

# About Training

## Outline

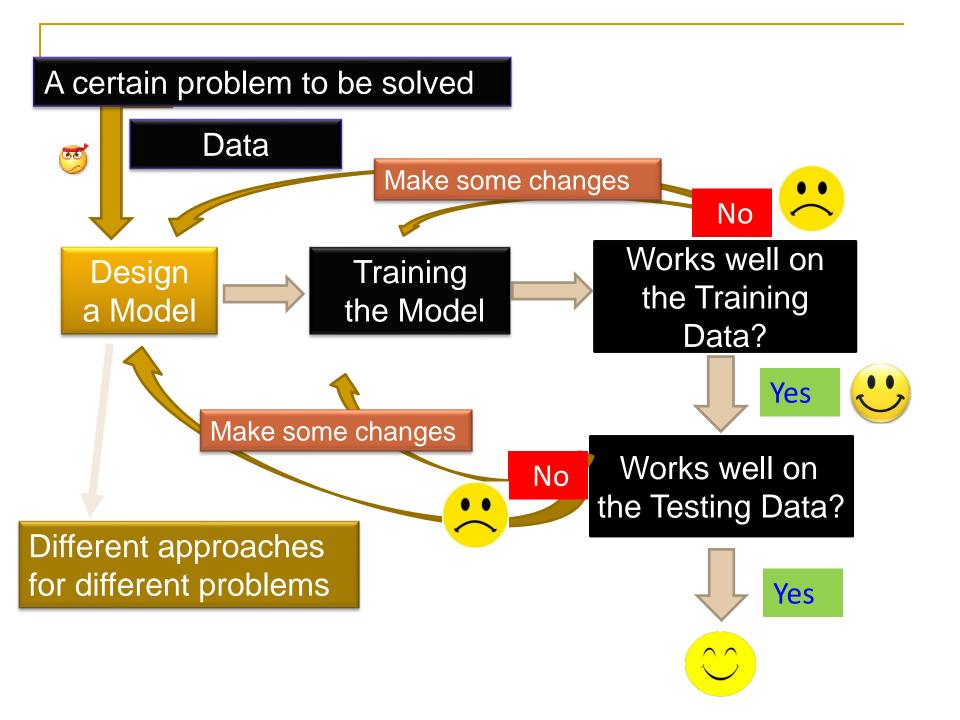
- Hyperparameters & Parameters
- Setting up the data
- Gradient Descent
- Learning rate
- Batch Normalization
- Early stopping
- Regularization
- Dropout
- Hyperparameter tuning

# Supervised Learning Task - Review

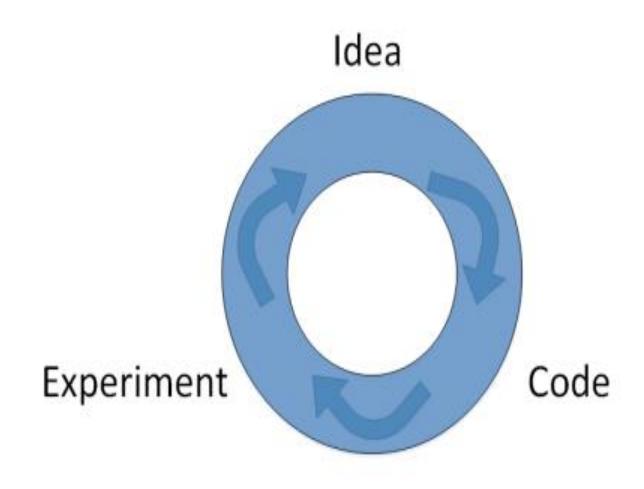
- ❖ Given: training data  $\{(x_i, y_i), i = 1, ..., n\}$  i.i.d. from distribution D
- ❖ Find  $y = f(x) \in \mathcal{H}$
- S.t. f works well on test data i.i.d. from distribution D
  - ♦ Find  $y=f(x) \in \mathcal{H}$  that minimizes

$$\widehat{L}(f) = \frac{1}{n} \sum_{i=1}^{n} l(f, x_i, y_i)$$

**Empirical loss** 



# The whole process is a cycle



# Underfitting & Overfitting

#### Diagnosis:

- If your model cannot even fit the training examples, then you have large bias Not train well
   Underfitting
- If you can fit the training data, but with large error on the testing data, then you probably have large variance

Overfitting

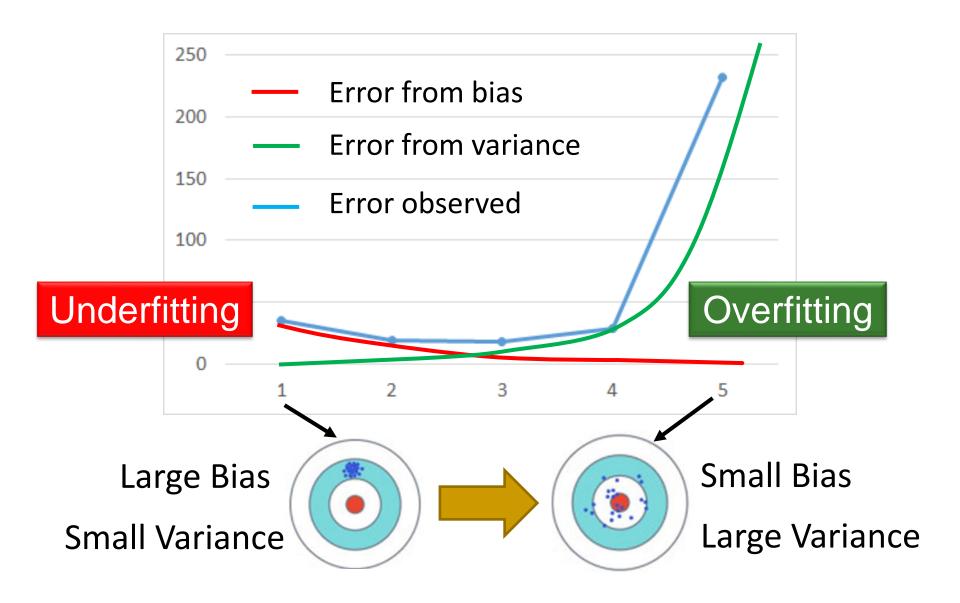
#### For large bias:

- Add more features as inputs
- Use a more complex model

#### For large variance:

- Use more data: Very effective, but not always practical
- Regularization: May increase bias

## Bias v.s. Variance



## Hyperparameters & Parameters







#### (Model Design + Hyperparameters) → Model Parameters

The building blocks:

- # Layers
- Activations
- Optimizers

The knobs that you can turn:

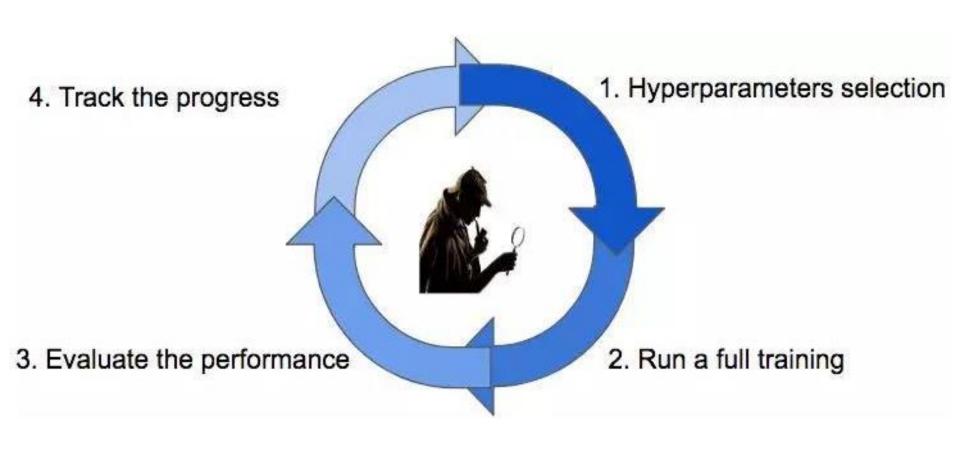
Learning Rate

Dropout

The variables learned from the data:

weights

...



## Outline

- Hyperparameters & Parameters
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# Setting the dataset

Idea #1: Choose hyperparameters that work best on the data

dataset

BAD: Always works perfectly on the training data

Idea #2: Split data into train and test, choose hyperparameters that work best on the test data

train test

BAD: The test set is a proxy for the generalization performance! No idea how algorithm will perform on new data

# Setting the dataset

Idea #3: Split data into train, validation, and test; choose hyperparameters on the validation data and evaluate on the test data.

|--|

❖ Better!

