

# Deep Learning

## Lecture 03: Optimization and Regularization

## 优化与正则化

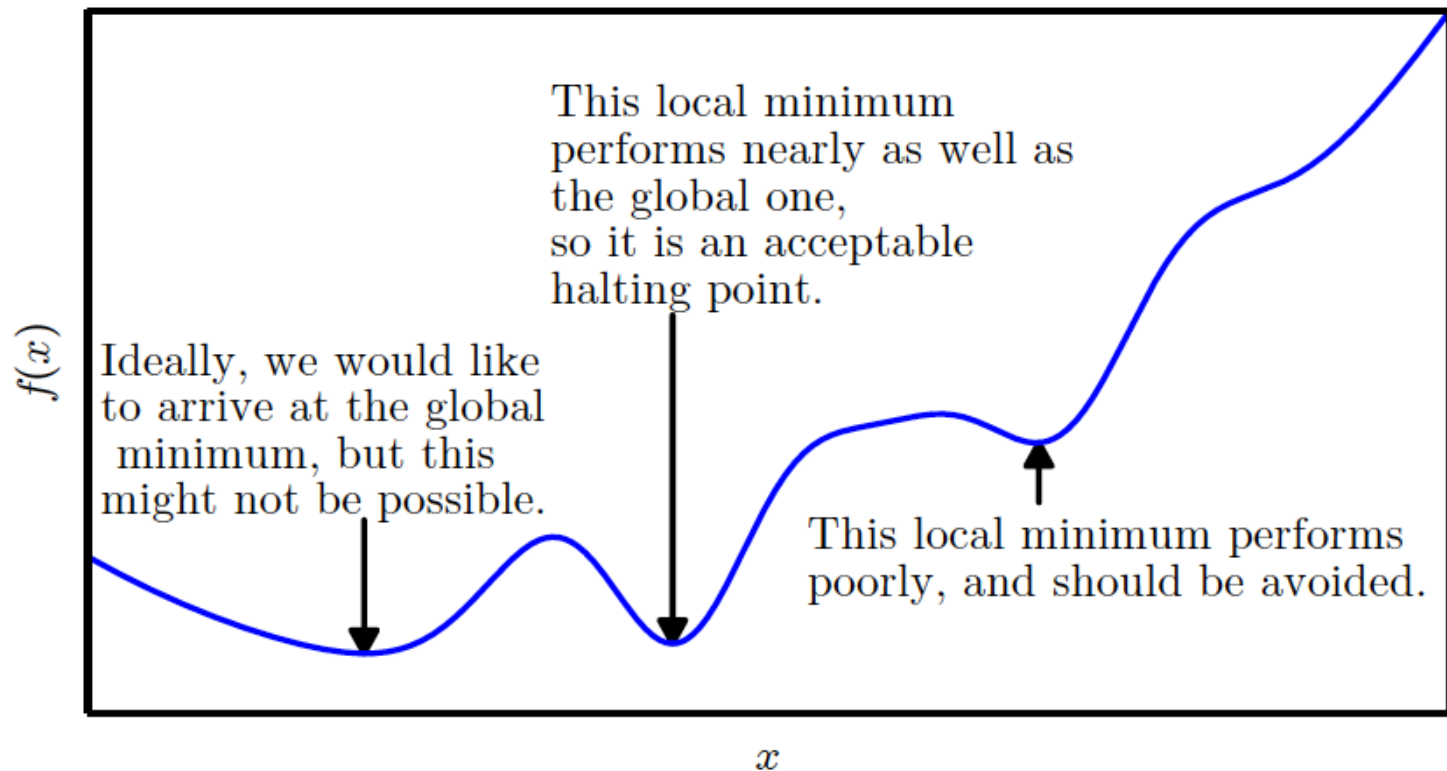
Wanxiang Che

# Optimization



# Challenges in NN Optimization

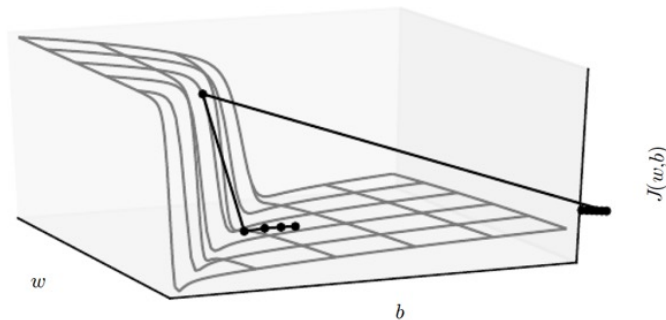
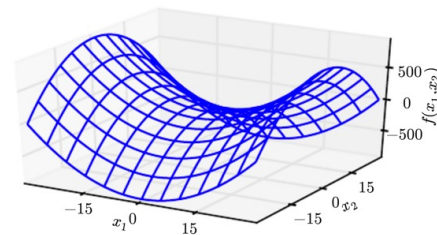
## Approximate minimization



