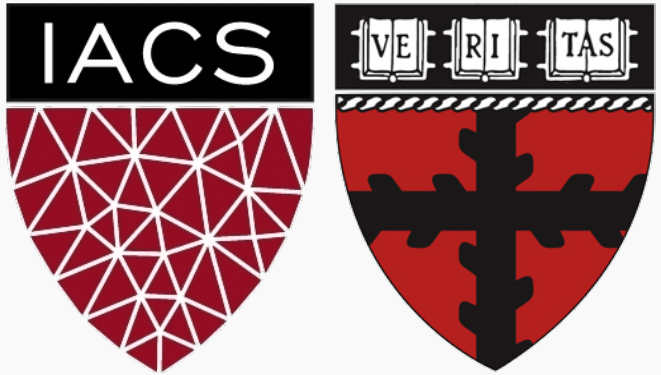
Lecture 21: Optimization and Regularization

CS109A Introduction to Data Science

Pavlos Protopapas, Kevin Rader and Chris Tanner



ANNOUNCEMENTS

- Homework 7 OH:

  y_out in 1.1 is just to get diimensions out

  - For conceptual questions: Kevin and Chris will continue their office hours.
  - If you have problems with TensorFlow please let us know on ED. We will arrange special OH to help if necessary.
- Project:
  - Milestone3 due on Wed. EDA and base model

Outline

Optimization

Regularization of NN

Outline

Optimization

- Challenges in Optimization
- Momentum
- Adaptive Learning Rate
- Parameter Initialization
- Batch Normalization

Regularization of NN

- Norm Penalties
- Early Stopping
- Data Augmentation
- Sparse Representation
- Dropout

Outline

Optimization

- **Challenges in Optimization** ways to improve SGD in NN
- Momentum
- Adaptive Learning Rate
- Parameter Initialization
- Batch Normalization

Regularization of NN preventing overfitting of NN

- Norm Penalties
- Early Stopping
- Data Augmentation
- Sparse Representation
- Dropout

Learning vs. Optimization

Goal of learning: minimize generalization error, or the loss function

input and weights

$$\mathcal{L}(W) = \mathbb{E}_{(x,y)\sim p_{data}}\left[L(f\left(x, W\right), y\right]$$

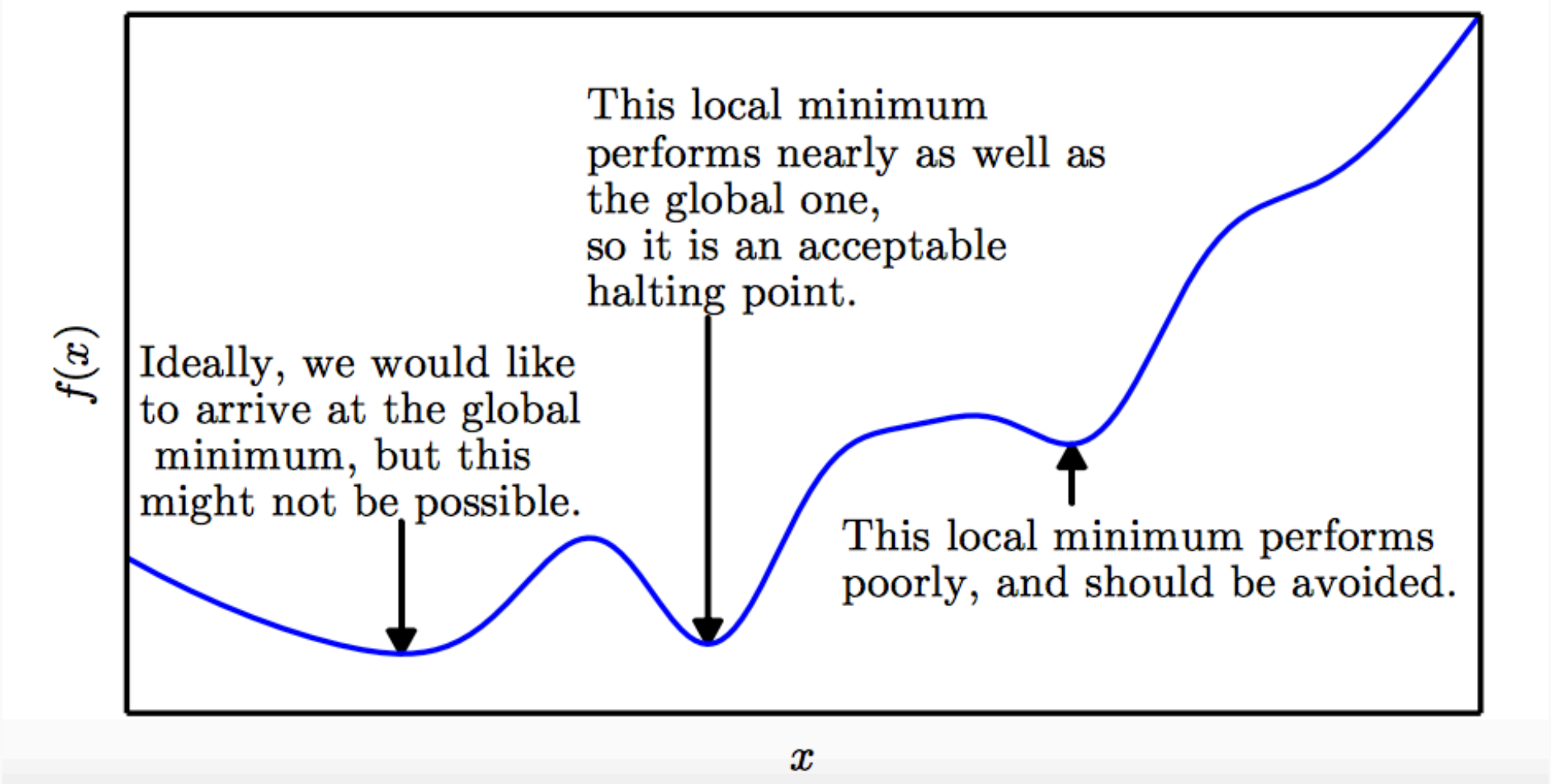
f is the neural network

In practice, empirical risk minimization:

$$\mathcal{L}(W) = \sum_i \left[L(f\left(x_i; W\right), y_i\right]$$

Quantity optimized different from the quantity we care about

Local Minima

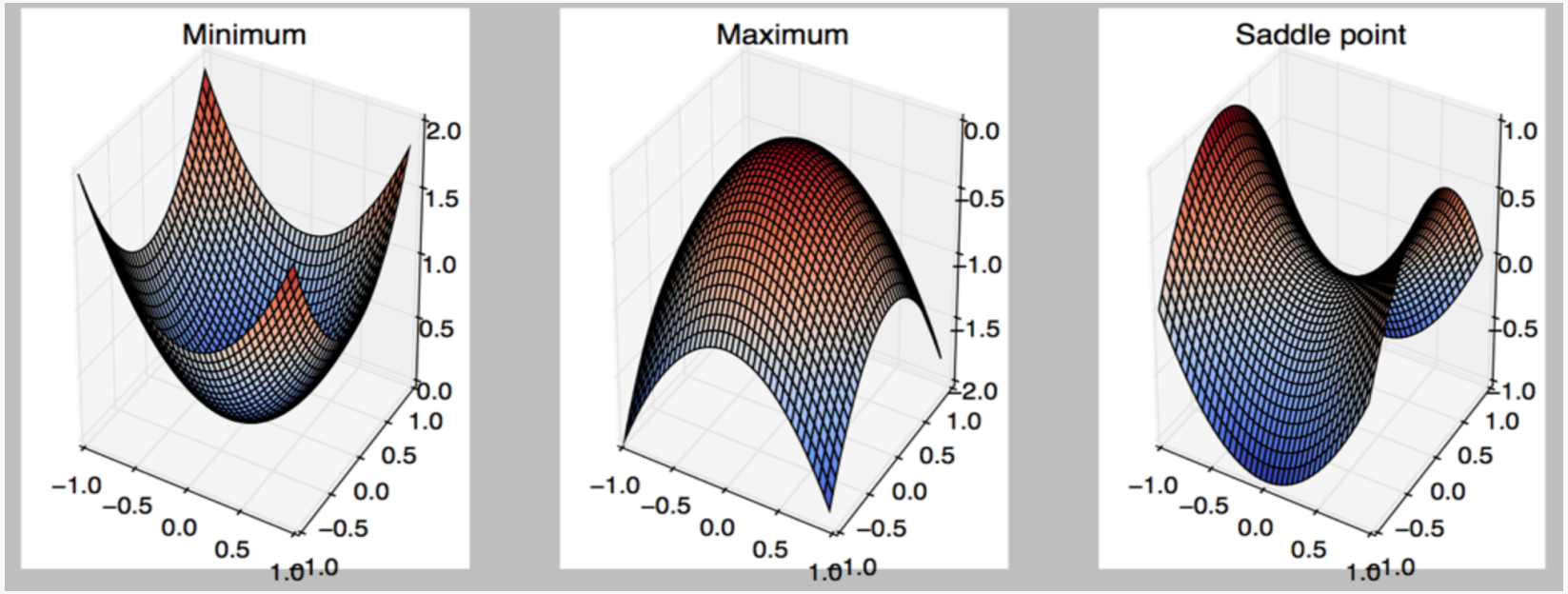


Goodfellow et al. (2016)

Critical Points

Points with zero gradient

2nd-derivate (Hessian) determines curvature



Goodfellow et al. (2016)

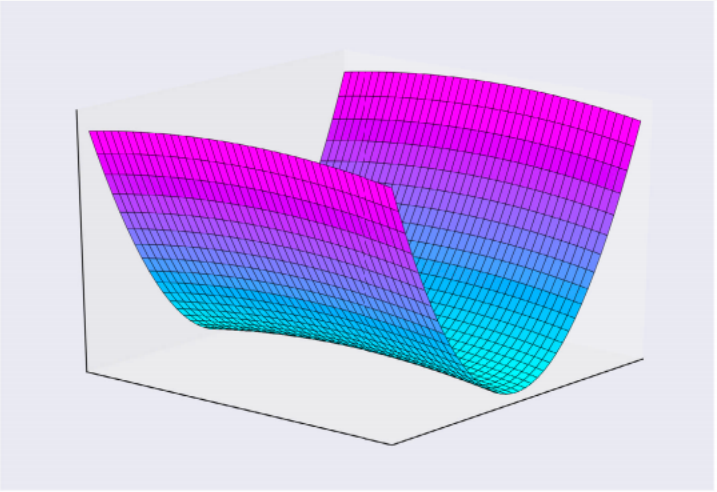
Local Minima

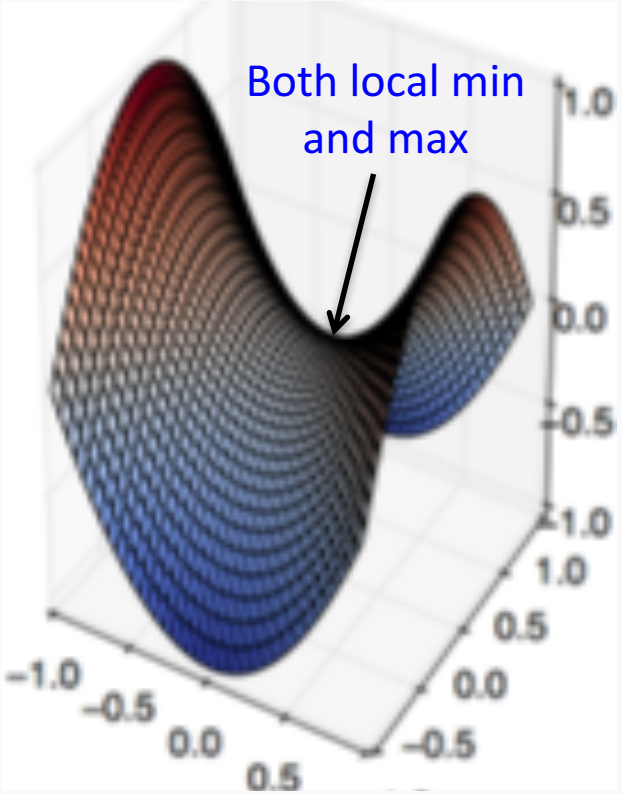
Old view: local minima is major problem in neural network training

Recent view:

- For sufficiently large neural networks, most local minima incur low cost
- Not important to find true global minimum

Saddle Points





Recent studies indicate that in high dim, saddle points are more likely than local min

Gradient can be very small near saddle points

Goodfellow et al. (2016)

Poor Conditioning

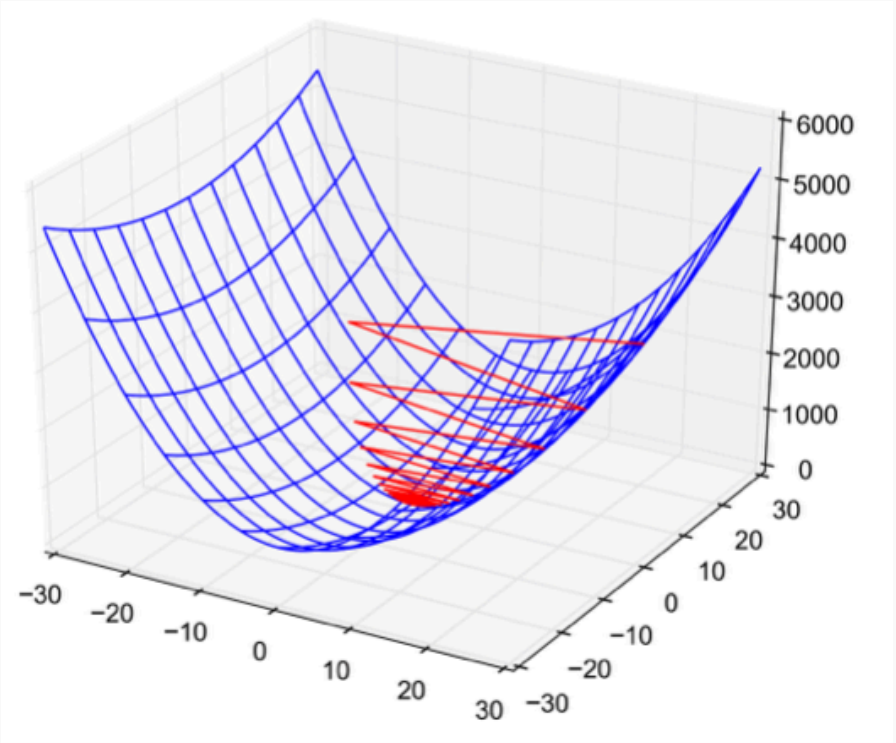
shape of likelihood surface is very complex

Poorly conditioned Hessian matrix

- High curvature: small steps leads to huge increase

Learning is slow despite strong gradients

Oscillations slow down progress

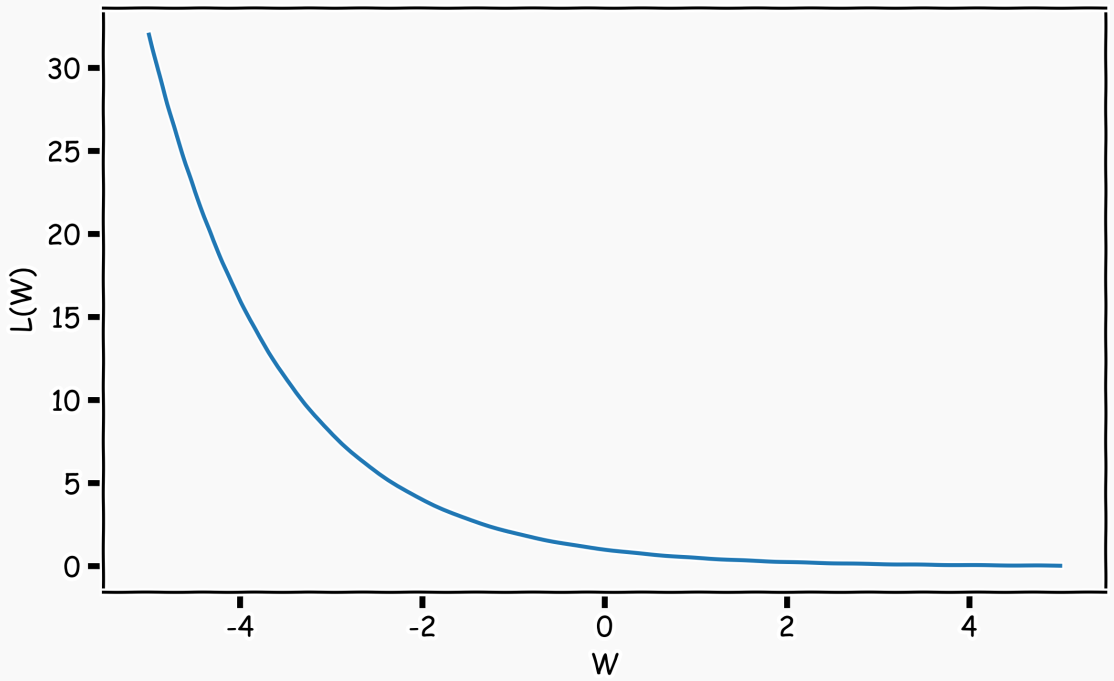


No Critical Points

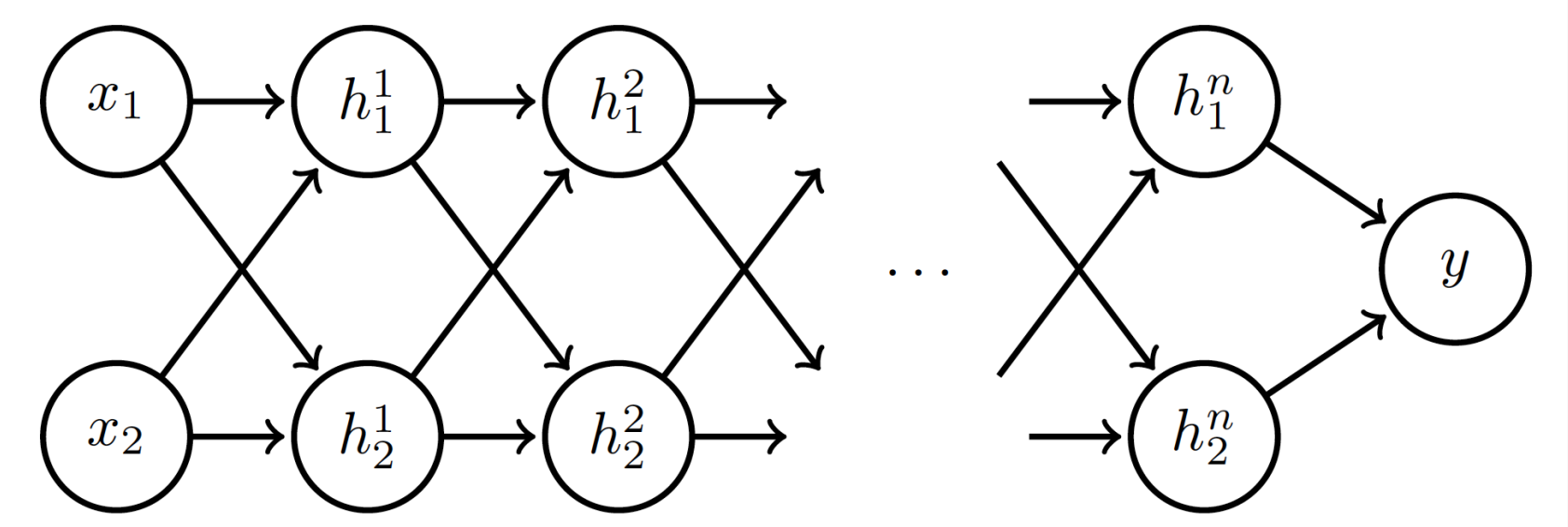
Some cost functions do not have critical points. In particular classification.