# Setting the dataset

Idea #4: Cross-Validation: Split data into folds, try each fold as validation and average the results

fold 1	fold 2	fold 3	fold 4	fold 5	test
fold 1	fold 2	fold 3	fold 4	fold 5	test
fold 1	fold 2	fold 3	fold 4	fold 5	test

> Especially useful for small datasets

# Hyperparameters Setting

- Choose hyperparameters using the validation set
- Only run on the test set once at the very end!
  - Measuring the generalization of the designed model

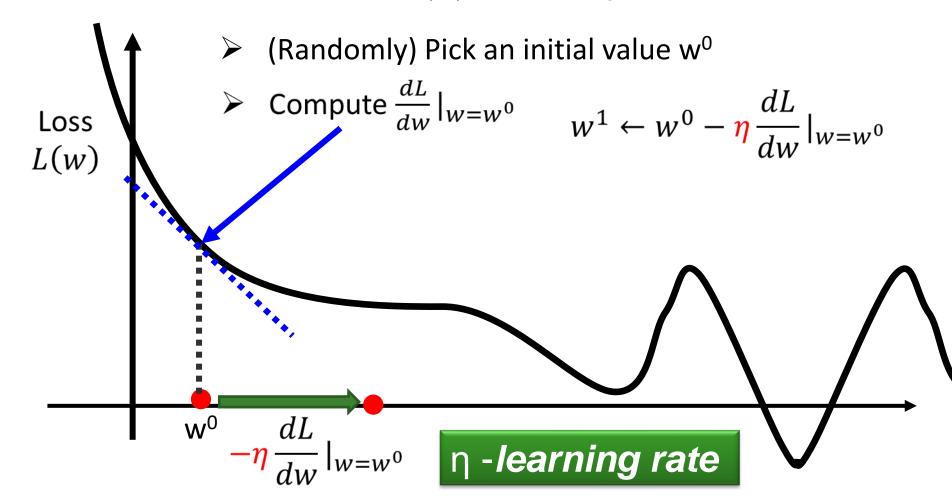
## Outline

- Hyperparameters & Parameters
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- Gradient descent
- Learning rate
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## Gradient Descent

$$w^* = \arg\min_{w} L(w)$$

 $\diamond$  Consider loss function L(w) with one parameter w:



## Gradient Descent

$$abla L = \begin{bmatrix} rac{\partial L}{\partial w} \\ rac{\partial L}{\partial b} \end{bmatrix}$$
 gradient

How about two parameters?

$$w^*, b^* = arg \min_{w,b} L(w,b)$$

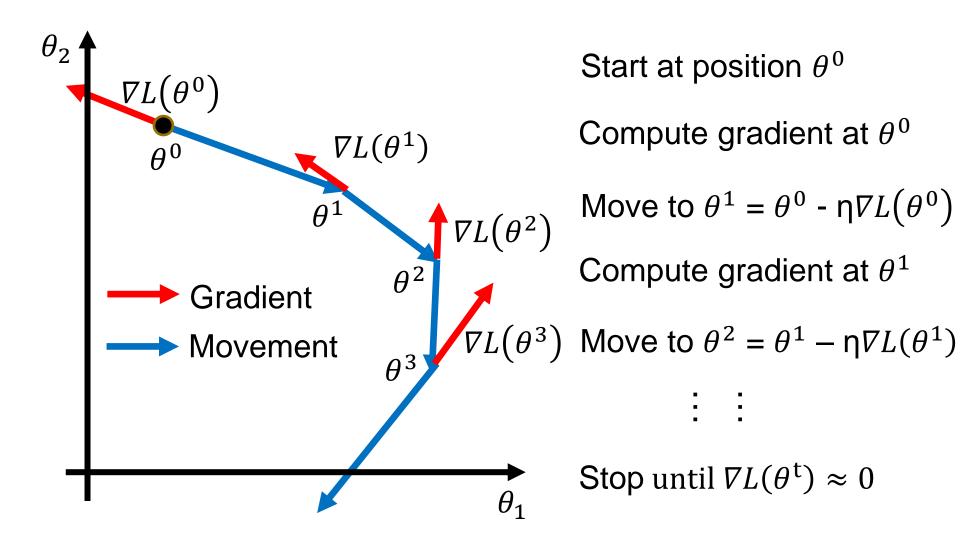
- ➤ (Randomly) Pick an initial value w<sup>0</sup>, b<sup>0</sup>
- ightharpoonup Compute  $\frac{\partial L}{\partial w}|_{w=w^0,b=b^0}$ ,  $\frac{\partial L}{\partial b}|_{w=w^0,b=b^0}$

$$w^{1} \leftarrow w^{0} - \frac{\partial L}{\partial w}|_{w=w^{0},b=b^{0}} \qquad b^{1} \leftarrow b^{0} - \frac{\partial L}{\partial b}|_{w=w^{0},b=b^{0}}$$

ightharpoonup Compute  $\frac{\partial L}{\partial w}|_{w=w^1,b=b^1}$ ,  $\frac{\partial L}{\partial b}|_{w=w^1,b=b^1}$ 

$$w^2 \leftarrow w^1 - \frac{\partial L}{\partial w}|_{w=w^1,b=b^1} \qquad b^2 \leftarrow b^1 - \frac{\partial L}{\partial b}|_{w=w^1,b=b^1}$$

## Gradient Descent



## Stochastic Gradient Descent

$$L = \sum_{n} \left( \hat{y}^n - \left( b + \sum_{i} w_i x_i^n \right) \right)^2$$

Loss is the summation over all training examples

Gradient Descent

$$\theta^i = \theta^{i-1} - \eta \nabla L(\theta^{i-1})$$

Stochastic Gradient Descent

Faster!

Pick an example x<sup>n</sup>

$$L^{n} = \left(\hat{y}^{n} - \left(b + \sum w_{i} x_{i}^{n}\right)\right)^{2} \theta^{i} = \theta^{i-1} - \eta \nabla L^{n}(\theta^{i-1})$$

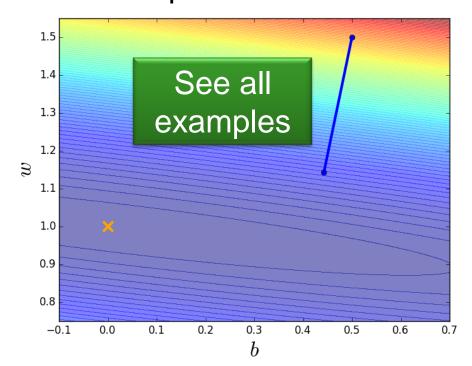
Loss for only one example

$$\theta^i = \theta^{i-1} - \eta \nabla L^n (\theta^{i-1})$$

## Stochastic Gradient Descent

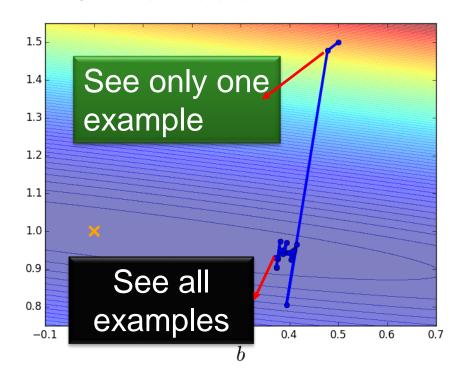
#### **Gradient Descent**

Update after seeing all examples



#### Stochastic Gradient Descent

Update for each example If there are 20 examples, 20 times faster.



## Mini-batch SGD

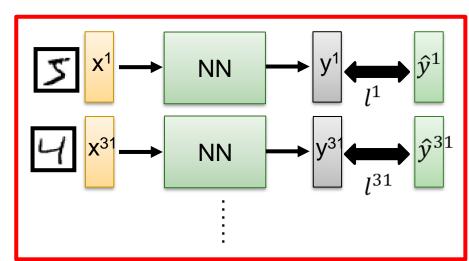
- Iterate over epochs
  - Iterate over dataset mini-batches  $(x_1, y_1), ..., (x_b, y_b)$ 
    - Compute gradient of the mini-batch loss:

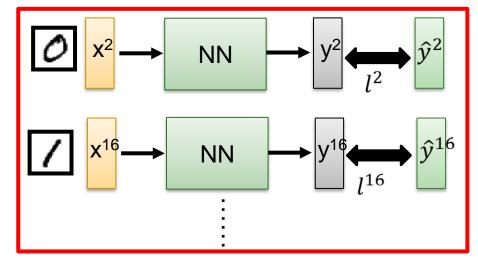
$$\nabla \hat{L} = \frac{1}{b} \sum_{i=1}^{b} \nabla l(w, x_i, y_i)$$

Update parameters:

$$w \leftarrow w - \eta \nabla \hat{L}$$

- Check for convergence, decide whether to decay learning rate
- What are the hyperparameters?
  - Mini-batch size, learning rate decay schedule, deciding when to stop





- Randomly initialize network parameters
- Pick the 1<sup>st</sup> batch  $L' = l^1 + l^{31} + \cdots$ Update parameters once
- Pick the  $2^{nd}$  batch  $L'' = l^2 + l^{16} + \cdots$  Update parameters once :
- Until all mini-batches have been picked

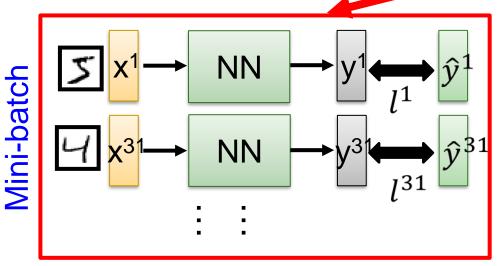
one epoch

Repeat the above process

## Mini-batch

Batch size influences both *speed* and *performance*. You have to tune it.

model.fit(x\_train, y\_train, batch size=100, nb epoch=20)



100 examples in a mini-batch Batch size = 1

Stochastic gradient descent

Pick the 1<sup>st</sup> batch

$$L' = l^1 + l^{31} + \cdots$$

Update parameters once

➢ Pick the 2<sup>nd</sup> batch

$$L'' = l^2 + l^{16} + \cdots$$

Update parameters once

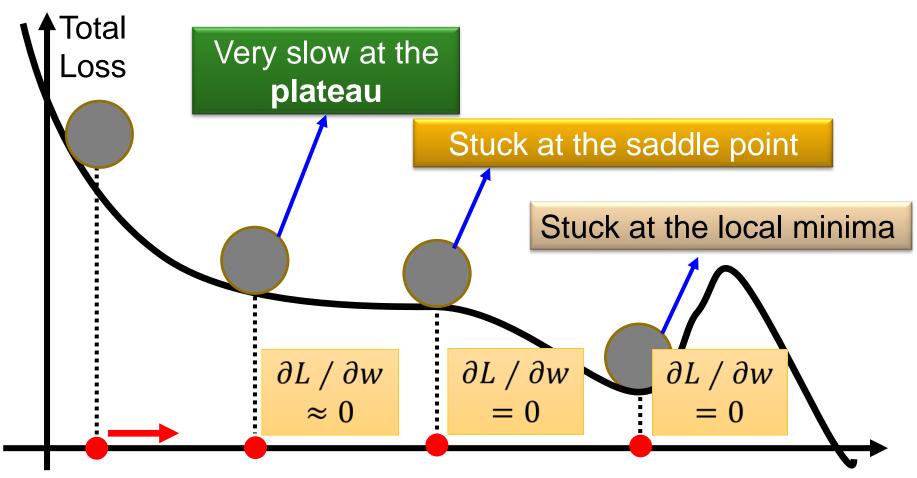
:

