MAE 688: Machine Learning for Mechanical Engineers

Lecture 4 - Training network: Maxout, Learning Rate, Momentum and Dropout

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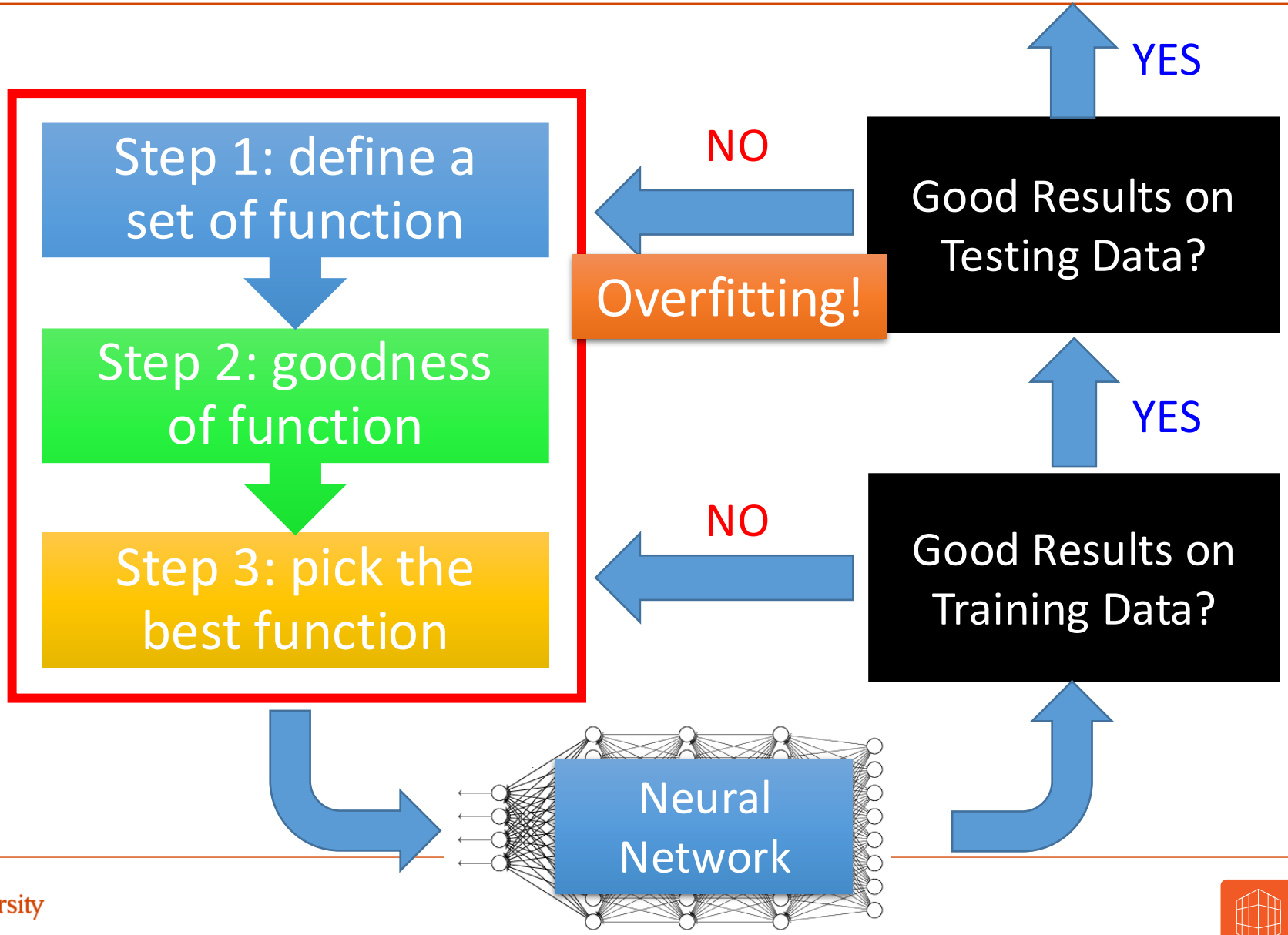
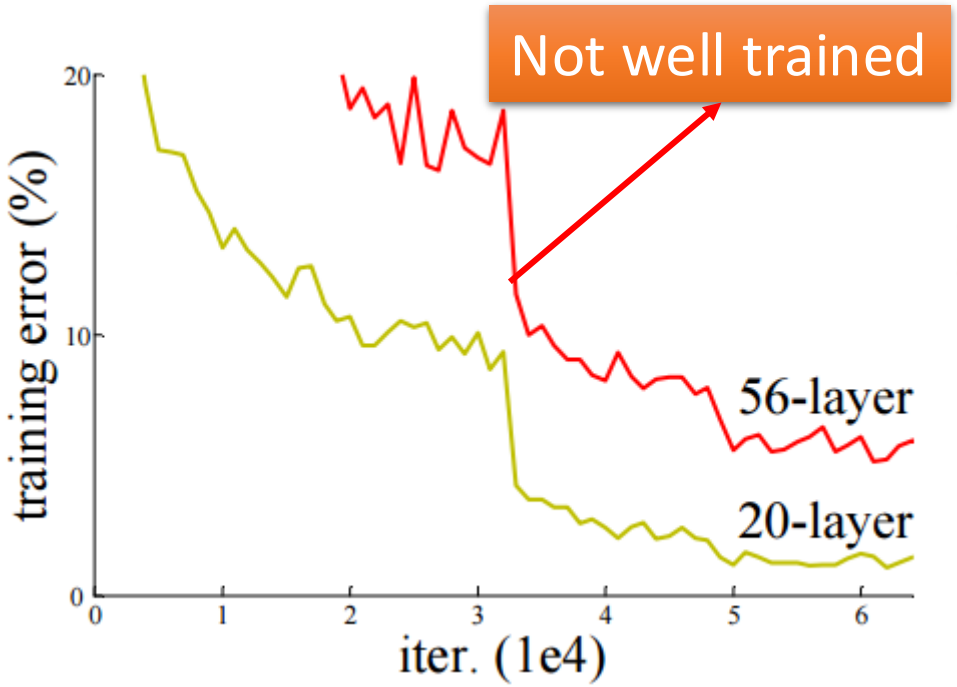
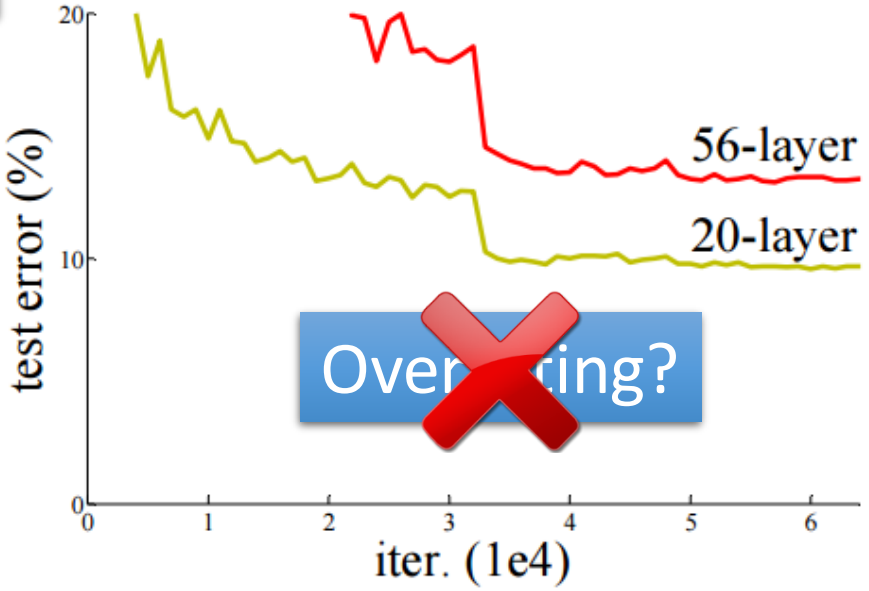
Recipe of Deep Learning



Do not always blame overfitting

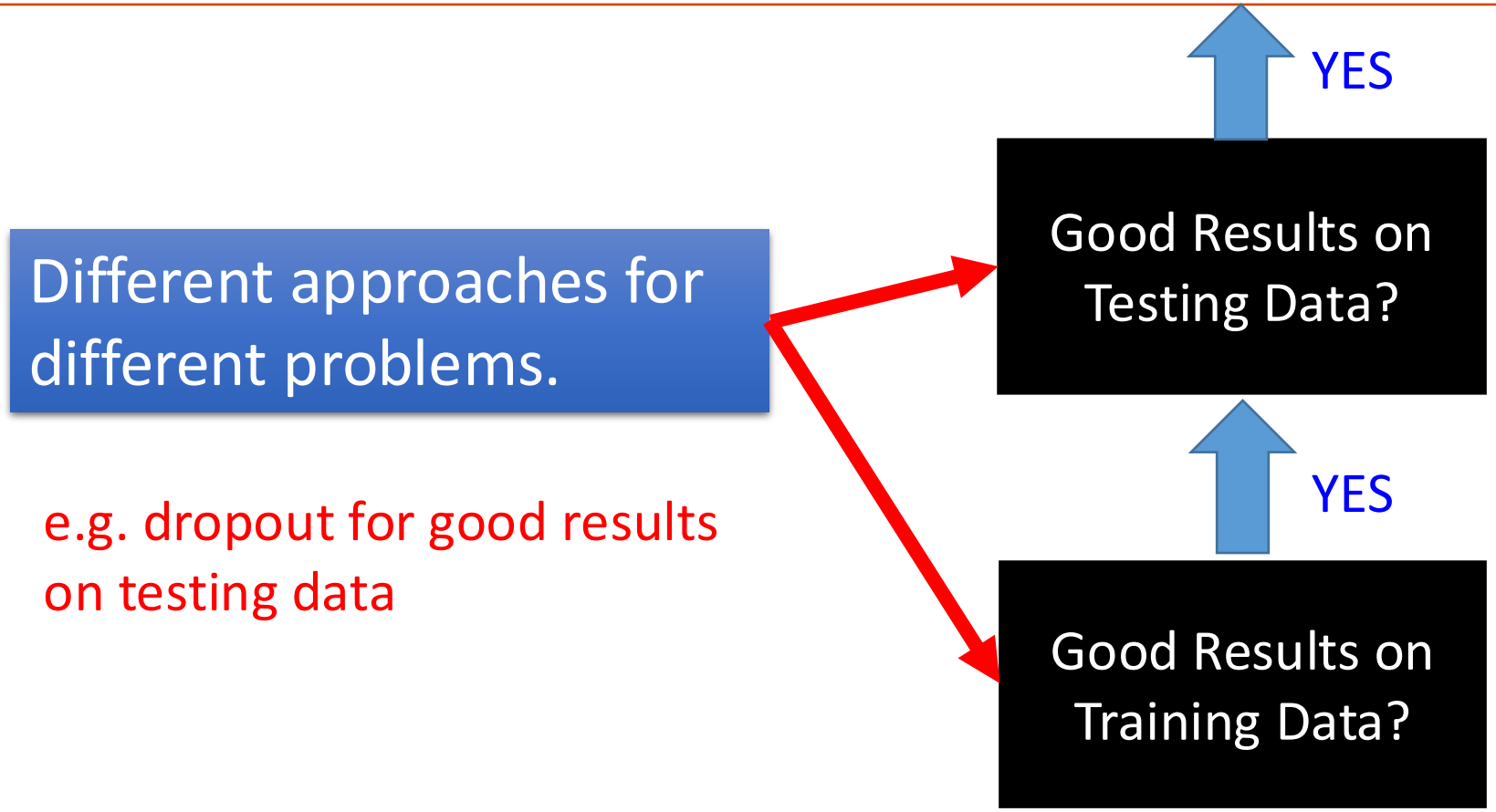


Training Data



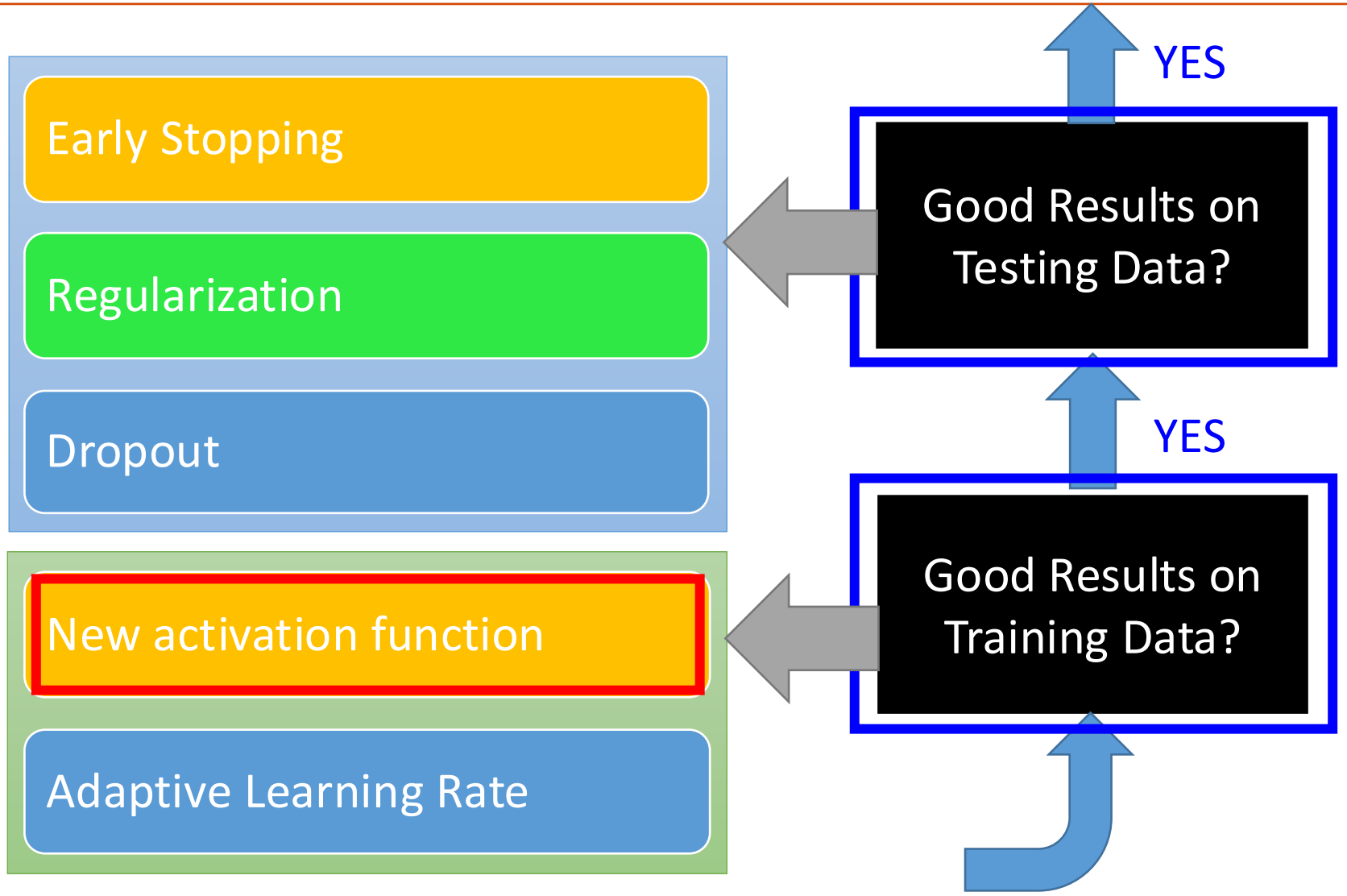
Testing Data

Recipe of Deep Learning

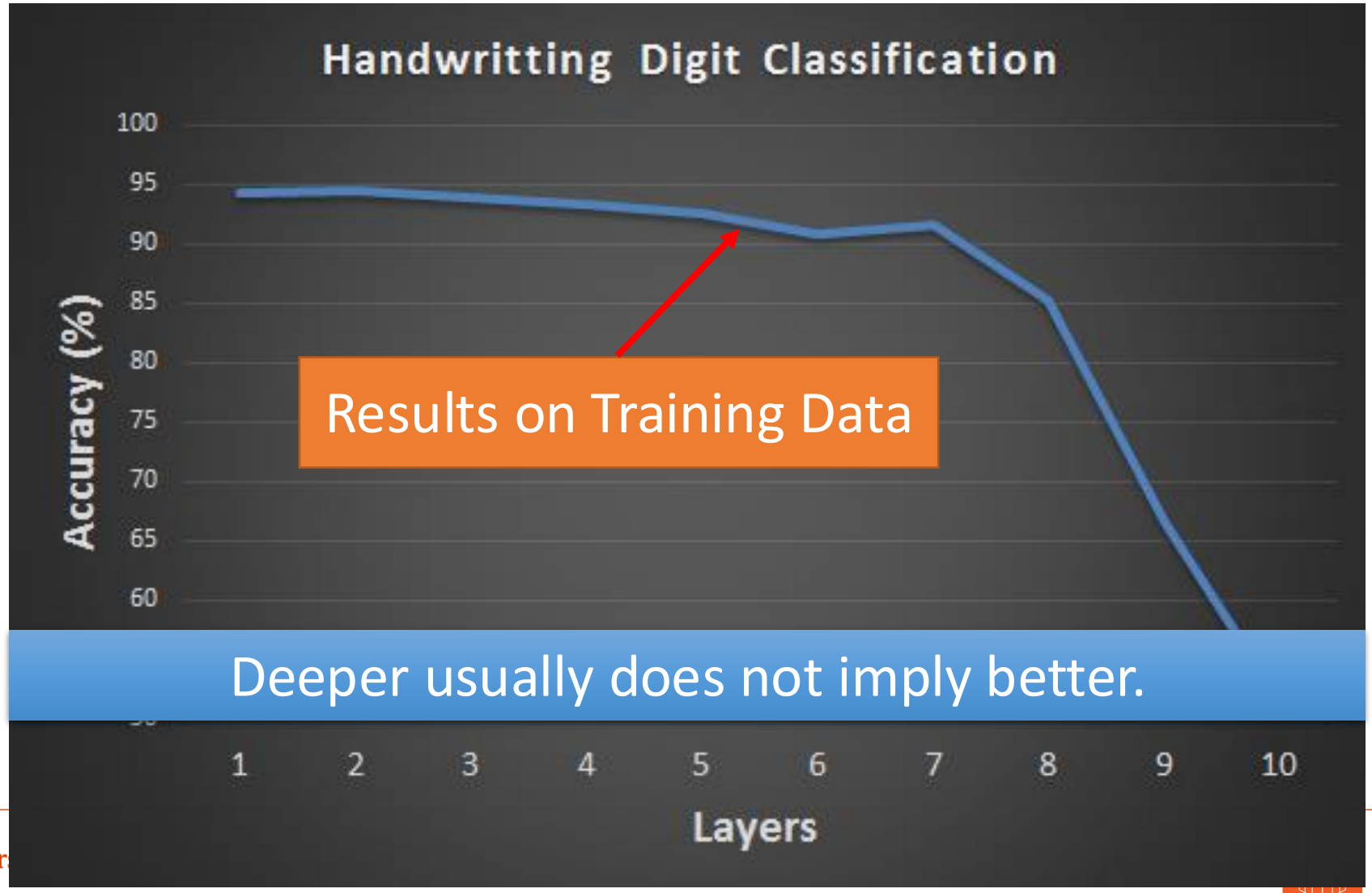


Maxout

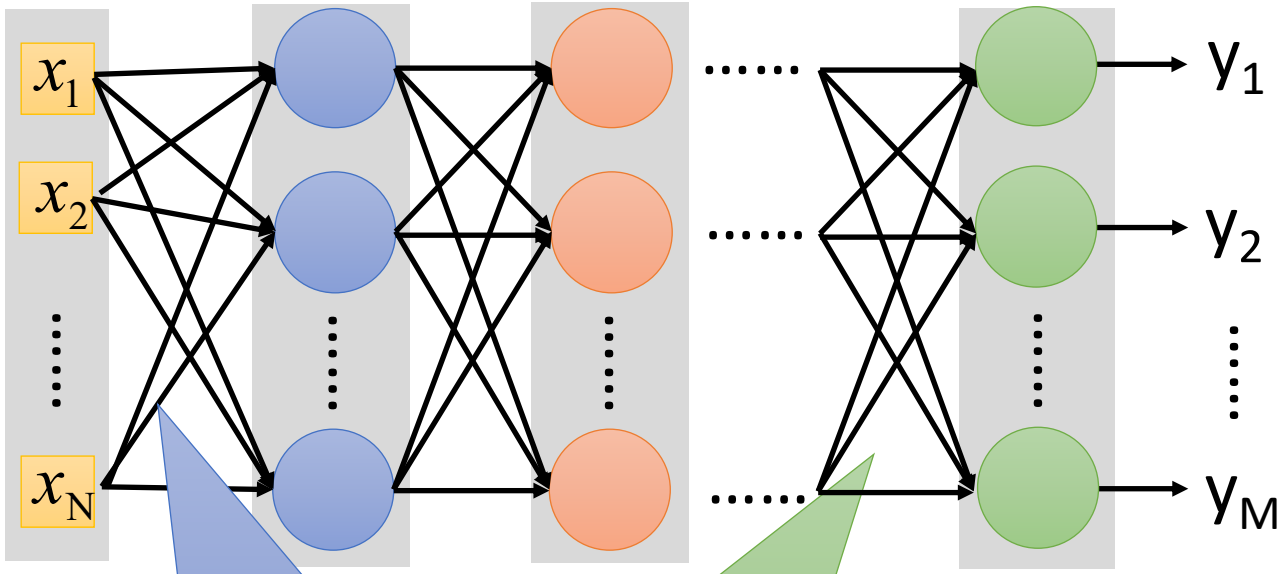
Recipe of Deep Learning



Hard to get the power of deep…



Vanishing Gradient Problem



Smaller gradients

Learn very slow

Almost random

Larger gradients

Learn very fast

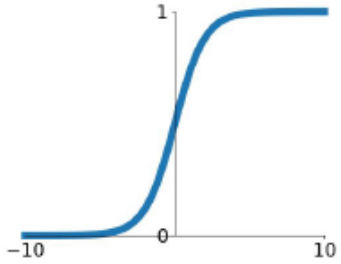
Already converge

based on random!?