# Challenges in NN Optimization

[Goodfellow et al., 2016. Section 8.2]

- Local Minima
- Plateaus, **Saddle Points** and Other Flat Regions
- Cliffs and Exploding Gradients
- Learning **Long-Term Dependencies**
  - Exploding or Vanishing Product Jacobians
- Inexact Gradients
- Theoretical Limits of Optimization



# Optimizing (Learning) Algorithms

- (Batch) Gradient Descent

$$\theta \leftarrow \theta + \epsilon \nabla_{\theta} \sum_t L(f(\mathbf{x}^{(t)}; \theta), \mathbf{y}^{(t)}; \theta)$$

- Stochastic Gradient Descent (SGD)
  - Online GD ( $m = 1$ ), Minibatch SGD ( $m > 1$ )

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**Algorithm 8.1** Stochastic gradient descent (SGD) update at training iteration  $k$

---

**Require:** Learning rate  $\epsilon_k$ .

**Require:** Initial parameter  $\theta$

**while** stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$  with corresponding targets  $\mathbf{y}^{(i)}$ .

    Compute gradient estimate:  $\hat{\mathbf{g}} \leftarrow +\frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

    Apply update:  $\theta \leftarrow \theta - \epsilon \hat{\mathbf{g}}$

**end while**

---

# Batch or Minibatch?

- Batch
  - Slow to estimate gradient
  - More exactly
- Minibatch
  - Fast to estimate gradient
  - Standard error of a mean estimated from  $n$  samples  $\hat{\sigma}/\sqrt{n}$ 
    - there are less than linear returns to using more examples to estimate the gradient
    - 100 examples vs. 10,000 examples

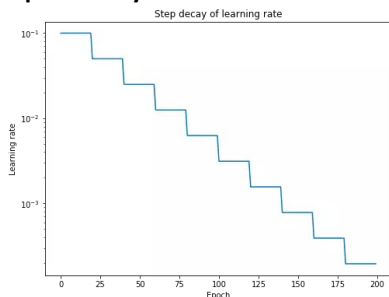
# Factors of Minibatch Sizes

- Larger batches provide a more accurate estimate of the gradient, but with less than linear returns
- Multicore architectures are usually underutilized by extremely small batches
- When using GPU, it is common for power of 2 batch sizes (32-256) to offer better runtime

# How to Choose Learning Rate (学习率)?

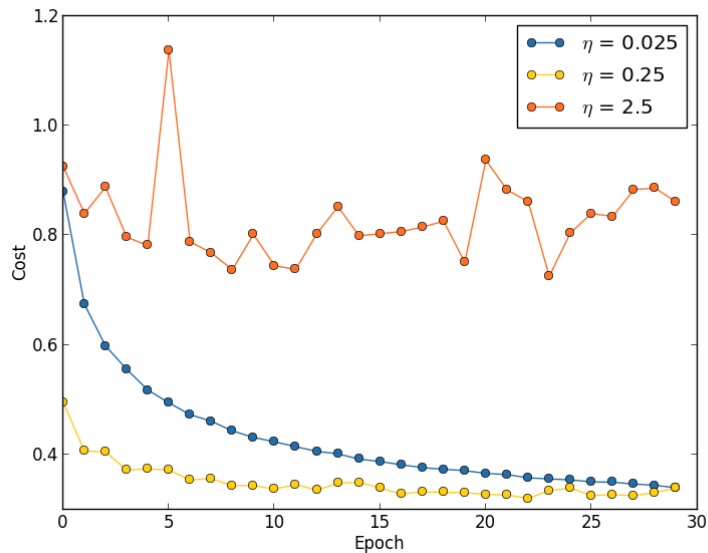
- Too high  $\rightarrow$  Oscillation; Too low  $\rightarrow$  Slow
- Gradually decrease the learning rate