Until all mini-batches have been picked

Repeat 20 times

one epoch

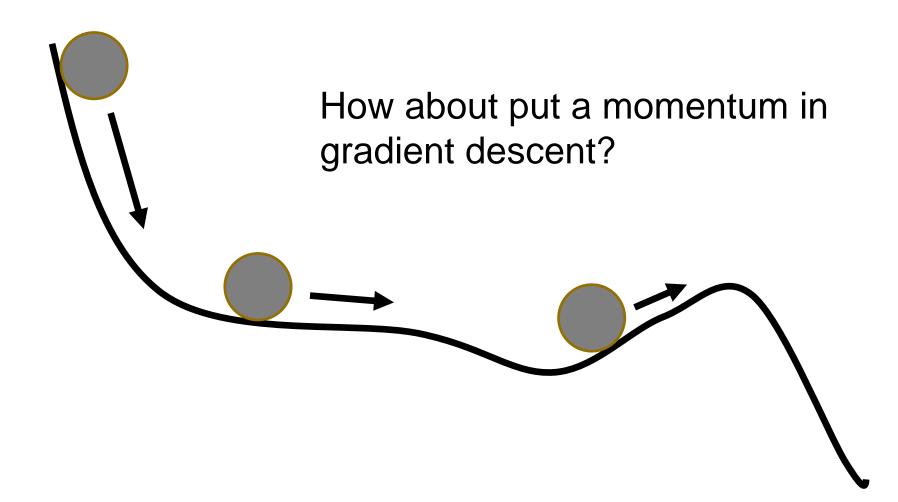
# Hard to find optimal network parameters



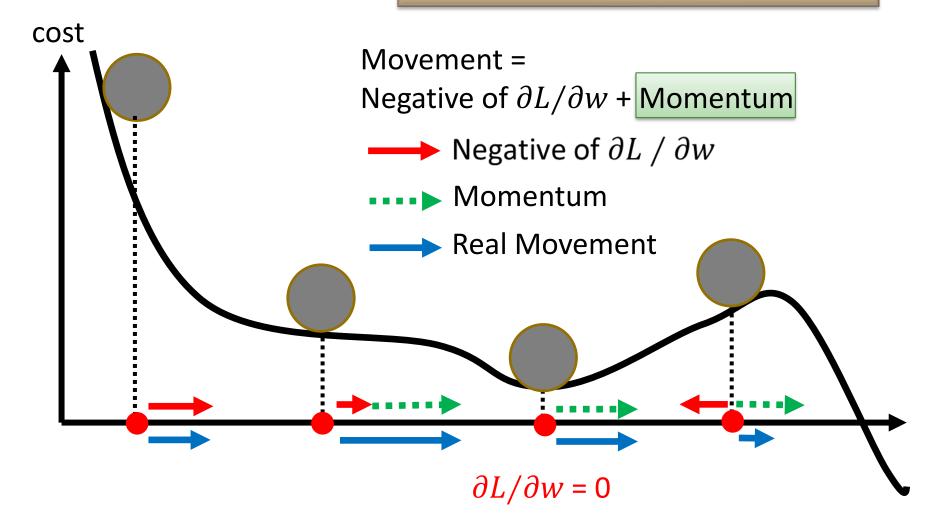
The value of a network parameter w

## In physical world .....

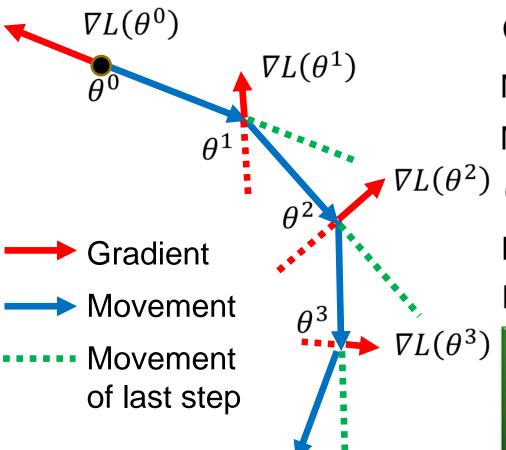
Momentum



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



Movement: movement of the last step minus the gradient at present



Start at point  $\theta^0$ 

Movement v<sup>0</sup>=0

Compute gradient at  $\theta^0$ 

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

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

Compute gradient at  $\theta^1$ 

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

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

Movement not just based on the gradient, but also on the previous

innov/almaamit

Movement: movement of last step minus the gradient at present

v<sup>i</sup> is actually the weighted sum of all the previous gradient:

$$\nabla L(\theta^0), \nabla L(\theta^1), \dots \nabla L(\theta^{i-1})$$

$$v^0 = 0$$

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

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

Start at point  $\theta^0$ 

Movement  $v^0=0$ 

Compute gradient at  $\theta^0$ 

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

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

Compute gradient at  $\theta^1$ 

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

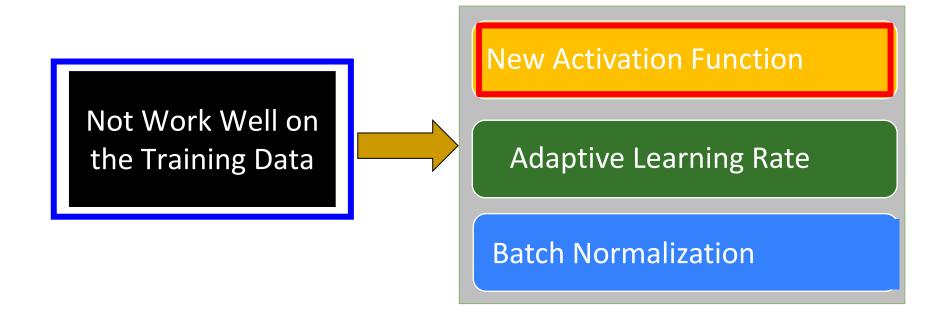
Move to  $\theta^2 = \theta^1 + v^2$ 

$$egin{aligned} v_{dw} &= eta v_{dw} + (1-eta)dW \ v_{db} &= eta v_{db} + (1-eta)db \end{aligned}$$

$$W=W-lpha v_{dw}$$
  $b=b-lpha v_{db}$ 

#### A certain problem to be solved Make some changes No Works well on Design **Training** the Training the Model a Model Data? Yes Make some changes Works well on No the Testing Data? Different approaches Yes for different problems

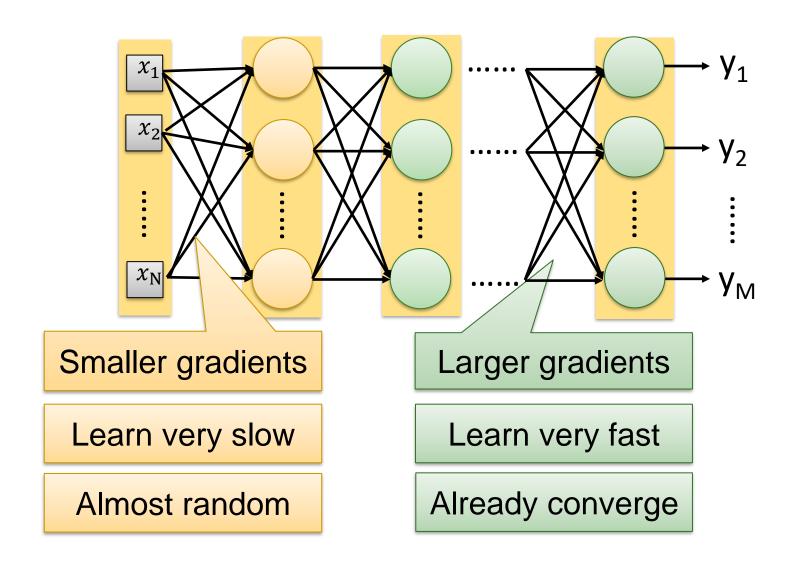
# Not Work Well on the Training Data



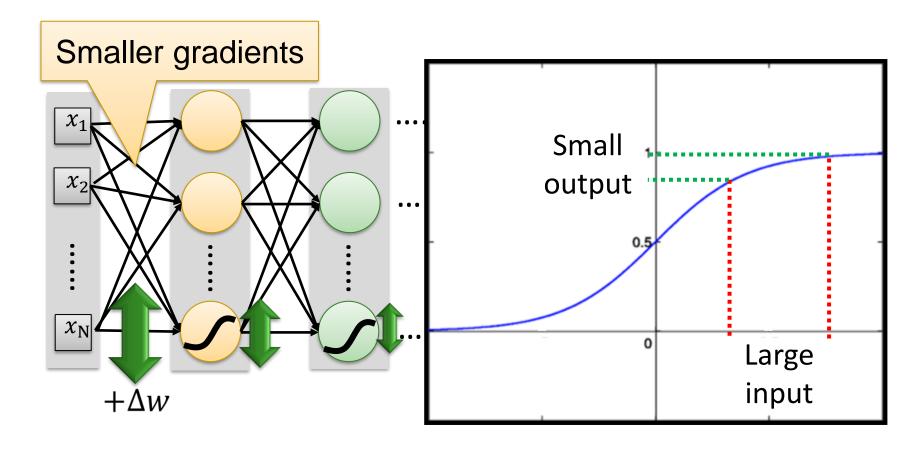
# Deeper usually does not imply better



## Vanishing Gradient Problem



## Vanishing Gradient Problem



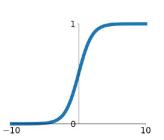
An intuitive way to compute the derivatives ...