Activation Functions

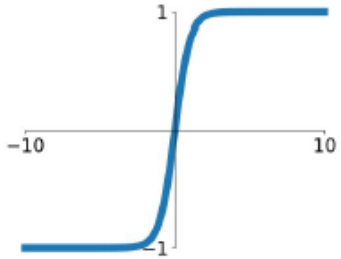
Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



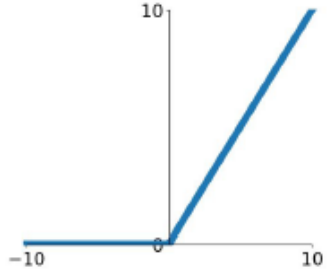
tanh

$$\tanh(x)$$



ReLU

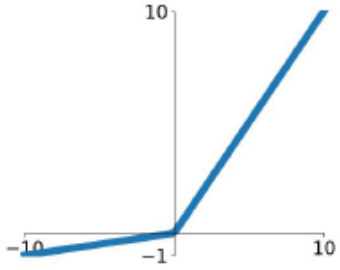
$$\max(0, x)$$



Rectified Linear Unit

Leaky ReLU

$$\max(0.1x, x)$$

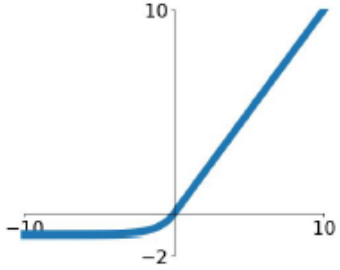


Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$

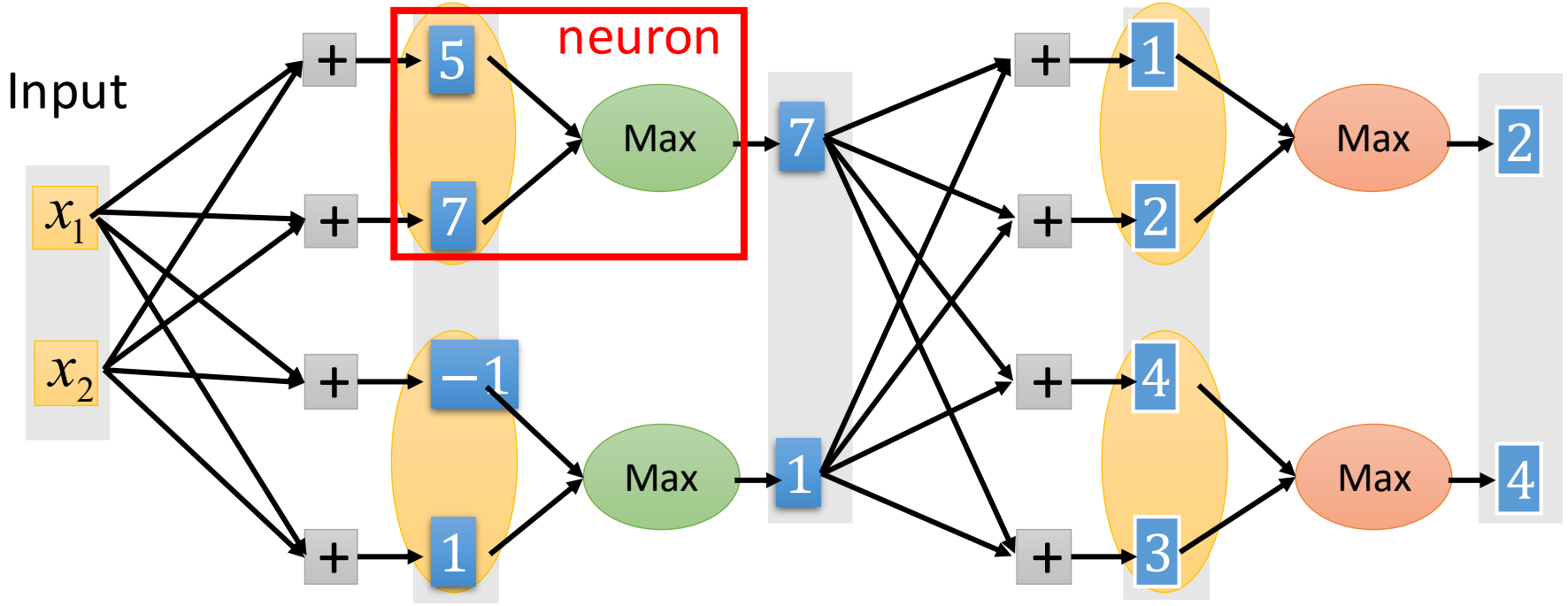


Exponential Linear Units

Maxout

ReLU is a special cases of Maxout

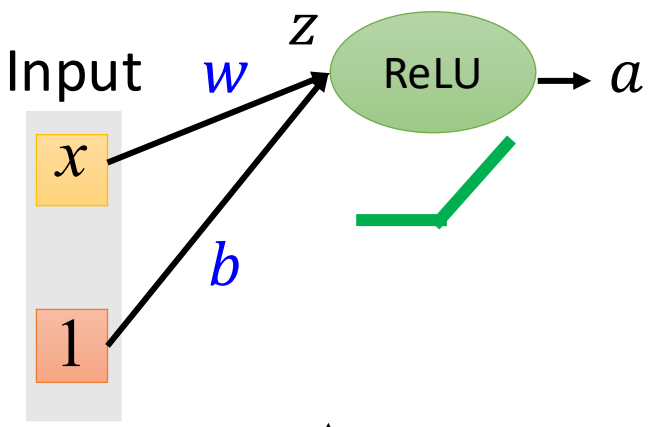
Learnable activation function [Ian J. Goodfellow, ICML'13]

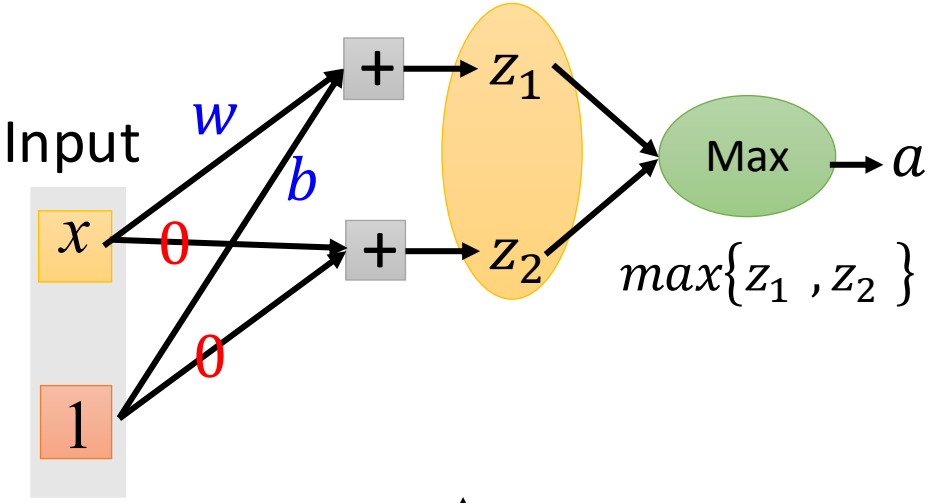


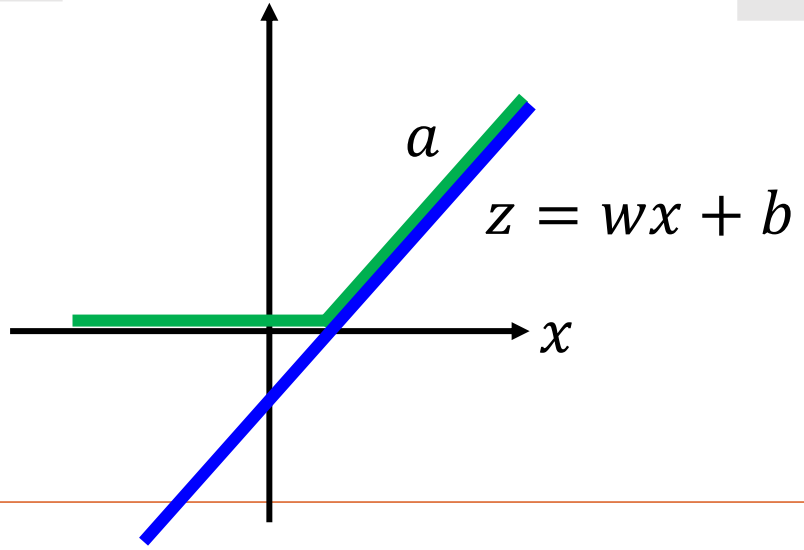
You can have more than 2 elements in a group.

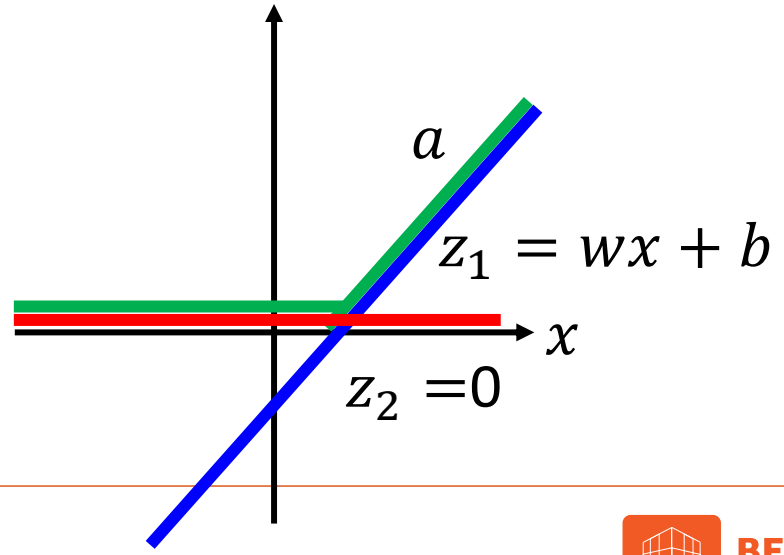
Maxout

ReLU is a special cases of Maxout



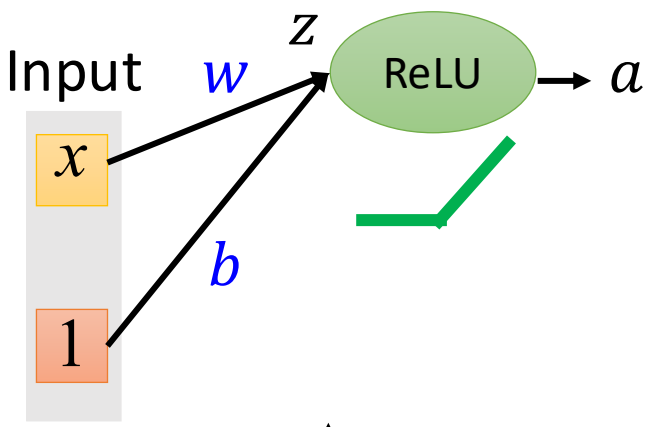


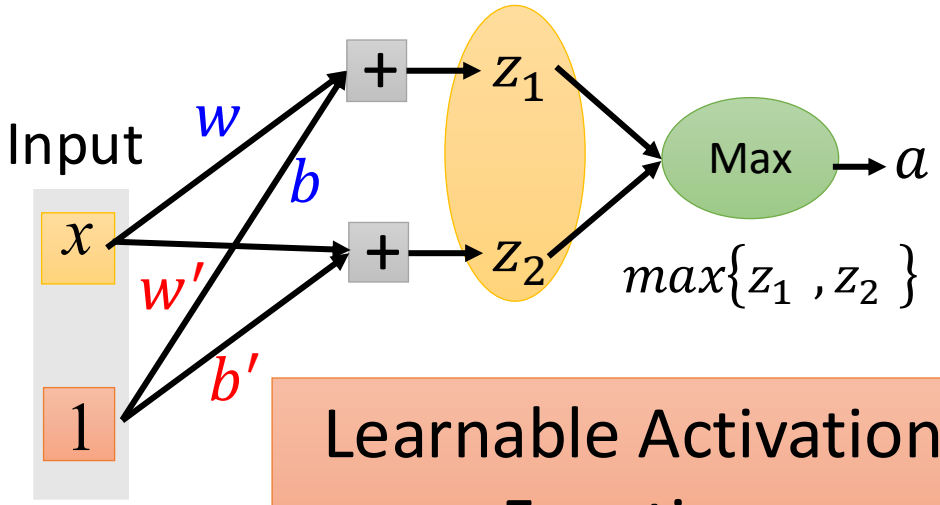




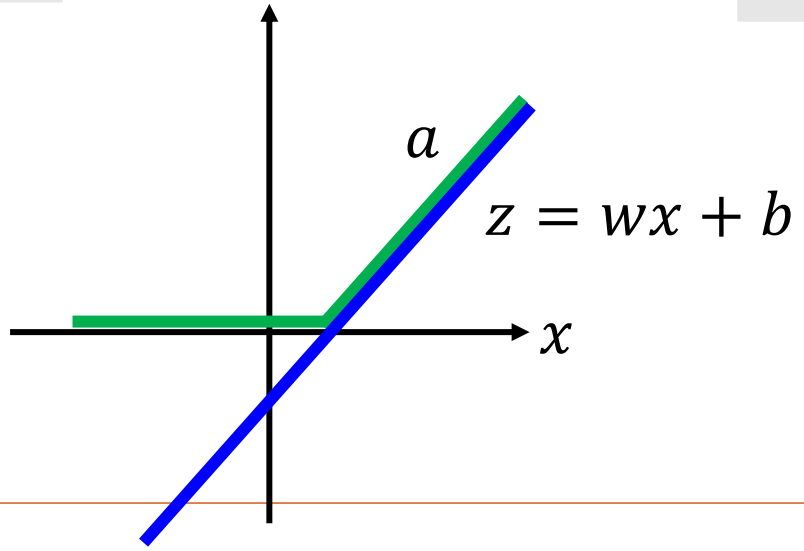
Maxout

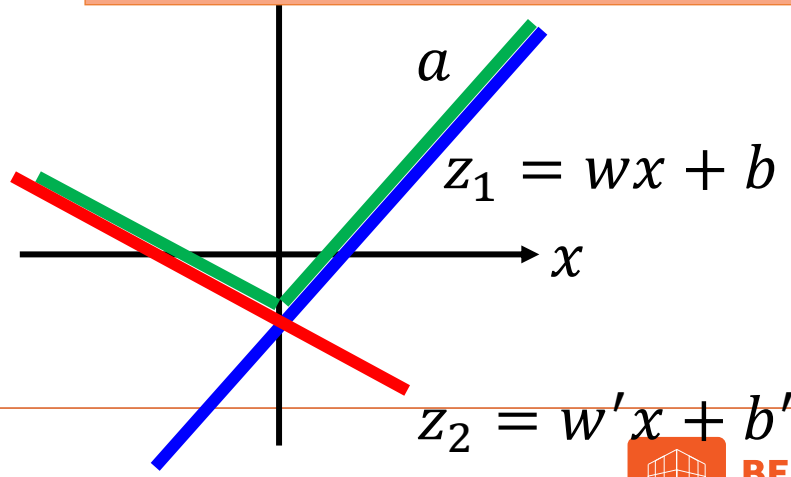
More than ReLU





Learnable Activation Function

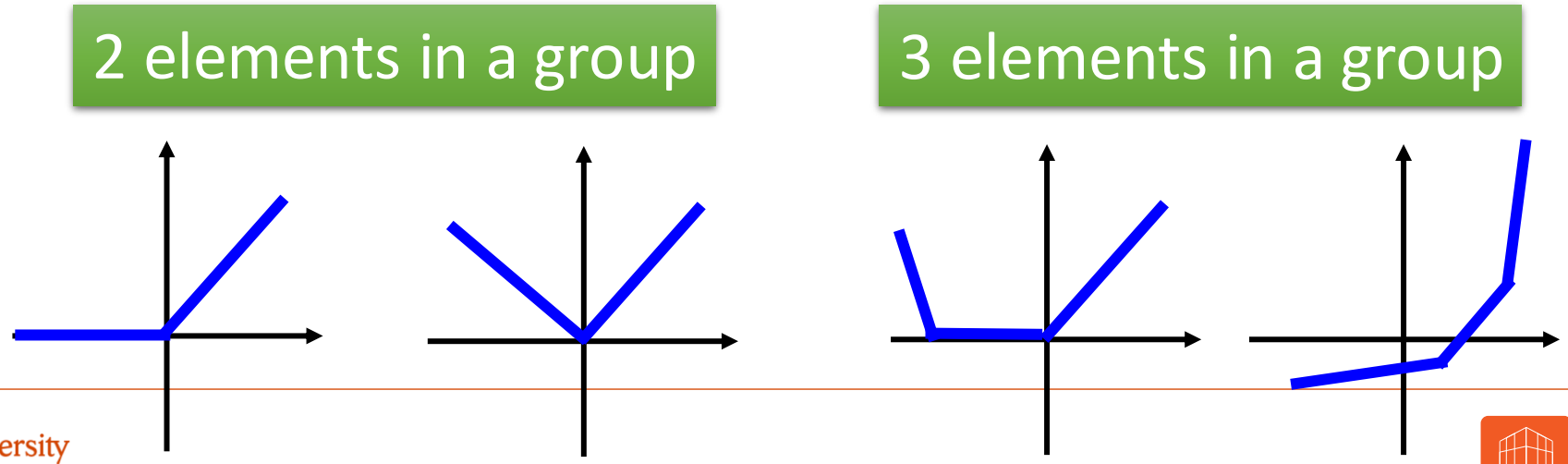




Maxout

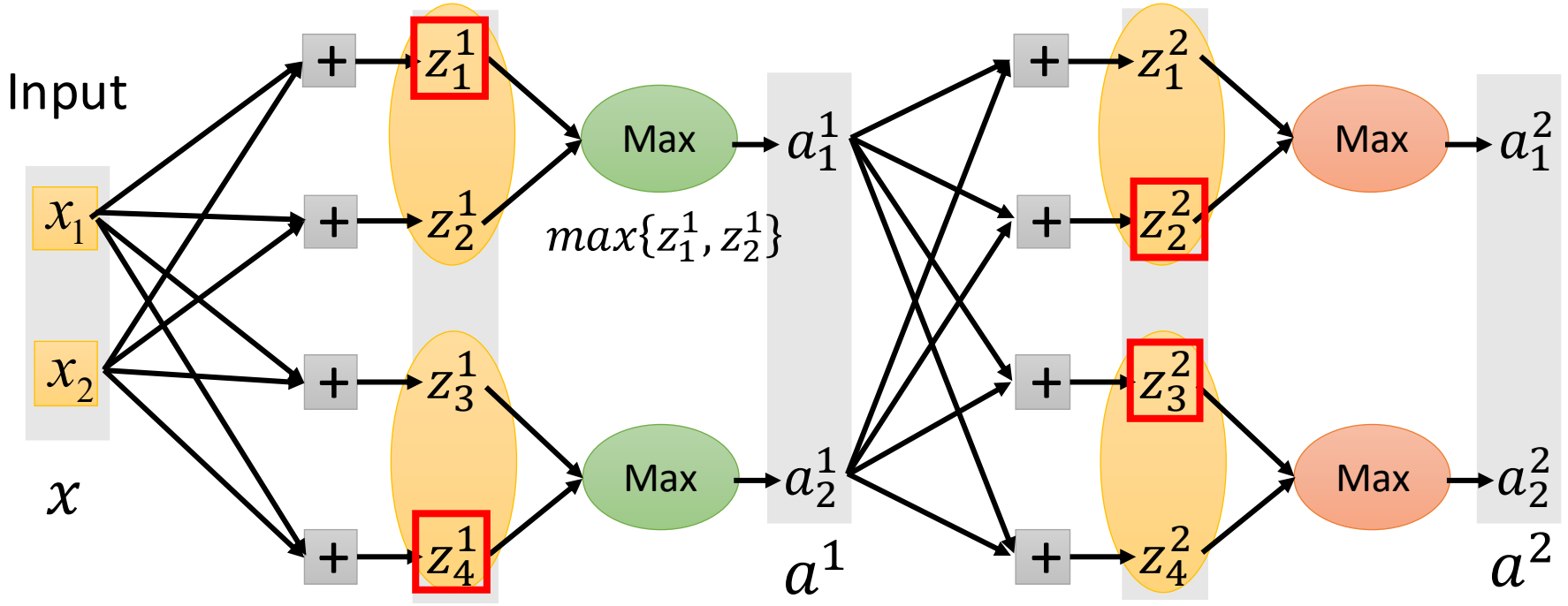
Learnable activation function [Ian J. Goodfellow, ICML'13]

- Activation function in maxout network can be any piecewise linear convex function
- How many pieces depending on how many elements in a group



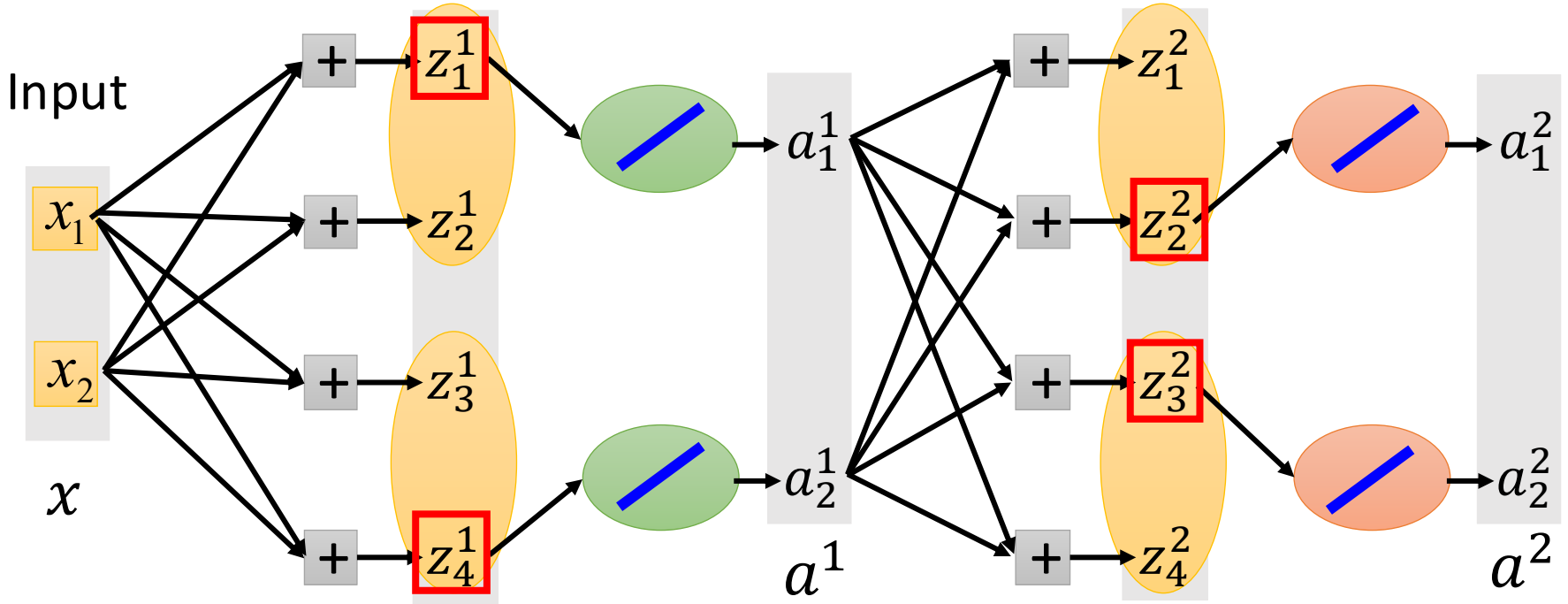
Maxout- Training

Given a training data x, we know which z would be the max



Maxout

- Given a training data x, we know which z would be the max

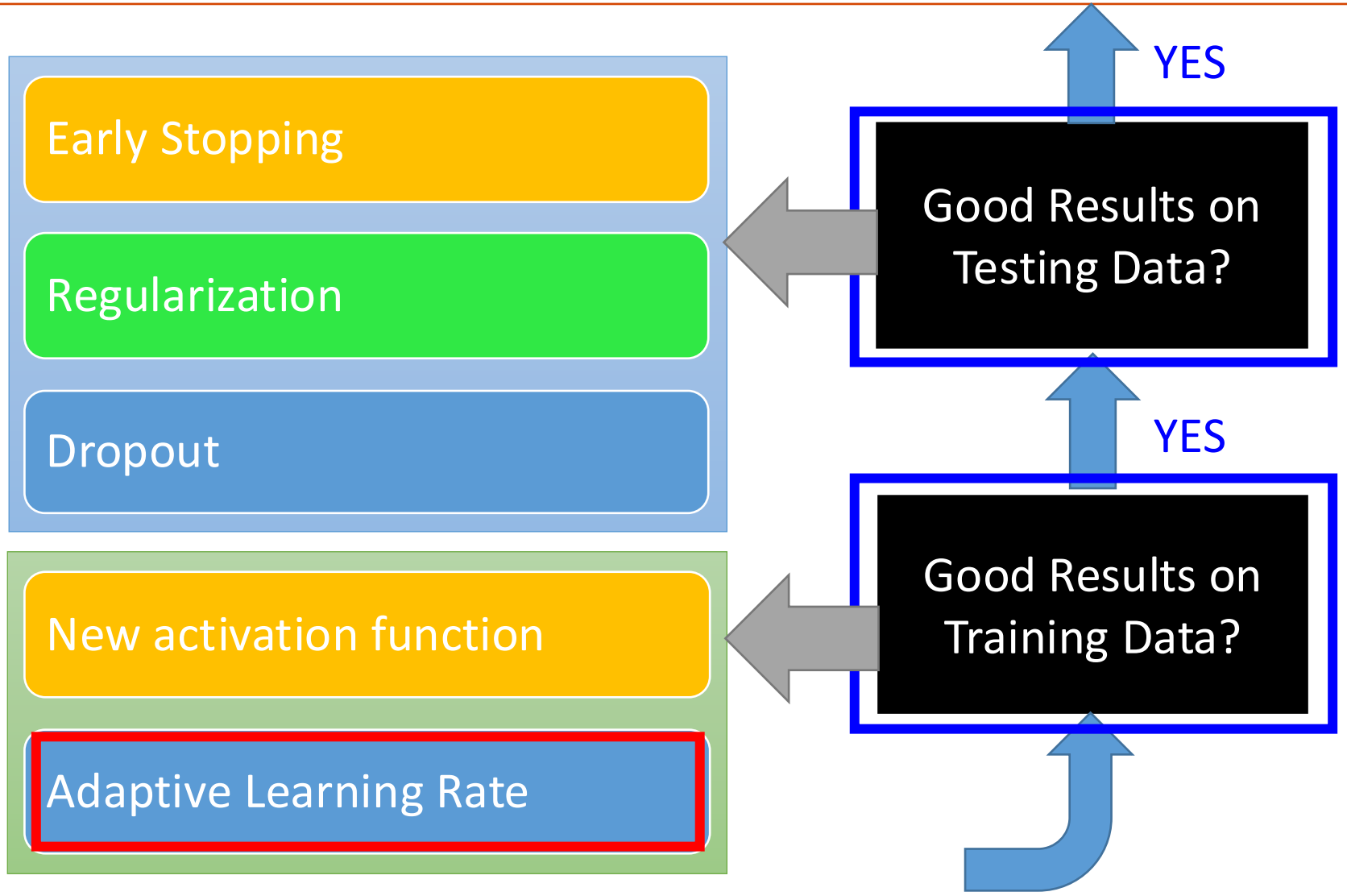


- Train this thin and linear network

Different thin and linear network for different examples

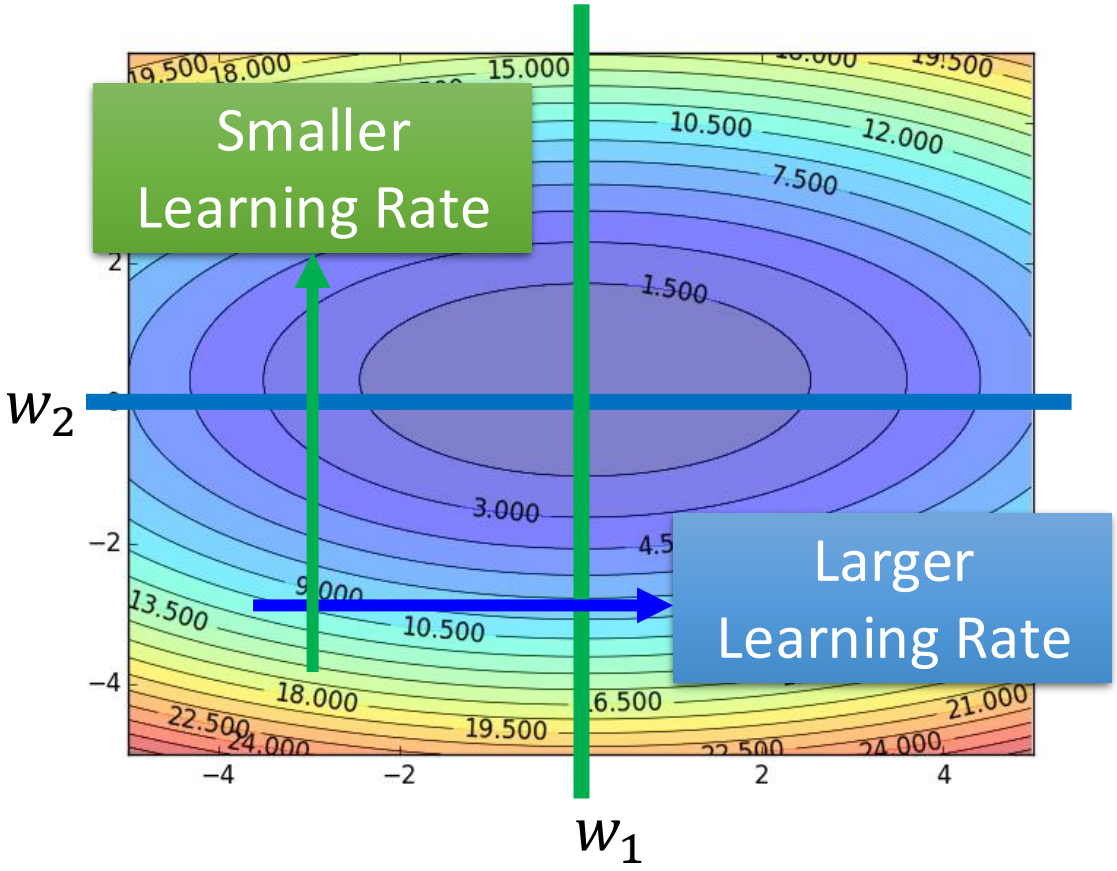
Adaptive Learning

Recipe of Deep Learning



Review

Adagrad



$$w^{t+1} \leftarrow w^t - \frac{\eta}{\sqrt{\sum_{i=0}^{t}(g^i)^2}} g^t$$

Use first derivative to estimate second derivative

Adagrad

σ^t: ***root mean square*** of the previous derivatives of parameter w

$$w^1 \leftarrow w^0 - \frac{\eta^0}{\sigma^0} g^0 \qquad \sigma^0 = \sqrt{(g^0)^2}$$

$$w^2 \leftarrow w^1 - \frac{\eta^1}{\sigma^1} g^1 \qquad \sigma^1 = \sqrt{\frac{1}{2}[(g^0)^2 + (g^1)^2]}$$