WHY?

this is because sigmoid fxn never reaches 0,1
minimum entropy is when probability matches class exactly
but sigmoid fxn will never reach probability 0 or 1



Exploding and Vanishing Gradients



Linear activation $h_i = Wx$

$h_i = Wh_{i-1}, \qquad i = 2, \ldots, n$

Exploding and Vanishing Gradients

$$\text{Suppose } \mathbf{W} = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}:$$

$$\begin{bmatrix} h_1^1 \\ h_2^1 \end{bmatrix} = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad \cdots \quad \begin{bmatrix} h_1^n \\ h_2^n \end{bmatrix} = \begin{bmatrix} a^n & 0 \\ 0 & b^n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

first layer

nth layer

Exploding and Vanishing Gradients

$$\text{Suppose } x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\text{Case 1: } a = 1,\ b = 2:$$

$$y \to 1, \quad \overset{\text{derivative}}{\nabla y \to} \begin{bmatrix} n \\ n2^{n-1} \end{bmatrix}$$

Explodes!

$$\text{Case 2: } a = 0.5,\ b = 0.9:$$

$$y \to 0, \quad \overset{\text{derivative}}{\nabla y \to} \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Vanishes!

this is why you don't want small derivatives in your layers
machine learning precision limits

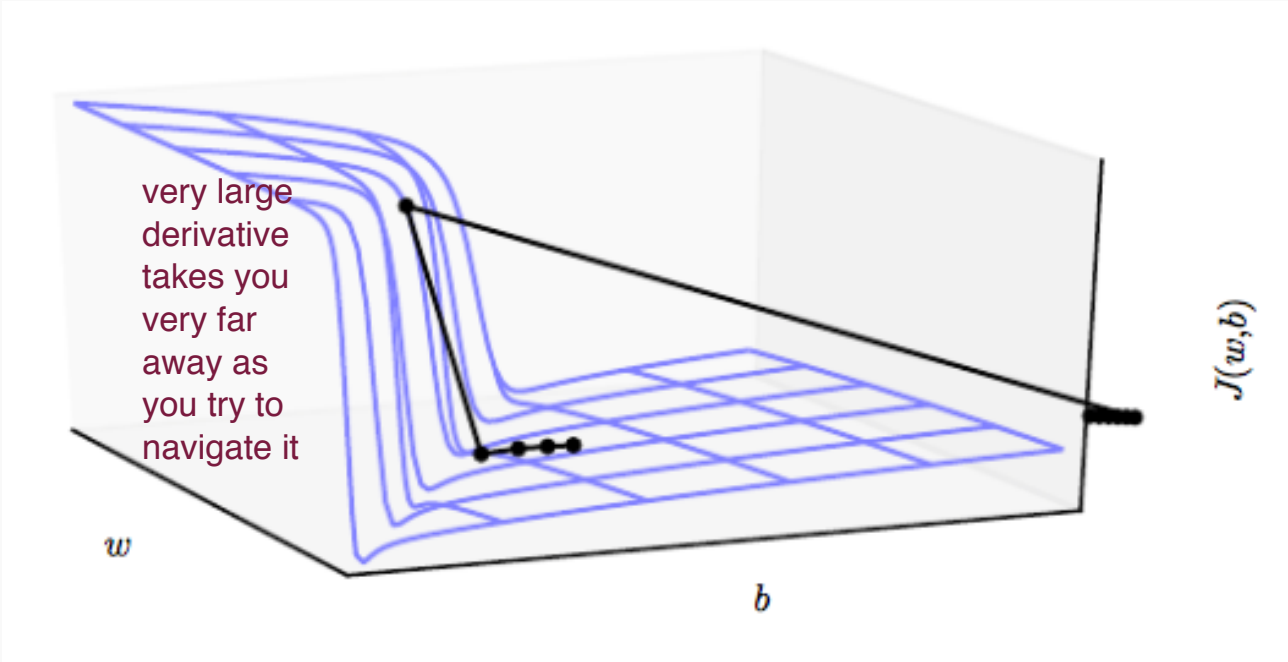
Exploding and Vanishing Gradients

Exploding gradients lead to cliffs

Can be mitigated using gradient clipping

$$\text{if } \|g\| > u$$

$$g \leftarrow \frac{gu}{\|g\|}$$



Goodfellow et al. (2016)

Outline

Optimization

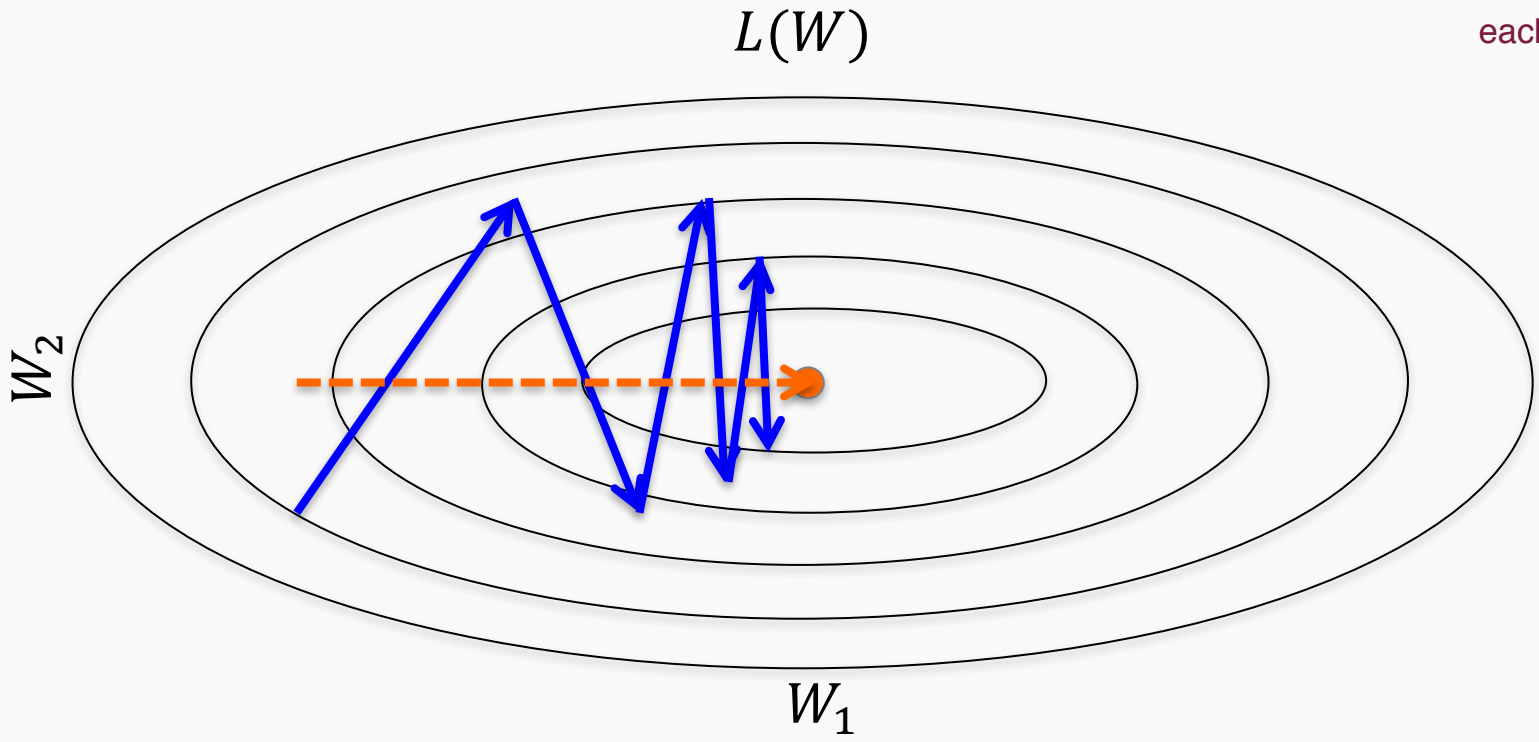
- Challenges in Optimization
- **Momentum** solve the problem of weird shapes
- Adaptive Learning Rate
- Parameter Initialization
- Batch Normalization

Regularization of NN

- Norm Penalties
- Early Stopping
- Data Augmentation
- Sparse Representation
- Dropout

Momentum

Oscillations because updates do not exploit curvature information



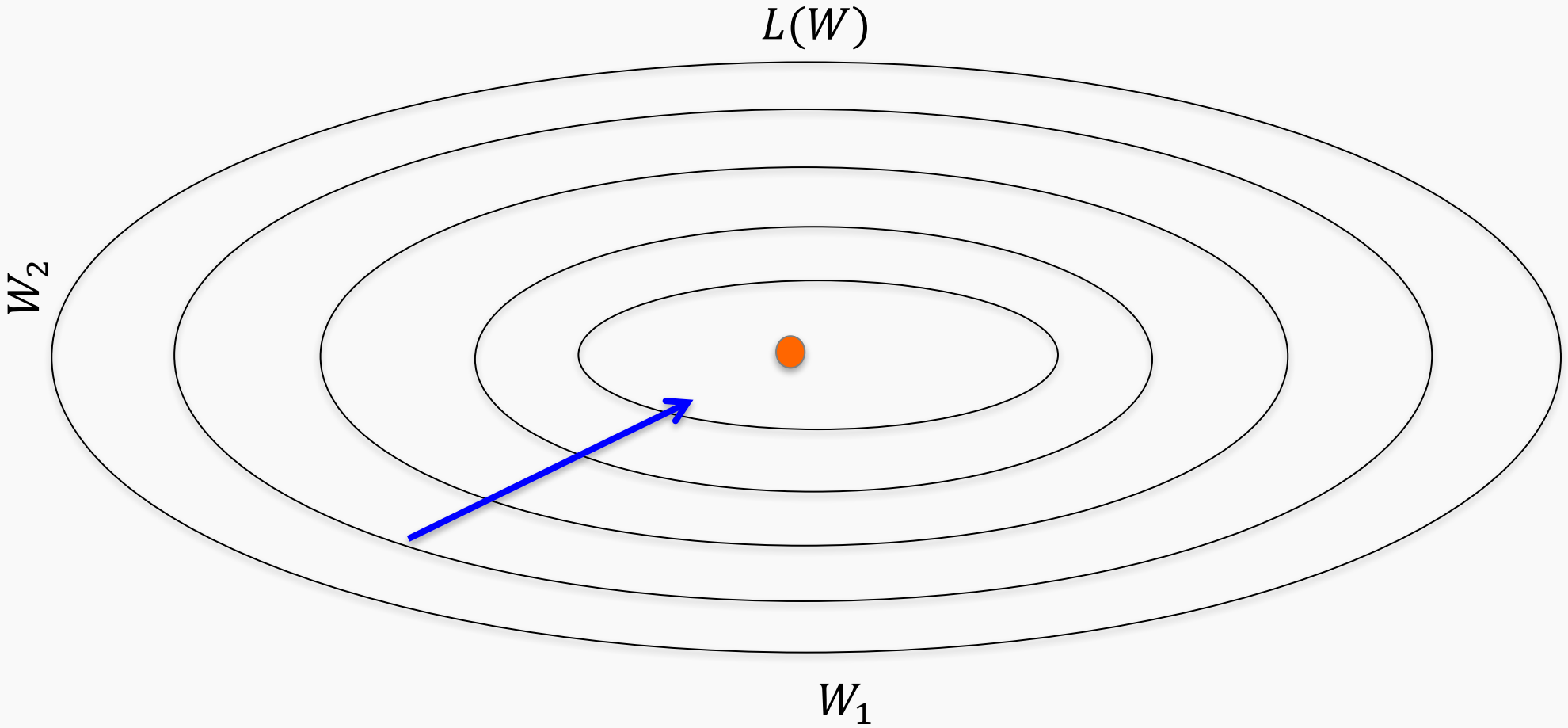
each line represents equal L(W)

Average gradient presents faster path to optimal: vertical components cancel out

Momentum

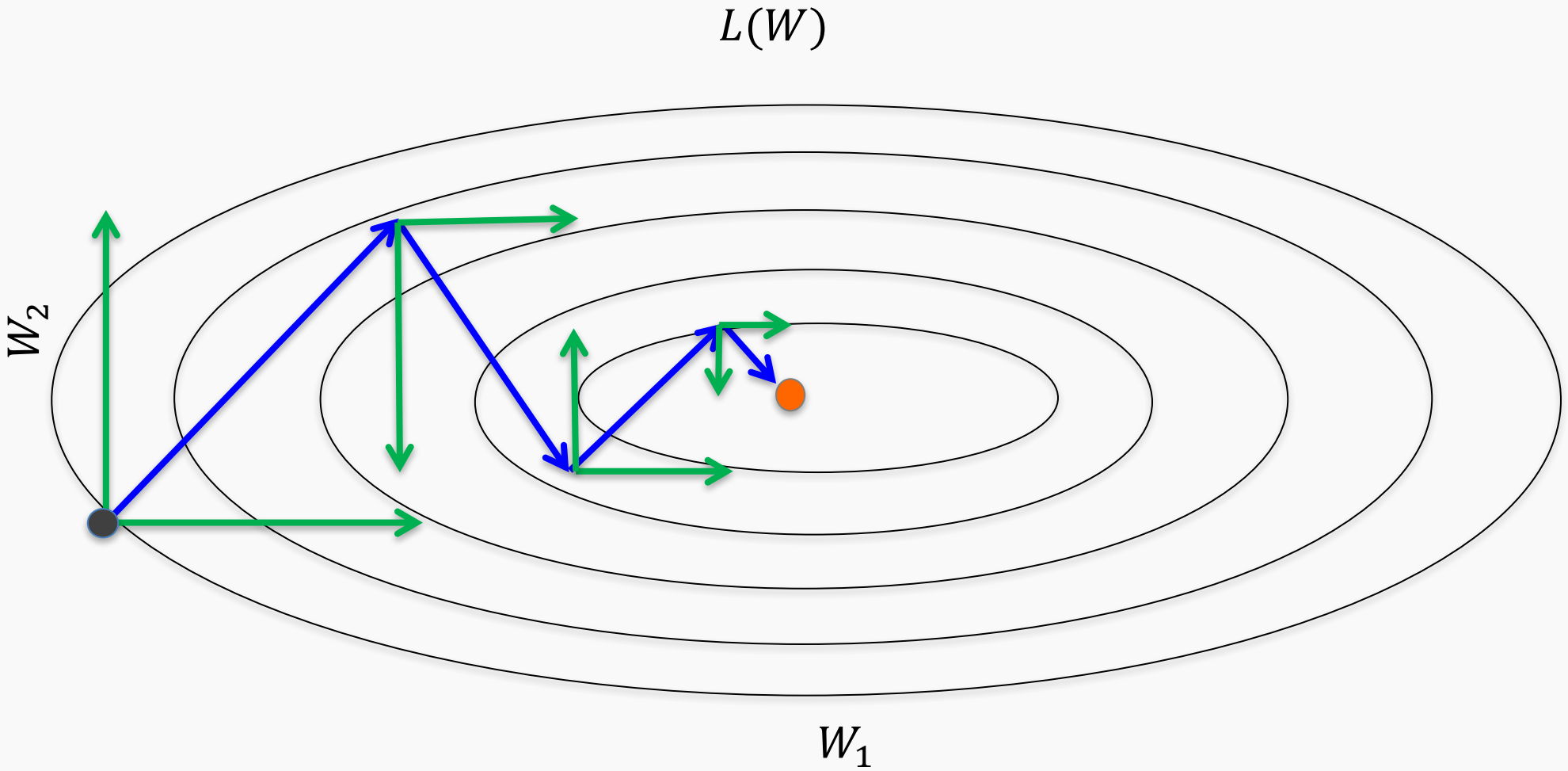
Question: Why not this?

general shape of L(W) - can be elongated, many parameters in practice, not just quadratic



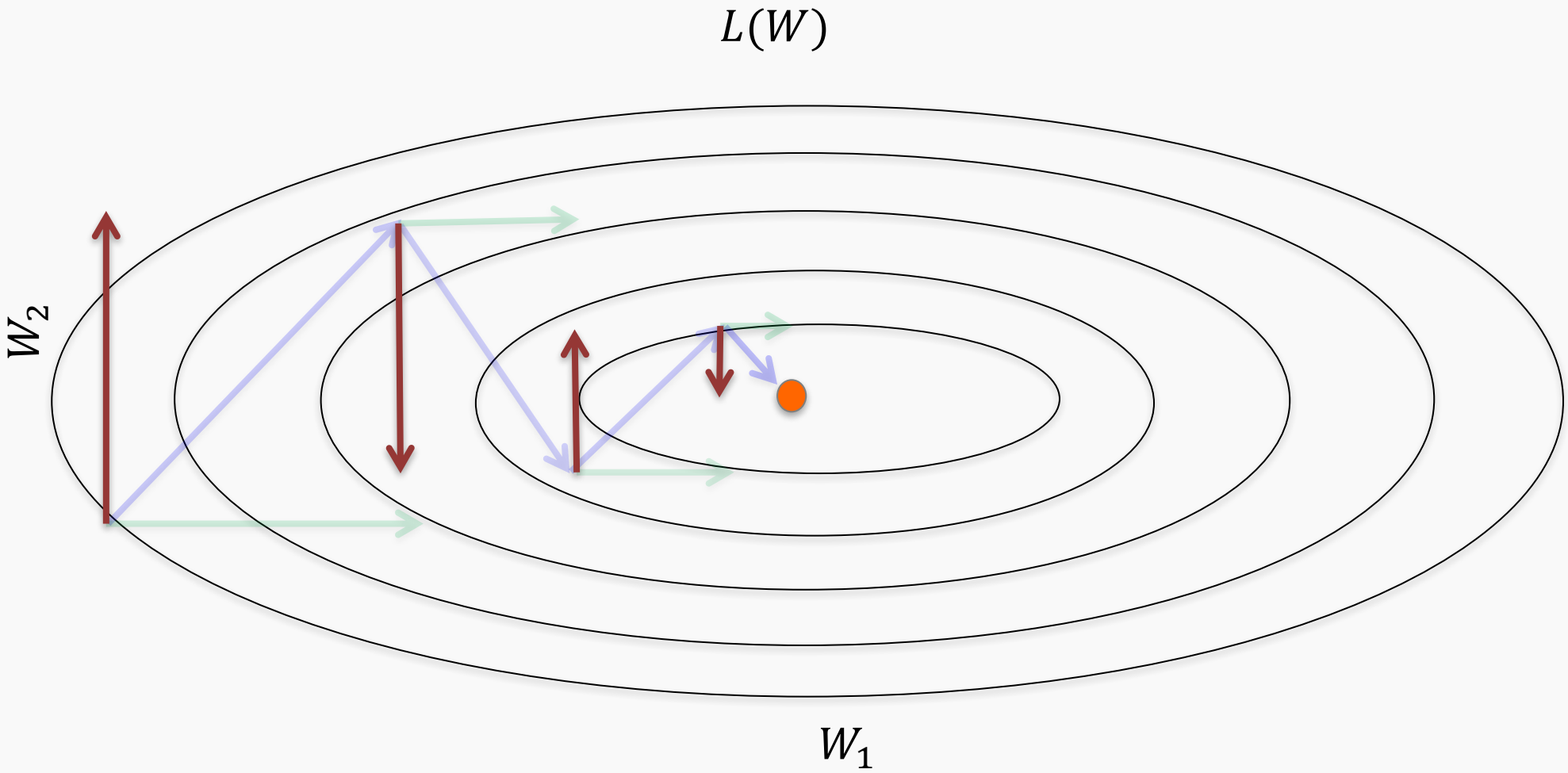
Momentum

Let us figure out an algorithm which will lead us to the minimum faster.