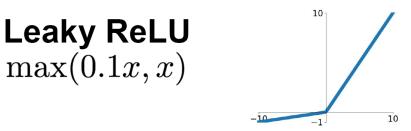
$$\frac{\partial l}{\partial w} = ? \frac{\Delta l}{\Delta w}$$

## Some Activation Functions

#### **Sigmoid**

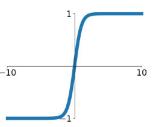
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$





#### tanh

tanh(x)

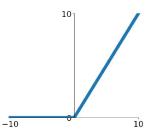


#### **Maxout**

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

#### ReLU

 $\max(0,x)$ 

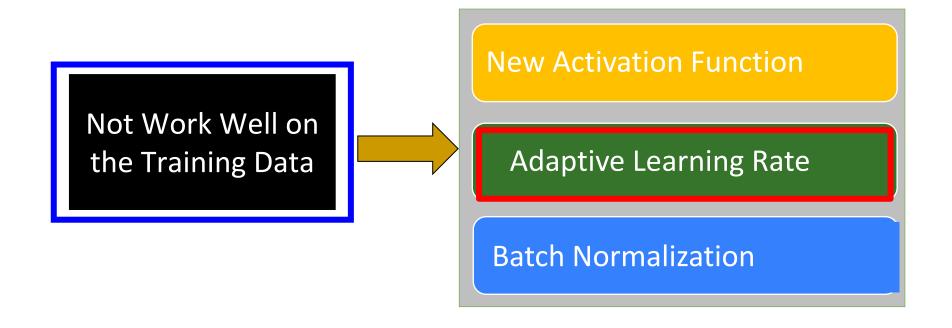


#### **ELU**

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

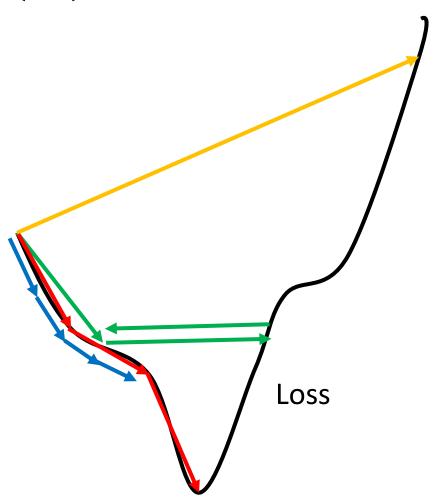
. . . . . .

# Not Work Well on the Training Data



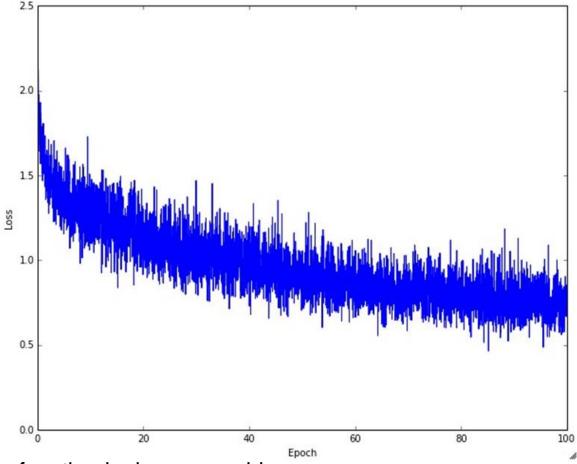
# Learning Rate

$$\theta^i = \theta^{i-1} - \eta \nabla L(\theta^{i-1})$$



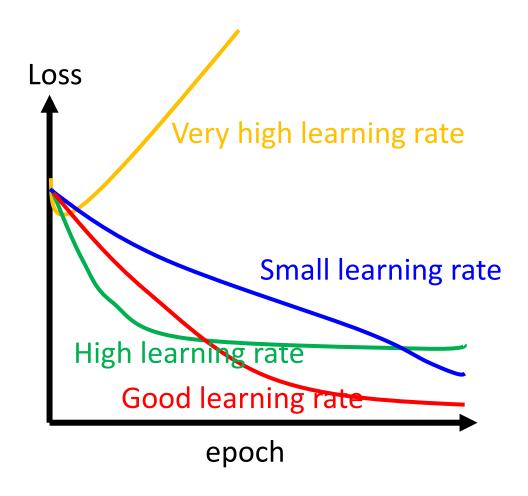
Set the learning rate  $\eta$  carefully

#### We can always visualize this.



- The loss function looks reasonable
- Might indicate a slightly too small learning rate based on its speed of decay
- The batch size might be a little too low (since the loss is a little too noisy)

# The effects of different learning rates



## Adaptive Learning Rates

- Popular & Simple Idea: Reduce the learning rate by some factor every few epochs.
  - At the beginning, we are far from the destination, so we use larger learning rate
  - After several epochs, we are close to the destination, so we reduce the learning rate
  - E.g. 1/t decay:  $\eta^t = \eta/\sqrt{t+1}$
- Learning rate cannot be one-size-fits-all
  - Giving different parameters different learning rates

$$\eta^t = \frac{\eta}{\sqrt{t+1}}$$
  $g^t = \frac{\partial L(\theta^t)}{\partial w}$ 

Divide the learning rate of each parameter by the root mean square of its previous deviation

### Vanilla Gradient descent

$$w^{t+1} \leftarrow w^t - \eta^t g^t$$

### **Adagrad**

$$w^{t+1} \leftarrow w^t - \frac{\eta^t}{\sigma^t} g^t$$

Parameter dependent

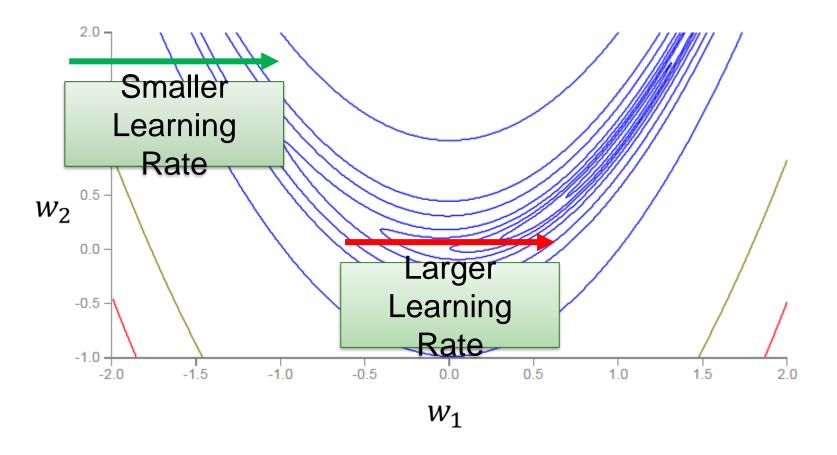
# Adagrad

Divide the learning rate of each parameter by the root mean square of its previous derivatives

where 
$$t$$
 is  $t$  in  $t$ 

## 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

# RMSProp

$$egin{align} s_{dw} &= eta s_{dw} + (1-eta) dW^2 \ s_{db} &= eta s_{db} + (1-eta) db^2 \ \end{align}$$

$$W=W-lpharac{dW}{\sqrt{s_{dw}}+arepsilon} \ b=b-lpharac{db}{\sqrt{s_{db}}+arepsilon}$$

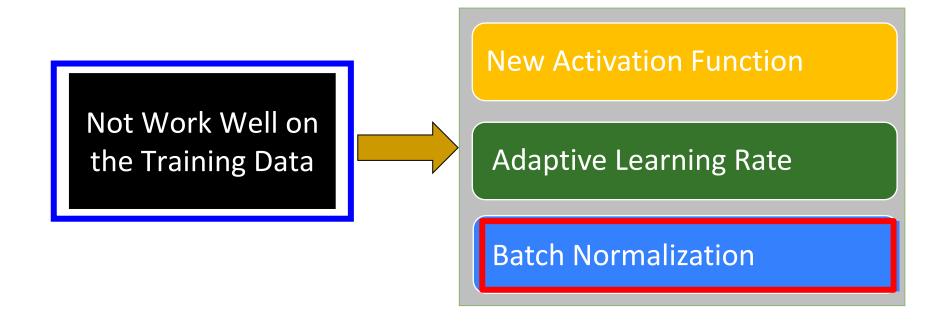
### Adam

### 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  $\beta_1^t$  and  $\beta_2^t$  we denote  $\beta_1$  and  $\beta_2$  to the power t.