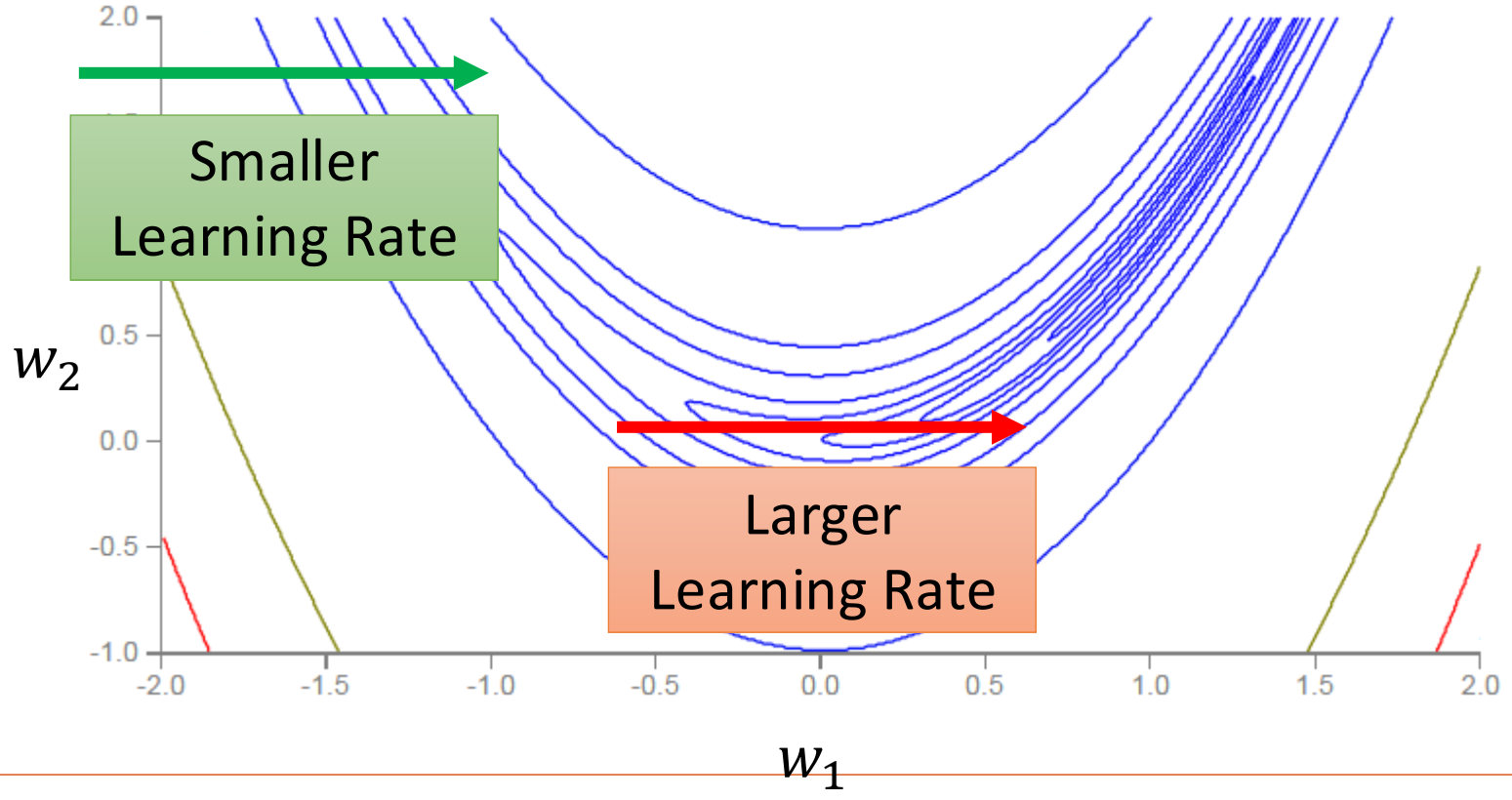
$$w^3 \leftarrow w^2 - \frac{\eta^2}{\sigma^2} g^2 \qquad \sigma^2 = \sqrt{\frac{1}{3}[(g^0)^2 + (g^1)^2 + (g^2)^2]}$$

$$\vdots$$

$$w^{t+1} \leftarrow w^t - \frac{\eta^t}{\sigma^t} g^t \qquad \sigma^t = \sqrt{\frac{1}{t+1}\sum_{i=0}^{t}(g^i)^2}$$

RMSProp

Error Surface can be very complex when training NN.



RMSProp

$$w^1 \leftarrow w^0 - \frac{\eta}{\sigma^0} g^0 \qquad \sigma^0 = g^0$$

$$w^2 \leftarrow w^1 - \frac{\eta}{\sigma^1} g^1 \qquad \sigma^1 = \sqrt{\alpha(\sigma^0)^2 + (1-\alpha)(g^1)^2}$$

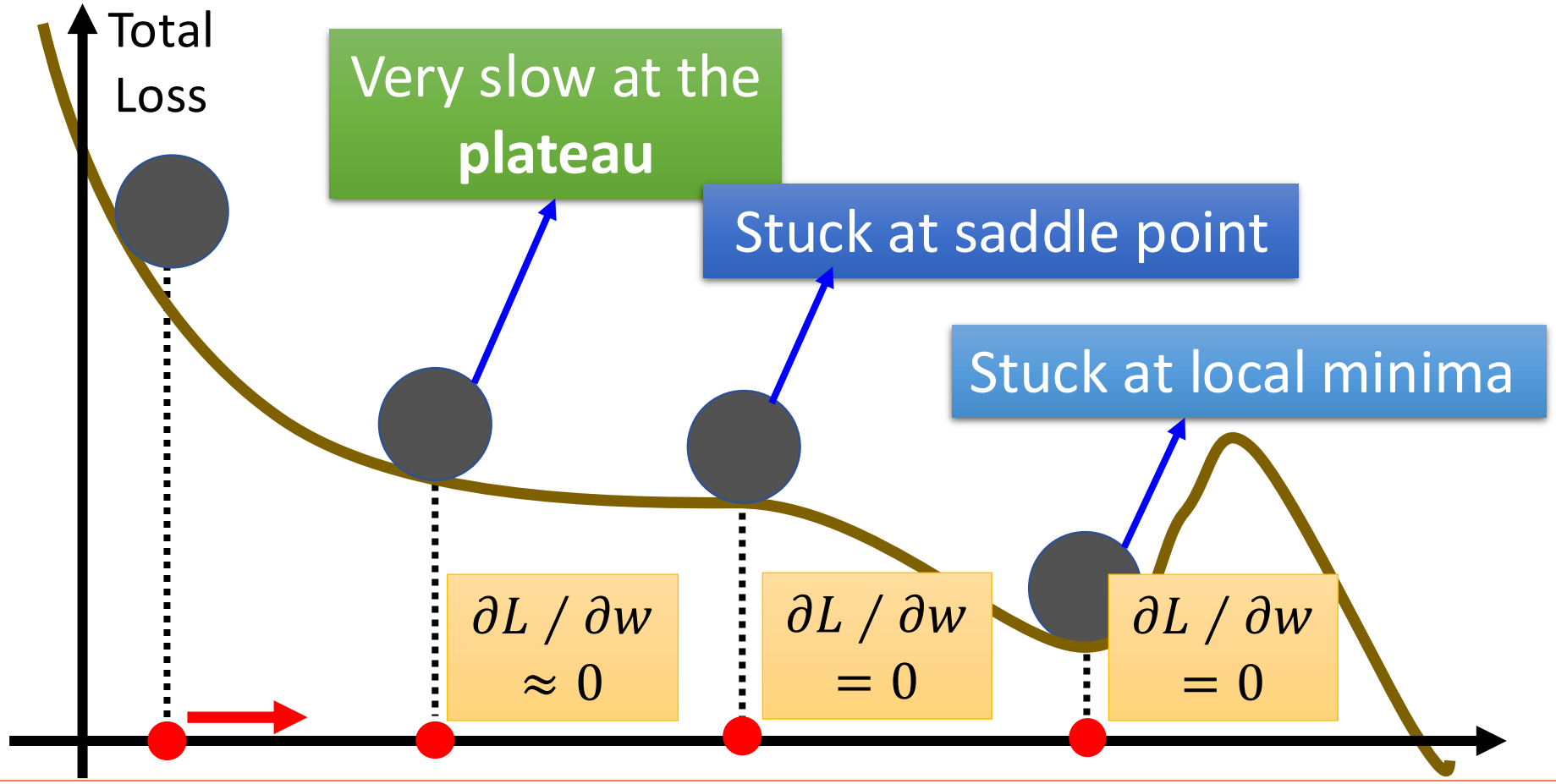
$$w^3 \leftarrow w^2 - \frac{\eta}{\sigma^2} g^2 \qquad \sigma^2 = \sqrt{\alpha(\sigma^1)^2 + (1-\alpha)(g^2)^2}$$

$$\vdots$$

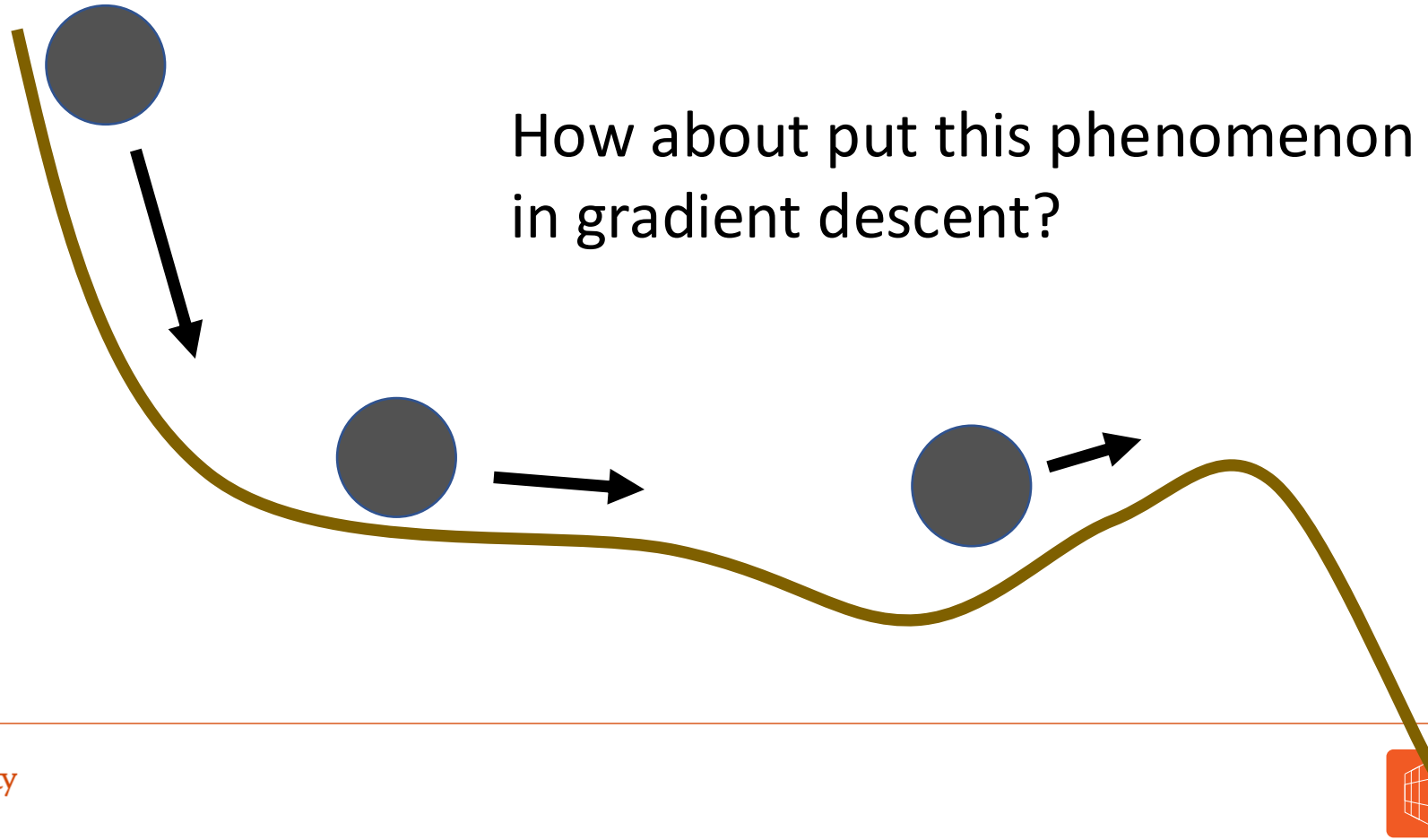
$$w^{t+1} \leftarrow w^t - \frac{\eta}{\sigma^t} g^t \qquad \sigma^t = \sqrt{\alpha(\sigma^{t-1})^2 + (1-\alpha)(g^t)^2}$$

Root Mean Square of the gradients with previous gradients being decayed

Hard to find optimal network parameters



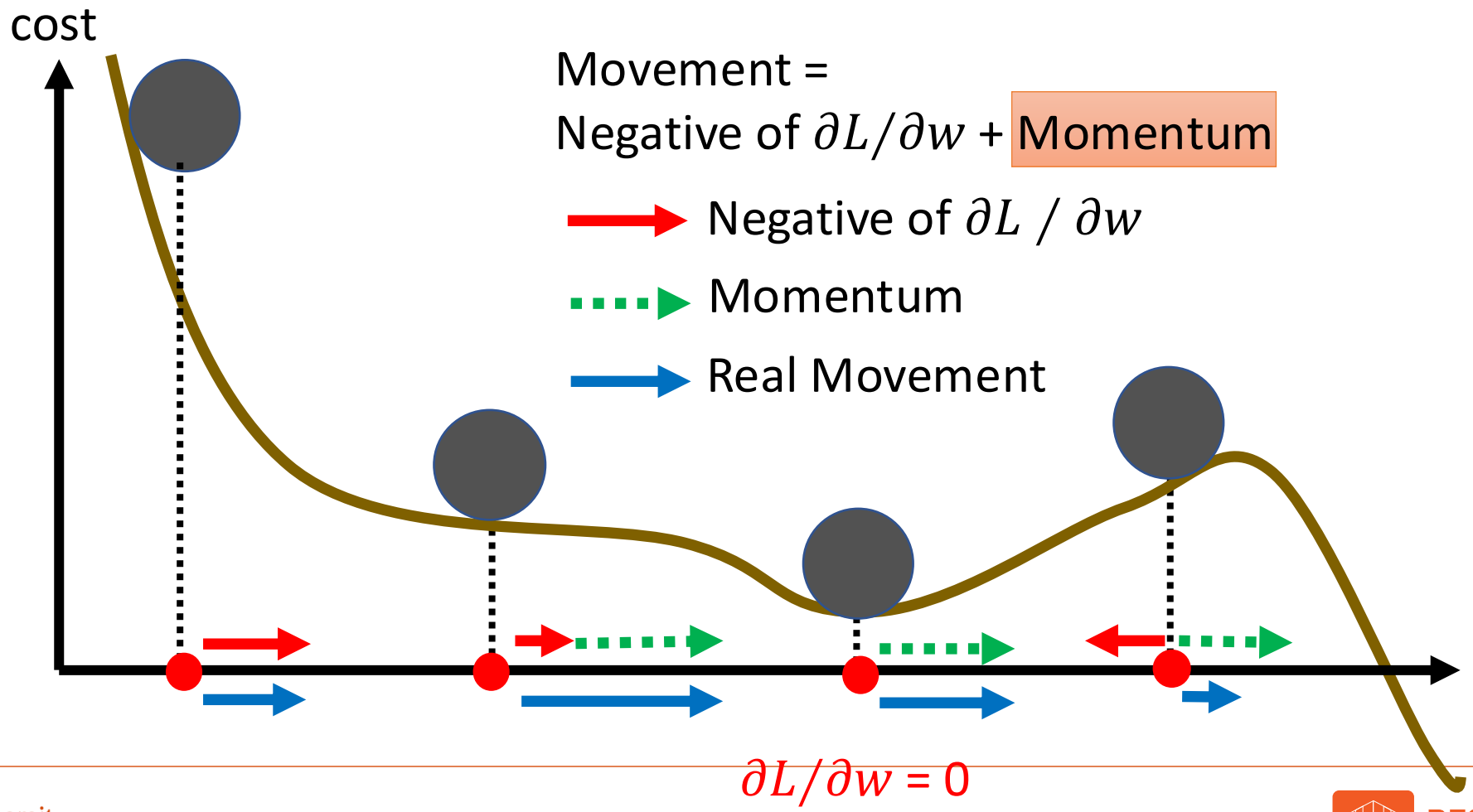
Momentum



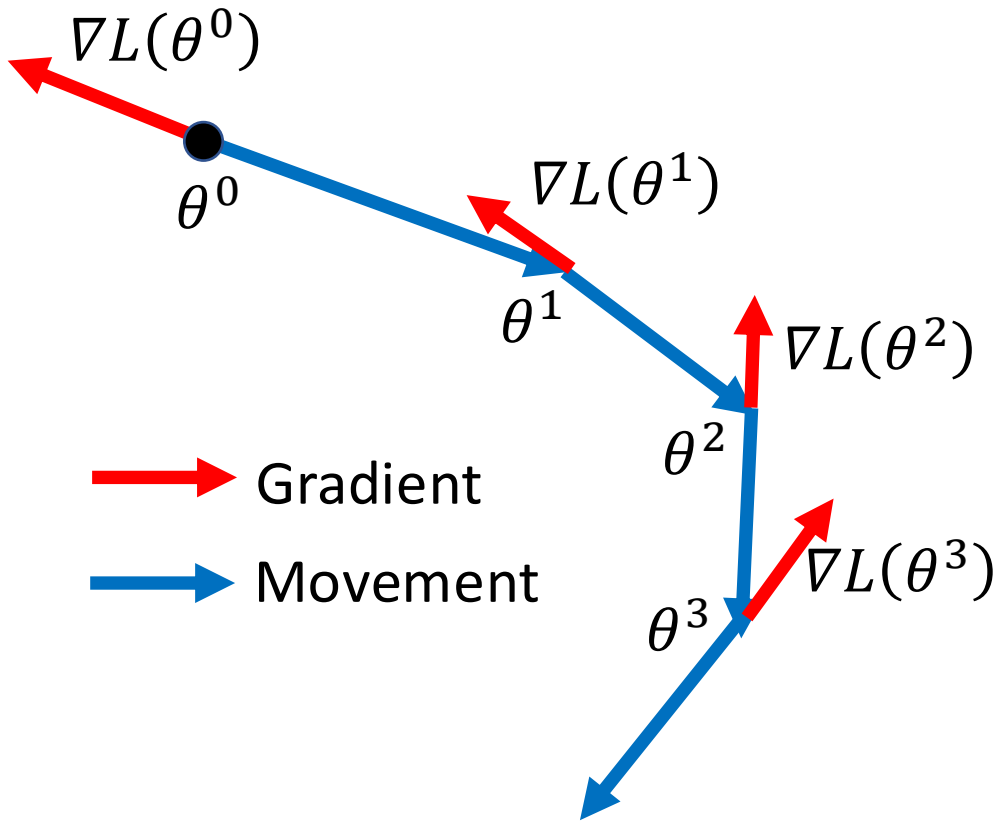
How about put this phenomenon in gradient descent?

Momentum

Still not guarantee reaching global minima, but give some hope ……



Review: Vanilla Gradient Descent



Start at position θ^0

Compute gradient at θ^0

Move to $\theta^1 = \theta^0 - \eta\nabla L(\theta^0)$

Compute gradient at θ^1

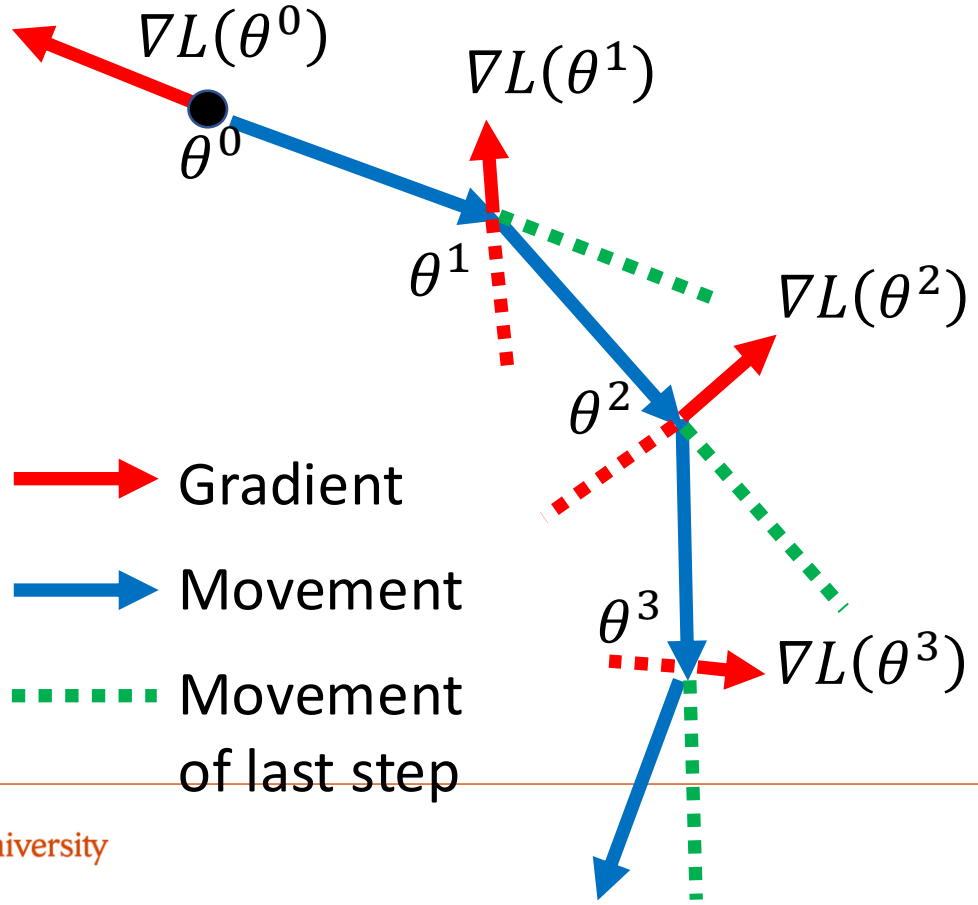
Move to $\theta^2 = \theta^1 - \eta\nabla L(\theta^1)$

⋮

Stop until $\nabla L(\theta^t) \approx 0$

Momentum

Movement: movement of last step minus gradient at present



Start at point θ^0

Movement $v^0=0$

Compute gradient at θ^0

Movement $v^1 = \lambda v^0 - \eta \nabla L(\theta^0)$

Move to $\theta^1 = \theta^0 + v^1$

Compute gradient at θ^1

Movement $v^2 = \lambda v^1 - \eta \nabla L(\theta^1)$

Move to $\theta^2 = \theta^1 + v^2$

Movement not just based on gradient, but previous movement.