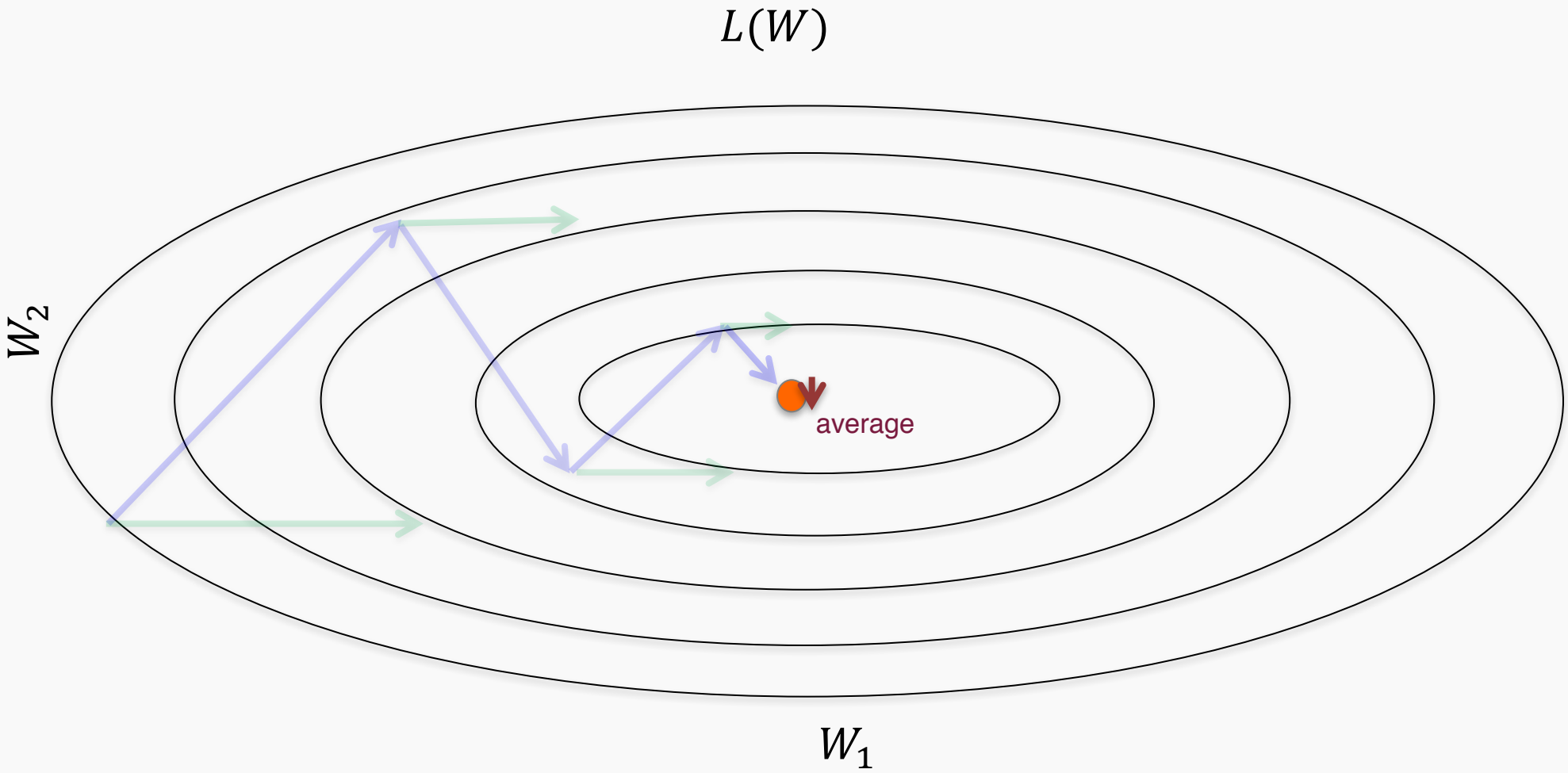
Momentum

Look each component at a time



Momentum

Let us figure out an algorithm



Momentum

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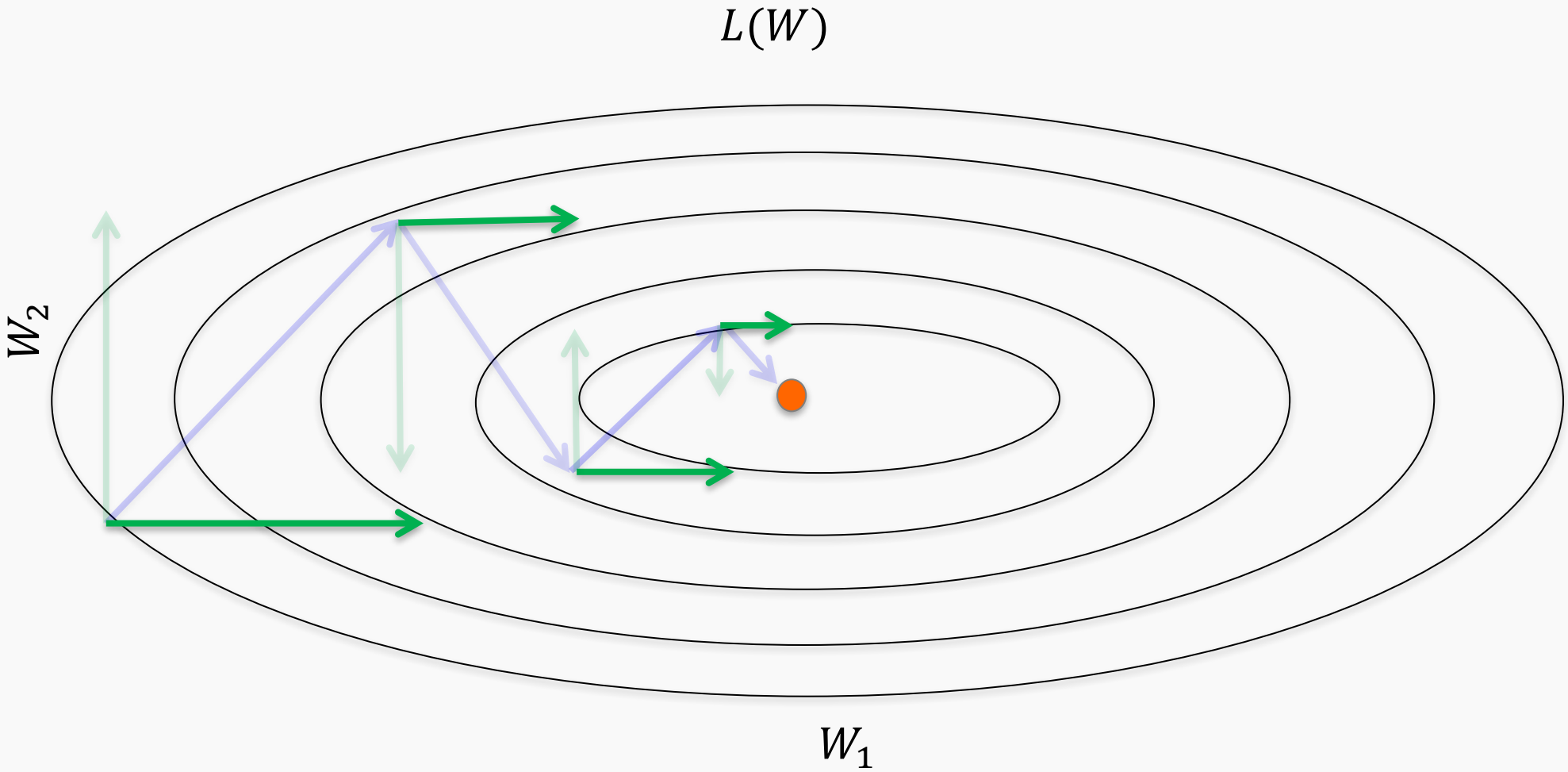
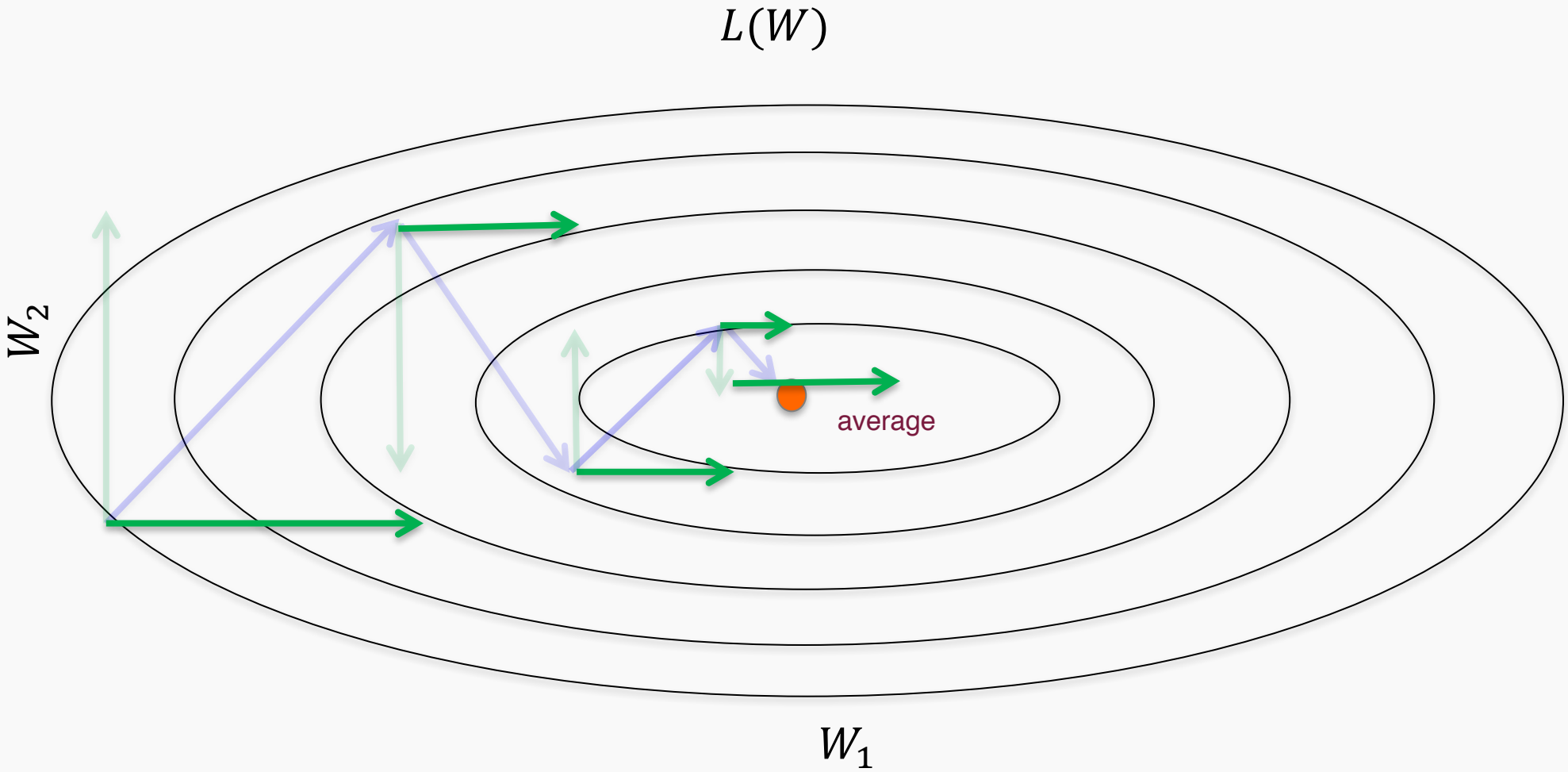


Momentum

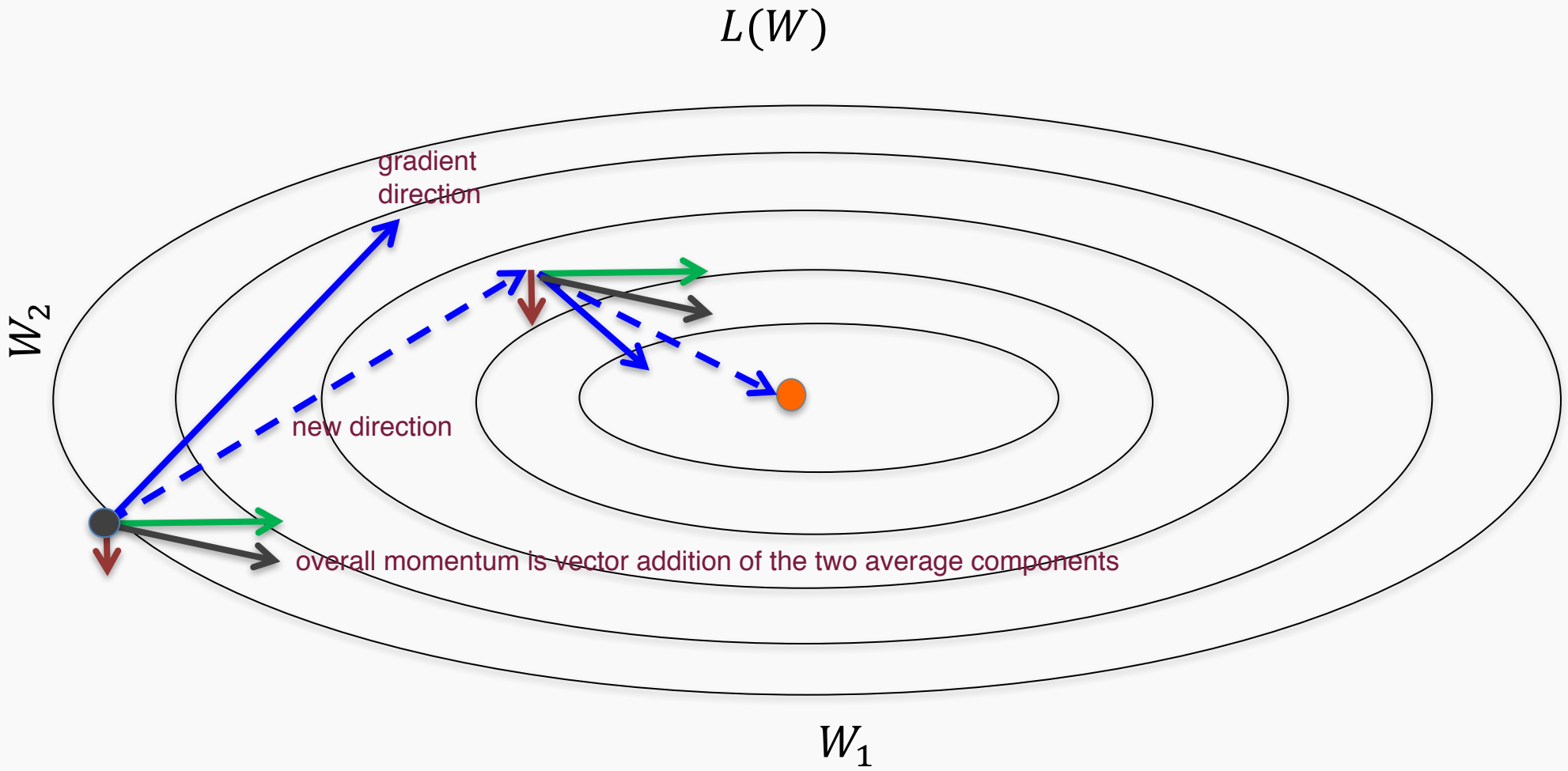
Let us figure out an algorithm



Momentum

oscillating direction average will wash out, but direction will remain

Let us figure out an algorithm



Momentum

f is the Neural Network

Old gradient descent:

$$g = \frac{1}{m}\sum_i \nabla_W L(f(x_i; W), y_i) \qquad W^* = W - \lambda g$$

$$g = g + average\ g\ from\ before$$

New gradient descent with momentum:

like a moving average, first steps oscillate a lot, but then you learn some momentum and your oscillations decrease and you go 'faster' to the local minimum (or global?)