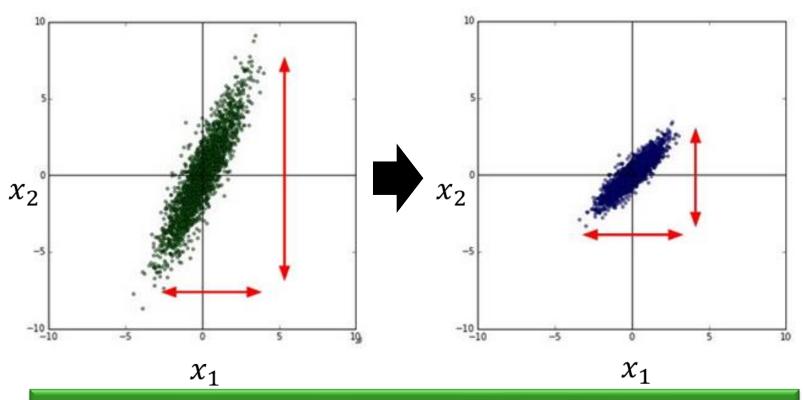
```
Require: \alpha: Stepsize
Require: \beta_1, \beta_2 \in [0, 1): Exponential decay rates for the moment estimates
Require: f(\theta): Stochastic objective function with parameters \theta
Require: \theta_0: Initial parameter vector
                                                              for momentum
   m_0 \leftarrow 0 (Initialize 1<sup>st</sup> moment vector)
   v_0 \leftarrow 0 (Initialize 2<sup>nd</sup> moment vector)
   t \leftarrow 0 (Initialize timestep)
                                                                 for RMSProp
   while \theta_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)
      \hat{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 \theta_t (Resulting parameters)
```

# Not Work Well on the Training Data



## Feature Scaling

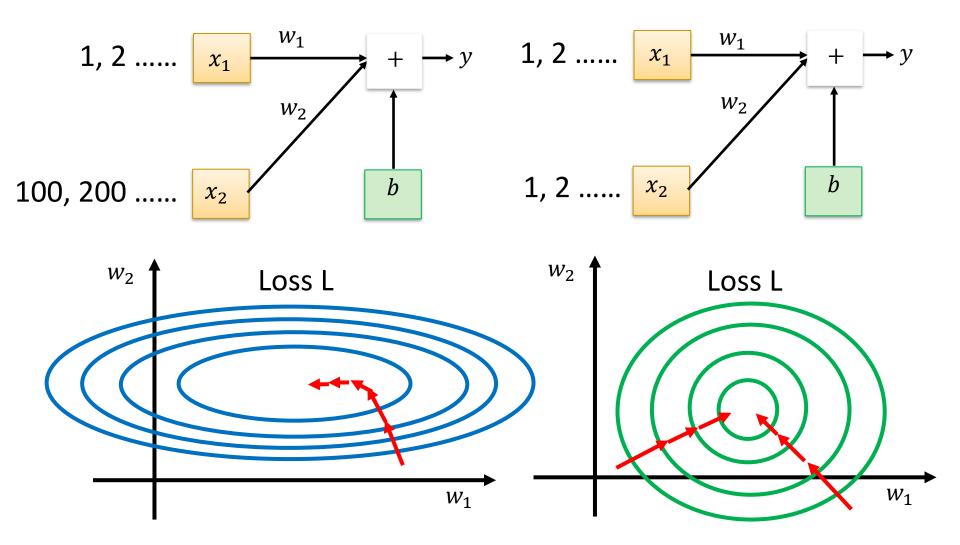
$$y = w_1 x_1 + w_2 x_2 + b$$



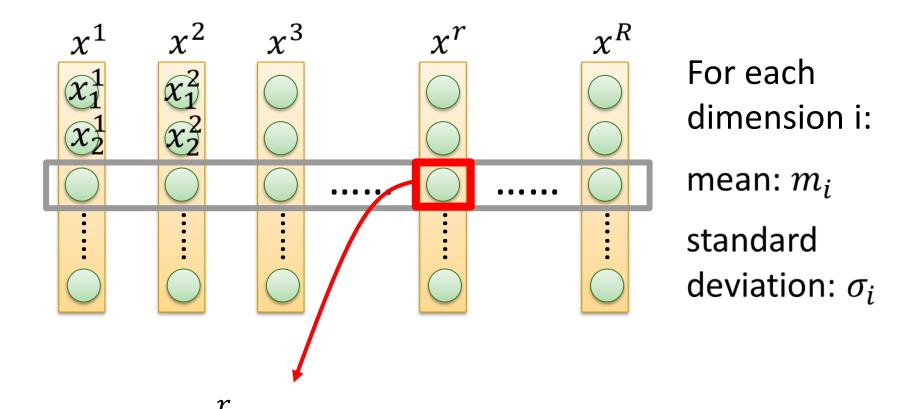
Make different features have the same scaling.

### Feature Scaling

$$y = w_1 x_1 + w_2 x_2 + b$$



## Feature Scaling

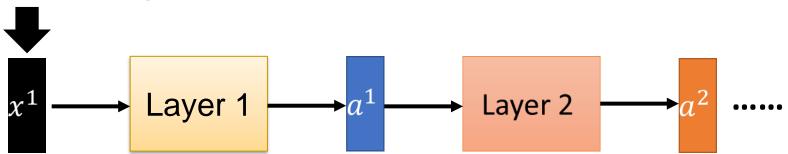


In general, gradient descent converges

much faster with feature scaling.

### How about Hidden Layer?

#### Feature Scaling



#### Internal Covariate Shift



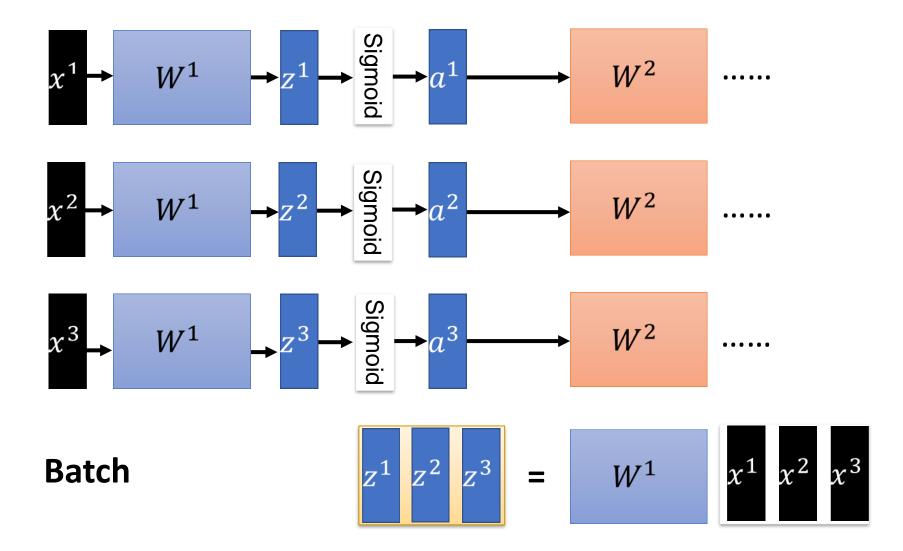
Smaller learning rate can be helpful, but the training would be slower.

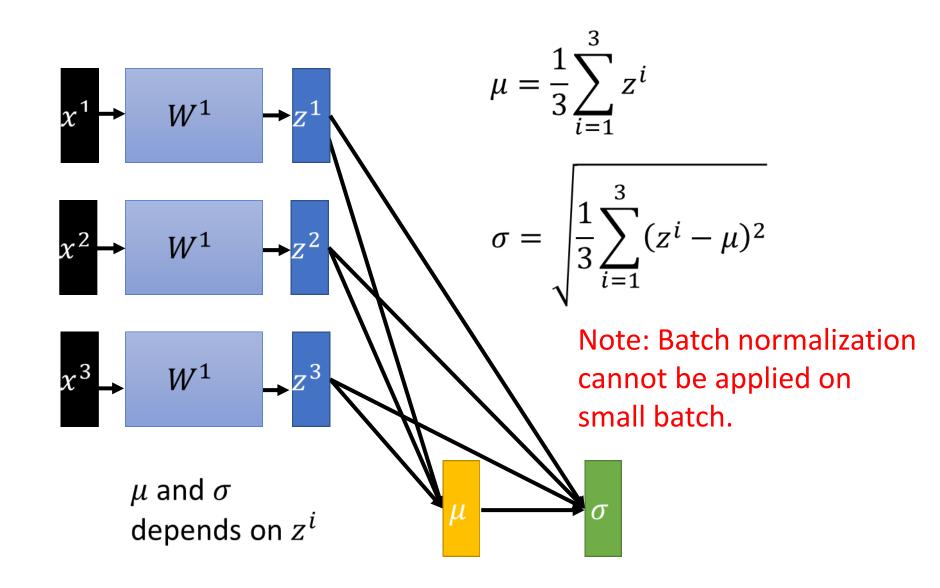


### **Batch normalization**

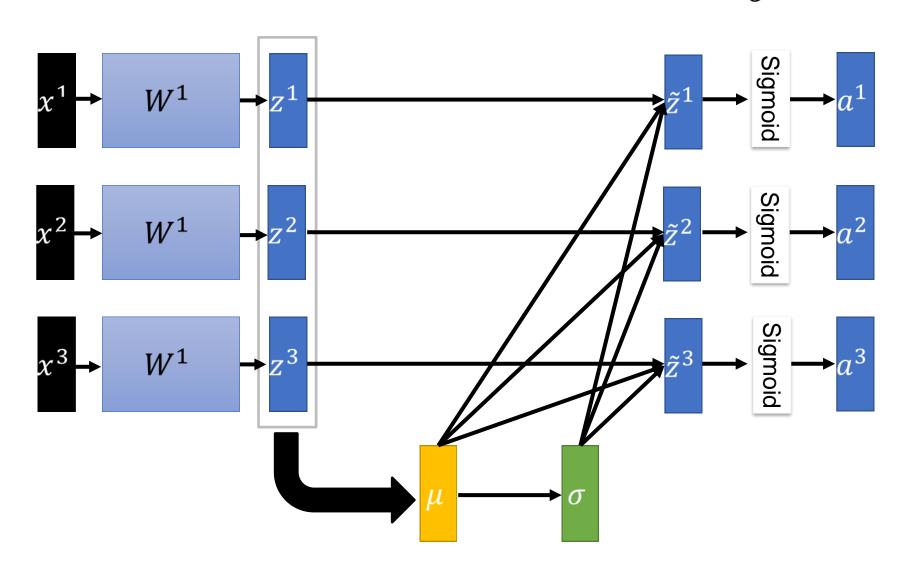
Sergey Ioffe, Christian Szegedy. Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift. 2015