– Step decay



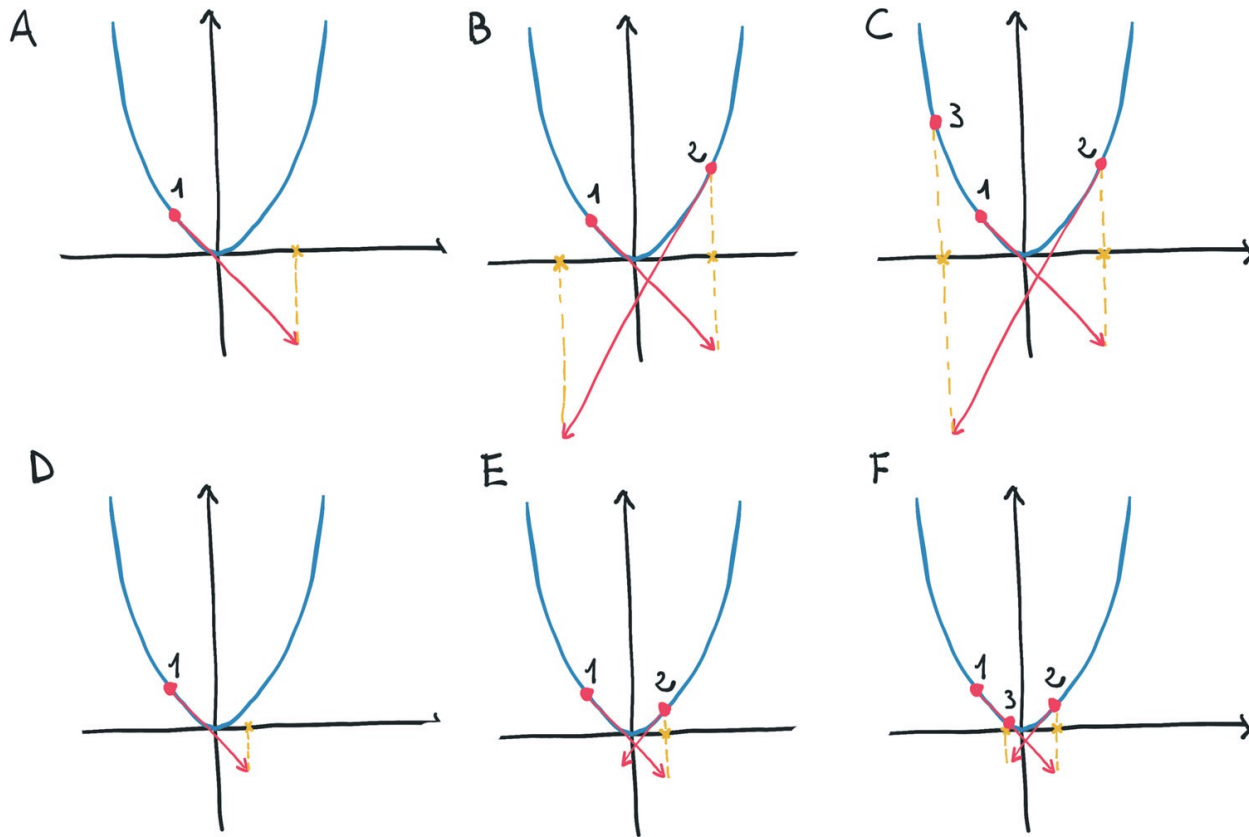
– Exponential decay:  $\alpha = \alpha_0 e^{-kt}$

– 1/t decay:  $\alpha = \alpha_0 / (1 + kt)$





# Illustration of different learning rates



# Momentum

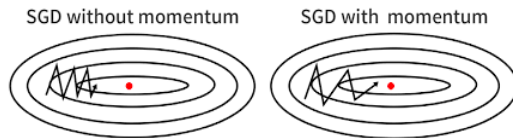
- SGD sometimes can be slow
  - high curvature, small but consistent gradients, or noisy gradients
- The method of momentum Polyak (1964) is designed to **accelerate learning**
- Intuition
  - Derived from a physical interpretation of the optimization process

# Momentum

- A variable  $v$  that plays the role of velocity (or momentum) that accumulates gradient

$$v \leftarrow +\alpha v + \eta \nabla_{\theta} \left( \frac{1}{m} \sum_{t=1}^m L(f(x^{(t)}; \theta), y^{(t)}) \right)$$

$$\theta \leftarrow \theta + v$$



```
sgd = keras.optimizers.SGD(lr=0.01, momentum=0.9)
```