$$v = \alpha v + (1-\alpha)\, g \qquad W^* = W - \lambda v$$

momentum of past gradients

alpha:
0 ignore momentum
1 only momentum, no current gradient

$\alpha \in [0,1)$ controls how quickly effect of past gradients decay

Nesterov Momentum

Apply an interim update:

$$\tilde{W} = W + \nu$$

Perform a correction based on gradient at the interim point:

$$g = \frac{1}{m}\sum_i \nabla_W L(f(x_i; \tilde{W}), y_i)$$

$$\nu = \alpha\nu - \varepsilon g$$

$$W = W + \nu$$

Momentum based on look-ahead slope

distill.pub/2017/momentum/

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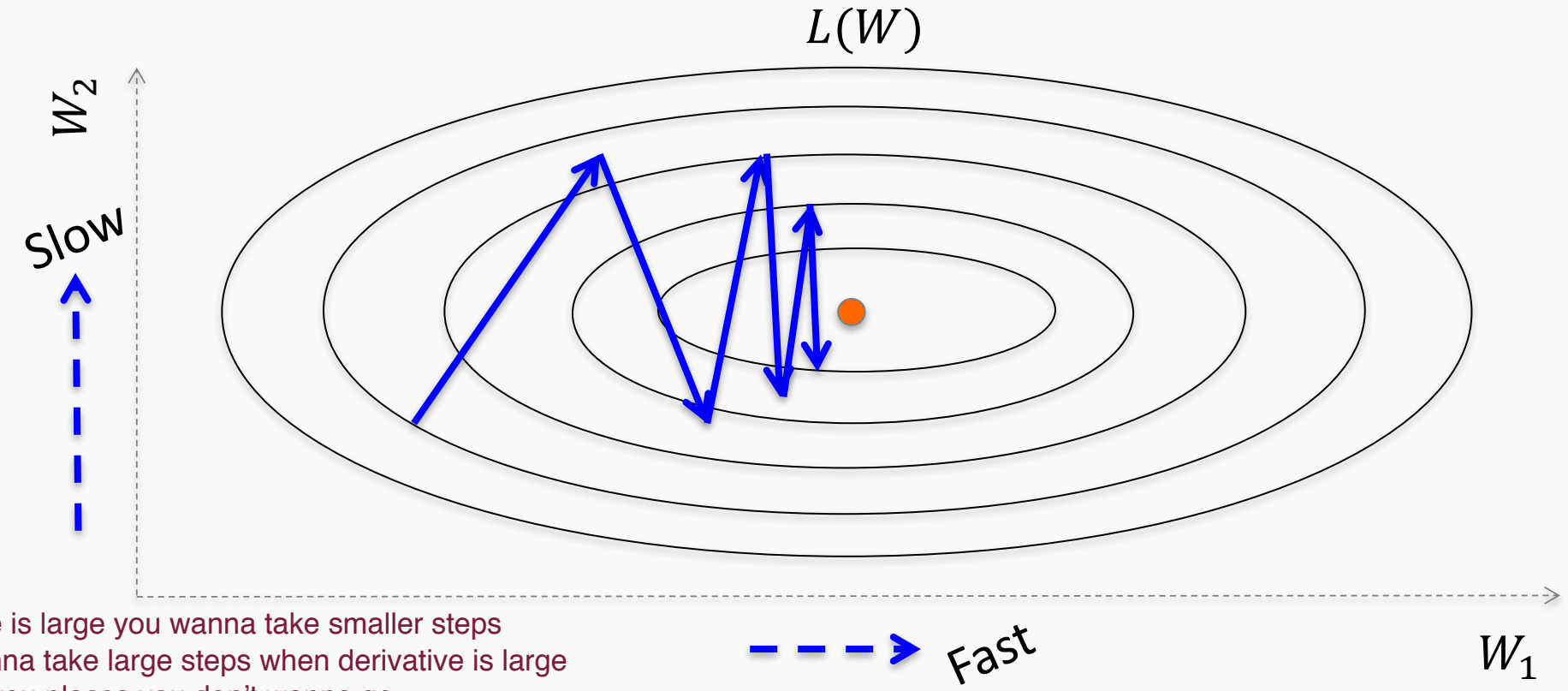
Adaptive Learning Rates



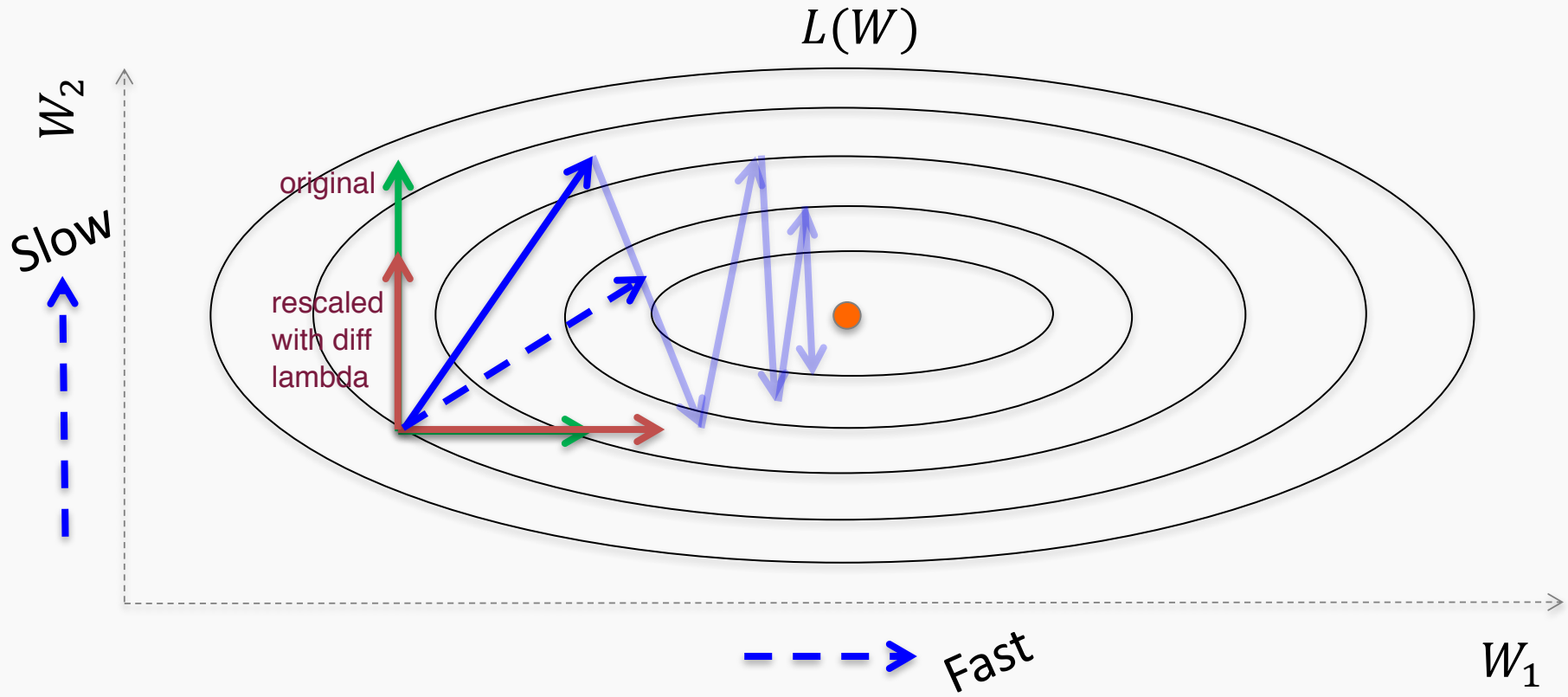
derivative is large you wanna take smaller steps
don't wanna take large steps when derivative is large
will take you places you don't wanna go

Oscillations along vertical direction

– Learning must be slower along parameter 2 to avoid big jumps

Use a different learning rate for each parameter?

Adaptive Learning Rates



Oscillations along vertical direction

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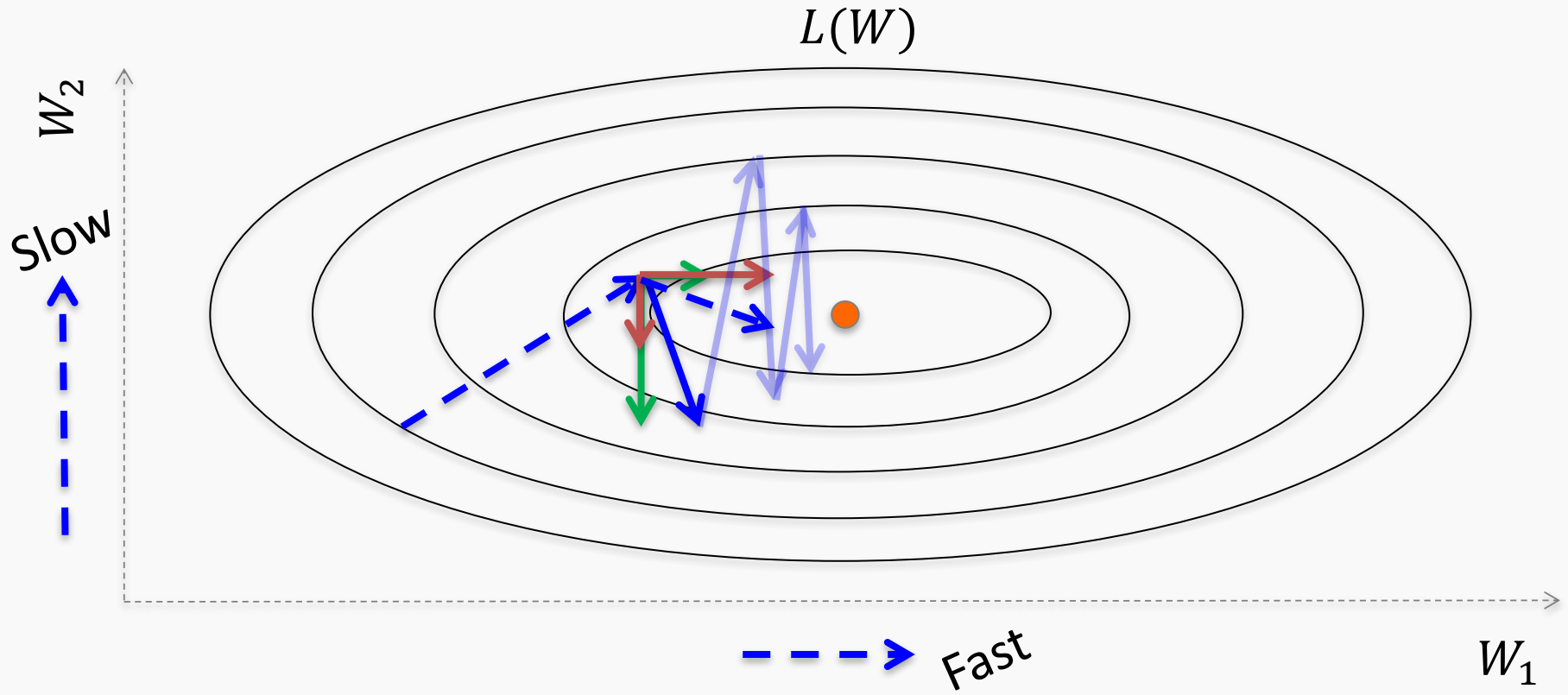
Adaptive Learning Rates



Oscillations along vertical direction

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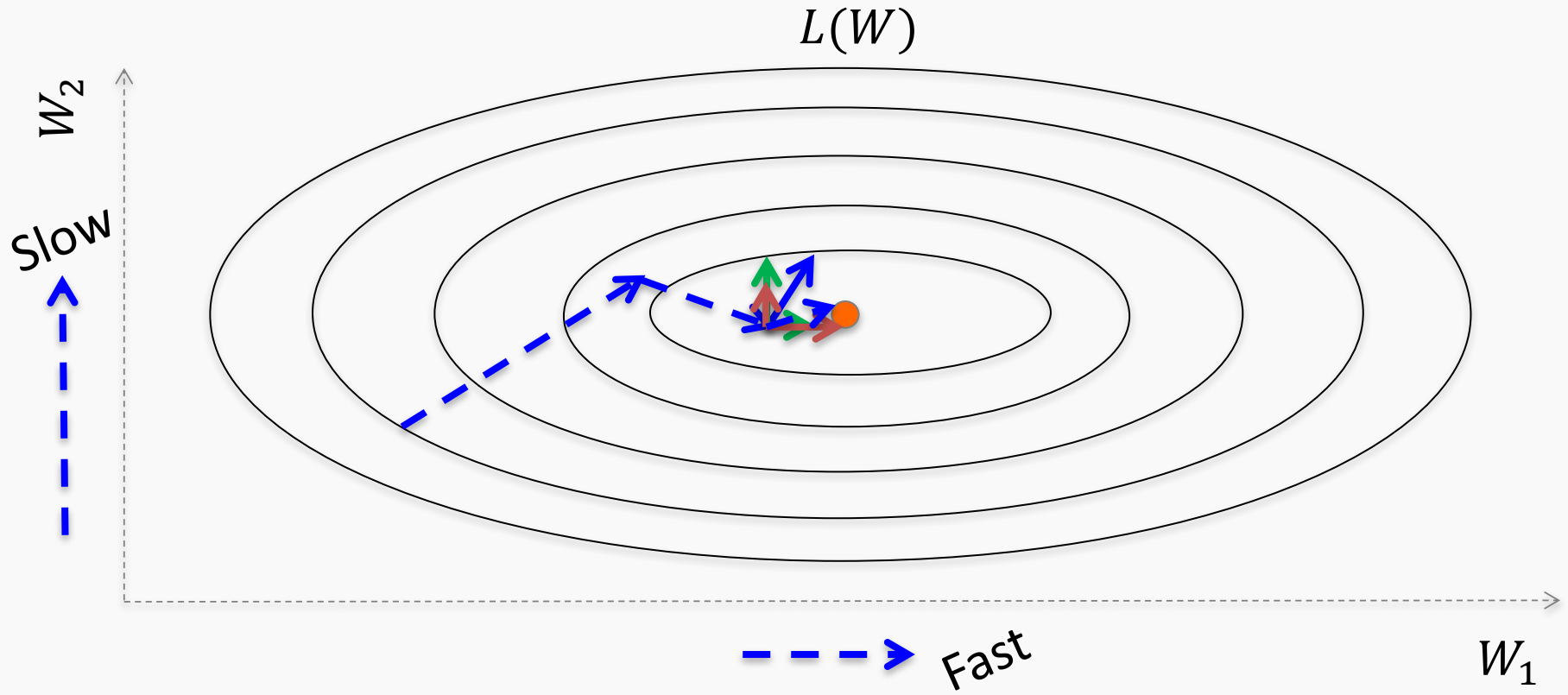
Adaptive Learning Rates

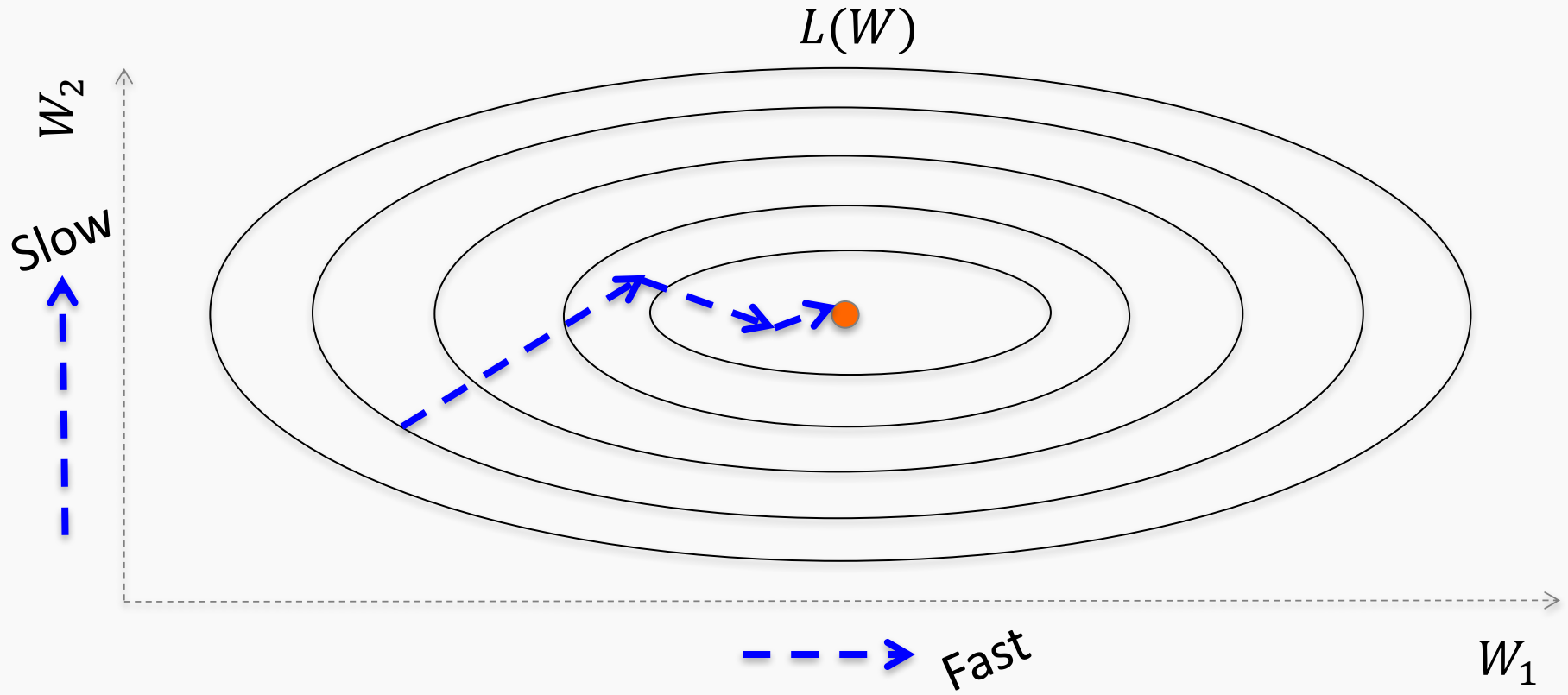


Oscillations along vertical direction

- Learning must be slower along parameter 2

Use a different learning rate for each parameter?

Adaptive Learning Rates



Oscillations along vertical direction

- Learning must be slower along parameter 2

Use a different learning rate for each parameter?