### Batch



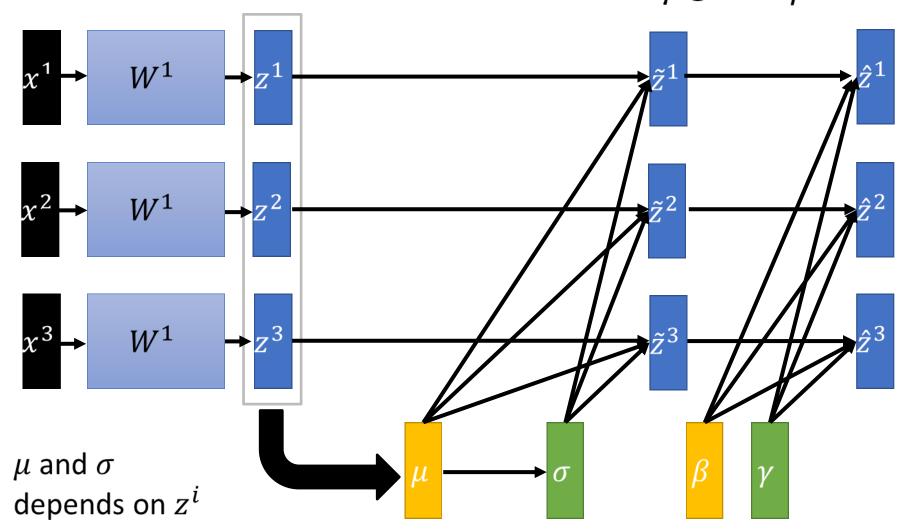


$$\tilde{z}^i = \frac{z^i - \mu}{\sigma}$$

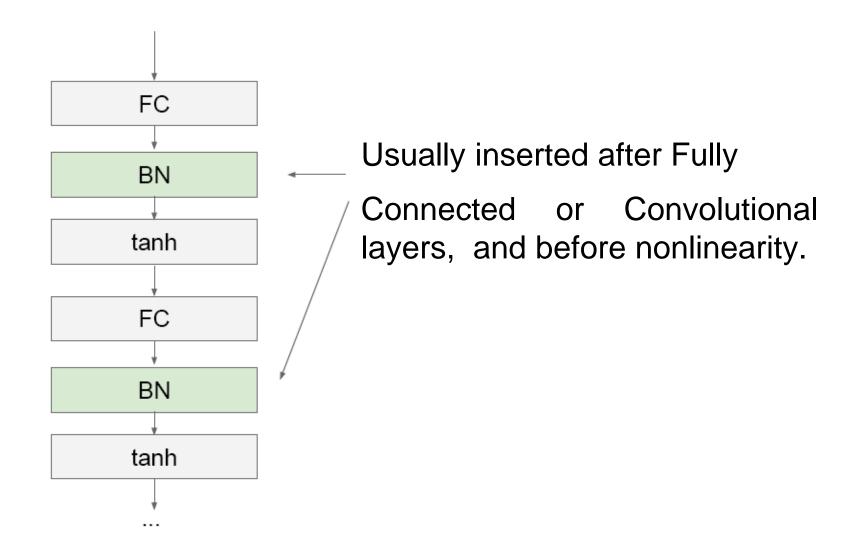


$$\tilde{z}^i = \frac{z^i - \mu}{\sigma}$$

$$\hat{z}^i = \gamma \odot \tilde{z}^i + \beta$$

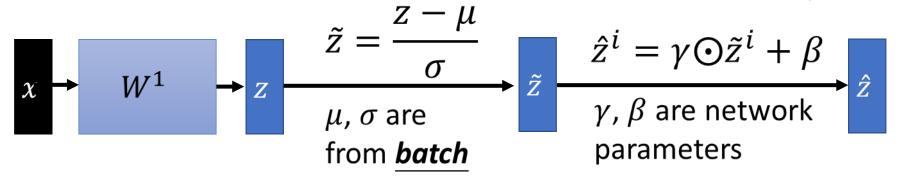


```
Input: Values of x over a mini-batch: \mathcal{B} = \{x_{1...m}\};
             Parameters to be learned: \gamma, \beta
Output: \{y_i = BN_{\gamma,\beta}(x_i)\}
  \mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^{m} x_i
                                                                  // mini-batch mean
   \sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2
                                                            // mini-batch variance
                                                                             // normalize
    y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv BN_{\gamma,\beta}(x_i)
                                                                      // scale and shift
```



Acc  $\mu_{100}$   $\mu_{300}$  Updates

At testing stage:



We do not have **batch** at testing stage.

#### Ideal solution:

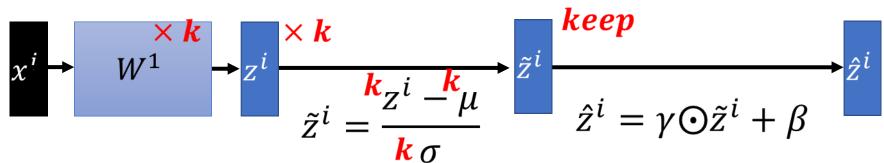
Computing  $\mu$  and  $\sigma$  using the whole training dataset.

#### Practical solution:

Computing the moving average of  $\mu$  and  $\sigma$  of the batches during training.

### Batch normalization - Benefit

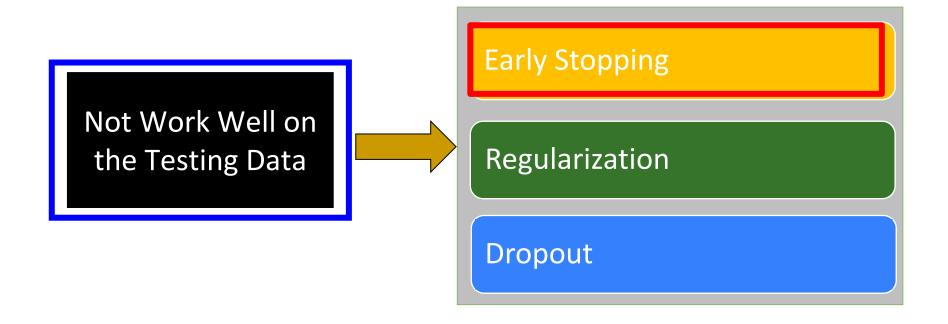
- BN reduces training times, and make very deep net trainable.
  - Because of less Covariate Shift, we can use larger learning rates.
  - Less exploding/vanishing gradients
    - Especially effective for sigmoid, tanh, etc.
- Learning is less affected by initialization.



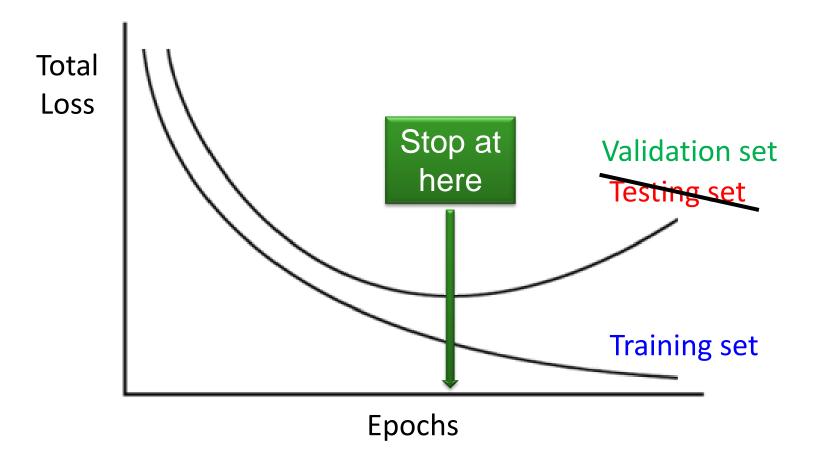
BN reduces the demand for regularization.

### A certain problem to be solved Make some changes No Works well on Design **Training** the Training the Model a Model Data? Yes Make some changes Works well on No the Testing Data? Different approaches for different problems Yes

## Not Work Well on the Testing Data

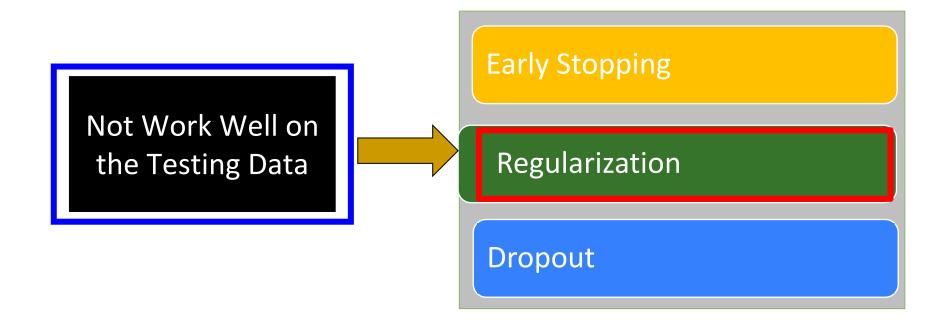


# Early Stopping



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

# Not Work Well on the Testing Data



# Regularization

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

$$L'(\theta) = L(\theta) + \lambda \frac{1}{2} ||\theta||_2 \longrightarrow \text{Regularization term}$$
 
$$\theta = \{w_1, w_2, \dots\}$$

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

L2 regularization:

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

(usually not consider biases)

# Regularization

### L2 regularization:

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

New loss function to be minimized

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

Update: 
$$w^{t+1} \leftarrow w^t - \eta \frac{\partial L'}{\partial w} = w^t - \eta \left( \frac{\partial L}{\partial w} + \lambda w^t \right)$$
$$= \underbrace{(1 - \eta \lambda)w^t}_{} - \eta \frac{\partial L}{\partial w}$$
 Weight Decay