Momentum

Movement: movement of last step minus gradient at present

v^i is actually the weighted sum of all the previous gradient: $\nabla L(\theta^0), \nabla L(\theta^1), \ldots \nabla L(\theta^{i-1})$

$v^0 = 0$

$v^1 = -\eta \nabla L(\theta^0)$

$v^2 = -\lambda \eta \nabla L(\theta^0) - \eta \nabla L(\theta^1)$

⋮

Start at point θ^0

Movement $v^0=0$

Compute gradient at θ^0

Movement $v^1 = \lambda v^0 - \eta \nabla L(\theta^0)$

Move to $\theta^1 = \theta^0 + v^1$

Compute gradient at θ^1

Movement $v^2 = \lambda v^1 - \eta \nabla L(\theta^1)$

Move to $\theta^2 = \theta^1 + v^2$

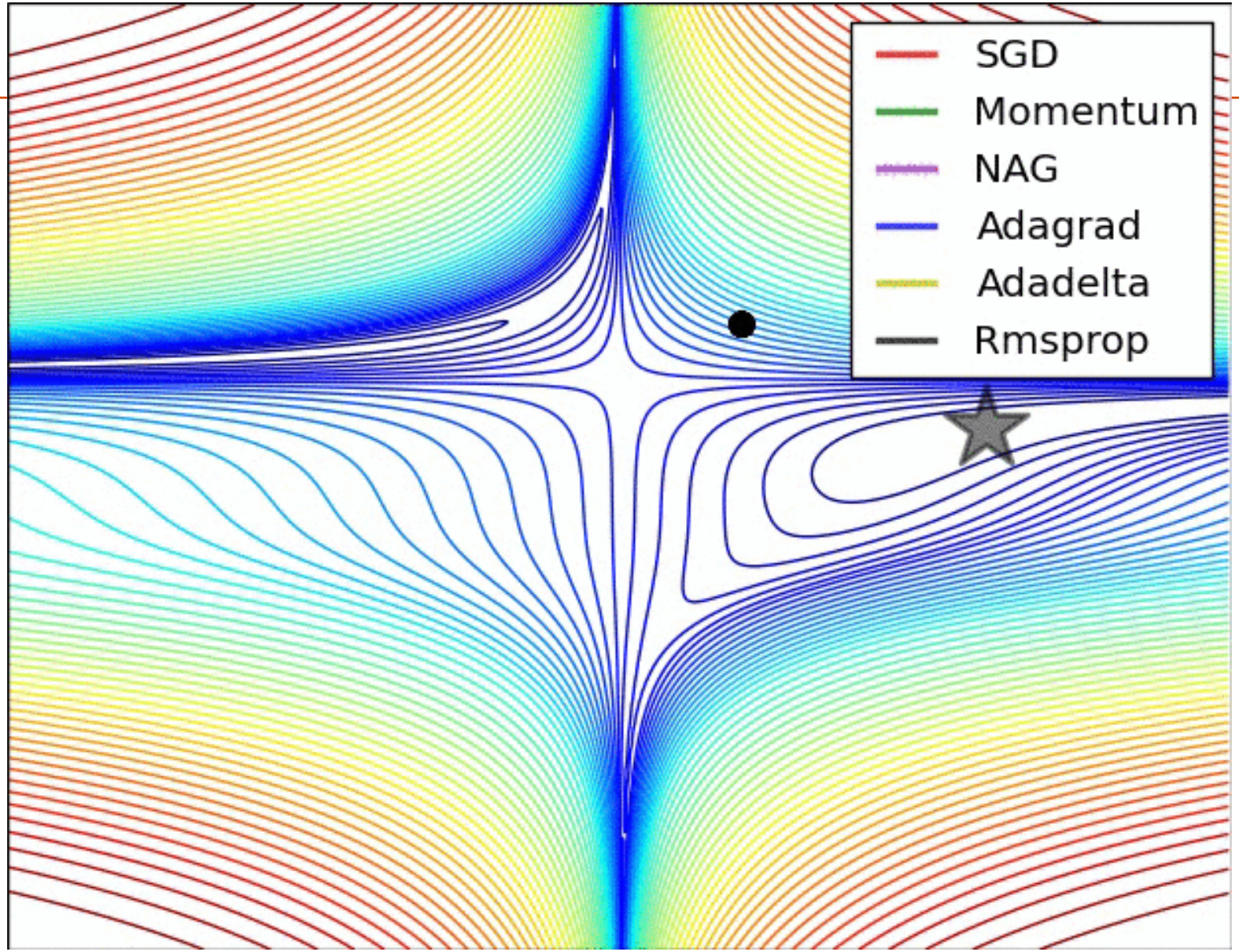
Movement not just based on gradient, but previous movement

Adam

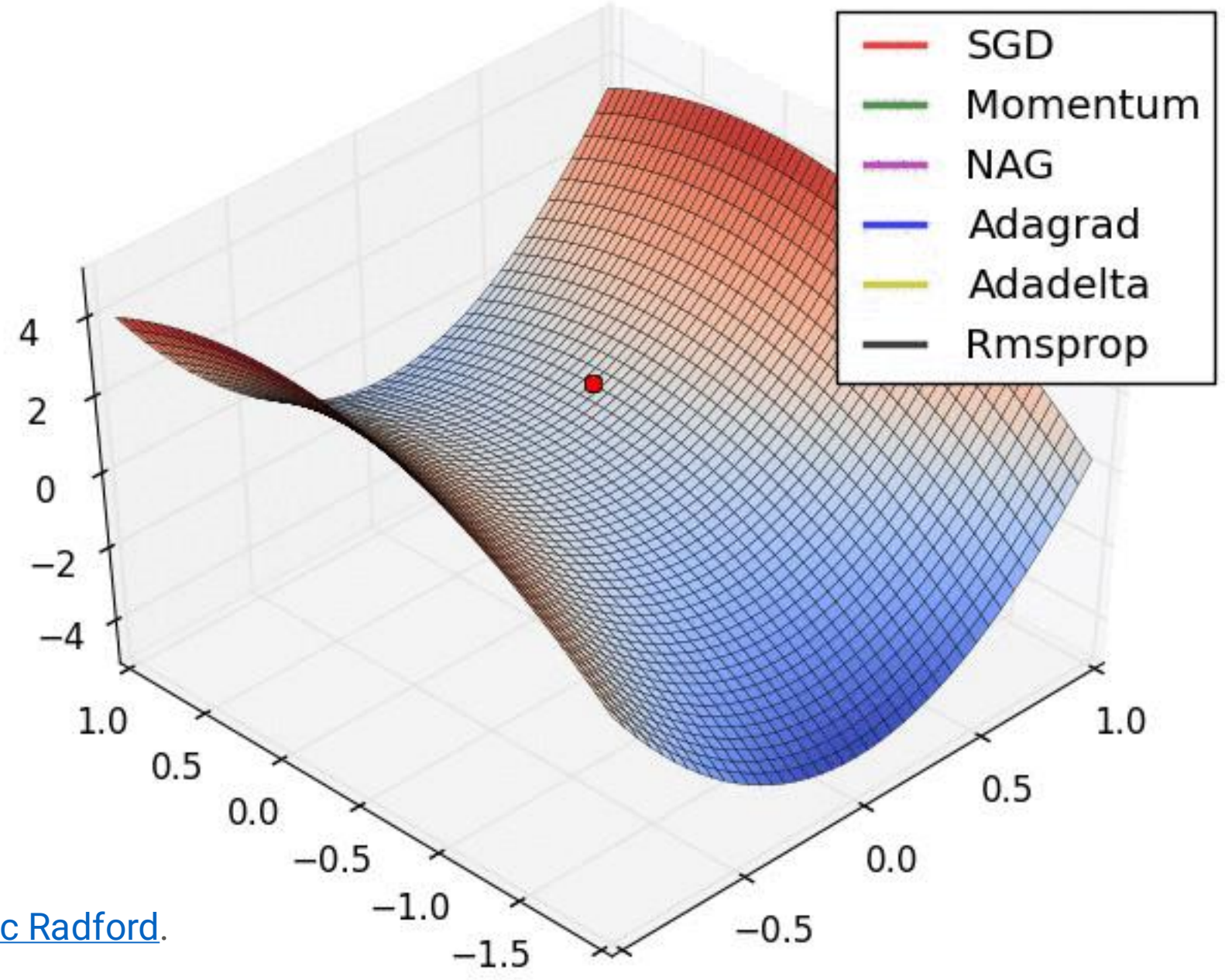
RMSProp + Momentum

Algorithm 1: *Adam*, our proposed algorithm for stochastic optimization. See section 2 for details, and for a slightly more efficient (but less clear) order of computation. g_t^2 indicates the elementwise square $g_t \odot g_t$. Good default settings for the tested machine learning problems are $\alpha = 0.001$, $\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\epsilon = 10^{-8}$. All operations on vectors are element-wise. With β_1^t and β_2^t we denote β_1 and β_2 to the power t.

Require: α: Stepsize
Require: $\beta_1, \beta_2 \in [0, 1)$: Exponential decay rates for the moment estimates
Require: $f(\theta)$: Stochastic objective function with parameters θ
Require: θ_0: Initial parameter vector
$m_0 \leftarrow 0$ (Initialize 1st moment vector) → for momentum
$v_0 \leftarrow 0$ (Initialize 2nd moment vector) → for RMSprop
$t \leftarrow 0$ (Initialize timestep)
while θ_t not converged **do**
$t \leftarrow t + 1$
$g_t \leftarrow \nabla_\theta f_t(\theta_{t-1})$ (Get gradients w.r.t. stochastic objective at timestep t)
$m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot g_t$ (Update biased first moment estimate)
$v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 - \beta_2) \cdot g_t^2$ (Update biased second raw moment estimate)
$\widehat{m}_t \leftarrow m_t / (1 - \beta_1^t)$ (Compute bias-corrected first moment estimate)
$\widehat{v}_t \leftarrow v_t / (1 - \beta_2^t)$ (Compute bias-corrected second raw moment estimate)
$\theta_t \leftarrow \theta_{t-1} - \alpha \cdot \widehat{m}_t / (\sqrt{\widehat{v}_t} + \epsilon)$ (Update parameters)
end while
return θ_t (Resulting parameters)



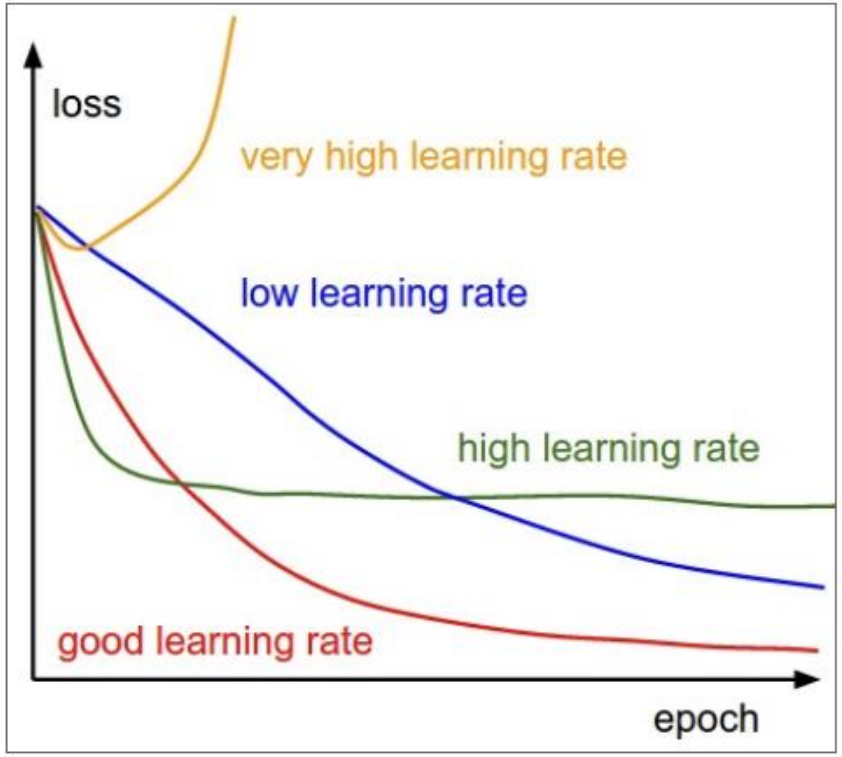
Images credit: Alec Radford.



Images credit: Alec Radford.

Learning Rate Decay

SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a hyperparameter.



Learning Rate Decay

SGD, SGD+Momentum, Adagrad, RMSProp, Adam
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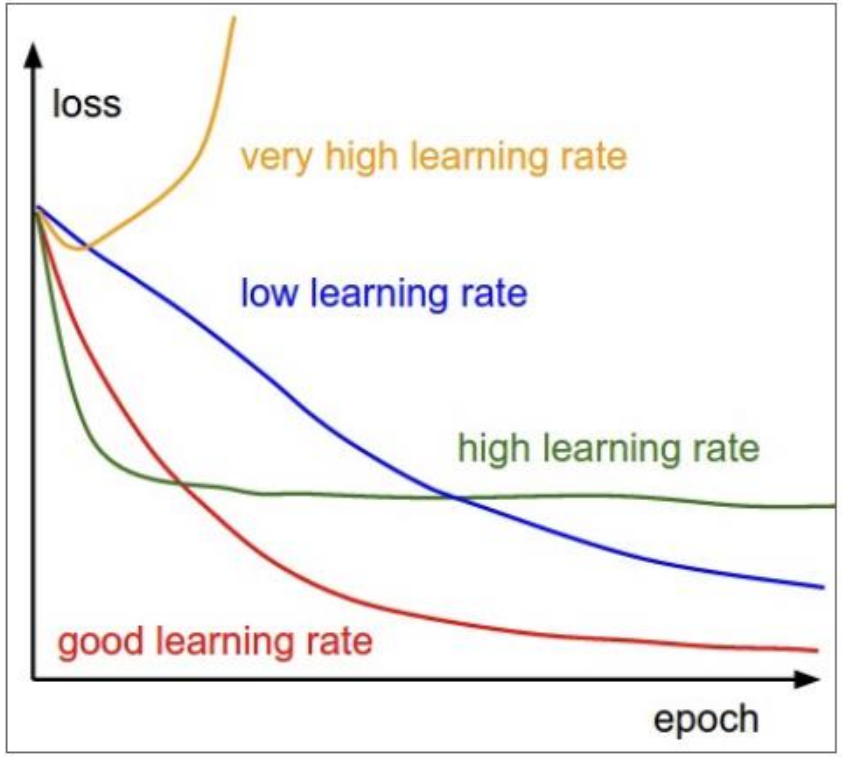
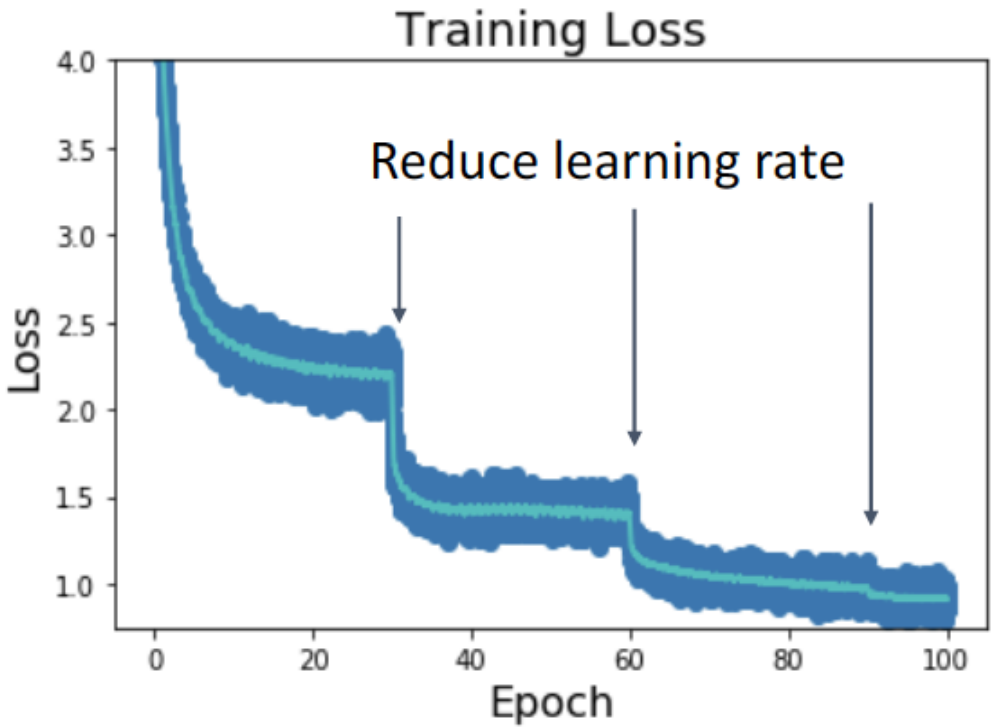


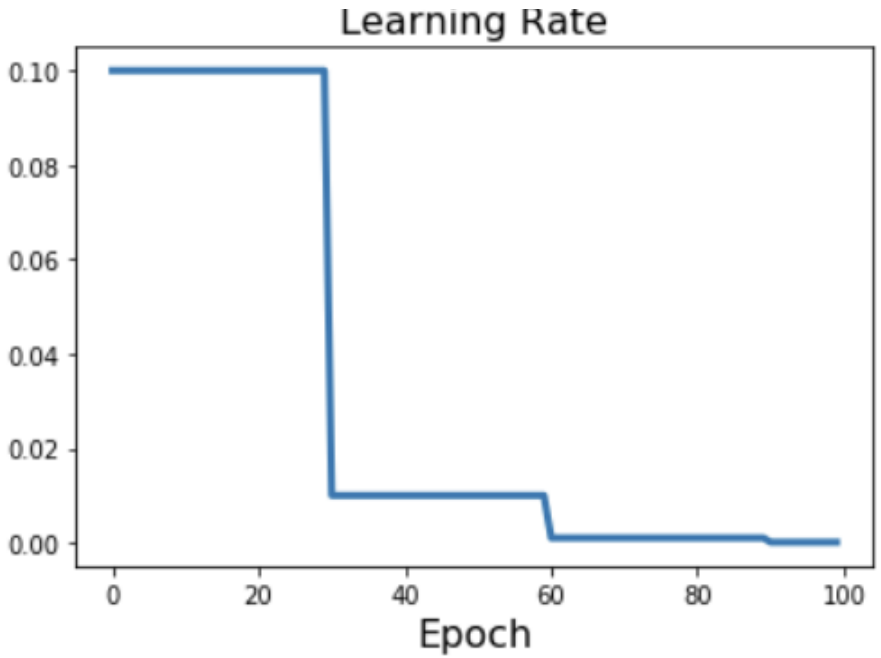
Q: Which one of these learning rates is best to use?

A: All of them! Start with large learning rate and decay over time

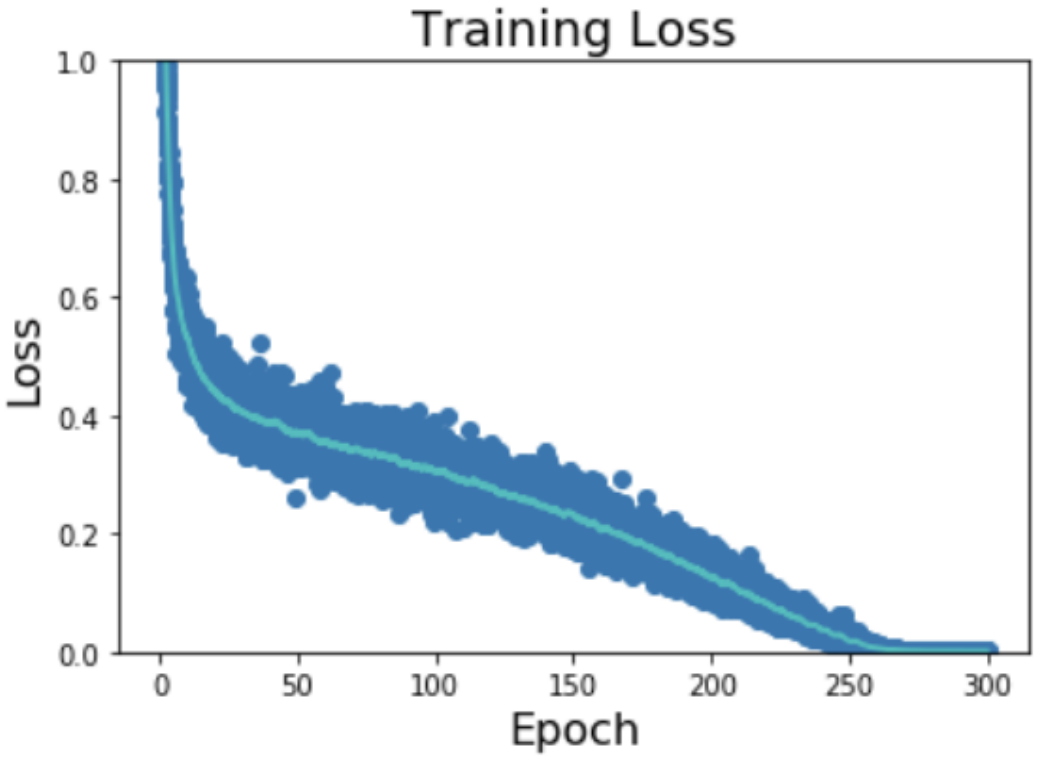
Learning Rate Decay: Step



Step: Reduce learning rate at a few fixed points. E.g. multiply Sigmoid function by 0.1 after epochs 30, 60, and 90.

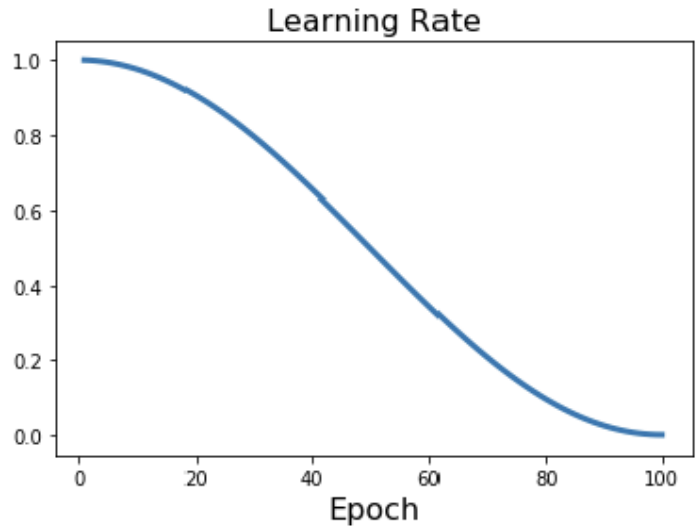


Learning Rate Decay: Cosine



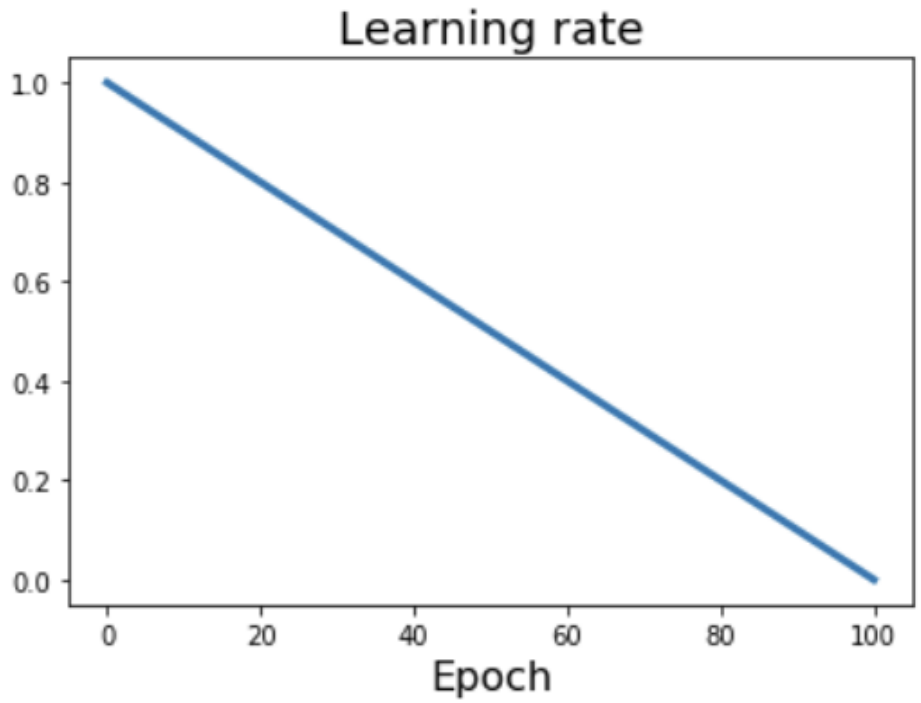
Step: Reduce learning rate at a few fixed points.
E.g. multiply Sigmoid function by 0.1 after epochs 30, 60, and 90.

Cosine: $\alpha_t = \frac{1}{2}\alpha_0 \left(1 + \cos(t\pi/T)\right)$



Loshchilov and Hutter, "SGDR: Stochastic Gradient Descent with Warm Restarts", ICLR 2017
Radford et al, "Improving Language Understanding by Generative Pre-Training", 2018
Feichtenhofer et al, "SlowFast Networks for Video Recognition", ICCV 2019
Radosavovic et al, "On Network Design Spaces for Visual Recognition", ICCV 2019
Child at al, "Generating Long Sequences with Sparse Transformers", arXiv 2019

Learning Rate Decay: Linear



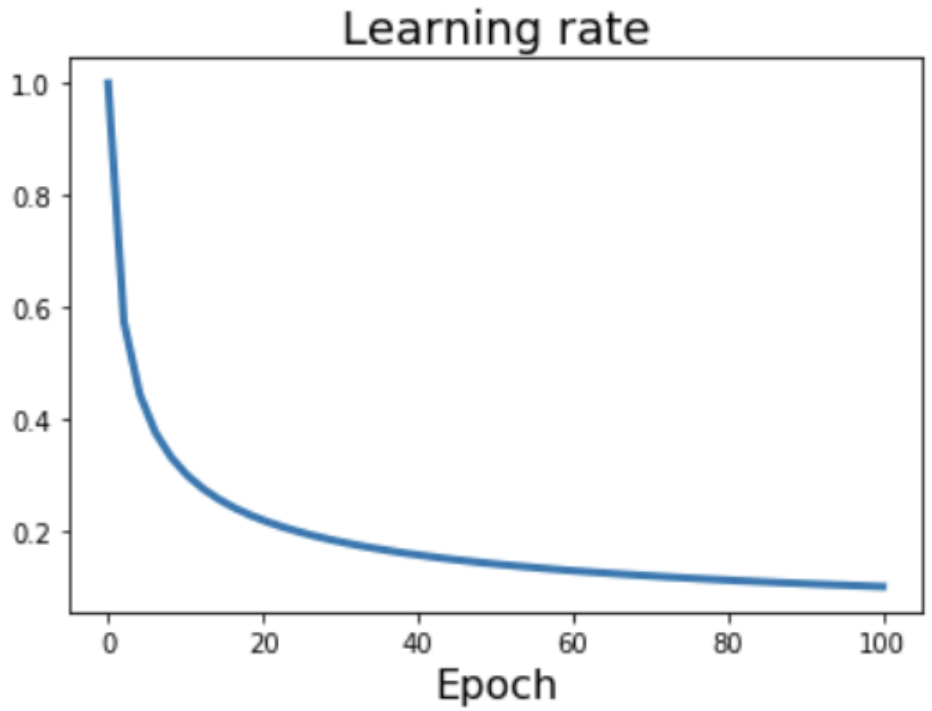
Step: Reduce learning rate at a few fixed points.
E.g. multiply Sigmoid function by 0.1 after epochs 30, 60, and 90.