AdaGrad

- Accumulate squared gradients:

$$r_i = r_i + g_i^2$$

g is the gradient

- Update each parameter:

$$W_i = W_i - \frac{\epsilon}{\delta + \sqrt{r_i}} g_i$$

Inversely proportional to cumulative squared gradient

- Greater progress along gently sloped directions

AdaGrad

δ is a small number, making sure this does not become too large

Old gradient descent:

$$g = \frac{1}{m}\sum_i \nabla_W L(f(x_i; W), y_i) \qquad W^* \quad W - \lambda g$$

We would like $\lambda's$ not to be the same and inversely proportion to the $|g_i|$

$$W_i^* = W_i - \lambda_i g_i \qquad \lambda_i \propto \frac{1}{|g_i|} = \frac{1}{\delta + |g_i|}$$

a little number here to prevent vanishing gradient

New gradient descent with adaptive learning rate:

$$r_i^* = r_i + g_i^2 \qquad W_i^* = W_i - \frac{\epsilon}{\delta + \sqrt{r_i}} \mathrm{g_i}$$

RMSProp

- For non-convex problems, AdaGrad can prematurely decrease learning rate
- Use exponentially weighted average for gradient accumulation

$$r_i = \rho r_i + (1-\rho) g_i^2$$

$$W_i = W_i - \frac{\epsilon}{\delta + \sqrt{r_i}} g_i$$

Adam classic optimizer in keras

- RMSProp + Momentum
- Estimate first moment:

momentum

$$v_i = \rho_1 v_i + (1-\rho_1) g_i$$

Also applies bias correction to v and r

- Estimate second moment:

$$r_i = \rho_2 r_i + (1-\rho_2) g_i^2$$

- Update parameters:

$$W_i = W_i - \frac{\epsilon}{\delta + \sqrt{r_i}} \nu_i$$

learning rate correction

Works well in practice, is fairly robust to hyper-parameters

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Parameter Initialization

- Goal: break symmetry between units
  - so that each unit computes a different function
- Initialize all weights (not biases) randomly
  - Gaussian or uniform distribution
- Scale of initialization?
  - *Large* -> grad explosion, *Small* -> grad vanishing

if we start with all weights same, each part of the NN can potentially learn the same feature - we want them to learn different features of the data

Xavier Initialization

- Heuristic for all outputs to have unit variance
- For a fully-connected layer with m inputs:

$$W_{ij} \sim N\left(0, \frac{1}{m}\right)$$

normal dist

- For ReLU units, it is recommended:

$$W_{ij} \sim N\left(0, \frac{2}{m}\right)$$

Normalized Initialization

- Fully-connected layer with m inputs, n outputs:

$$W_{ij} \sim U\left(-\sqrt{\frac{6}{m+n}}, \sqrt{\frac{6}{m+n}}\right)$$

uniform dist

- Heuristic trades off between initialize all layers have same activation and gradient variance
- Sparse variant when m is large
  - Initialize k nonzero weights in each unit

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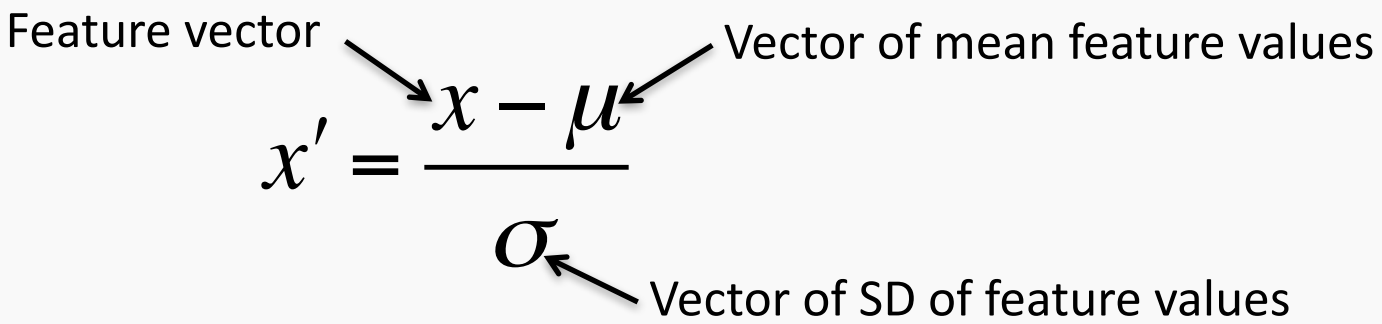
Feature Normalization

Good practice to normalize features before applying learning algorithm:



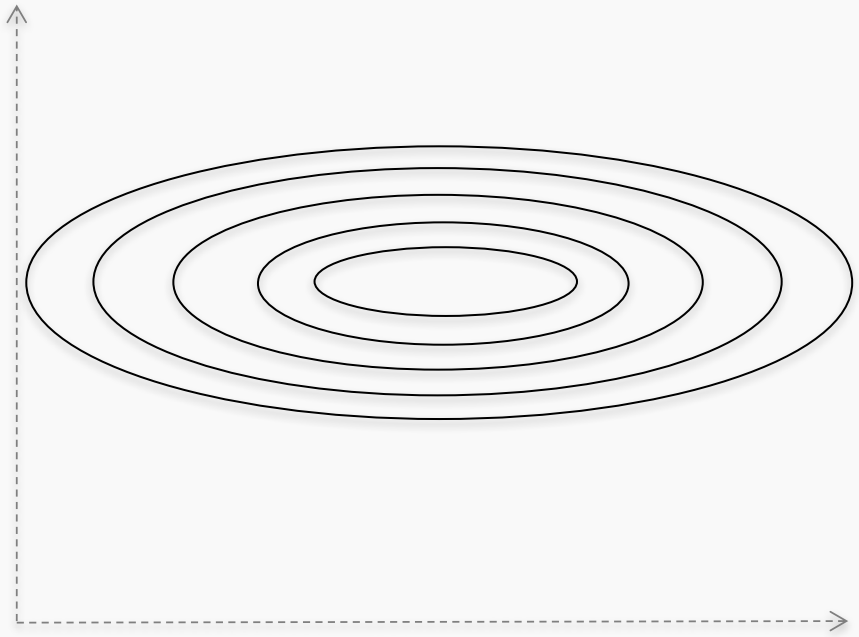
Features in same scale: mean 0 and variance 1

- Speeds up learning

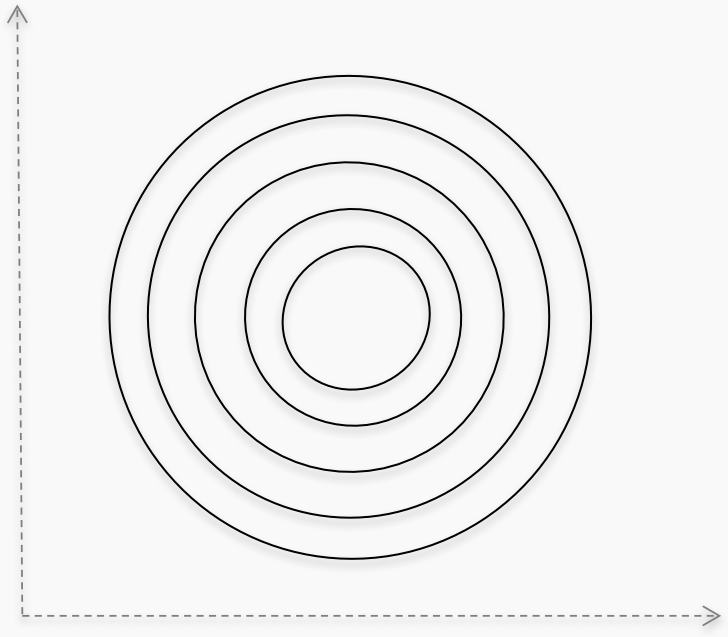
standard scaler in sklearn

Feature Normalization

$L(W)$



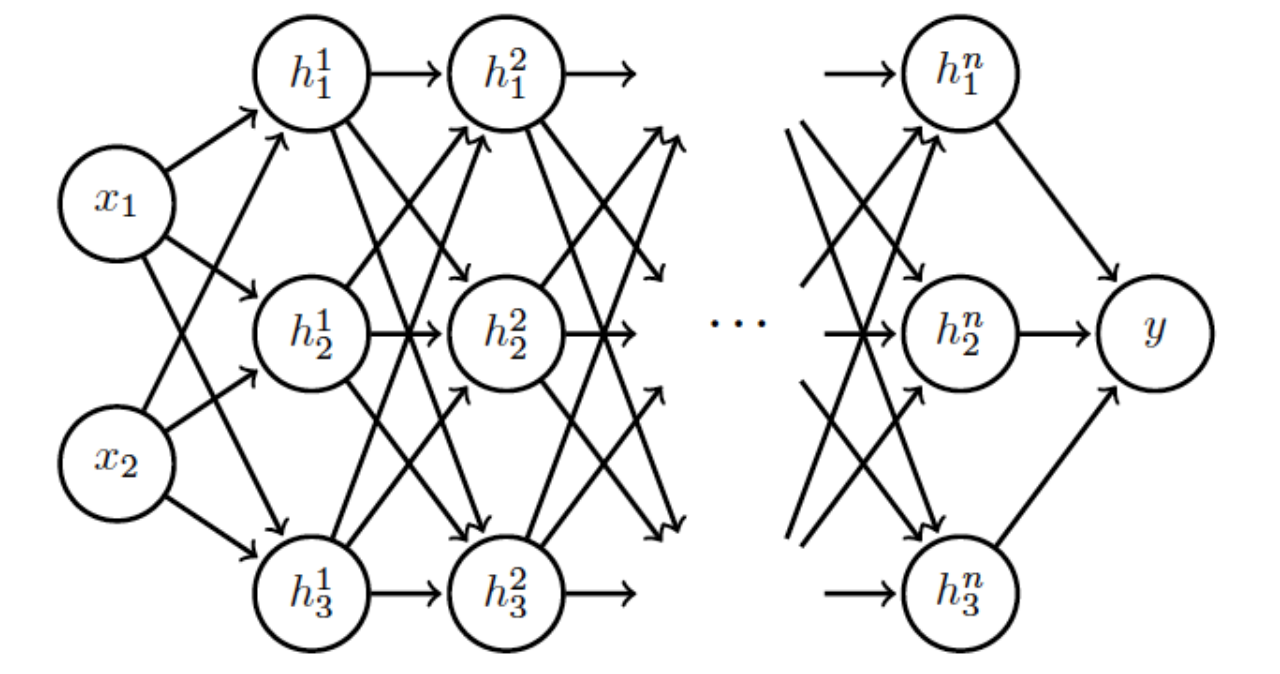
Before normalization



After normalization

Internal Covariance Shift

Each hidden layer changes distribution of inputs to next layer: *slows down learning*



Batch Normalization

Training time:

– Mini-batch of activations for layer to normalize

$$H = \begin{bmatrix} H_{11} & \cdots & H_{1K} \\ \vdots & \ddots & \vdots \\ H_{N1} & \cdots & H_{NK} \end{bmatrix}$$

K hidden layer activations

N data points in mini-batch

Batch Normalization

Training time:

- Mini-batch of activations for layer to normalize

where

$$H' = \frac{H - \mu}{\sigma}$$

$$\mu = \frac{1}{m}\sum_i H_{i,:} \qquad \sigma = \sqrt{\frac{1}{m}\sum_i (H - \mu)_i^2 + \delta}$$

Vector of mean activations across mini-batch

Vector of SD of each unit across mini-batch

Batch Normalization

Training time:

- Normalization can reduce expressive power
- Instead use:

$$\gamma H' + \beta$$

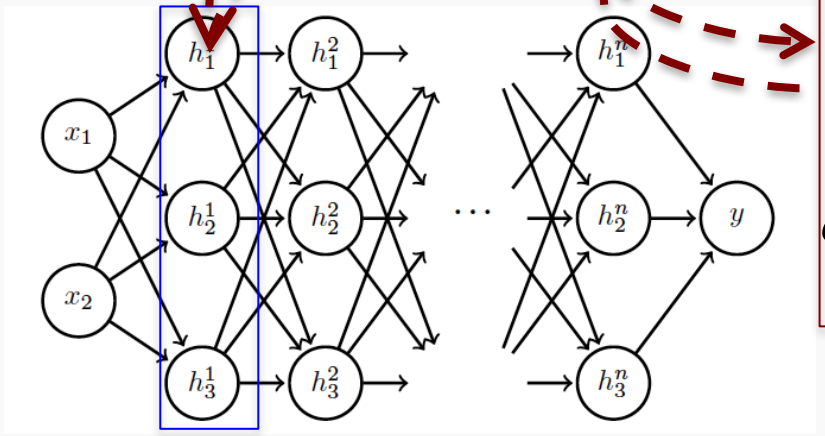
Learnable parameters

- Allows network to control range of normalization

Batch Normalization

you do scaling inside the network

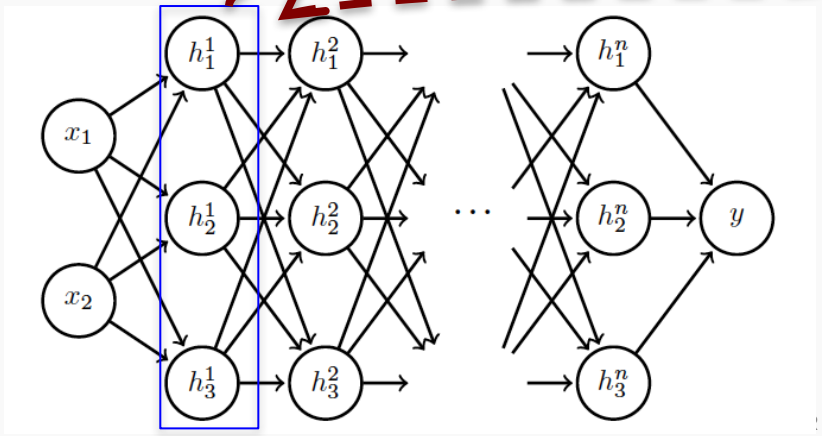
Batch 1



$$\mu^1 = \frac{1}{m}\sum_i H_{i,:}$$

$$\sigma^1 = \sqrt{\frac{1}{m}\sum_i (H-\mu)_i^2 + \delta}$$

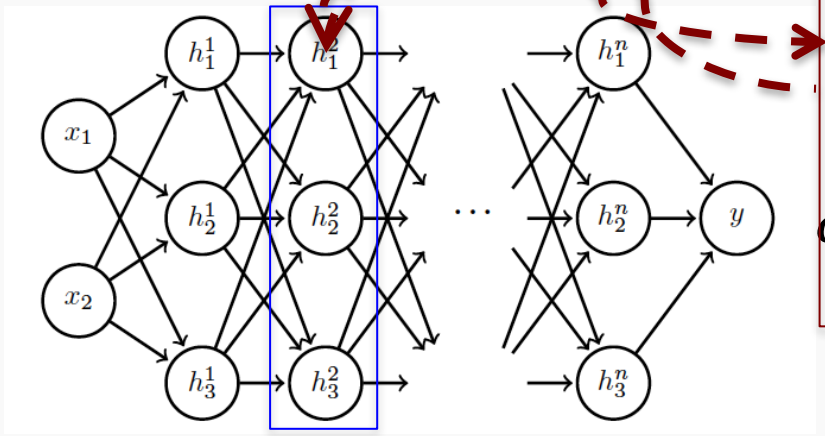
Batch *N*



Add normalization operations for layer 1

Batch Normalization

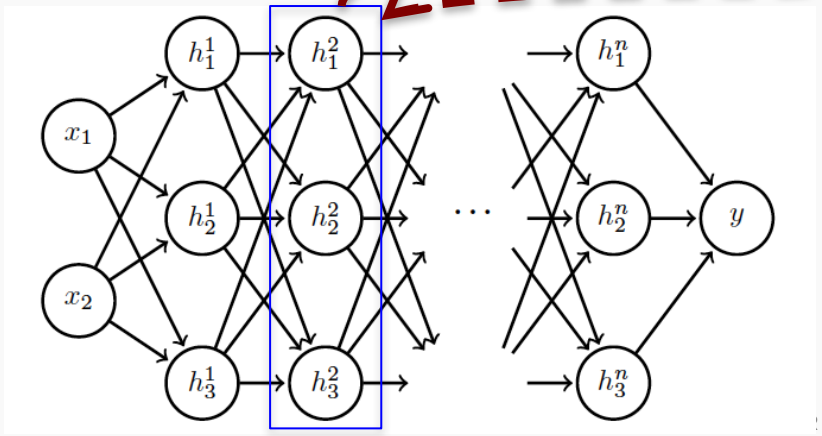
Batch 1



$$\mu^2 = \frac{1}{m}\sum_i H_{i,:}$$

$$\sigma^2 = \sqrt{\frac{1}{m}\sum_i (H-\mu)_i^2 + \delta}$$

Batch *N*



Add normalization operations for layer 2 and so on …

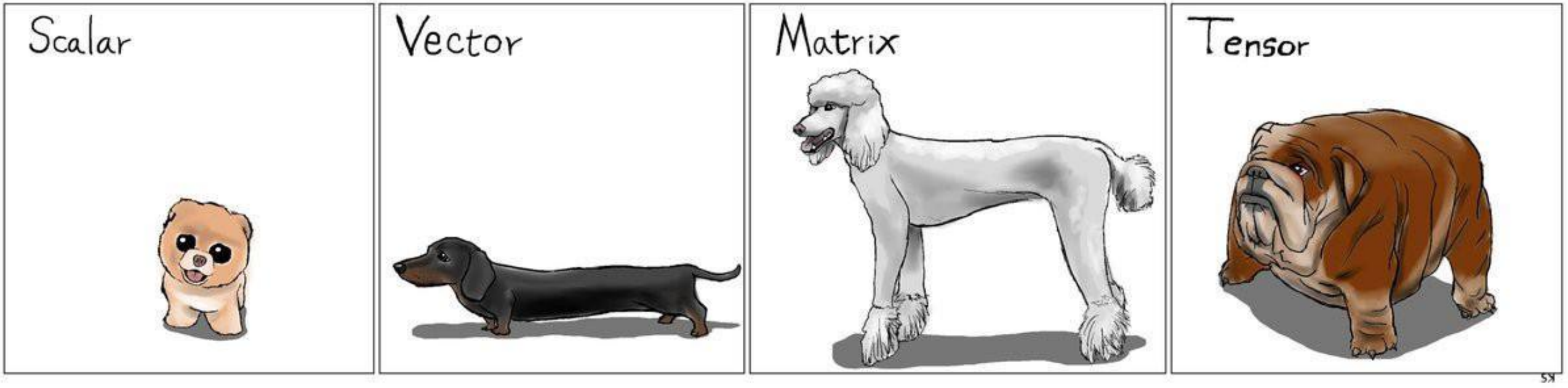
Batch Normalization

Differentiate the joint loss for N mini-batches

Back-propagate *through* the norm operations

Test time:

- Model needs to be evaluated on a *single example*
- Replace μ and σ with running averages collected during training


Scalar
Vector
Matrix
Tensor

Outline

Optimization

- Challenges in Optimization
- Momentum
- Adaptive Learning Rate
- Parameter Initialization
- Batch Normalization

Regularization of NN

- Norm Penalties
- Early Stopping
- Data Augmentation
- Sparse Representation
- Dropout

pruning, bagging, RF

L2, L1 penalties

Regularization

Regularization is any modification we make to a learning algorithm that is intended to **reduce its generalization error** but not its training error.