Close to zero

# Regularization

### L1 regularization:

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

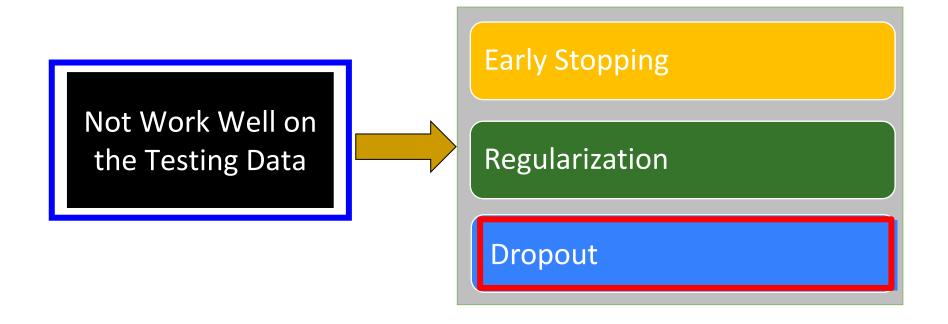
New loss function to be minimized

$$L'(\theta) = L(\theta) + \lambda \|\theta\|_1 \qquad \frac{\partial L'}{\partial w} = \frac{\partial L}{\partial w} + \lambda \operatorname{sgn}(w)$$

Update:

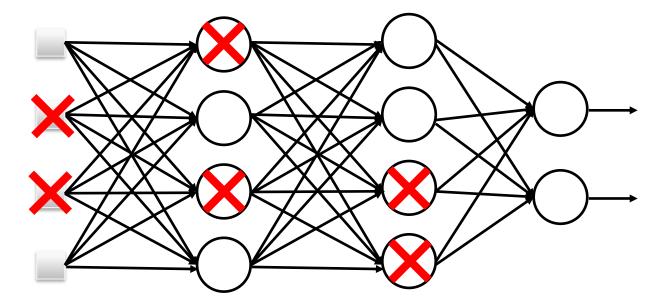
$$w^{t+1} \leftarrow w^t - \eta \frac{\partial L'}{\partial w} = w^t - \eta \left( \frac{\partial L}{\partial w} + \lambda \operatorname{sgn}(w^t) \right)$$
$$= w^t - \eta \lambda \operatorname{sgn}(w^t) - \eta \frac{\partial L}{\partial w}$$

## Not Work Well on the Testing Data



## Dropout

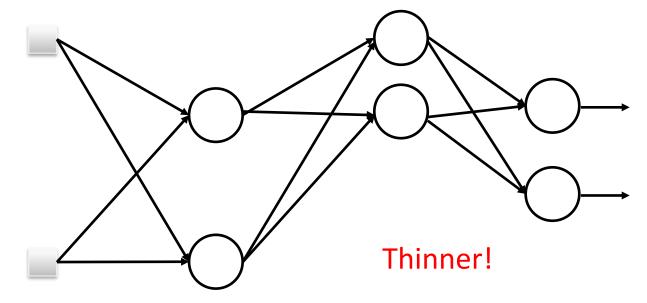
### **Training:**



- > Each time before updating the parameters
  - Each neuron has a probability of p to be dropouted

## Dropout

### **Training:**

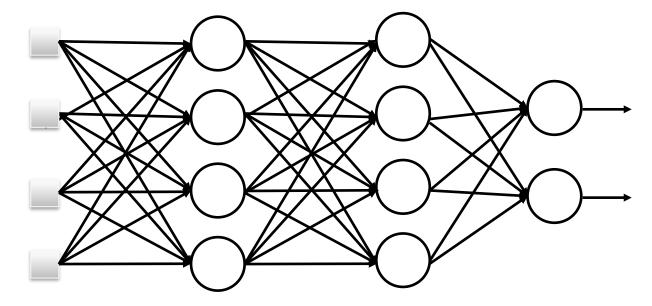


- > Each time before updating the parameters
  - Each neuron has a probability of p to be dropouted
    - The structure of the network is changed.
  - Using the new network for training

For each mini-batch, we resample the dropout neurons.

## Dropout

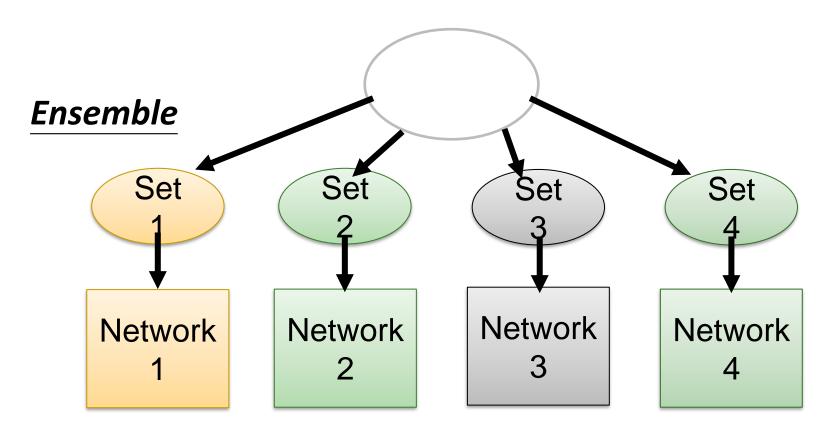
### **Testing:**



### No dropout

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

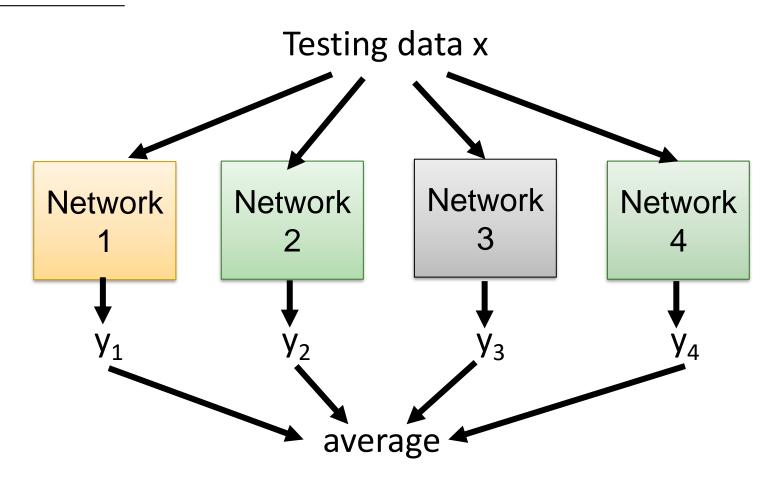
### Dropout is a kind of ensemble.



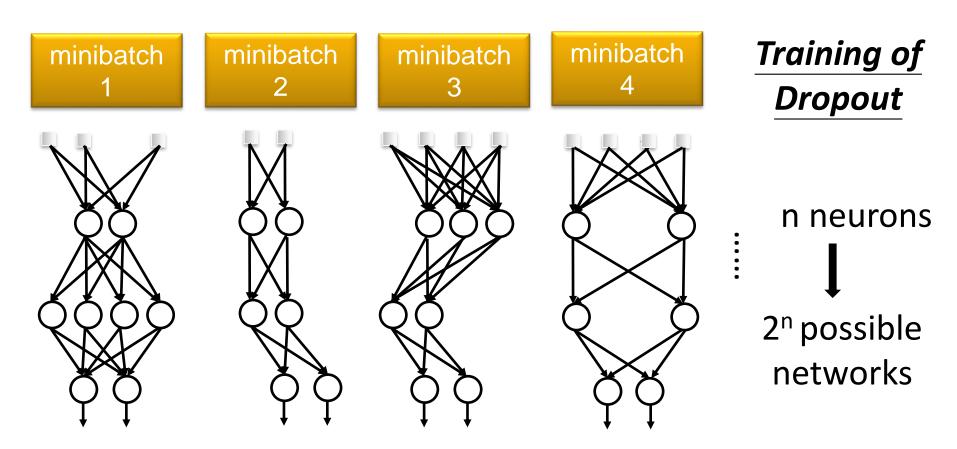
Train a bunch of networks with different structures

## Dropout is a kind of ensemble.

### **Ensemble**

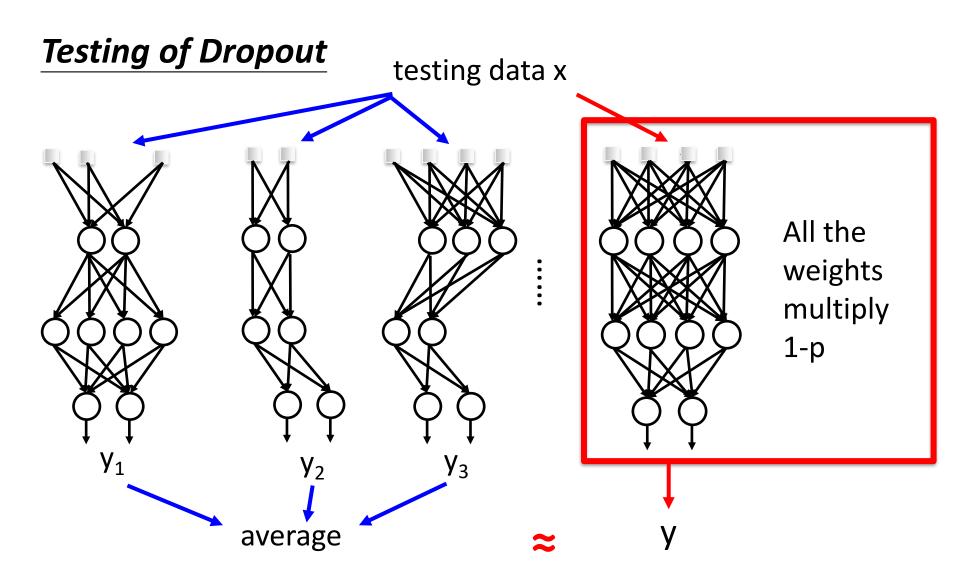


## Dropout is a kind of ensemble.



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

## Dropout is a kind of ensemble.



### Outline

- Hyperparameters & Parameters
- Setting up the data
- Gradient Descent
- Learning rate
- Batch Normalization
- Early stopping
- Regularization
- Dropout
- Hyperparameter tuning