Cosine: $\alpha_t = \frac{1}{2}\alpha_0 \left(1 + \cos(t\pi/T)\right)$

Linear: $\alpha_t = \alpha_0(1 - t/T)$

Devlin et al, "BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding", NAACL 2018
Liu et al, "RoBERTa: A Robustly Optimized BERT Pretraining Approach", 2019
Yang et al, "XLNet: Generalized Autoregressive Pretraining for Language Understanding", NeurIPS 2019

Learning Rate Decay: Inverse Sqrt



Step: Reduce learning rate at a few fixed points.
E.g. multiply Sigmoid function by 0.1 after epochs 30, 60, and 90.

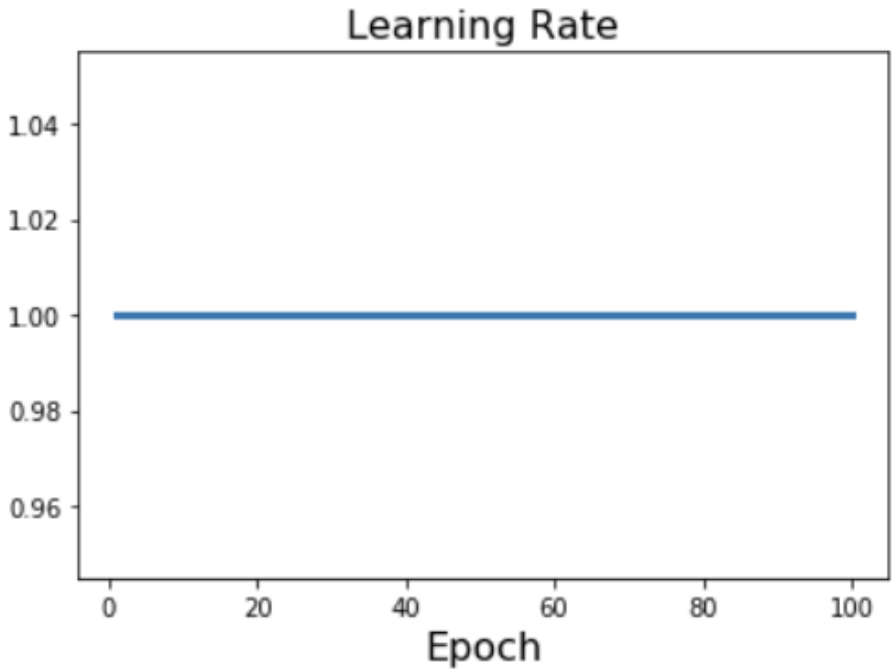
Cosine: $\alpha_t = \frac{1}{2}\alpha_0 \left(1 + \cos(t\pi/T)\right)$

Linear: $\alpha_t = \alpha_0(1 - t/T)$

Inverse sqrt: $\alpha_t = \alpha_0/\sqrt{t}$

Vaswani et al, "Attention is all you need", NIPS 2017

Learning Rate Decay: Constant!



Step: Reduce learning rate at a few fixed points.
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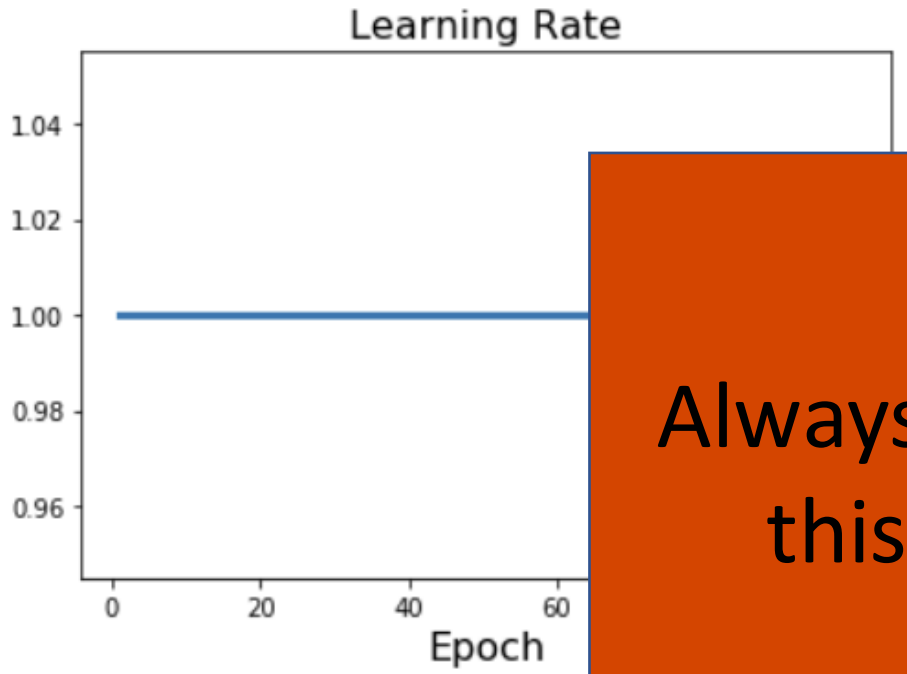
Inverse sqrt: $\alpha_t = \alpha_0/\sqrt{t}$

Constant: $\alpha_t = \alpha_0$

Brock et al, "Large Scale GAN Training for High Fidelity Natural Image Synthesis", ICLR 2019
Donahue and Simonyan, "Large Scale Adversarial Representation Learning", NeurIPS 2019

Learning Rate Decay: Constant!



Step: Reduce learning rate at a few fixed points.
E.g. multiply Sigmoid function by 0.1 after epochs

Always try to run this first!!!!

$$\frac{1}{2}\alpha_0\left(1+\cos(t\pi/T)\right)$$

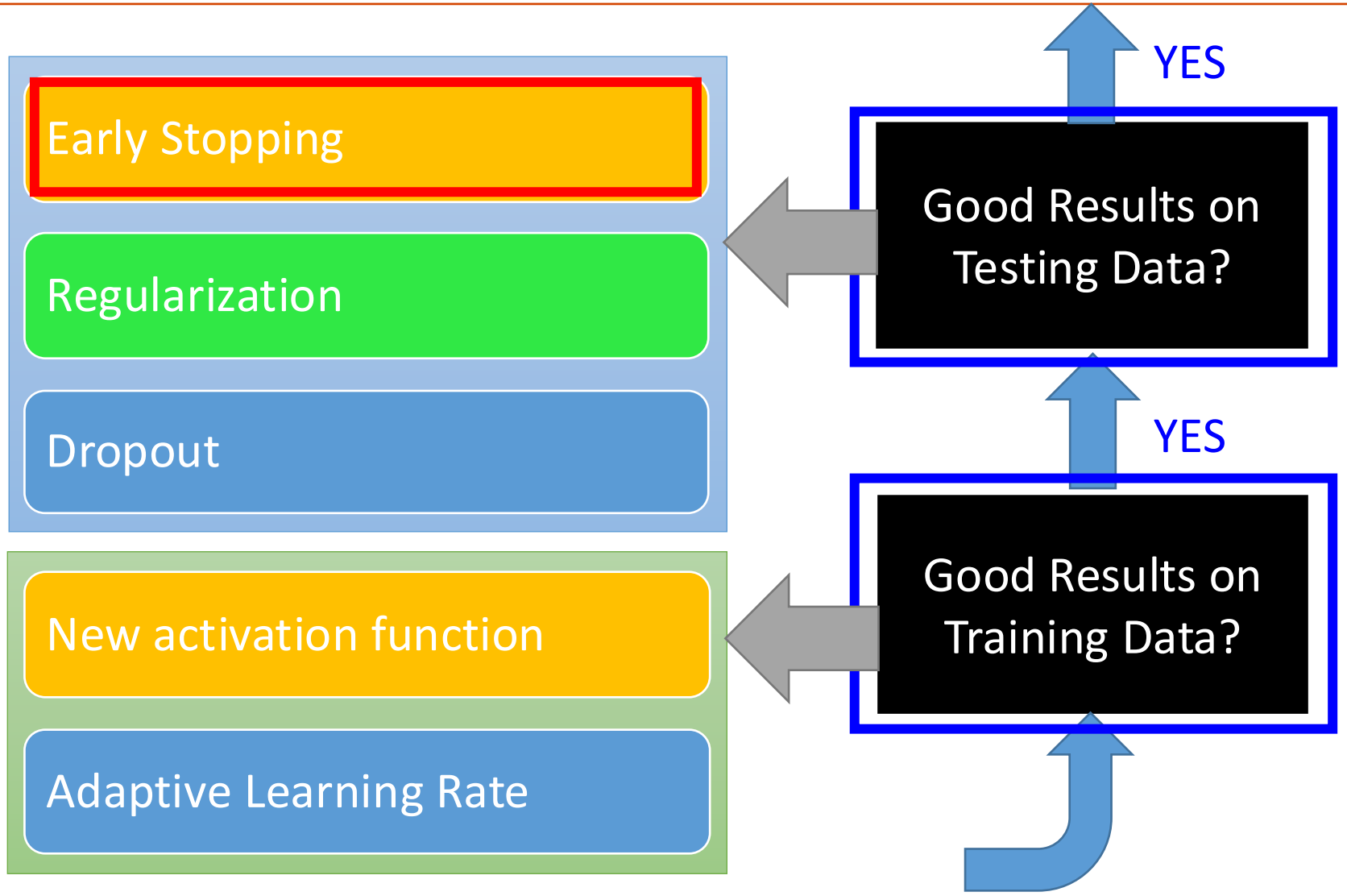
$$\alpha_0(1-t/T)$$

$$\alpha_t = \alpha_0/\sqrt{t}$$

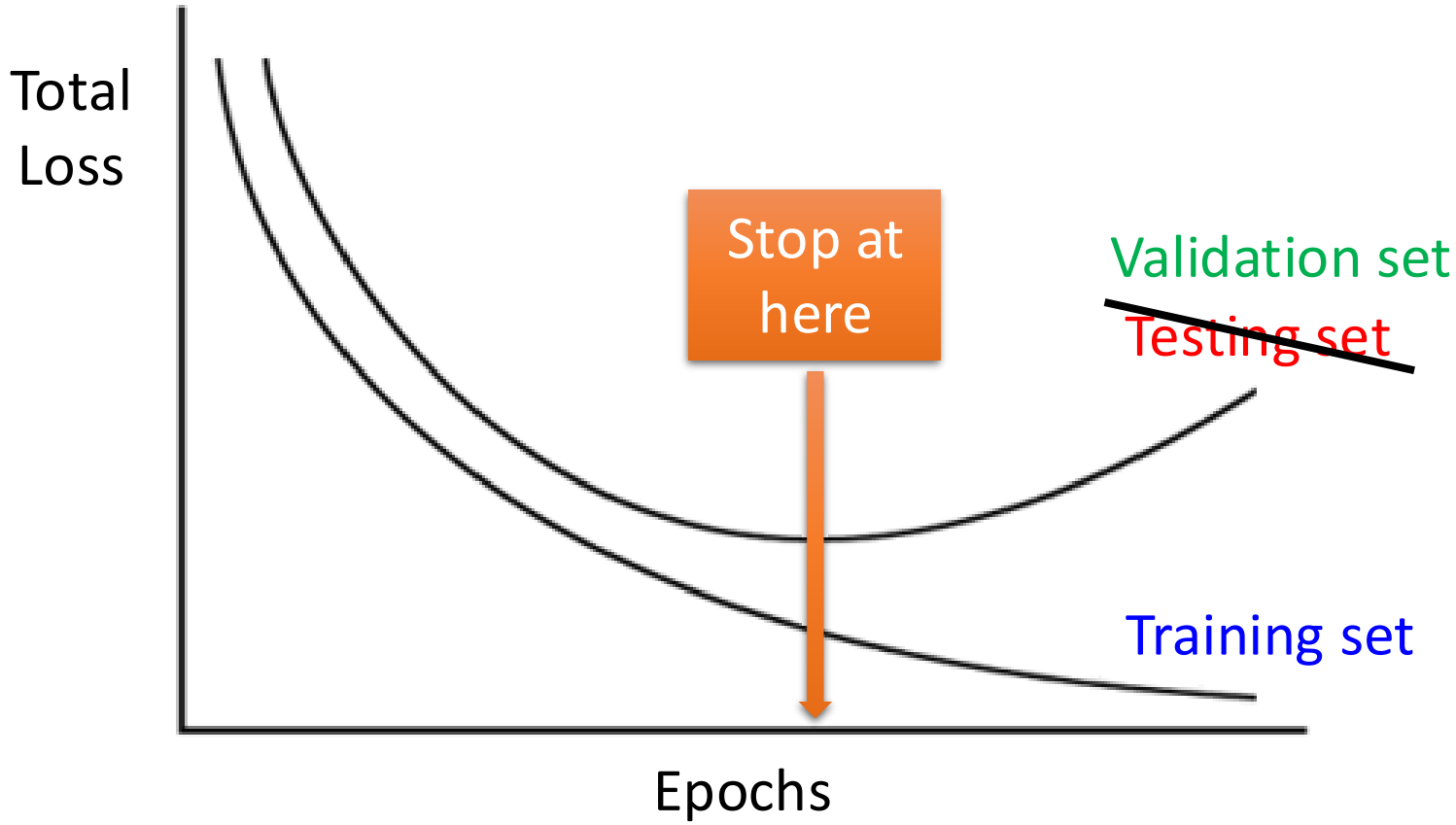
$$\alpha_t = \alpha_0$$

Brock et al, "Large Scale GAN Training for High Fidelity Natural Image Synthesis", ICLR 2019
Donahue and Simonyan, "Large Scale Adversarial Representation Learning", NeurIPS 2019

Recipe of Deep Learning

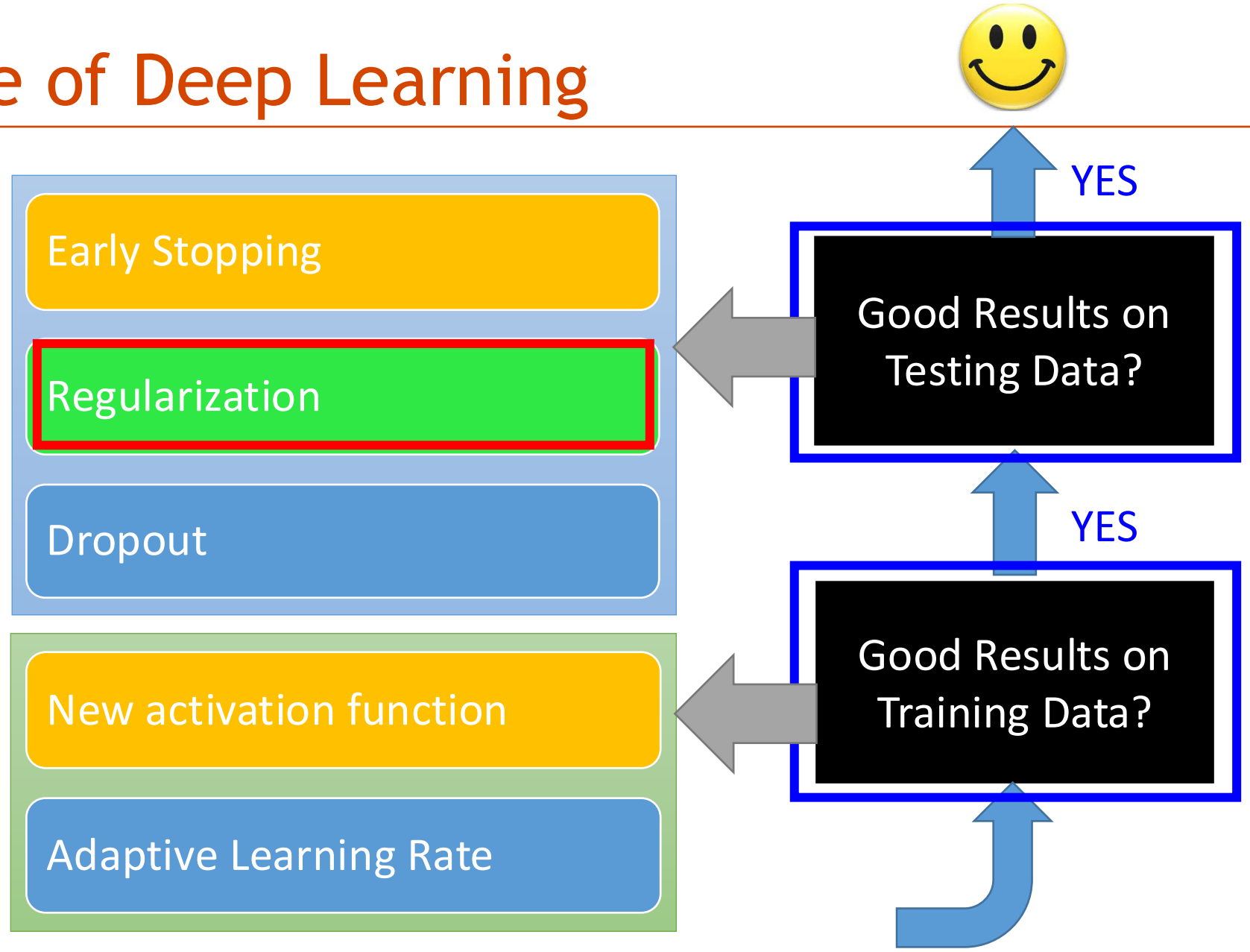


Early Stopping



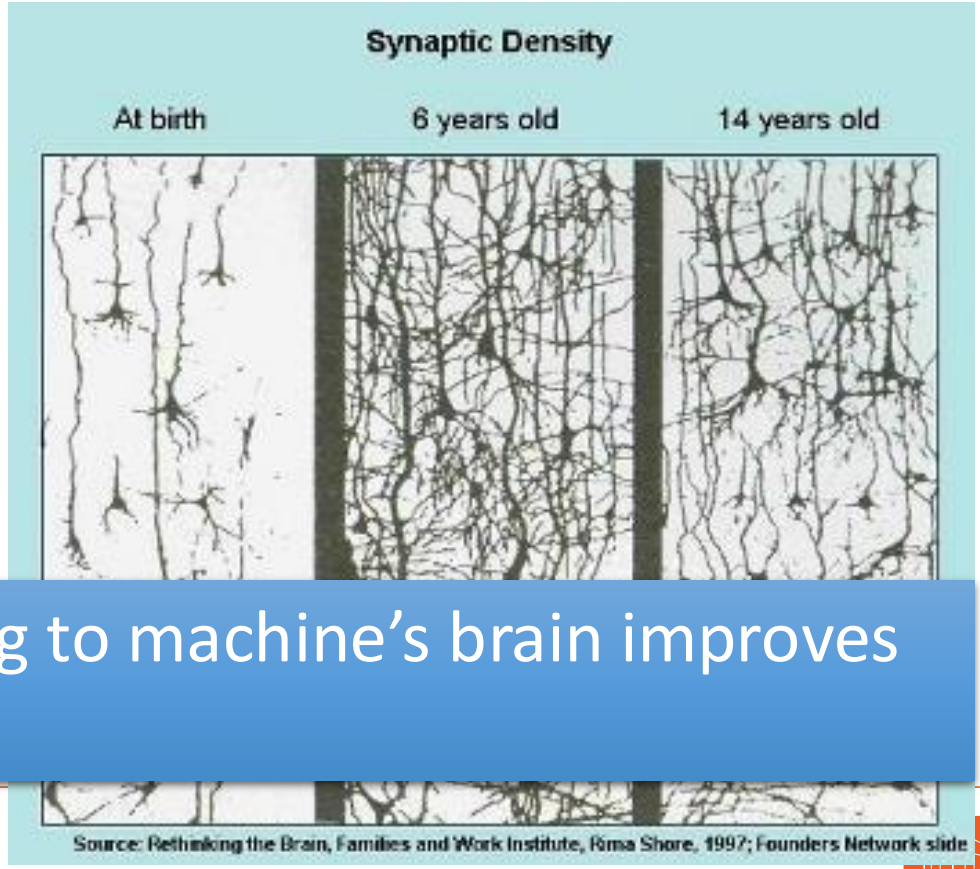
Keras: http://keras.io/getting-started/faq/#how-can-i-interrupt-training-when-the-validation-loss-isnt-decreasing-anymore

Recipe of Deep Learning



Regularization - Weight Decay

Our brain prunes out the useless link between neurons.



Doing the same thing to machine's brain improves the performance.

Regularization

- New loss function to be minimized
  - Find a set of weight not only minimizing original cost but also close to zero

$$L'(\theta) = L(\theta) + \lambda \frac{1}{2} \|\theta\|_2$$

→ Regularization term

$$\theta = \{w_1, w_2, \ldots\}$$

Original loss
(e.g. minimize square error, cross entropy …)

L2 regularization:

$$\|\theta\|_2 = (w_1)^2 + (w_2)^2 + \ldots$$

(usually not consider biases)

Regularization

L2 regularization:

$$\|\theta\|_2 = (w_1)^2 + (w_2)^2 + \dots$$

New loss function to be minimized

$$\mathrm{L}'(\theta) = L(\theta) + \lambda \frac{1}{2} \|\theta\|_2$$ Gradient: $$\frac{\partial \mathrm{L}'}{\partial w} = \frac{\partial \mathrm{L}}{\partial w} + \lambda w$$

Update: $$w^{t+1} \rightarrow w^t - \eta \frac{\partial \mathrm{L}'}{\partial w} = w^t - \eta \left(\frac{\partial \mathrm{L}}{\partial w} + \lambda w^t \right)$$

$$= (1 - \eta\lambda) w^t - \eta \frac{\partial \mathrm{L}}{\partial w}$$

Weight Decay

Closer to zero

Regularization

L1 regularization:

$$\|\theta\|_1 = |w_1| + |w_2| + \dots$$

New loss function to be minimized

$$\mathrm{L}'(\theta) = L(\theta) + \lambda \frac{1}{2}\|\theta\|_1 \qquad \frac{\partial \mathrm{L}'}{\partial w} = \frac{\partial \mathrm{L}}{\partial w} + \lambda \,\mathrm{sgn}(w)$$

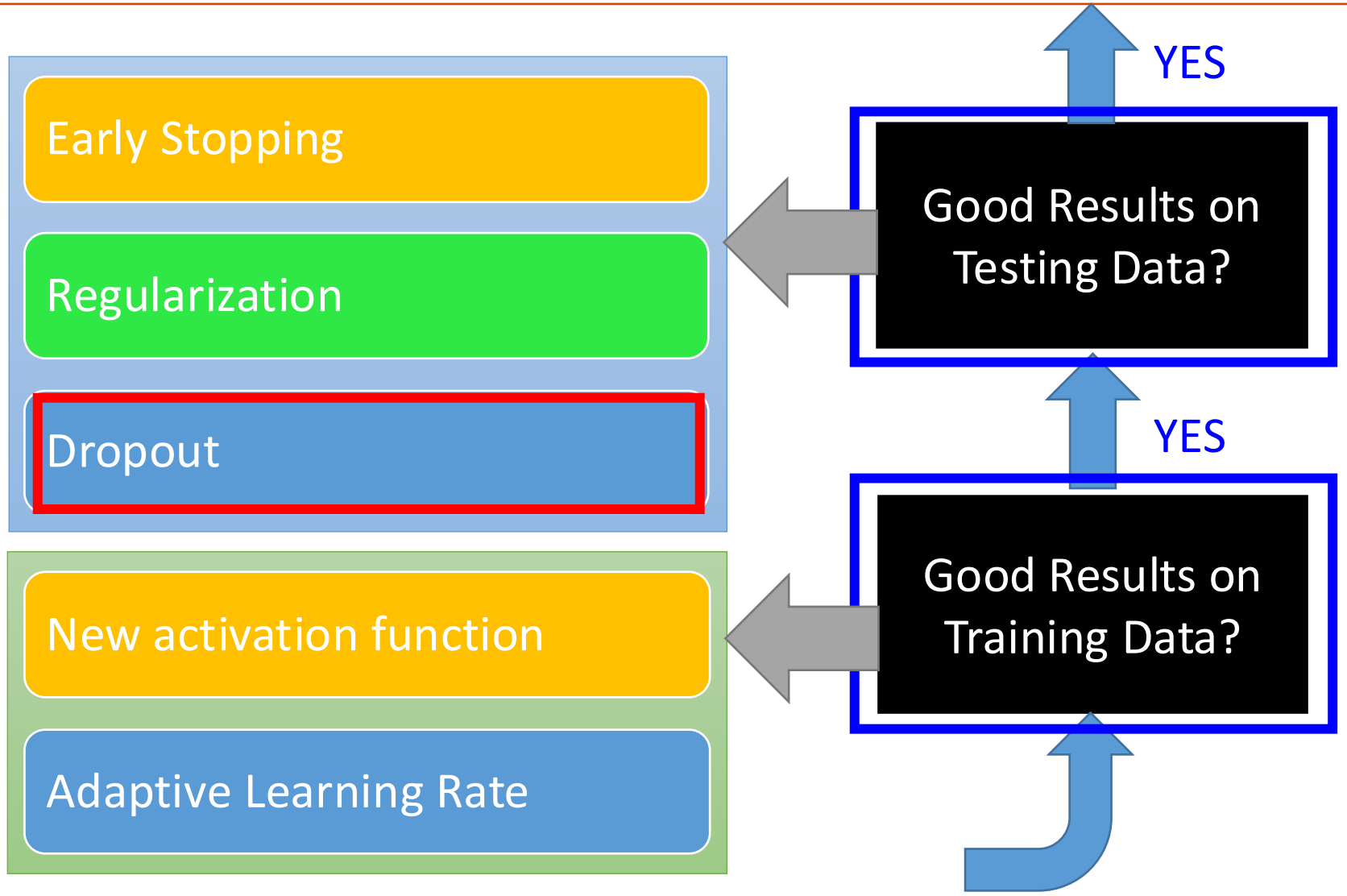
Update:

$$w^{t+1} \to w^t - \eta \frac{\partial \mathrm{L}'}{\partial w} = w^t - \eta\left(\frac{\partial \mathrm{L}}{\partial w} + \lambda \,\mathrm{sgn}\left(w^t\right)\right)$$

$$= w^t - \eta \frac{\partial \mathrm{L}}{\partial w} - \eta\lambda \,\mathrm{sgn}\left(w^t\right)$$