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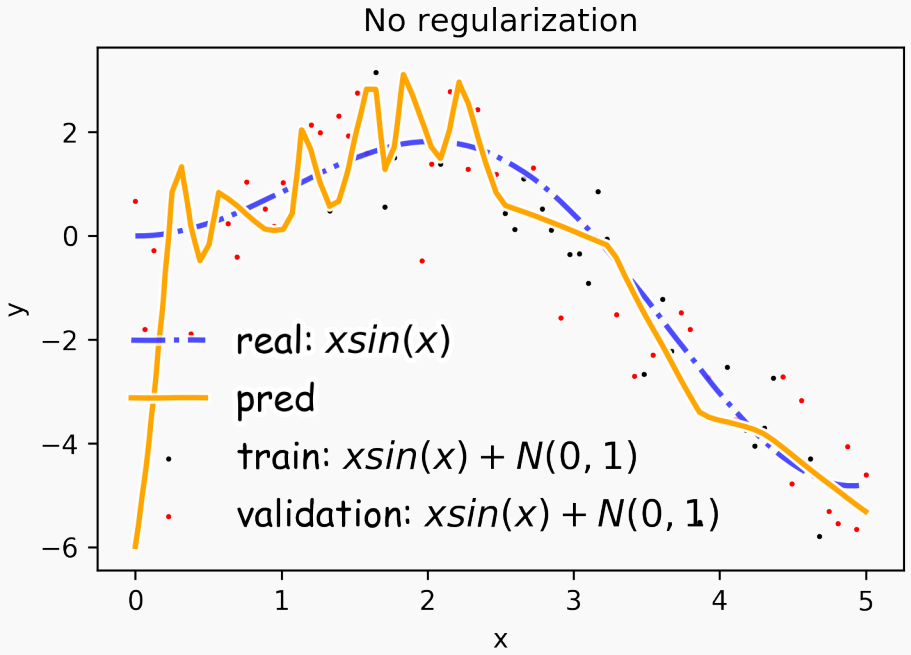
Overfitting

Fitting a deep neural network with 5 layers and 100 neurons per layer can lead to a very good prediction on the training set but poor prediction on validations set.



Norm Penalties

We used to optimize:

$$L(W; X, y)$$

Change to …

$$L_R(W; X, y) = L(W; X, y) + \alpha\Omega(W)$$

regularize the weights of the neural network

make sure weights are within reason

alpha tuned via CV - CV is very expensive - most often just do validation

L_2 regularization:

- Weights decay
- MAP estimation with Gaussian prior

$$\Omega(W) = \frac{1}{2} \| W \|_2^2$$

L_1 regularization:

- encourages sparsity
- MAP estimation with Laplacian prior

$$\Omega(W) = \frac{1}{2} \| W \|_1$$

Norm Penalties

We used to optimize:

$$W^{(i+1)} = W^{(i)} - \lambda \frac{\partial L}{\partial W}$$

Change to …

$$L_R(W; X, y) = L(W; X, y) + \frac{1}{2}\alpha W^2$$

$$W^{(i+1)} = W^{(i)} - \lambda \frac{\partial L}{\partial W} - \lambda\alpha\, W$$

original gradient descent term

Weights decay in proportion to size

Biases not penalized

L_2 regularization:

- **Decay of weights**
- MAP estimation with Gaussian prior

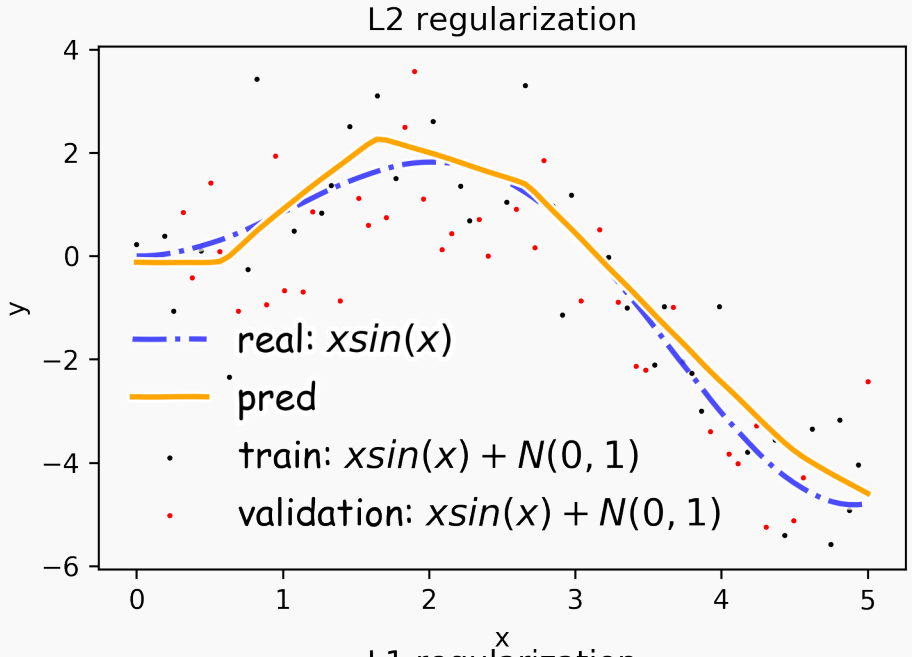
$$\Omega(W) = \frac{1}{2} \| W \|_2^2$$

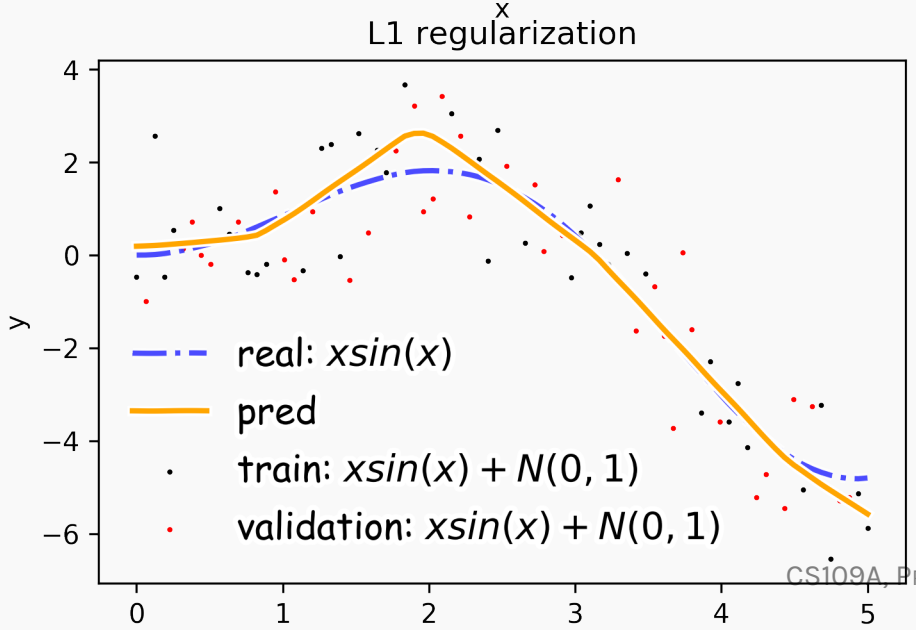
L_1 regularization:

- encourages sparsity
- MAP estimation with Laplacian prior

$$\Omega(W) = \frac{1}{2} \| W \|_1$$

Norm Penalties





$$\Omega(W) = \frac{1}{2} \| W \|_2^2$$

overfitting is better than underfitting - overfit first and then regularize because then you know your bias is low

$$\Omega(W) = \frac{1}{2} \| W \|_1$$

Norm Penalties as Constraints

$$\min_{\Omega(W) \leq K} J(W; X, y)$$

Useful if K is known in advance

Optimization:

- Construct Lagrangian and apply gradient descent
- Projected gradient descent

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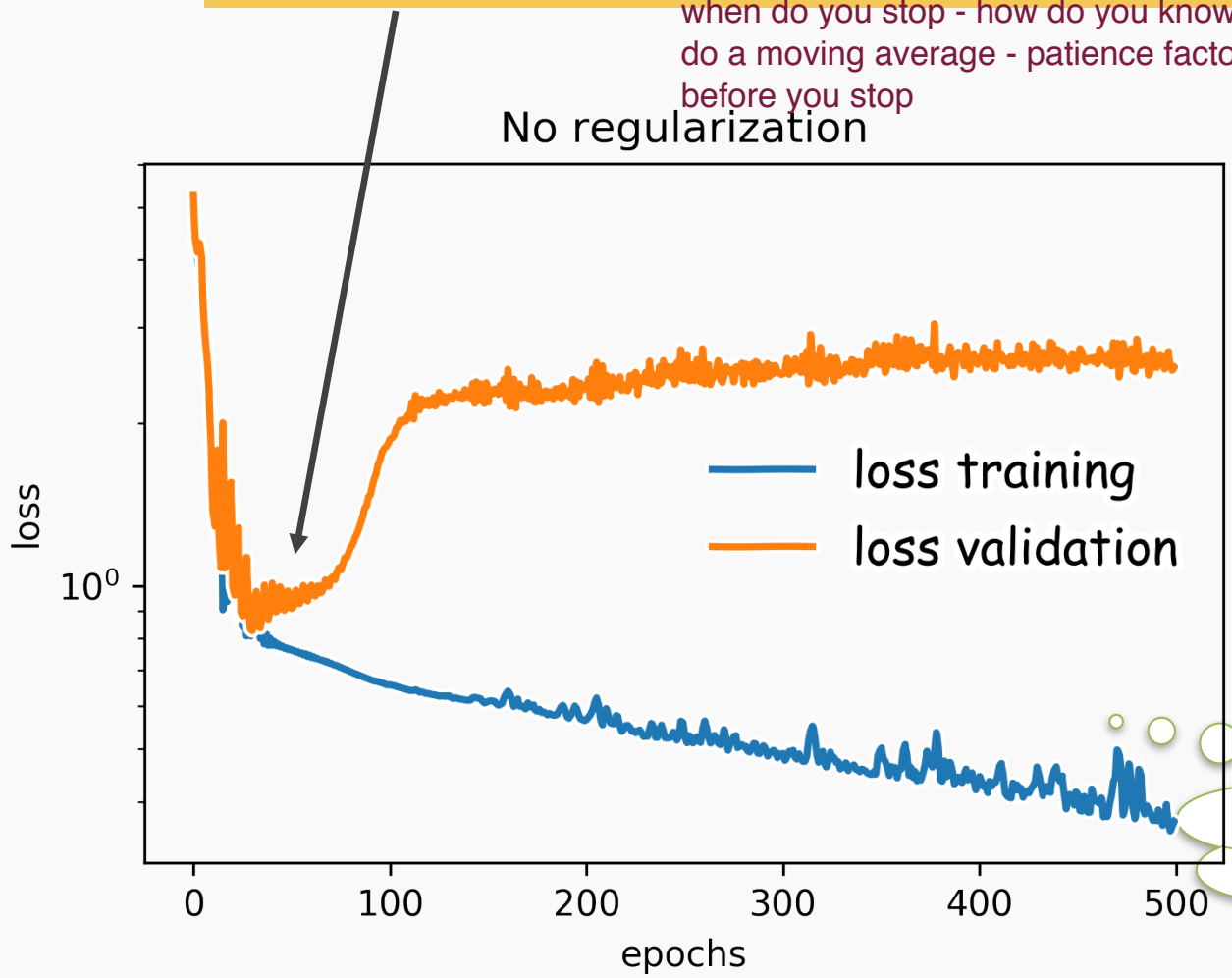
Early Stopping

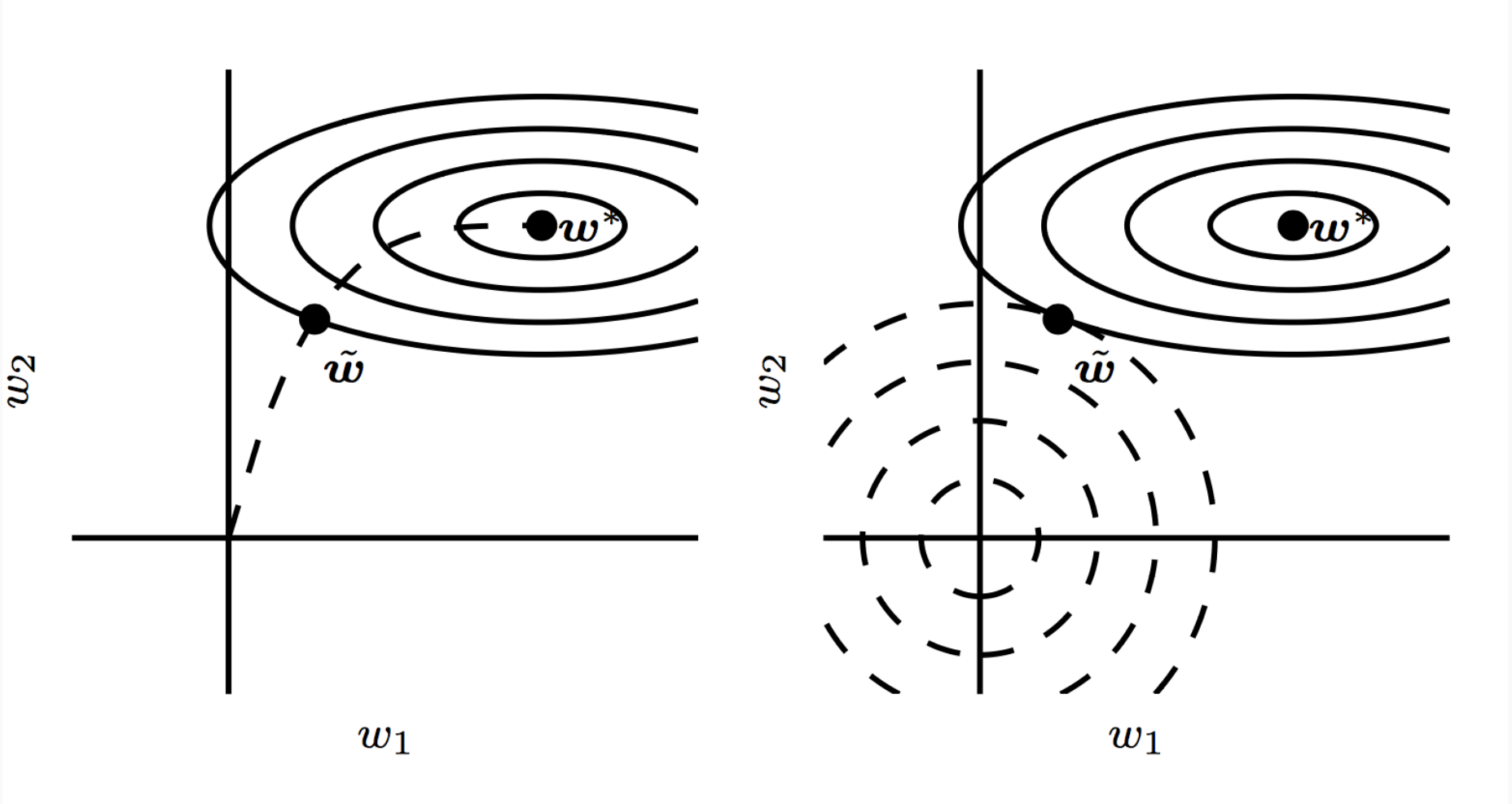
Early stopping: terminate while validation set performance is better

when do you stop - how do you know you reached the minimum
do a moving average - patience factor to decide how long you have to go up before you stop



Training time can be treated as a hyperparameter

Early Stopping



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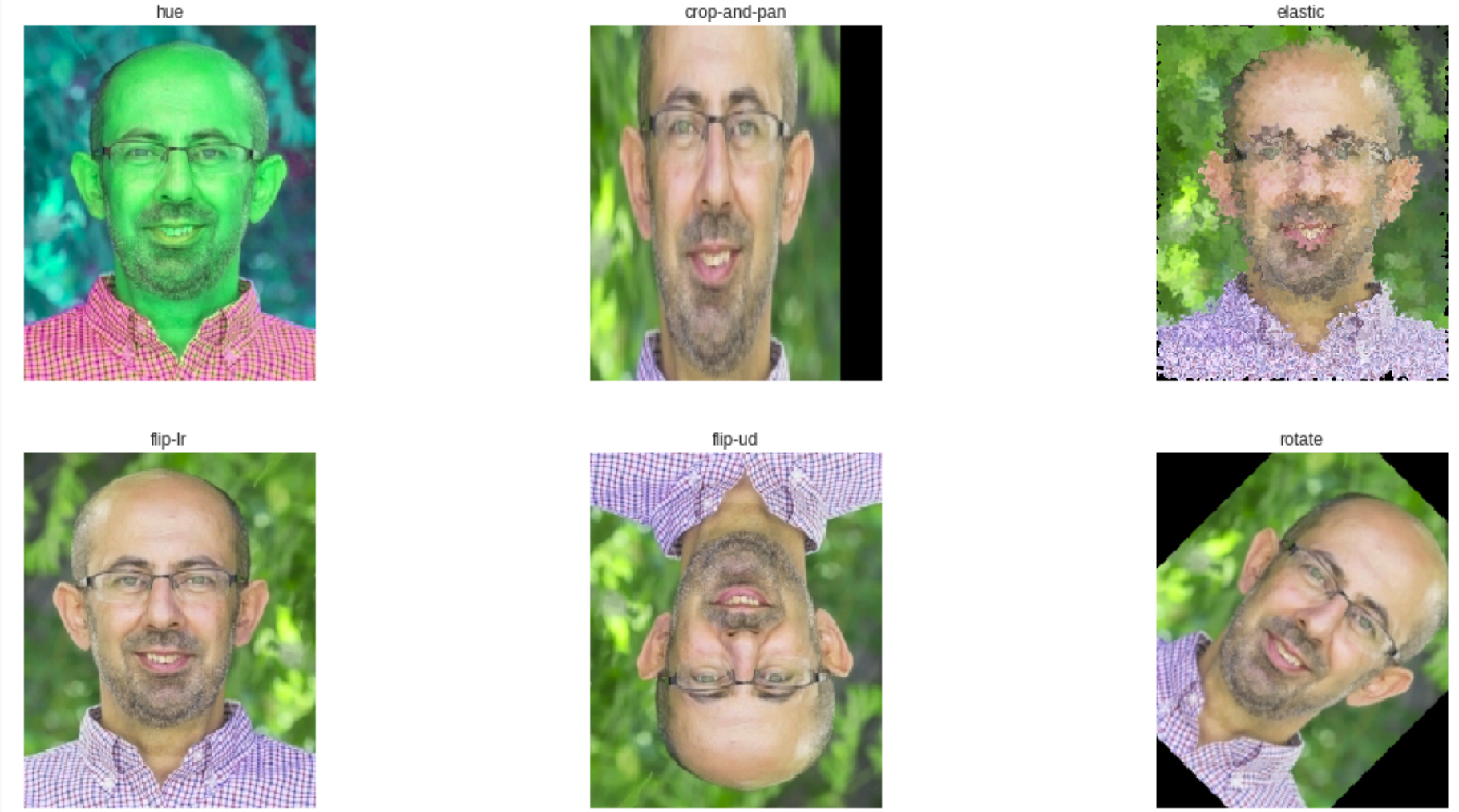
Data Augmentation