# Hyperparameter Tuning

- ☐ Choices about the algorithm that we set rather than learn
- Come up very often in the design of many Machine Learning algorithms that learn from data.
- ☐ Often not obvious & Very problem-dependent : (
- Just try and try and try and see what works best (e.g. the predicted class scores are consistent with the ground truth labels)

# Four main strategies for searching for the best configuration

- Babysitting
- Grid Search
- Random Search
- Automatic Hyperparameter Tuning

# Babysitting: Manually

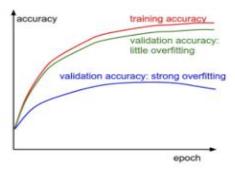


Data

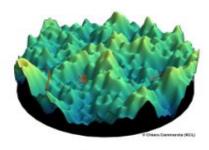


Act/Grad/Filter





Metric



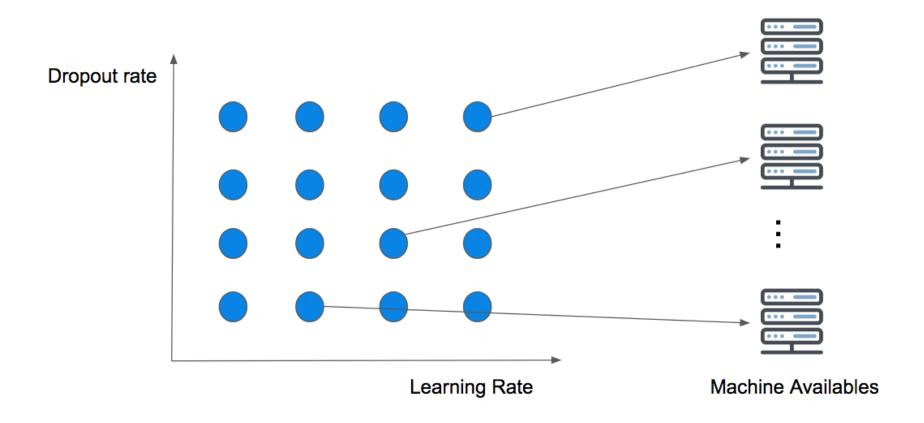
Space

## Grid Search

#### Workflow:

- ◆ Define a grid on n dimensions, where each of these maps is for an hyperparameter.
  - e.g. n = (learning\_rate, dropout\_rate, batch\_size)
- For each dimension, define the range of possible values:
  - e.g. batch\_size = [4, 8, 16, 32, 64, 128, 256]
- Search for all the possible configurations and wait for the results to establish the best one:
  - e.g. C1 = (0.1, 0.3, 4) -> acc = 92%, C2 = (0.1, 0.35, 4) -> acc = 92.3%, etc...

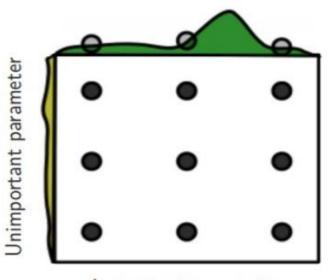
A simple grid search on two dimensions for the Dropout and Learning rate



- This strategy is embarrassingly parallel because it doesn't take into account the computation history.
- Pain point: the curse of dimensionality
  - It's common to use this approach when the dimensions are less than or equal to 4

## Grid Search vs Random Search

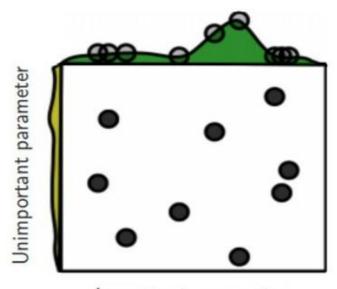
#### **Grid Layout**



Important parameter

Bad on high spaces

#### Random Layout



Important parameter

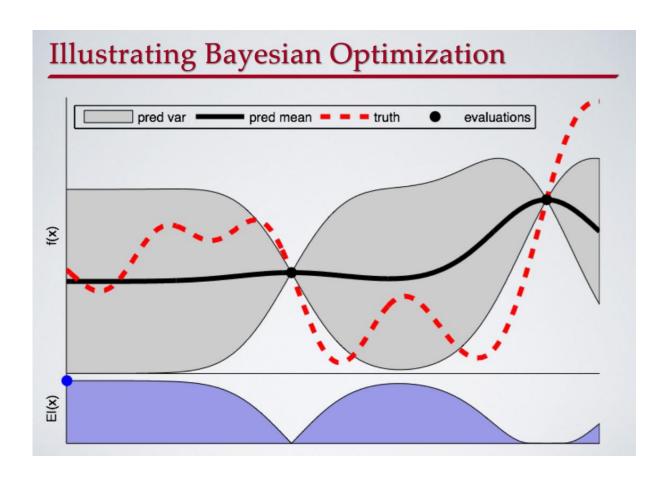
It doesn't guarantee to find the best hyperparameters

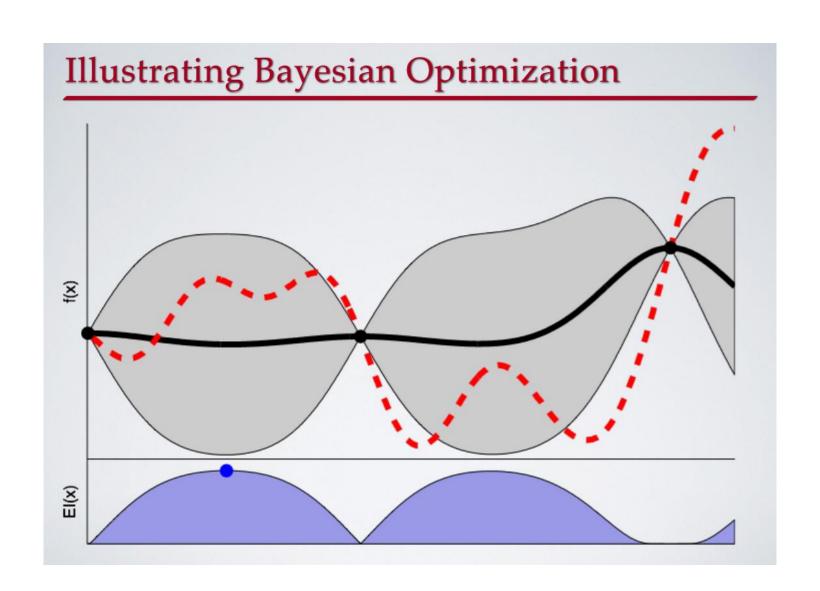
Good on high spaces

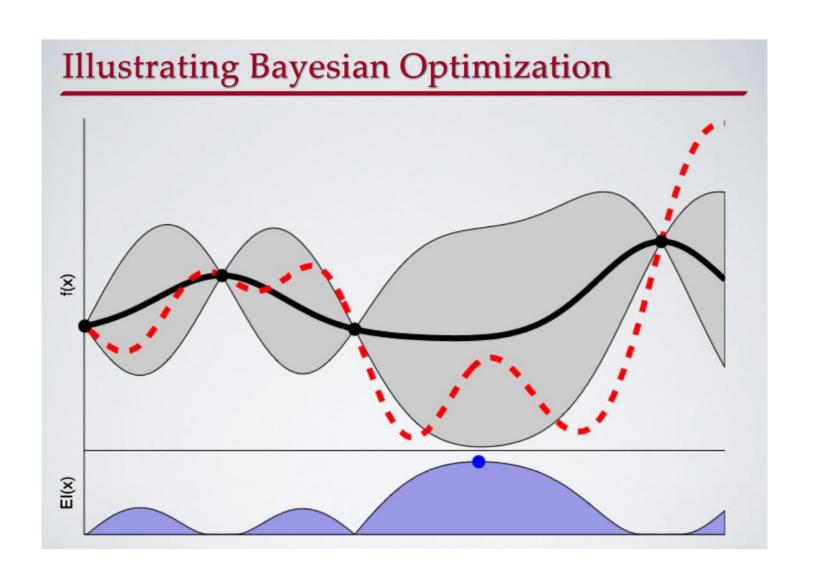
Give better results in less iterations

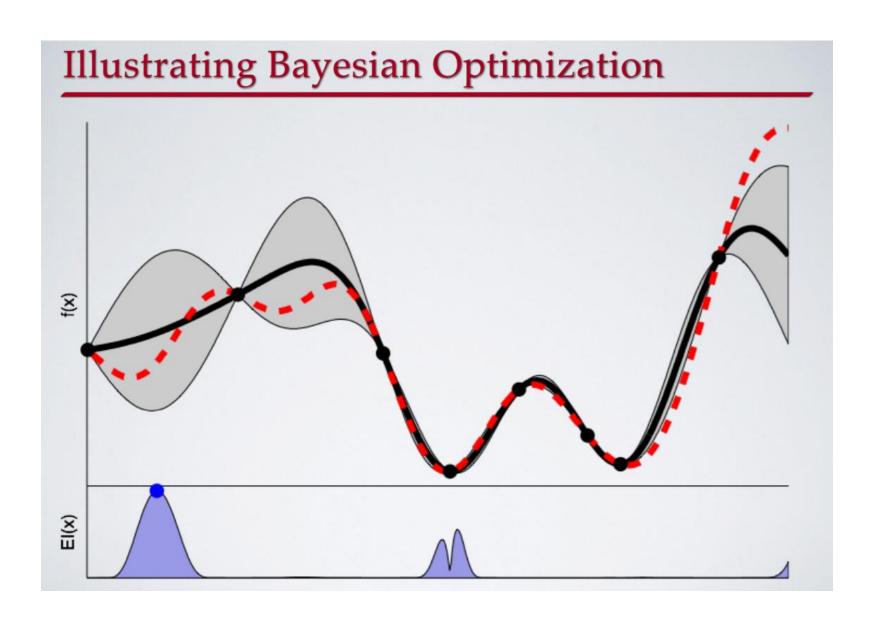
## Bayesian Optimization

-Automatic Hyperparameter Tuning









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