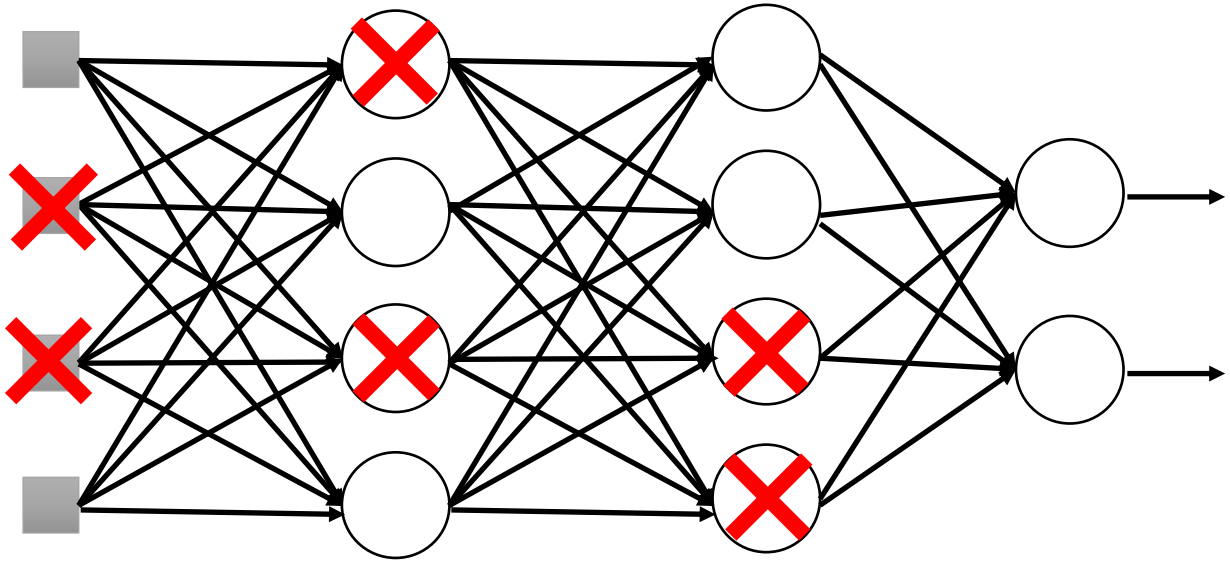
$$= (1 - \eta\lambda) w^t - \eta \frac{\partial \mathrm{L}}{\partial w}$$ L2

Recipe of Deep Learning



Dropout

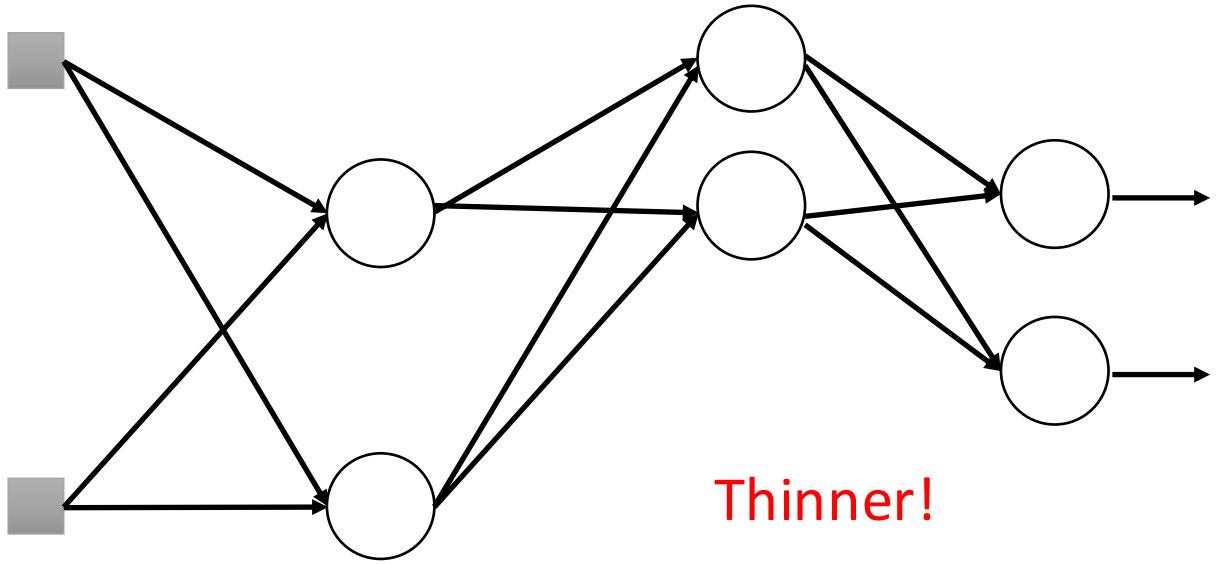
Training:



- **Each time before updating the parameters**
  - Each neuron has p% to dropout

Dropout

Training:



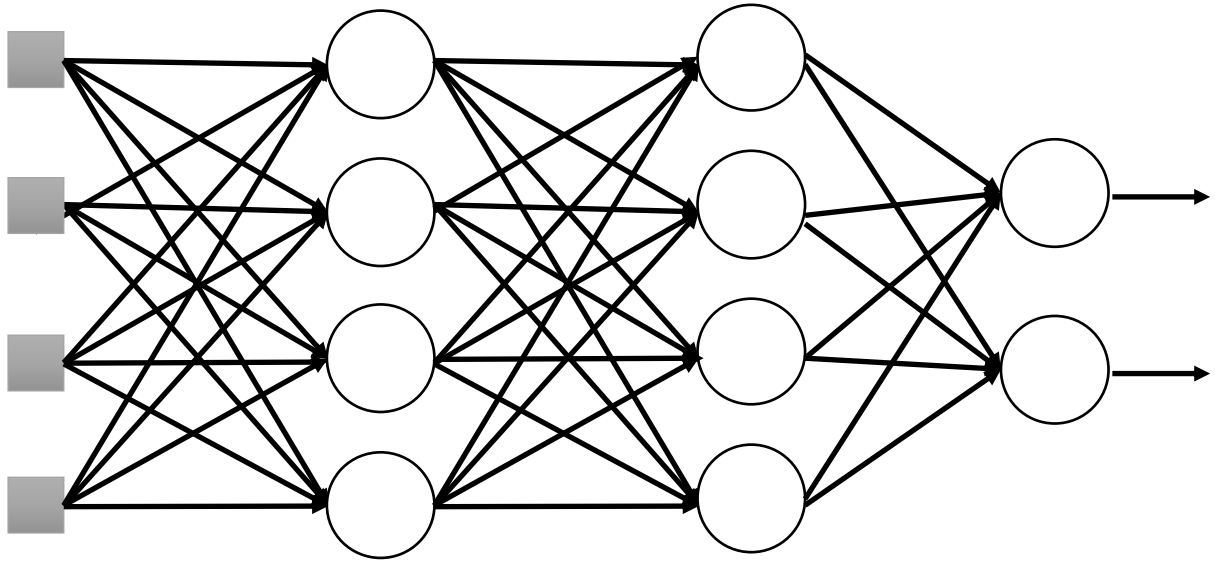
- **Each time before updating the parameters**
  - Each neuron has p% to dropout

    The structure of the network is changed.
  - Using the new network for training

For each mini-batch, we resample the dropout neurons

Dropout

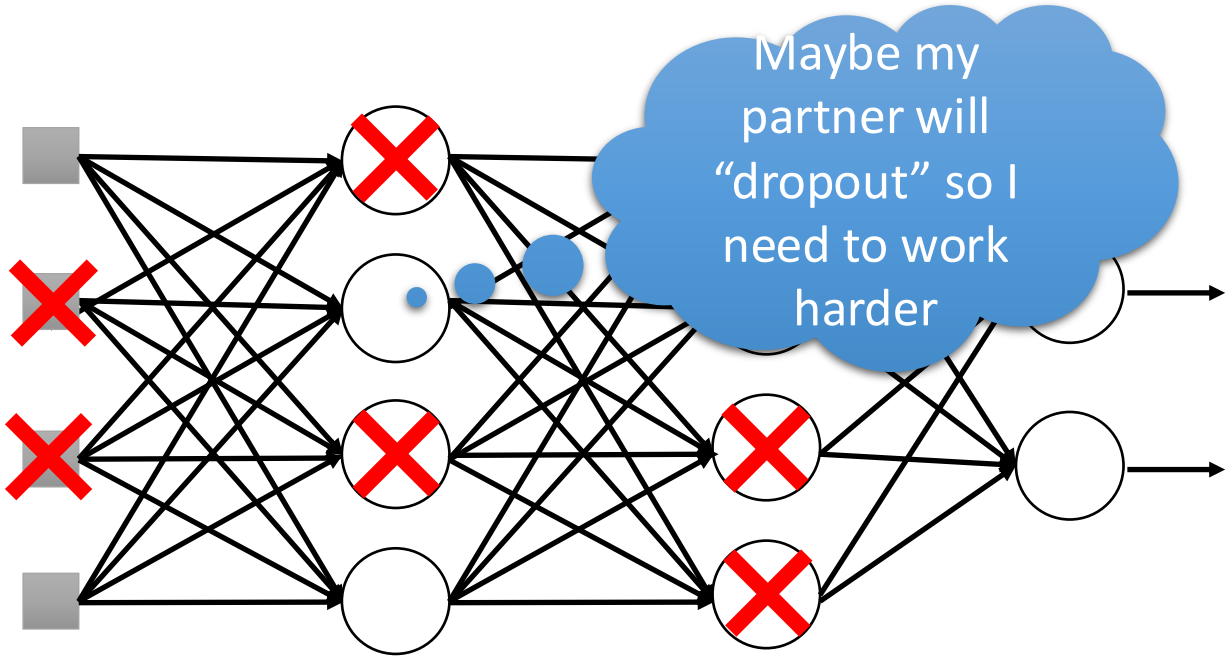
Testing:



➢ **No dropout**

- If the dropout rate at training is p%, all the weights times 1-p%
- Assume that the dropout rate is 50%. If a weight $w = 1$ by training, set $w = 0.5$ for testing.

Dropout – Intuitive Reason



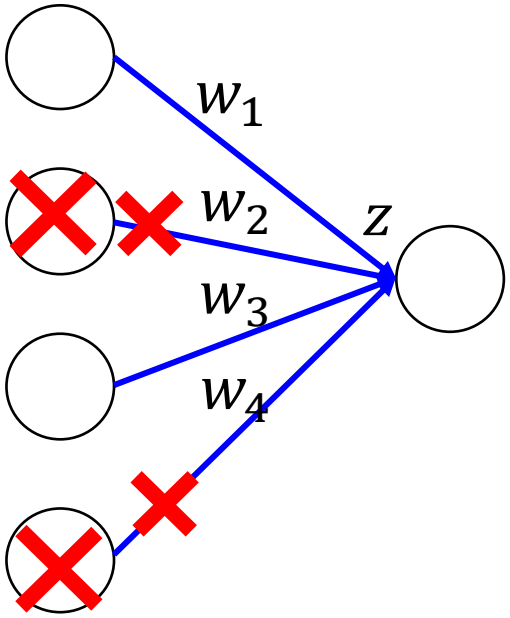
- When teams up, if everyone expect the partner will do the work, nothing will be done finally.
- However, if you know your partner will dropout, you will do better.
- When testing, no one dropout actually, so obtaining good results eventually.

Dropout – Intuitive Reason

Why the weights should multiply (1-p)% (dropout rate) when testing?

Training of Dropout

Assume dropout rate is 50%

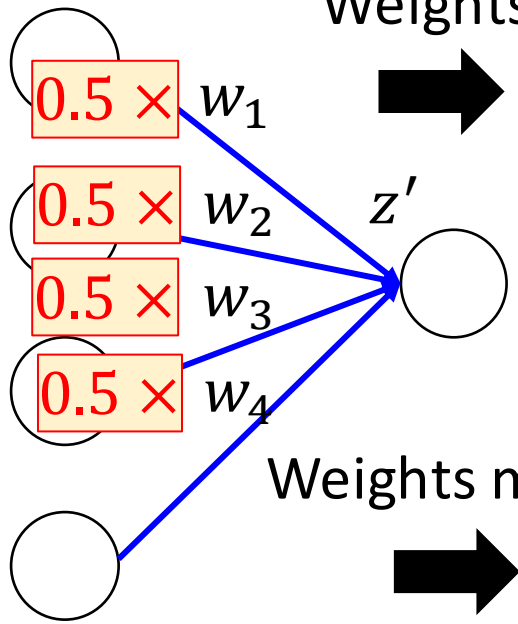


Testing of Dropout

No dropout

Weights from training

$z' \approx 2z$

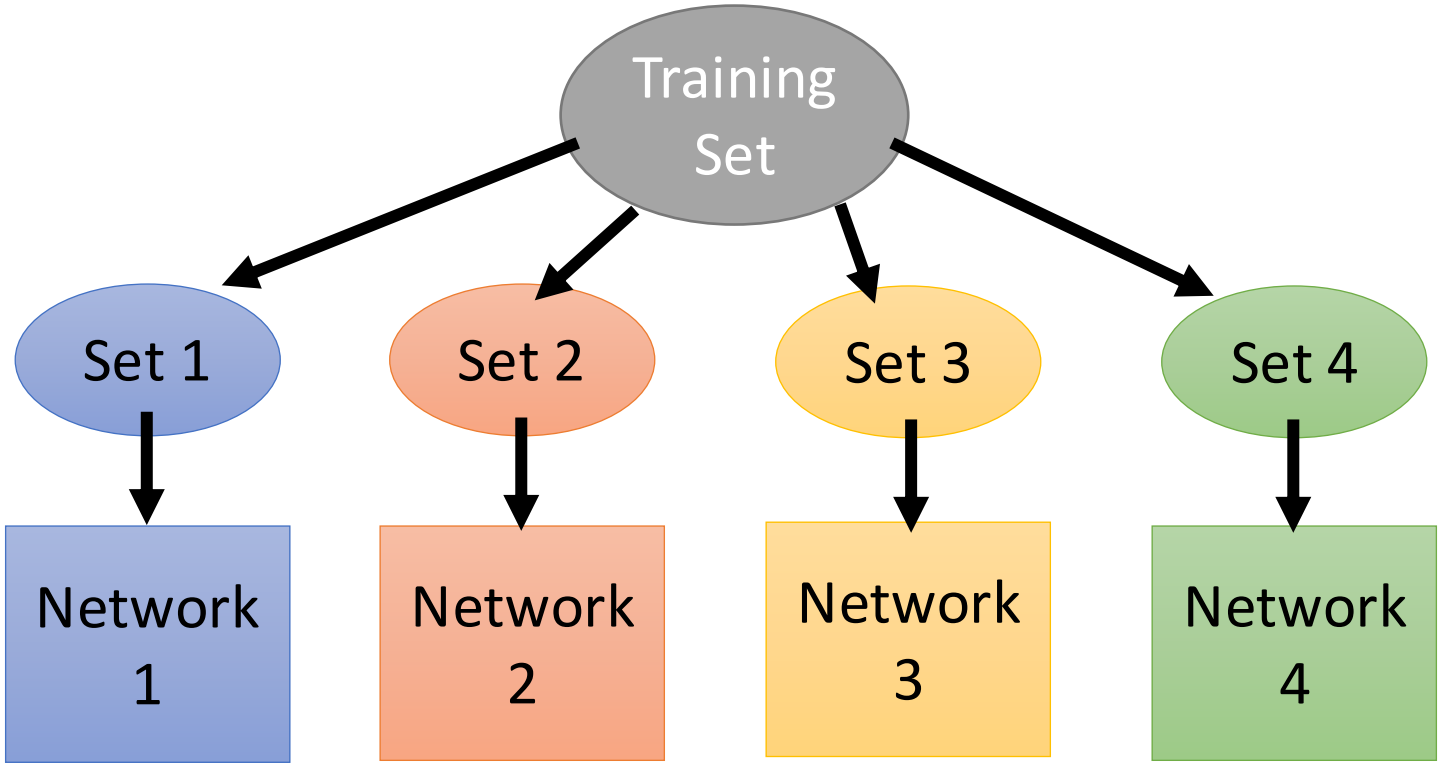


Weights multiply 1-p%

$z' \approx z$

Dropout is a kind of ensemble.

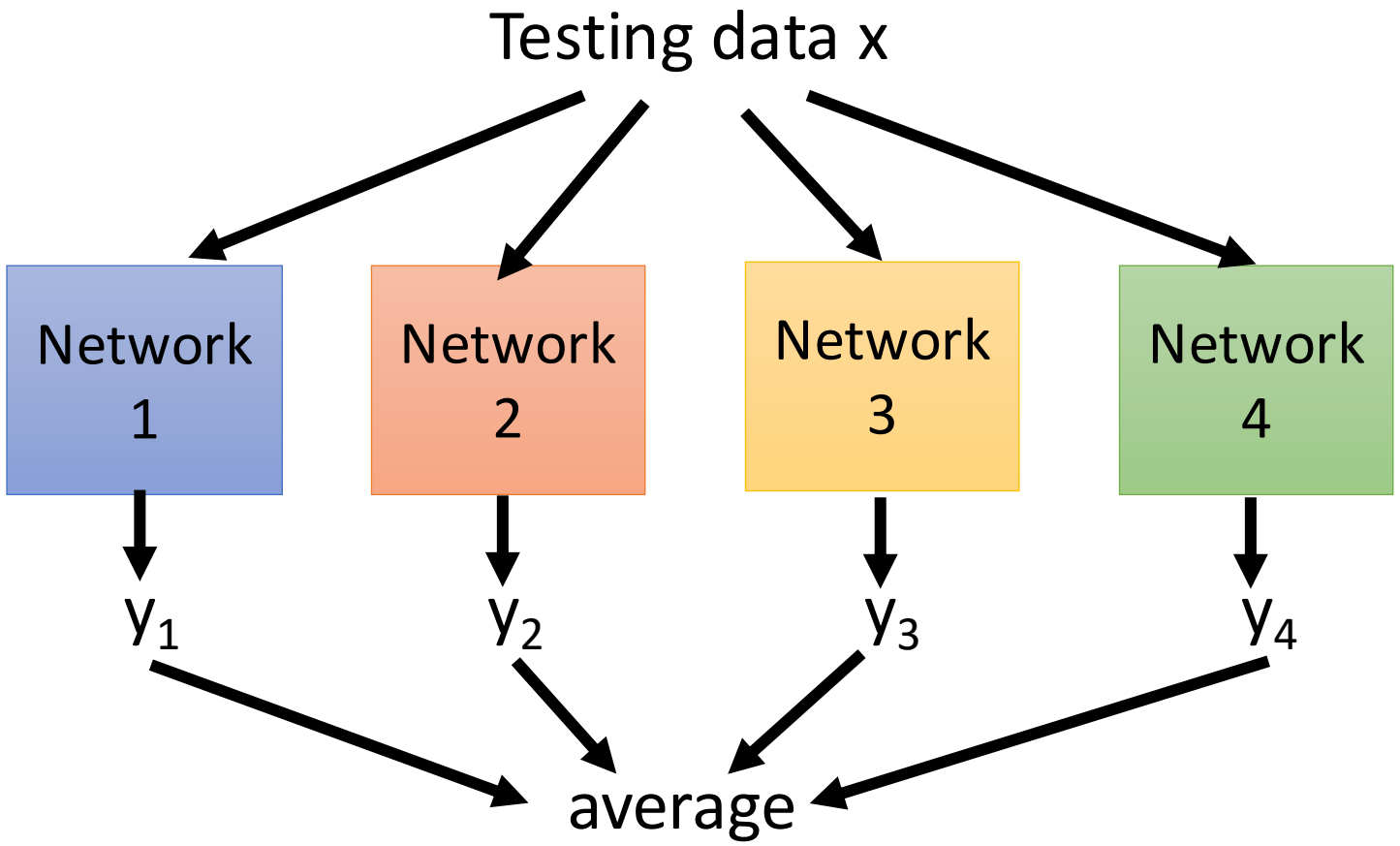
Ensemble



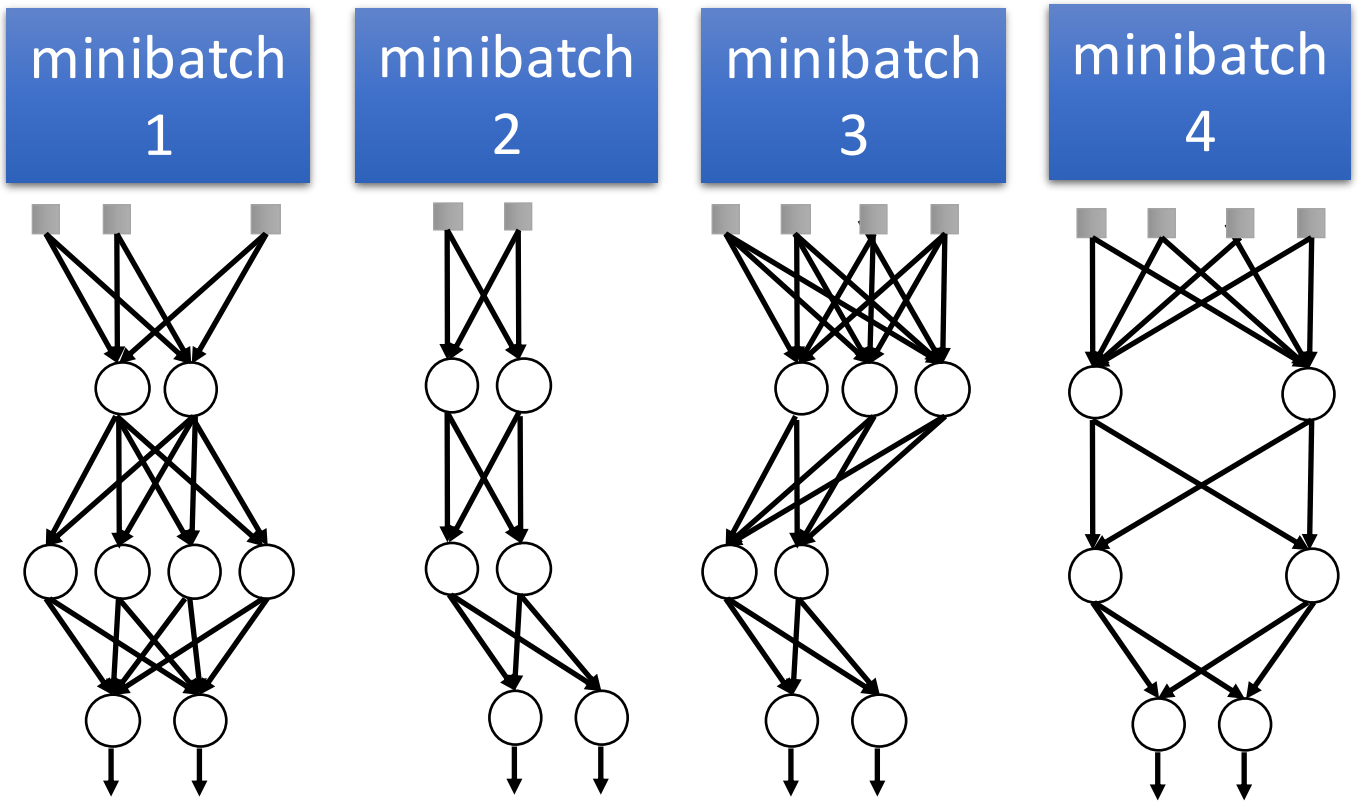
Train a bunch of networks with different structures

Dropout is a kind of ensemble.

Ensemble



Dropout is a kind of ensemble.