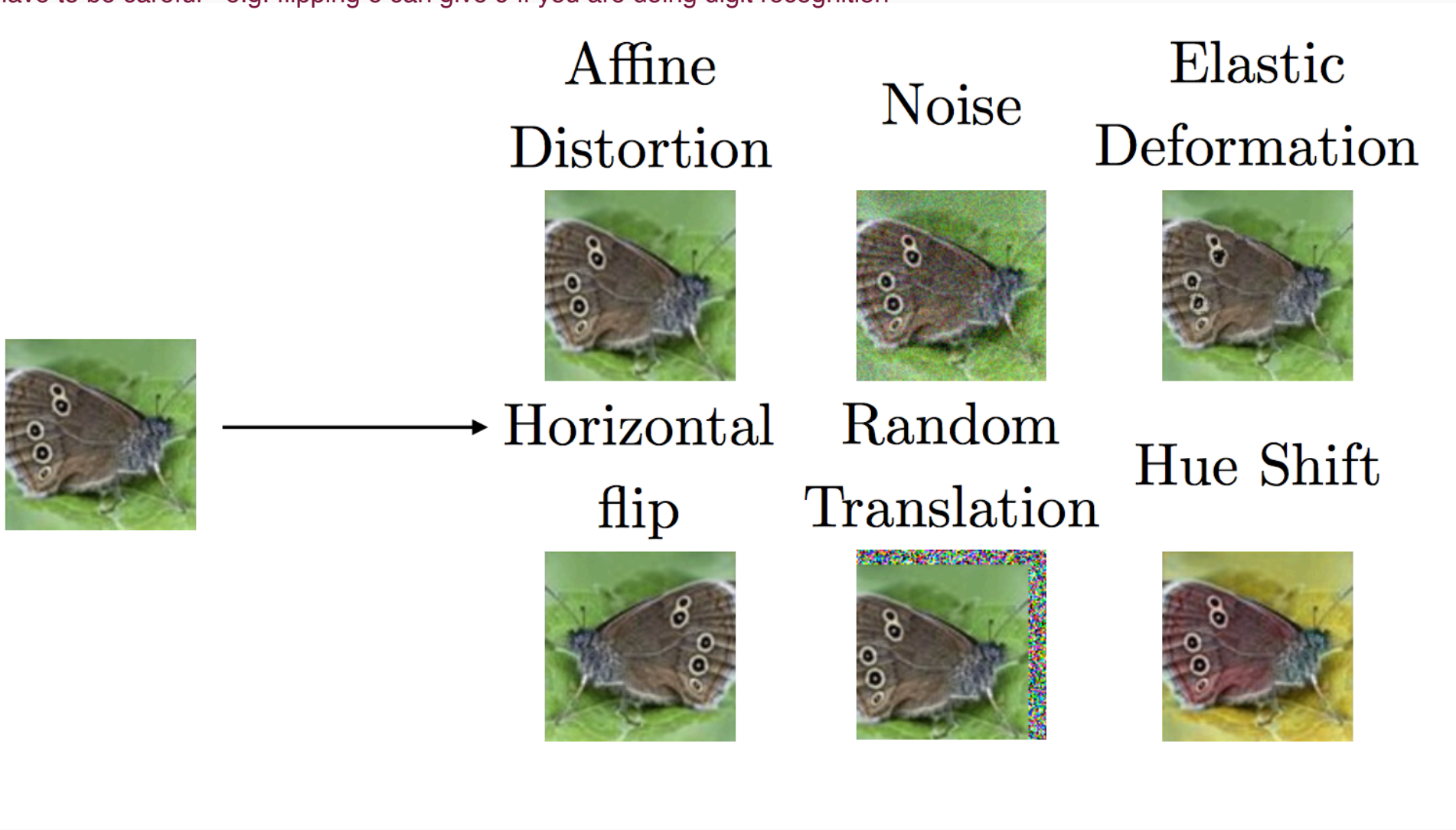
a lot of data can prevent overfitting - model cannot have enough parameters to overfit
can we make data? do data transforms to make different manifestations of the data

can be very powerful



Data Augmentation

have to be careful - e.g. flipping 6 can give 9 if you are doing digit recognition



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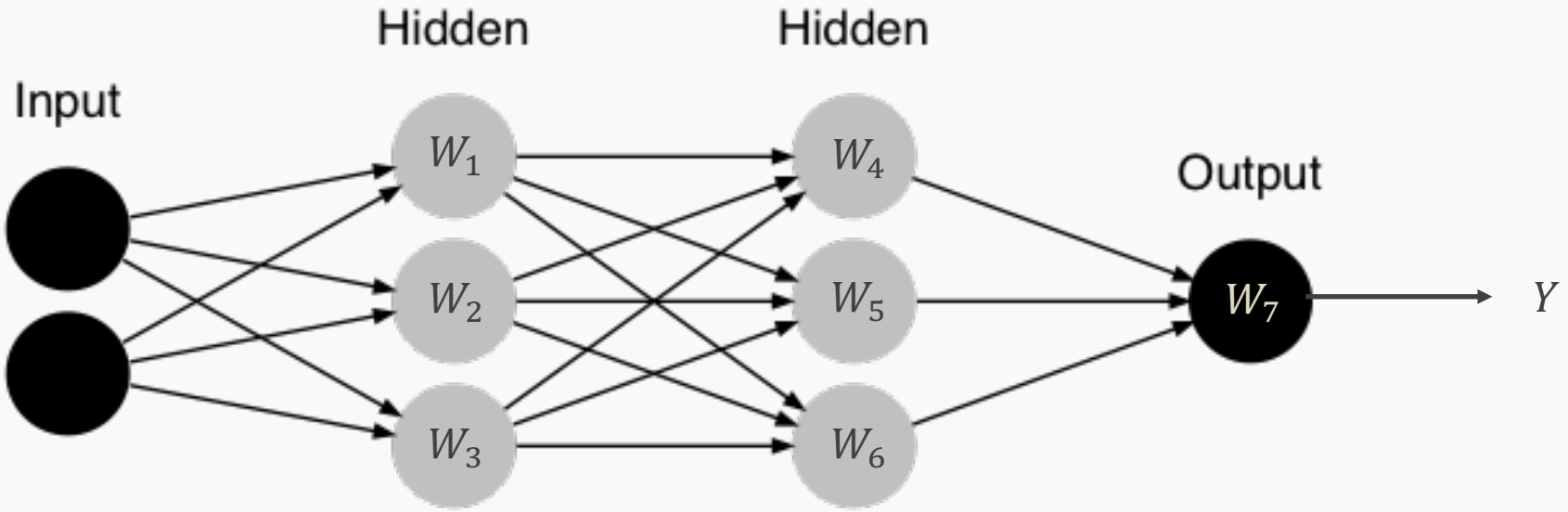
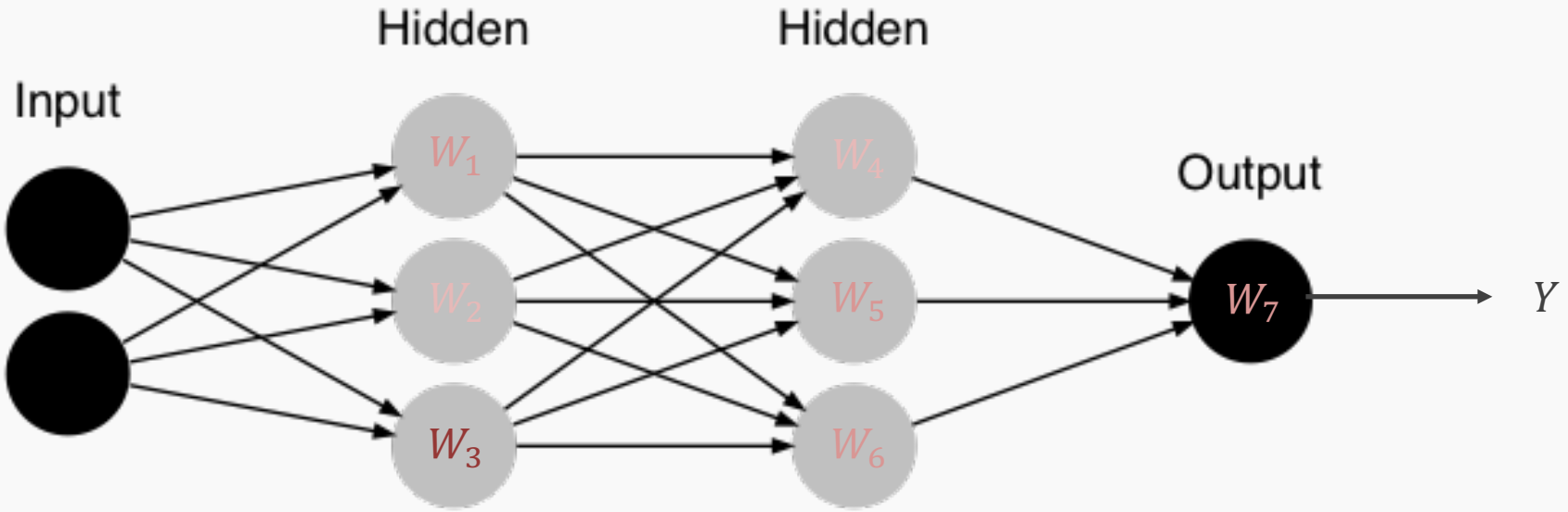
Sparse Representation



$$L(\theta; X, y)$$

$$[4.34] = \underbrace{[3.2 \quad 2.0 \quad 1.8]}_{W_7} \begin{bmatrix} 2 \\ -2.2 \\ 1.3 \end{bmatrix}$$

Sparse Representation

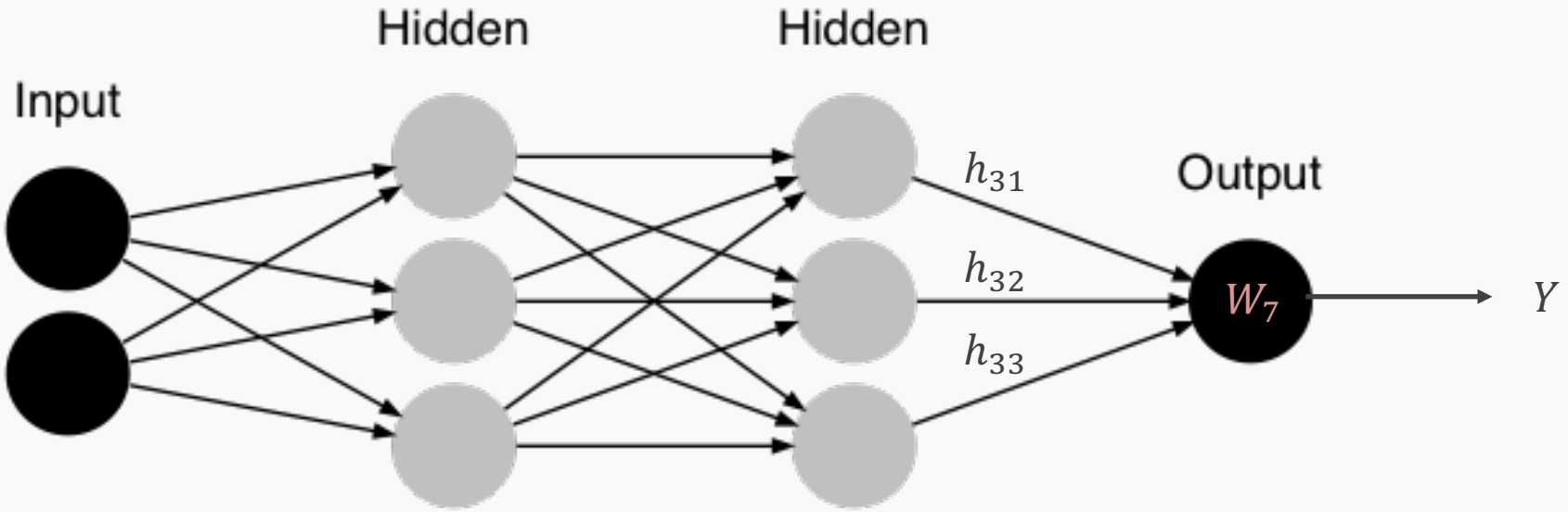


$$L_R(W; X, y) = L(\theta; X, y) + \alpha\Omega(W)$$

$$[0.69] = \underbrace{[0.5 \quad .2 \quad 0.1]}_{W_7} \begin{bmatrix} 2 \\ -2.2 \\ 1.3 \end{bmatrix}$$

Weights in output layer

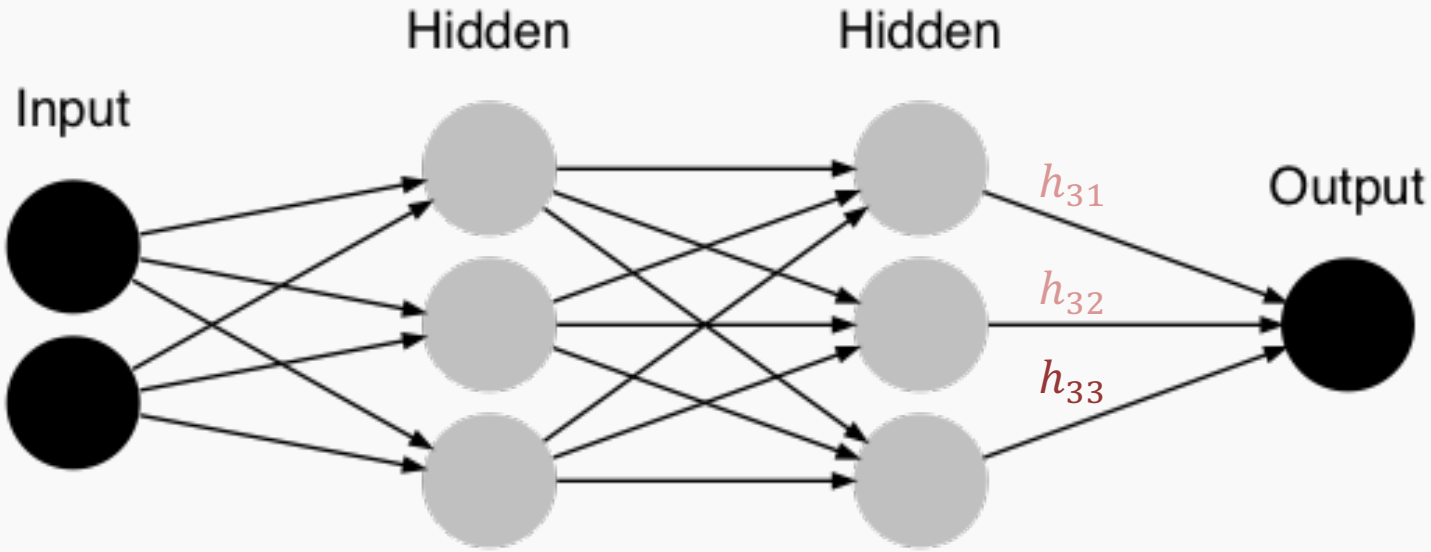
Sparse Representation



$$L(\theta; X, y)$$

$$[4.34] = [3.2 \quad 2 \quad 1] \left[\begin{matrix} 2 \\ -2.2 \\ 1.3 \end{matrix}\right] \Big\} \; h_{31}, h_{32}, h_{33}$$

Sparse Representation



regularize the output instead - not the weights
'pruning' the network

$$L_R(W; X, y) = L(\theta; X, y) + \alpha\Omega(h)$$

$$[1.3] = [3.2 \quad 2 \quad 1] \begin{bmatrix} 0 \\ -0.2 \\ .9 \end{bmatrix} \Big\} \; h_{31}, h_{32}, h_{33}$$

Output of hidden layer

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Noise Robustness

Random perturbation of network weights

- Gaussian noise: Equivalent to minimizing loss with regularization term
- Encourages smooth function: small perturbation in weights leads to small changes in output

