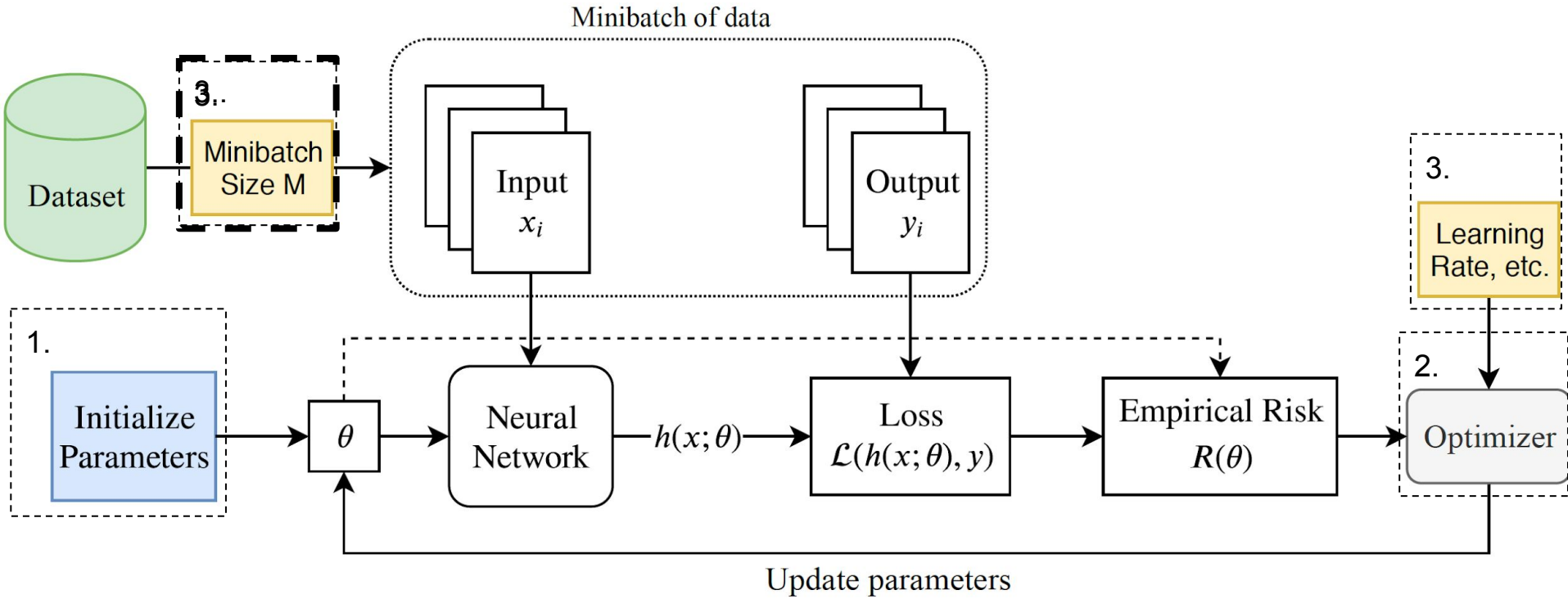
Iteration number

Hyperparam

3. **1/t decay:**

$$\eta(t) = \frac{\eta_0}{1+kt}$$

Neural Network Training Loop



Batch Size

Minibatch Size M

Batch Size: the number of training data points for computing the empirical risk at each iteration.

- Typical small batches are powers of 2: 32, 64, 128, 256, 512,
- Large batches are in the thousands

Large Batch Size has:

- **Fewer frequency of updates**
- More **accurate** gradient
- More **parallelization** efficiency / accelerates wallclock training
- **May hurt generalization,** perhaps by causing the algorithm to find poorer local optima/plateau.

Batch Size

Minibatch Size M

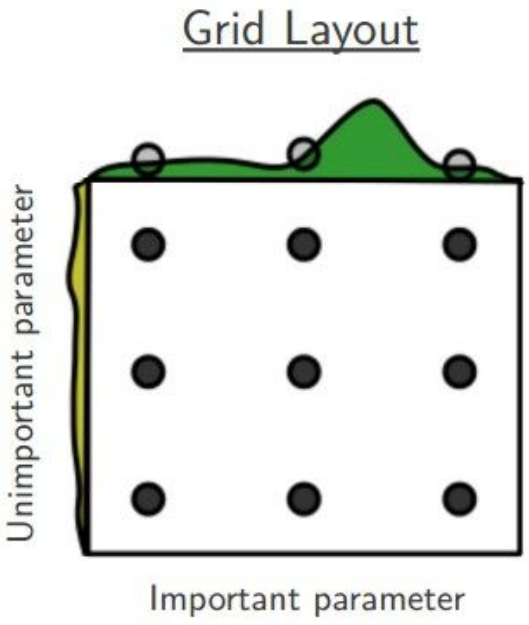
Related papers on batch size:

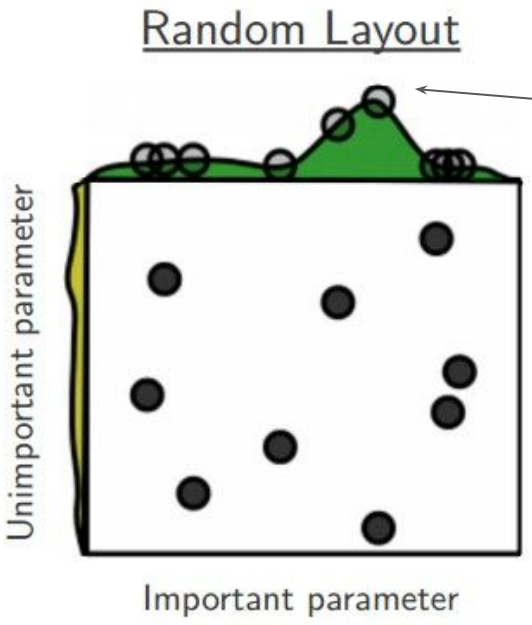
- Goyal et al., Accurate, large minibatch SGD
  - Proposes to increase the learning rate by of the minibatch size
- Hoffer et al., Train longer generalize better
  - Proposes to increase the learning rate by **square root** of the minibatch size
- Smith et al., Don't decay the learning rate, increase the batch size
  - Increasing batch size reduce noise, while maintaining same step size

Hyperparameter Tuning

Minibatch Size M

Several approaches for tuning multiple hyperparameters together:





Prefer **random search** over grid search, higher chance of finding better performing hyper param

Image source: [Random Search for Hyper-Parameter Optimization]

Hyperparameter Tuning

Search hyperparameter on **log scale:**

- `learning_rate = 10 ** uniform(-6, 1)`
  - Learning rate and regularization strength have multiplicative effects on the training dynamics
- Start from coarse ranges then narrow down, or expand range if near the boundary of range

One validation fold vs cross-validation:

- Simplifies code base to just use one (sizeable) validation set vs doing cross validation

Jupyter/Colab Demo in PyTorch

See Colab notebook

References

- Notes and tutorials from other courses:
  - ECE521 (Winter 2017) tutorial on Training neural network
  - Stanford's CS231n notes on Stochastic Gradient Descent, Setting up data and loss, and Training neural networks
  - Deeplearning.ai's interactive notes on Initialization and Parameter optimization in neural networks
  - Jimmy Ba's Talk for Optimization in Deep Learning at Deep Learning Summer School 2019
- Academic/white papers:
  - SGD tips and tricks from Leon Bottou
  - Efficient BackProp from Yann LeCun
  - Practical Recommendations for Gradient-Based Training of Deep Architectures from Yoshua Bengio