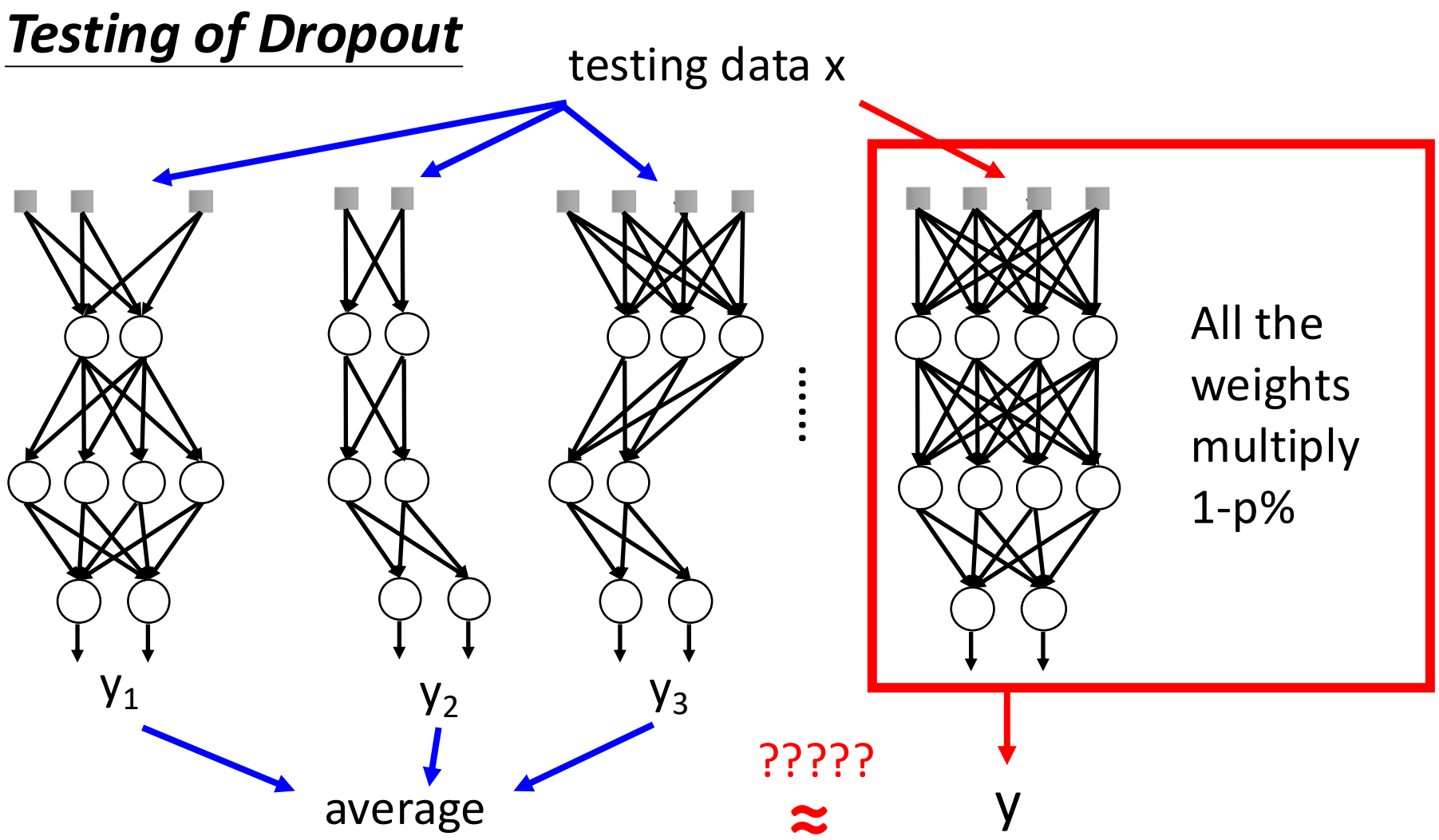
Training of Dropout

M neurons

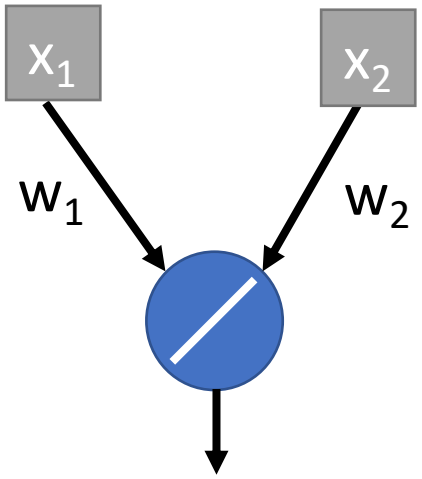
2^M possible networks

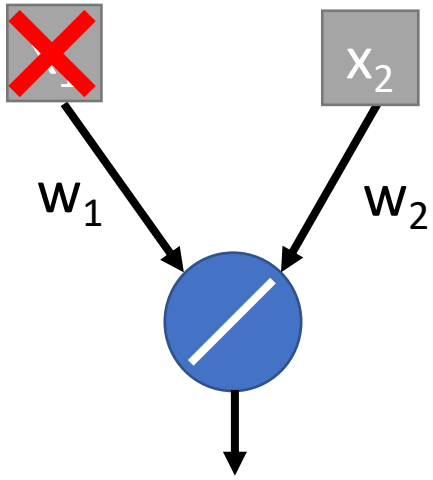
- Using one mini-batch to train one network
- Some parameters in the network are shared

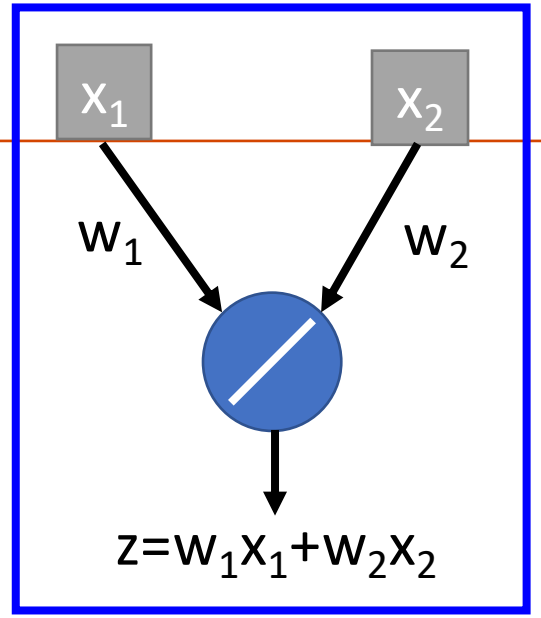
Dropout is a kind of ensemble.

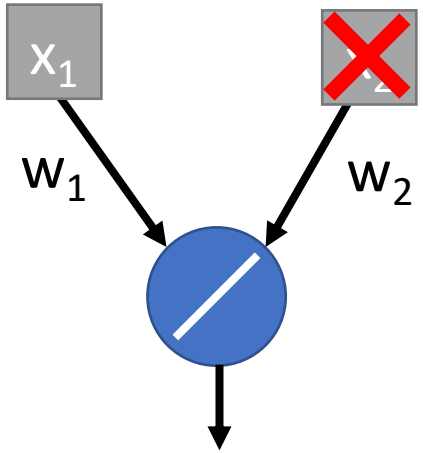


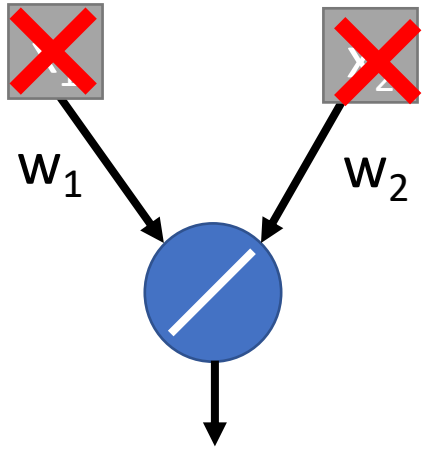
Testing of Dropout

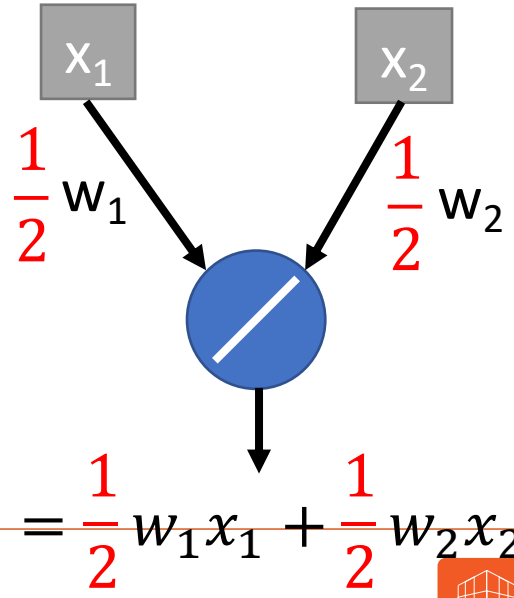












Dropout Summary

```
""" Vanilla Dropout: Not recommended implementation (see notes below) """

p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
  """ X contains the data """

  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = np.random.rand(*H1.shape) < p # first dropout mask
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = np.random.rand(*H2.shape) < p # second dropout mask
  H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3

  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)

def predict(X):
  # ensembled forward pass
  H1 = np.maximum(0, np.dot(W1, X) + b1) * p # NOTE: scale the activations
  H2 = np.maximum(0, np.dot(W2, H1) + b2) * p # NOTE: scale the activations
  out = np.dot(W3, H2) + b3
```

drop in forward pass

scale at test time

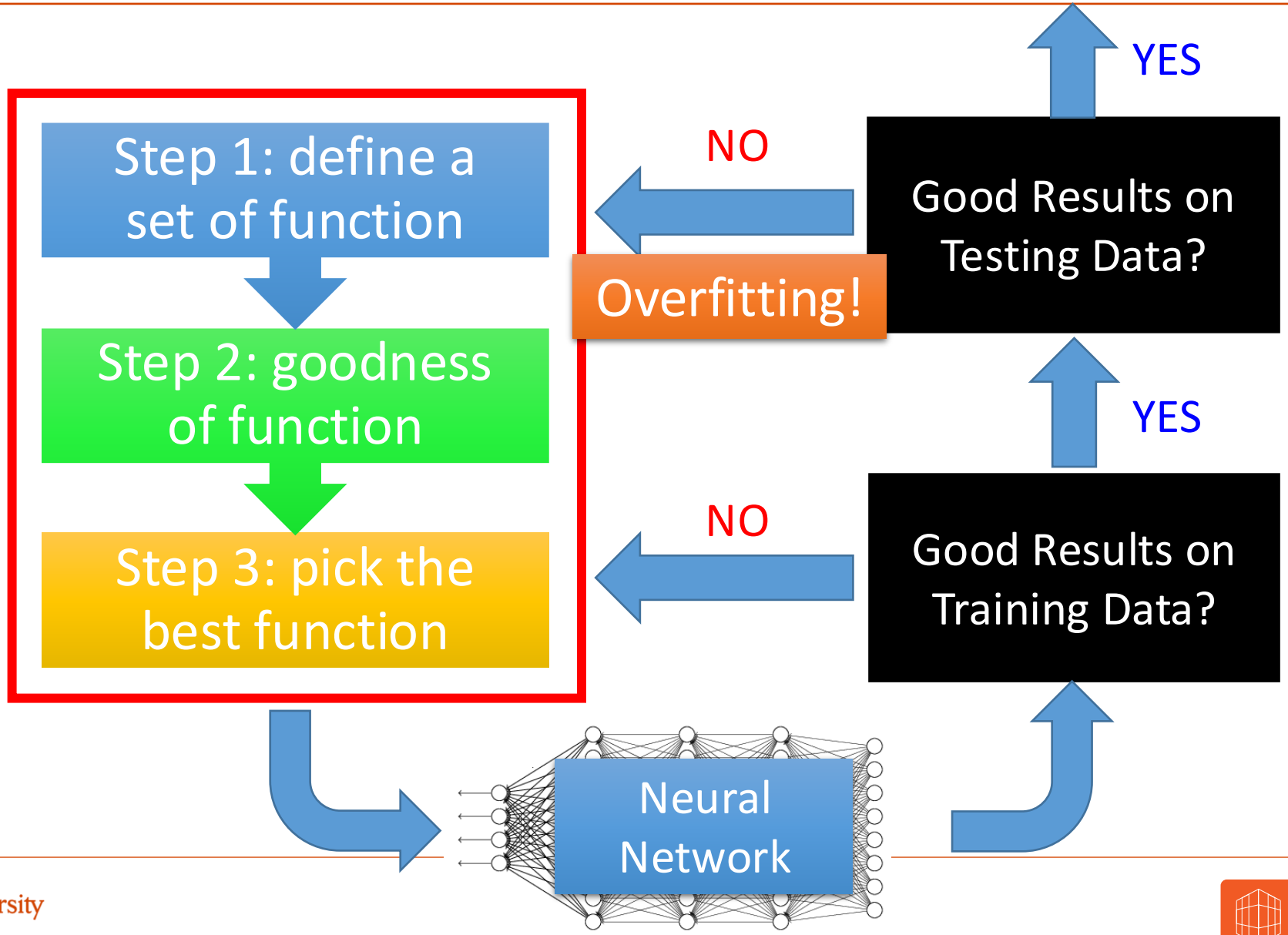
A More Common Implementation: Inverted Dropout

```python
p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = (np.random.rand(*H1.shape) < p) / p # first dropout mask. Notice /p!
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = (np.random.rand(*H2.shape) < p) / p # second dropout mask. Notice /p!
  H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3

  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)

def predict(X):
  # ensembled forward pass
  H1 = np.maximum(0, np.dot(W1, X) + b1) # no scaling necessary
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  out = np.dot(W3, H2) + b3
```

Drop and scale during training

test time is unchanged!

Recipe of Deep Learning



Choosing Hyperparameters

Choosing Hyperparameters: Grid Search

Choose several values for each hyperparameter
(Often space choices log-linearly)

Example:
Weight decay: [$1x10^{-4}$, $1x10^{-3}$, $1x10^{-2}$, $1x10^{-1}$]
Learning rate: [$1x10^{-4}$, $1x10^{-3}$, $1x10^{-2}$, $1x10^{-1}$]

Evaluate all possible choices on this
hyperparameter grid

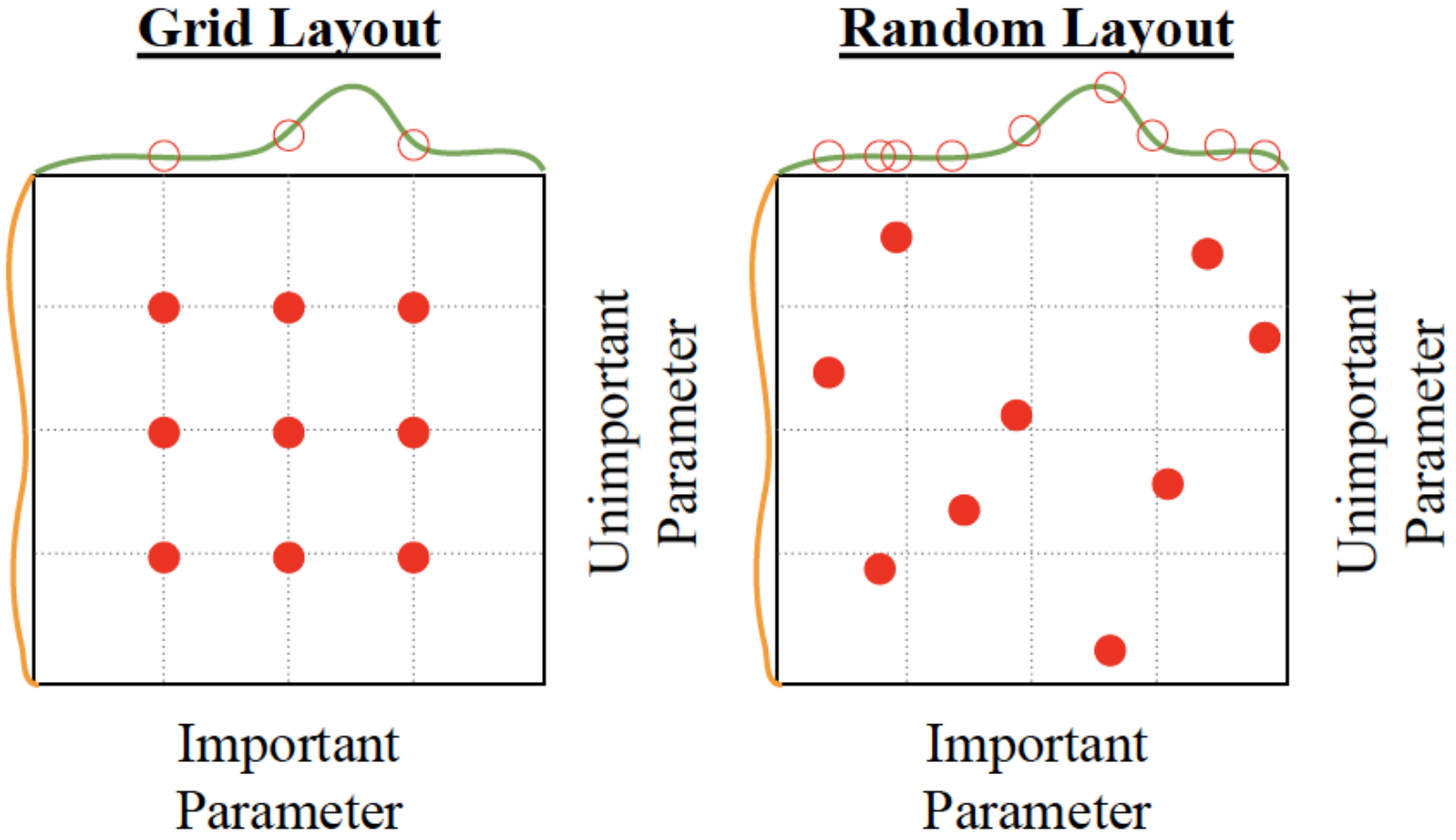
Choosing Hyperparameters: Random Search

Choose several values for each hyperparameter
(Often space choices log-linearly)

Example:
Weight decay: log-uniform on $[1x10^{-4}, 1x10^{-1}]$
Learning rate: log-uniform on $[1x10^{-4}, 1x10^{-1}]$

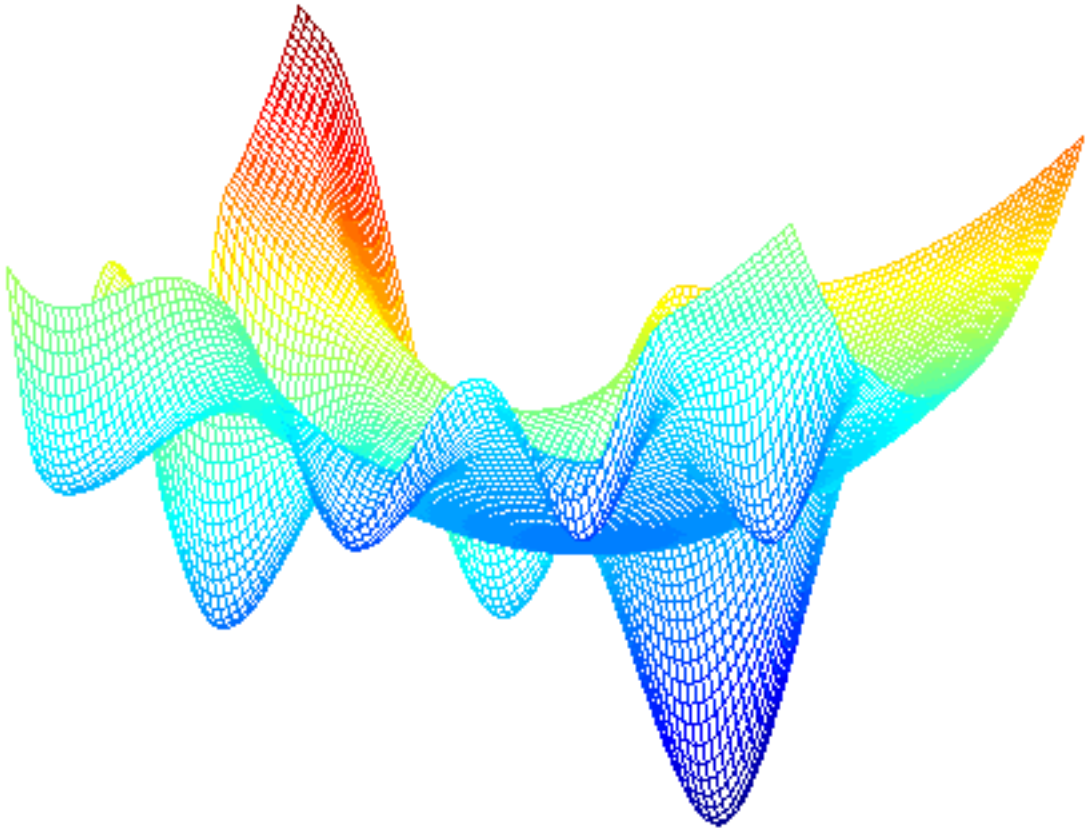
Run many different trials

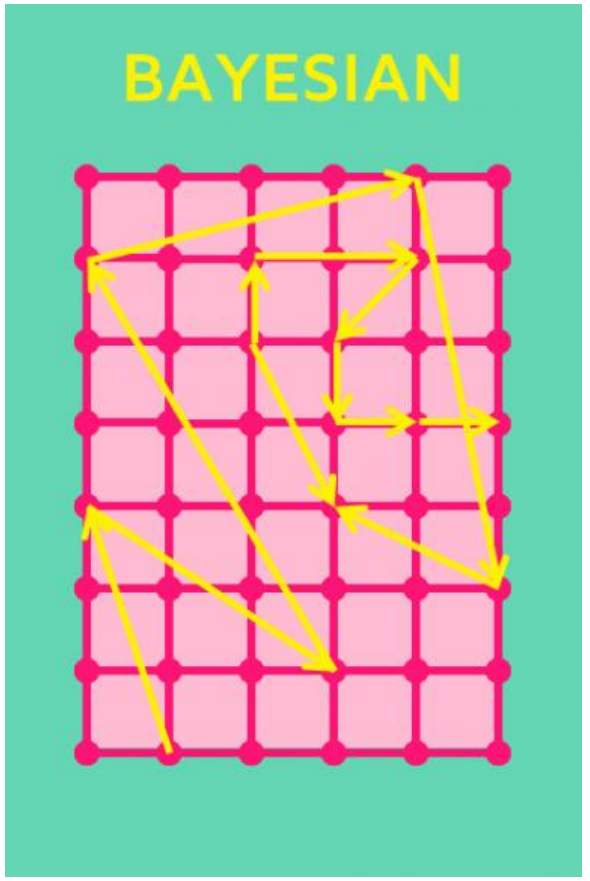
Hyperparameters: Random v.s. Grid Search



Bergstra and Bengio, "Random Search for Hyper-Parameter Optimization", JMLR 2012

Hyperparameters: Bayesian Optimization





https://github.com/fmfn/BayesianOptimization

Choosing Hyperparameters (without tons of GPUs)

Step 1: Check initial loss

Turn off weight decay, sanity check loss at initialization
e.g. log(C) for softmax with C classes

Choosing Hyperparameters

Step 1: Check initial loss
Step 2: Overfit a small sample

Try to train to 100% training accuracy on a small sample of training data (~5-10 minibatches); fiddle with architecture, learning rate, weight initialization. Turn off regularization.