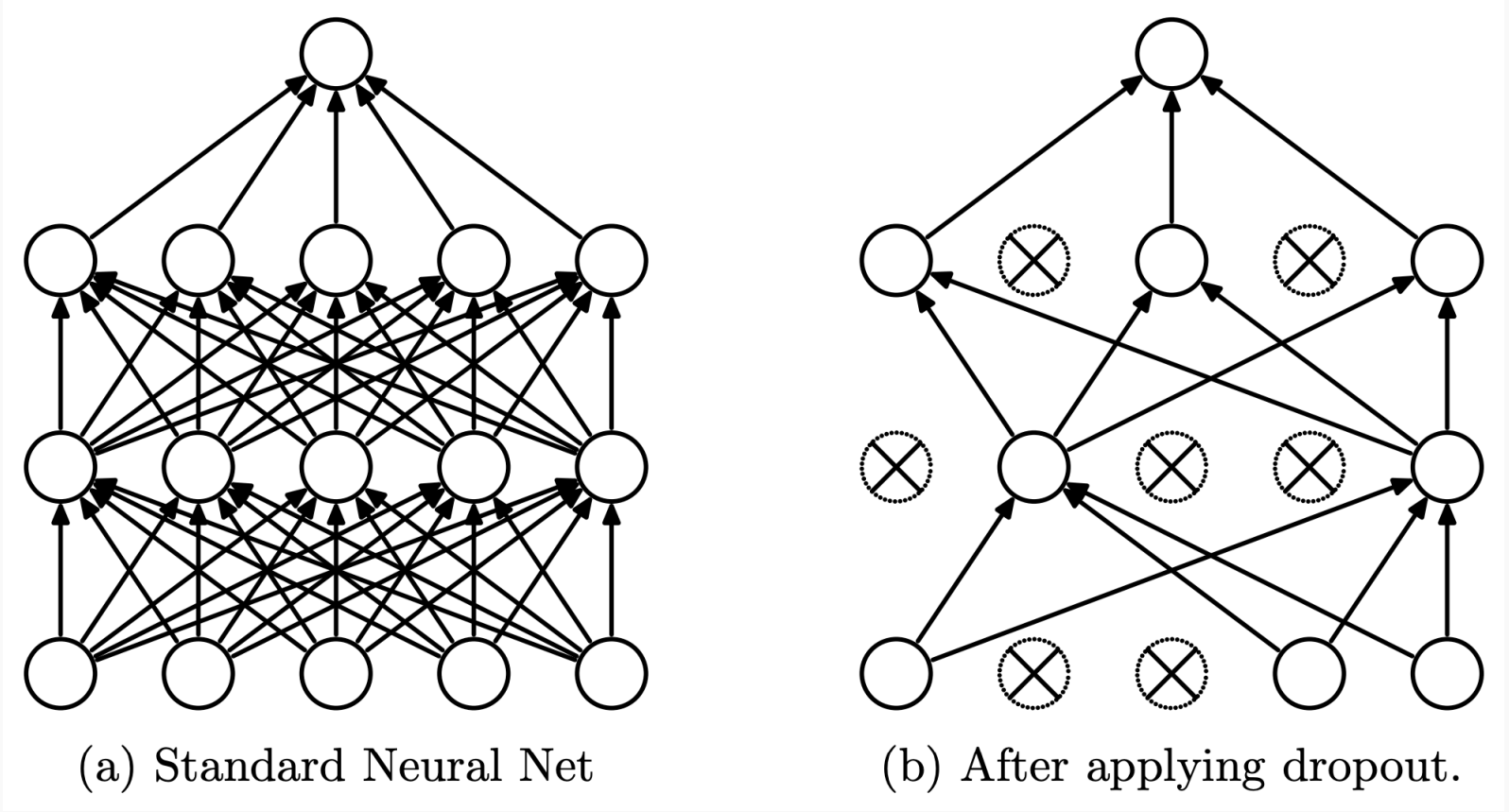
Injecting noise in output labels

- Better convergence: prevents pursuit of hard probabilities

Dropout

instead of bootstrapping data, let's bootstrap network - more efficient
take a network, set some neuron weights to 0, loss function, backpropagation —> do this for every batch in SGD

- Randomly set some neurons and their connections to zero (i.e. "dropped")
- Prevent overfitting by reducing co-adaptation of neurons
- Like training many random sub-networks

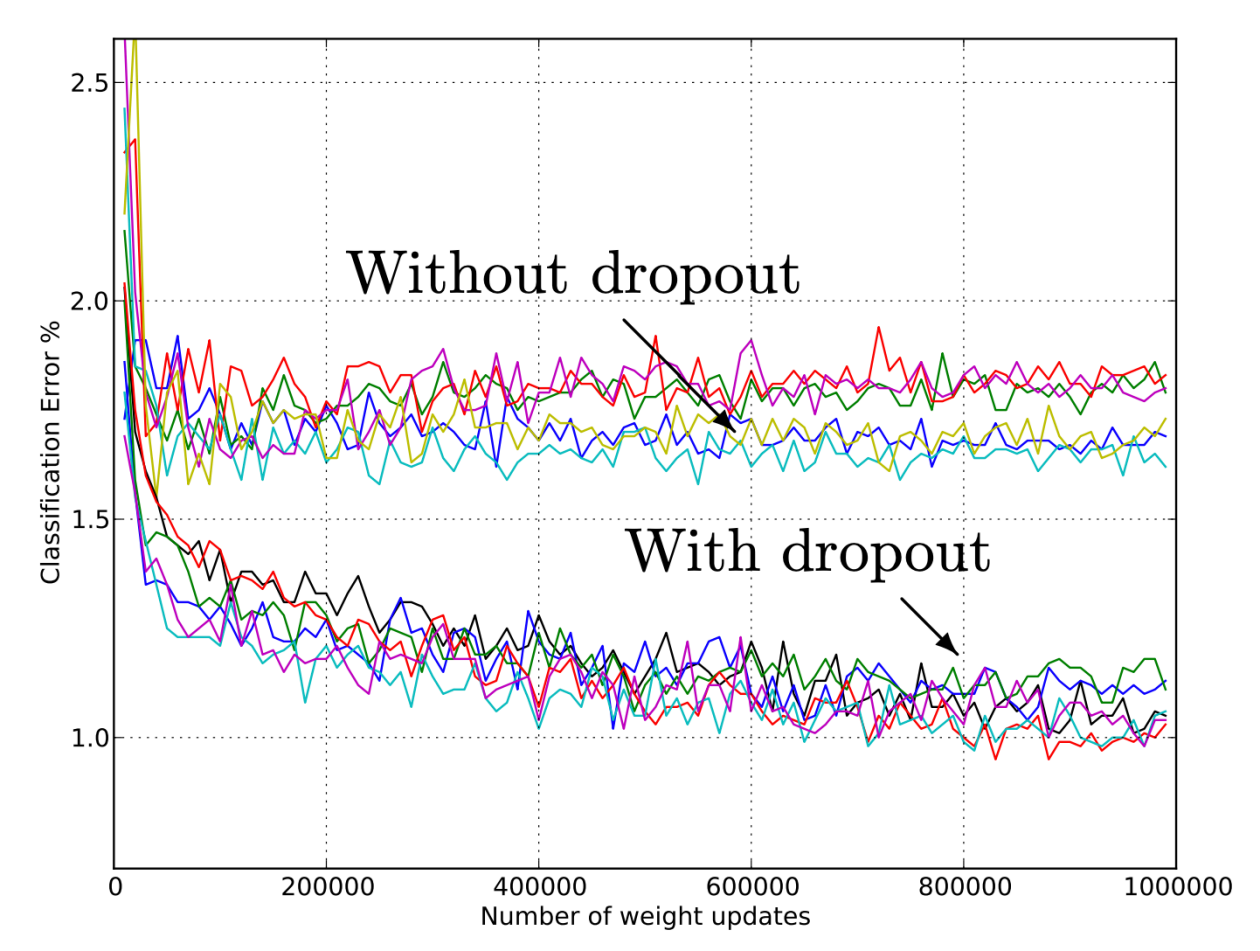


(a) Standard Neural Net

(b) After applying dropout.

Dropout

- Widely used and highly effective
- Proposed as an alternative to ensembling, which is too expensive for neural nets



Test error for different architectures with and without dropout. The networks have 2 to 4 hidden layers each with 1024 to 2048 units.

http://jmlr.org/papers/volume15/srivastava14a/srivastava14a.pdf

Dropout: Stochastic GD

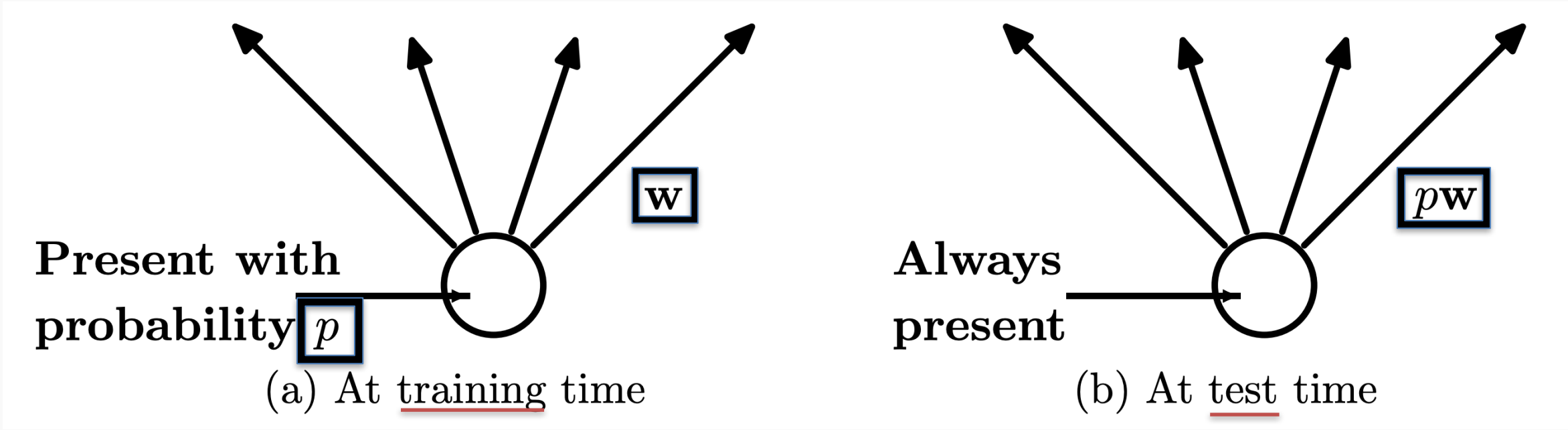
For each new example/mini-batch:

- Randomly sample a binary mask μ independently, where μ_i indicates if input/hidden node i is included
- Multiply output of node i with μ_i, and perform gradient update

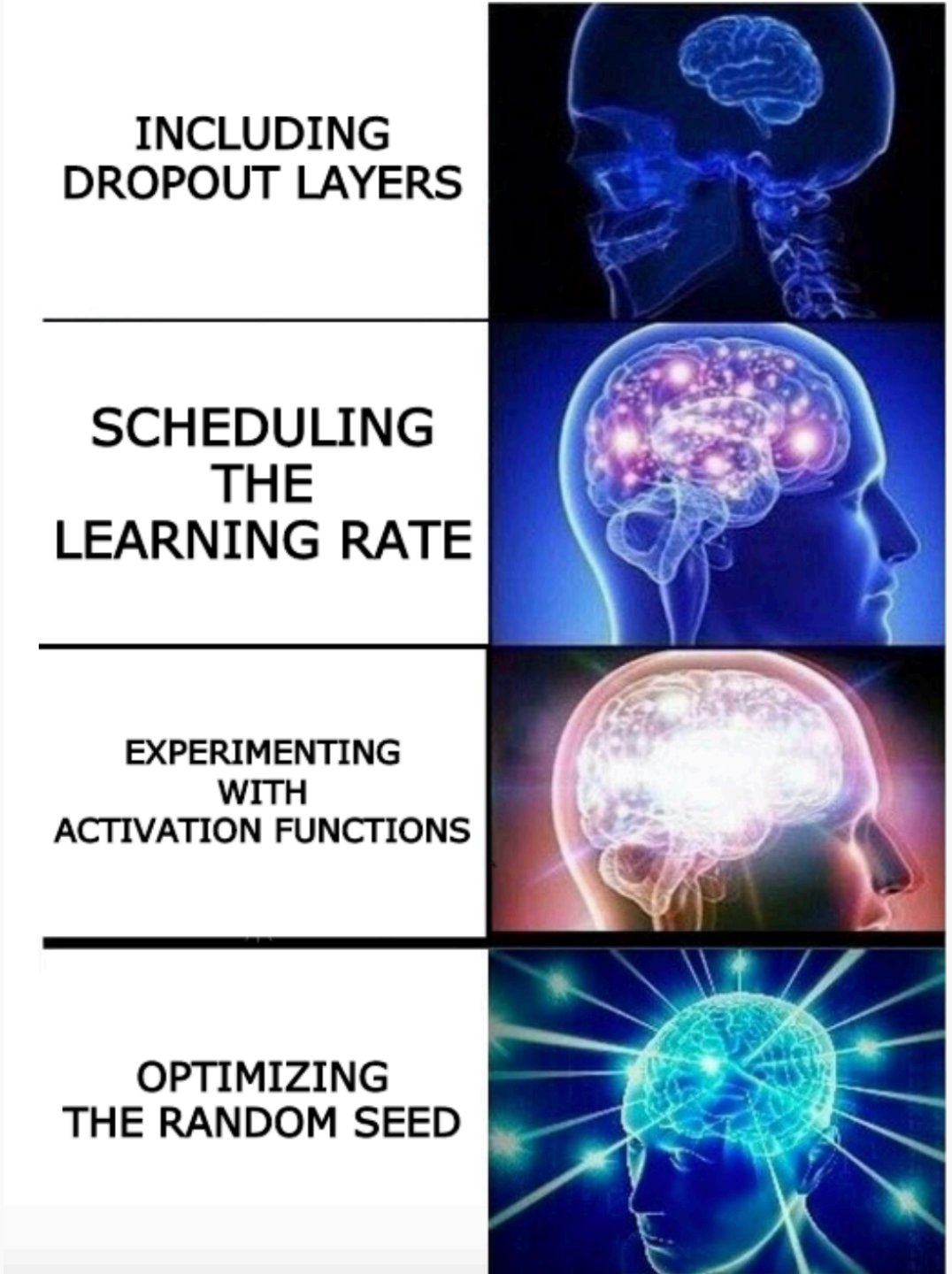
Typically, an input node is **included** with **prob=0.8**, hidden node with **prob=0.5.**

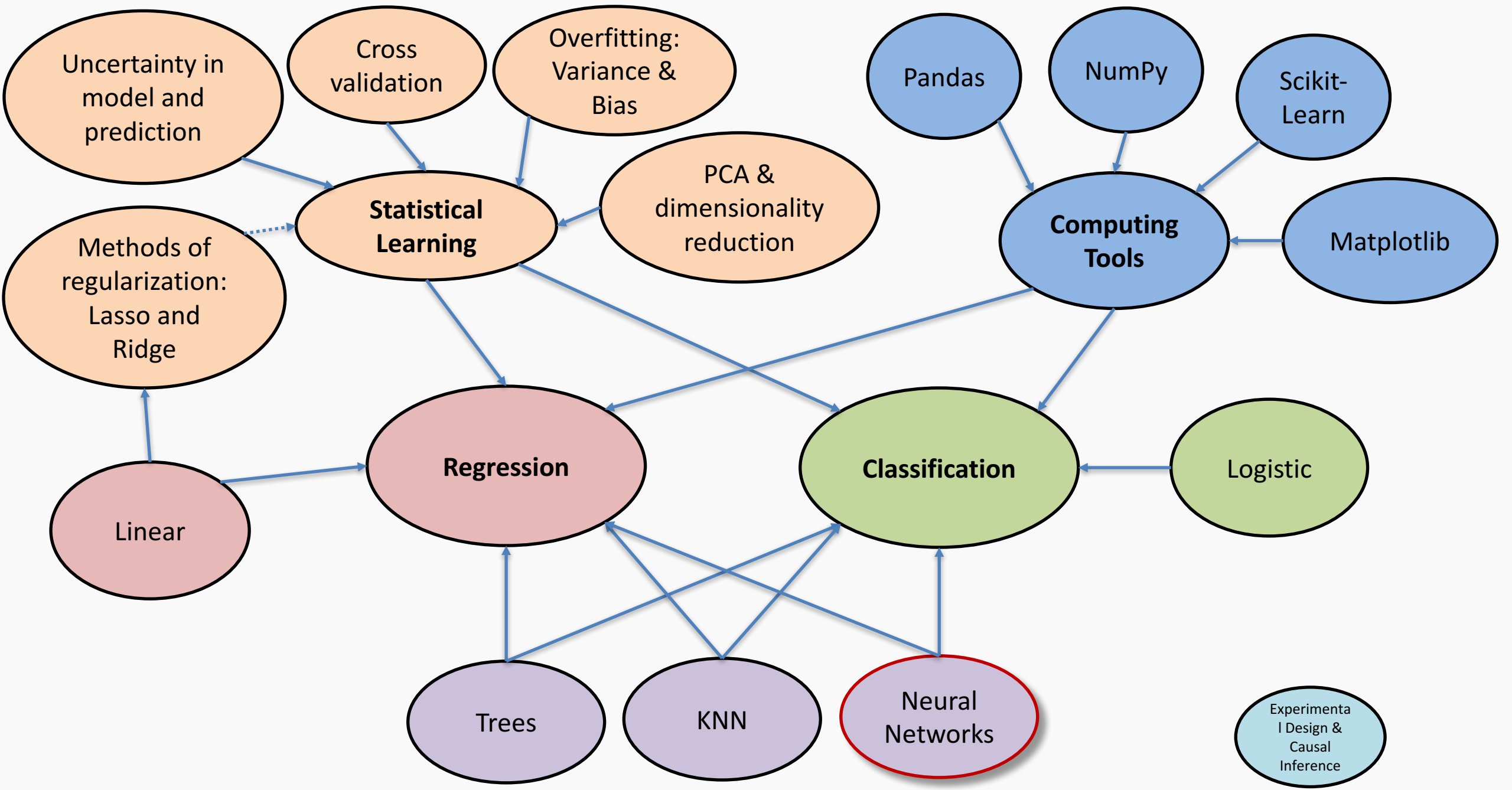
Dropout: Weight Scaling

- We can think of dropout as training many of sub-networks
- At **test time**, we can "aggregate" over these sub-networks by **reducing connection weights in proportion to dropout probability, *p***



nodes that are dropped a lot shouldn't be included because they haven't been trained a lot


INCLUDING
DROPOUT LAYERS
SCHEDULING
THE
LEARNING RATE
EXPERIMENTING
WITH
ACTIVATION FUNCTIONS
OPTIMIZING
THE RANDOM SEED


Uncertainty in model and prediction
Cross validation
Overfitting: Variance & Bias
Pandas
NumPy
Scikit-Learn
Statistical Learning
PCA & dimensionality reduction
Computing Tools
Matplotlib
Methods of regularization: Lasso and Ridge
Regression
Classification
Logistic
Linear
Trees
KNN
Neural Networks
Experimental Design & Causal Inference