Loss not going down? LR too low, bad initialization
Loss explodes to Inf or NaN? LR too high, bad initialization

Choosing Hyperparameters

Step 1: Check initial loss
Step 2: Overfit a small sample
Step 3: Find LR that makes loss go down

Use the architecture from the previous step, use all training data, turn on small weight decay, find a learning rate that makes the loss drop significantly within ~100 iterations

Good learning rates to try: 1e-1, 1e-2, 1e-3, 1e-4

Choosing Hyperparameters

Step 1: Check initial loss
Step 2: Overfit a small sample
Step 3: Find LR that makes loss go down
Step 4: Coarse grid, train for ~1-5 epochs

Choose a few values of learning rate and weight decay around what worked from Step 3, train a few models for ~1-5 epochs

Good weight decay to try: 1e-4, 1e-5, 0

Choosing Hyperparameters

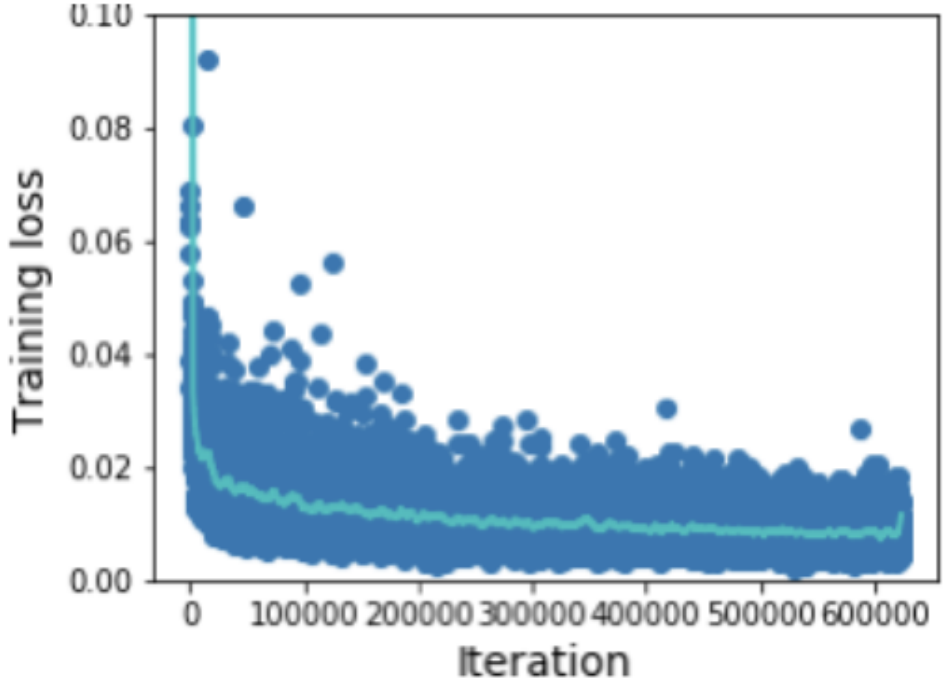
Step 1: Check initial loss
Step 2: Overfit a small sample
Step 3: Find LR that makes loss go down
Step 4: Coarse grid, train for ~1-5 epochs
Step 5: Refine grid, train longer

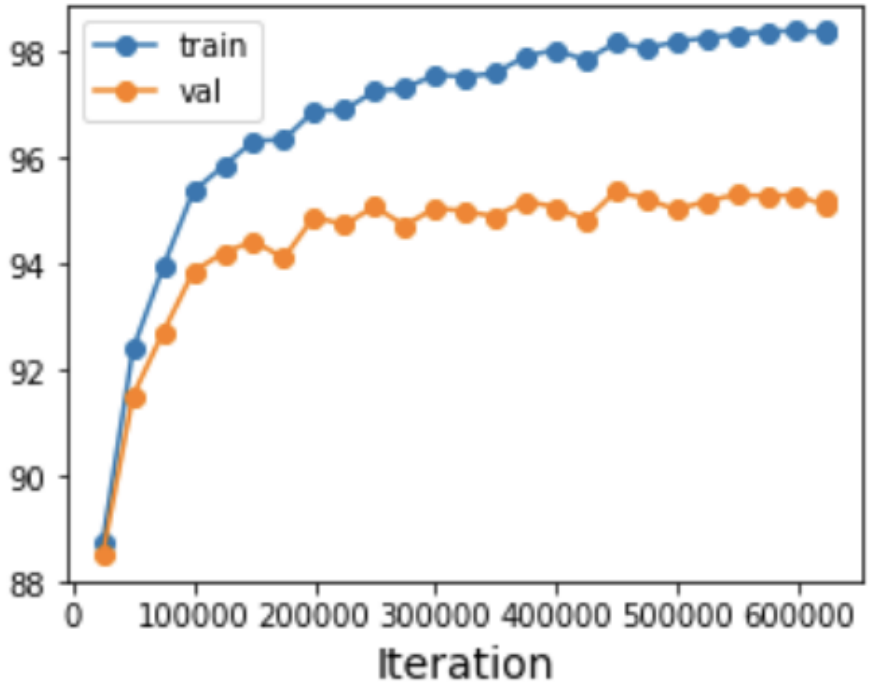
Pick best models from Step 4, train them for longer (~10-20 epochs) without learning rate decay

Choosing Hyperparameters

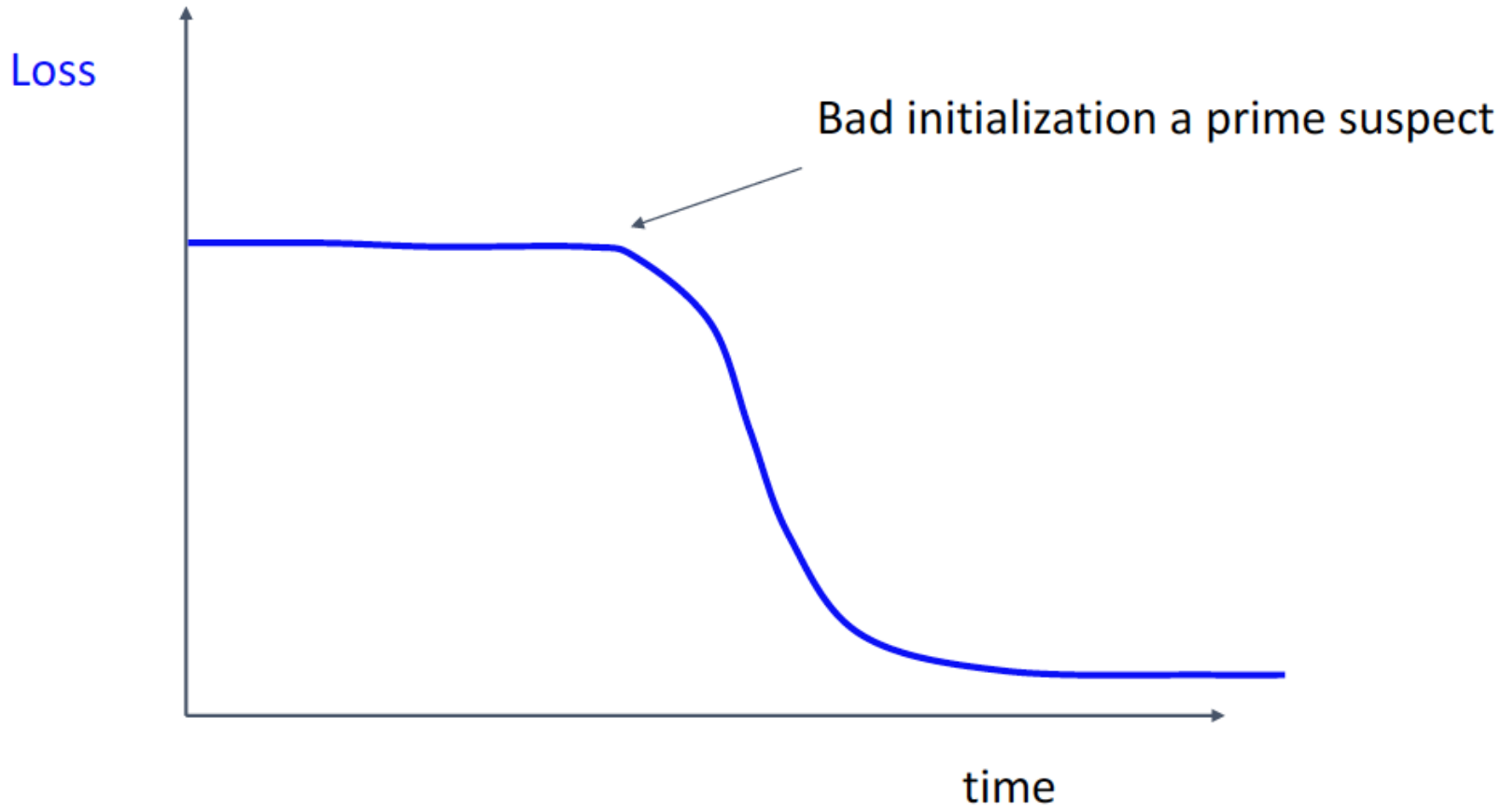
Step 1: Check initial loss
Step 2: Overfit a small sample
Step 3: Find LR that makes loss go down
Step 4: Coarse grid, train for ~1-5 epochs
Step 5: Refine grid, train longer
Step 6: Look at the learning curves

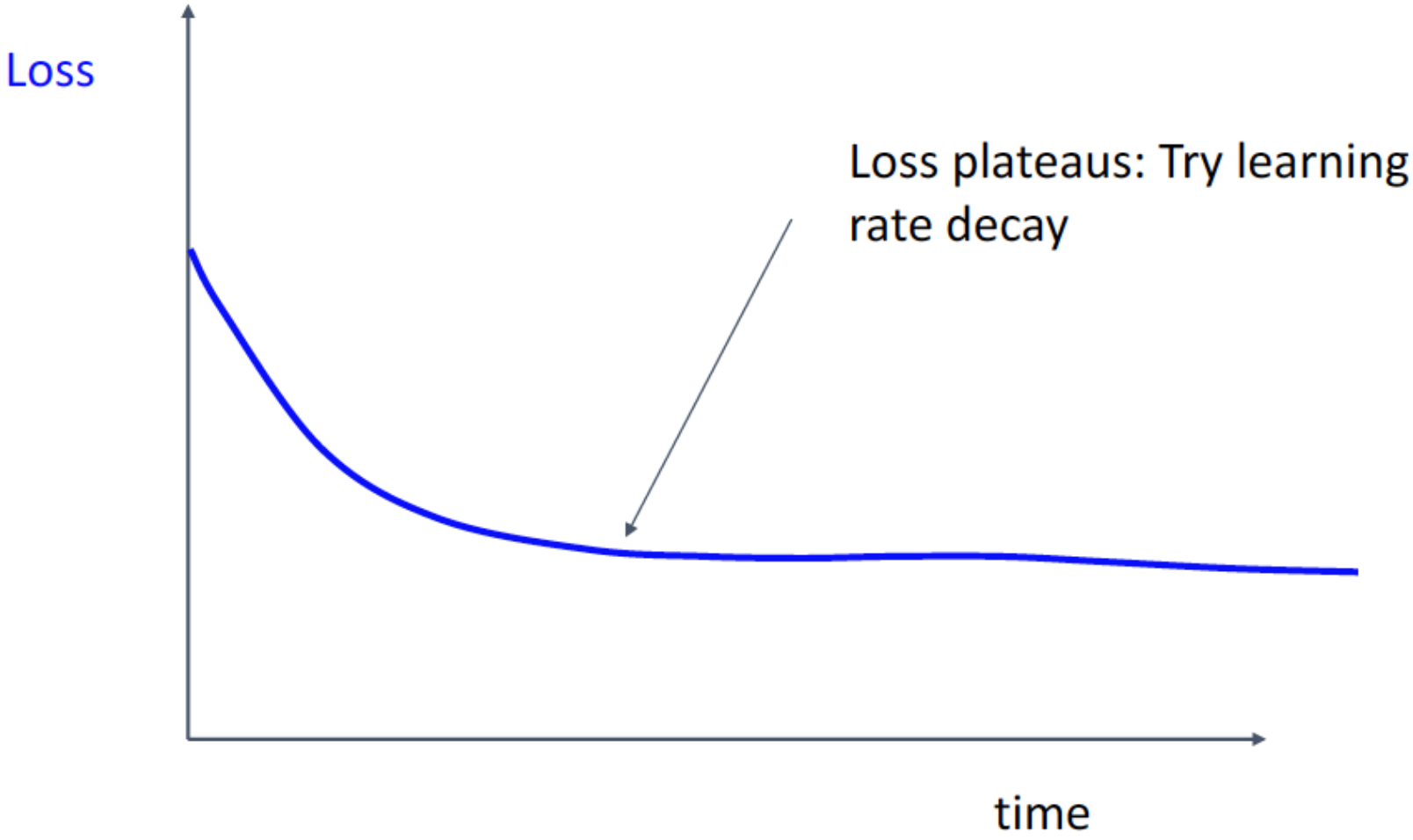
Look at Learning Curves!

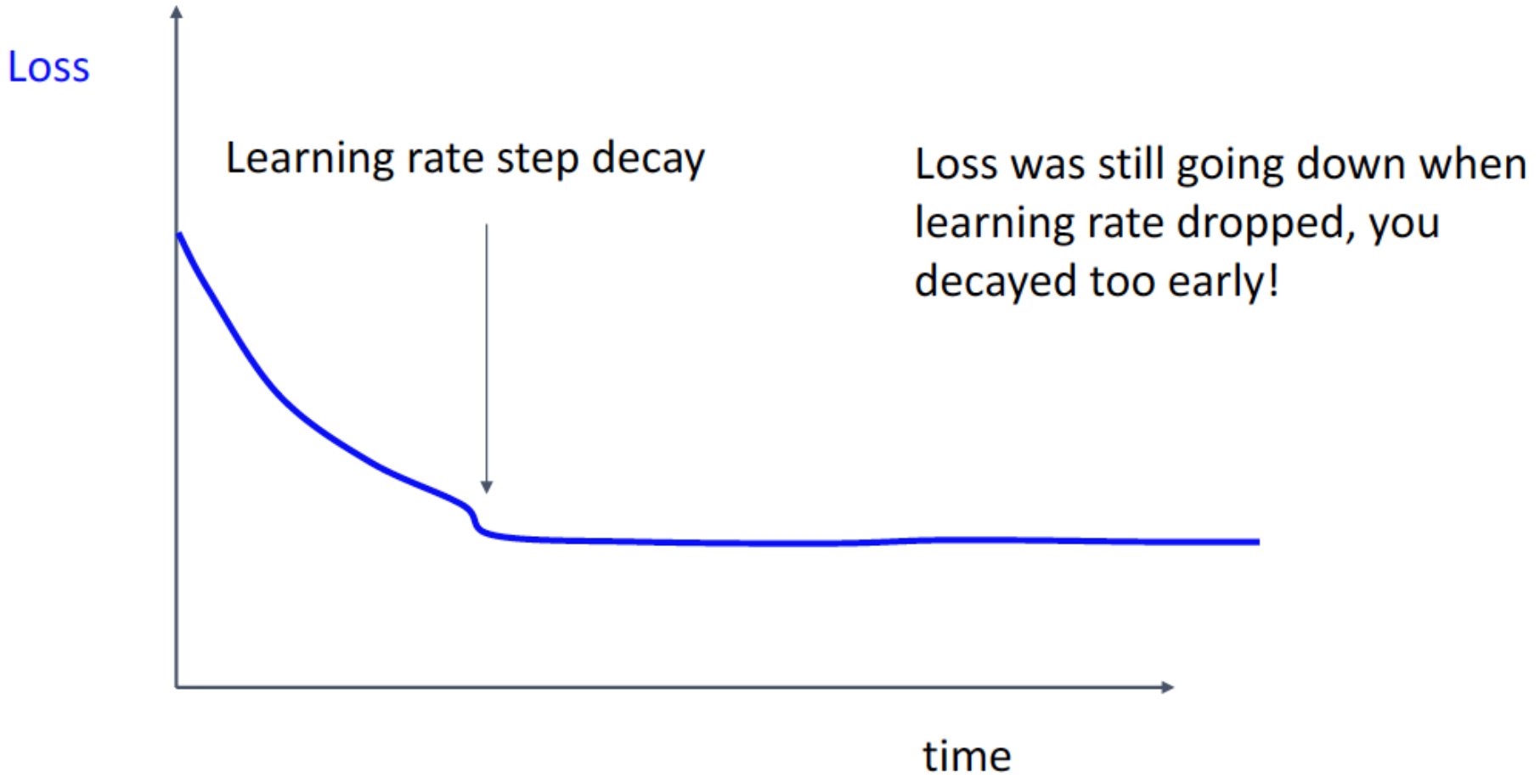


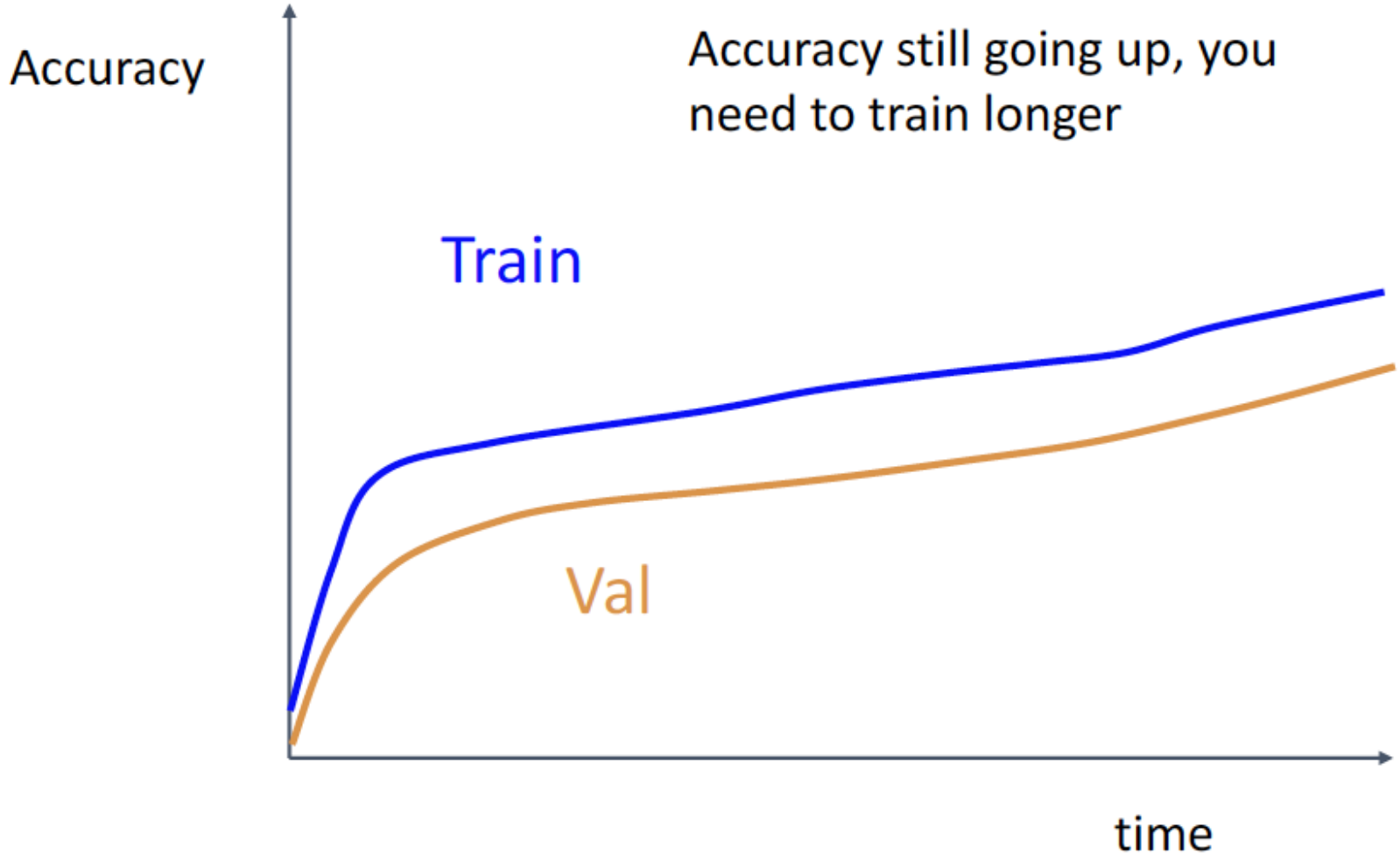


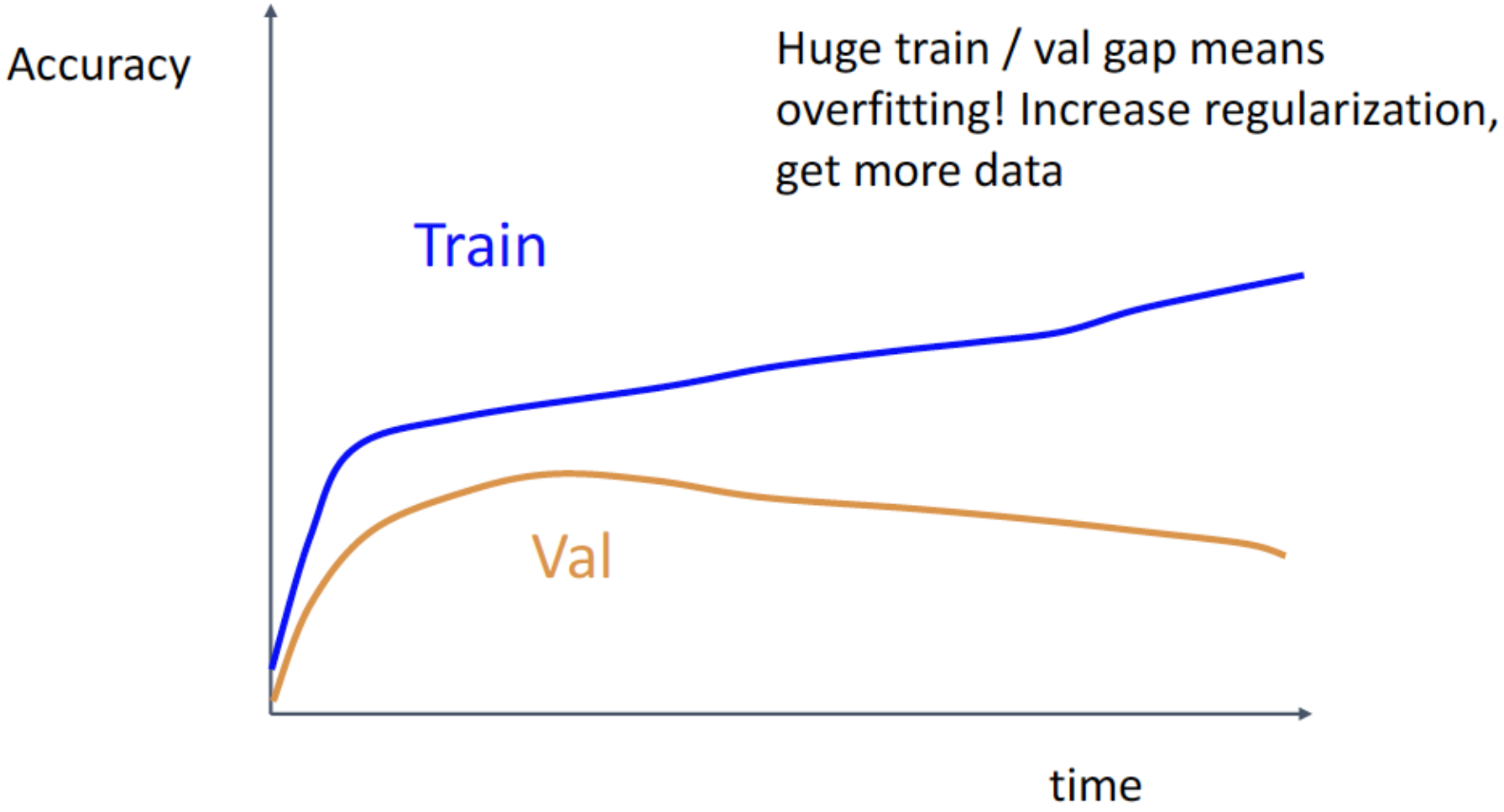
Losses may be noisy, use a scatter plot and also plot moving average to see trends better


Loss
Bad initialization a prime suspect
time

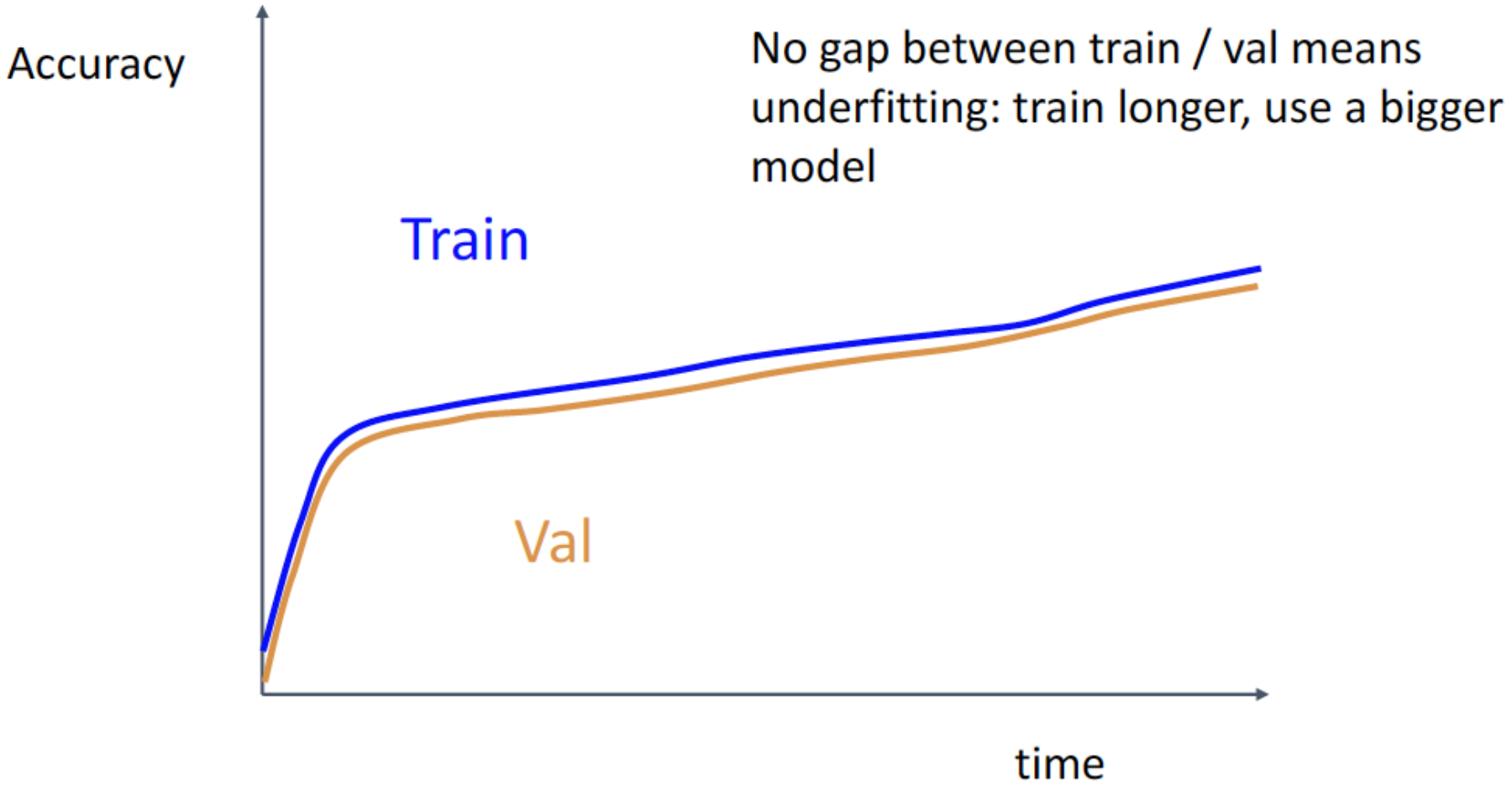

Loss
Loss plateaus: Try learning rate decay
time


Loss
Learning rate step decay
Loss was still going down when learning rate dropped, you decayed too early!
time


Accuracy
Accuracy still going up, you need to train longer
Train
Val
time


Accuracy
Huge train / val gap means overfitting! Increase regularization, get more data
Train
Val
time

Choosing Hyperparameters



Choosing Hyperparameters

Step 1: Check initial loss
Step 2: Overfit a small sample
Step 3: Find LR that makes loss go down
Step 4: Coarse grid, train for ~1-5 epochs
Step 5: Refine grid, train longer
Step 6: Look at the learning curves
Step 7: GO BACK to step 5

Summary: Choosing Hyperparameters

- network architecture
- learning rate, its decay schedule, update type
- regularization (L2/Dropout strength)

Summary: Choosing Hyperparameters

- network architecture
- learning rate, its decay schedule, update type
- regularization (L2/Dropout strength)

Use Tensor Board

Any Questions?

bidong@syr.edu