Acc: ~98%

# Nesterov Momentum (Sutskever *et al.* 2013)

$$\begin{array}{ll} v \leftarrow +\alpha v + \eta \nabla_{\theta} \left( \frac{1}{m} \sum_{t=1}^m L(f(\mathbf{x}^{(t)}; \theta), \mathbf{y}^{(t)}) \right) & \Rightarrow v \leftarrow +\alpha v + \eta \nabla_{\theta} \left[ \frac{1}{m} \sum_{t=1}^m L(f(\mathbf{x}^{(t)}; \theta + \alpha v), \mathbf{y}^{(t)}) \right] \\ \theta \leftarrow \theta + v & \theta \leftarrow \theta + v, \end{array}$$

---

**Algorithm 8.3** Stochastic gradient descent (SGD) with Nesterov momentum

---

**Require:** Learning rate  $\epsilon$ , momentum parameter  $\alpha$ .

**Require:** Initial parameter  $\theta$ , initial velocity  $v$ .

**while** stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$  with corresponding labels  $\mathbf{y}^{(i)}$ .

    Apply interim update:  $\tilde{\theta} \leftarrow \theta + \alpha v$

    Compute gradient (at interim point):  $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \tilde{\theta}), \mathbf{y}^{(i)})$

    Compute velocity update:  $v \leftarrow \alpha v - \epsilon \mathbf{g}$

    Apply update:  $\theta \leftarrow \theta + v$

**end while**

---

```
sgd = keras.optimizers.SGD(lr=0.01, decay=1e-6, momentum=0.9, nesterov=True)
```

Acc: ~98%

# AdaGrad

- **Individually** adapts the learning rates of all model parameters by scaling them inversely proportional to an accumulated sum of squared partial derivatives over all training iterations
- Empirically, AdaGrad results in a premature and excessive decrease in the effective learning rate

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**Algorithm 8.4** The Adagrad algorithm

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**Require:** Global learning rate  $\eta$ ,

**Require:** Initial parameter  $\theta$

Initialize gradient accumulation variable  $\mathbf{r} = \mathbf{0}$ ,

**while** Stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ .

    Set  $\mathbf{g} = \mathbf{0}$

**for**  $i = 1$  to  $m$  **do**

        Compute gradient:  $\mathbf{g} \leftarrow \mathbf{g} + \nabla_{\theta} L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

**end for**

    Accumulate gradient:  $\mathbf{r} \leftarrow \mathbf{r} + \mathbf{g}^2$  (square is applied element-wise)

    Compute update:  $\Delta\theta \leftarrow -\frac{\eta}{\sqrt{\mathbf{r}}} \mathbf{g}$ .   % ( $\frac{1}{\sqrt{r}}$  applied element-wise)

    Apply update:  $\theta \leftarrow \theta + \Delta\theta_t$

**end while**

---

# RMSprop (Hinton, 2012)

- Addresses the deficiency of AdaGrad by changing the gradient accumulation into an **exponentially** weighted moving average

---

## Algorithm 8.5 The RMSprop algorithm

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**Require:** Global learning rate  $\eta$ , decay rate  $\rho$ .

**Require:** Initial parameter  $\theta$

Initialize accumulation variables  $\mathbf{r} = \mathbf{0}$

**while** Stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ .

    Set  $\mathbf{g} = \mathbf{0}$

**for**  $i = 1$  to  $m$  **do**

        Compute gradient:  $\mathbf{g} \leftarrow \mathbf{g} + \nabla_{\theta} L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

**end for**

    Accumulate gradient:  $\mathbf{r} \leftarrow \rho \mathbf{r} + (1 - \rho) \mathbf{g}^2$

    Compute parameter update:  $\Delta \theta = -\frac{\eta}{\sqrt{\mathbf{r}}} \odot \mathbf{g}$ .   % ( $\frac{1}{\sqrt{\mathbf{r}}}$  applied element-wise)

    Apply update:  $\theta \leftarrow \theta + \Delta \theta$

**end while**

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## Algorithm 8.6 RMSprop algorithm with Nesterov momentum

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**Require:** Global learning rate  $\eta$ , decay rate  $\rho$ , momentum coefficient  $\alpha$ .

**Require:** Initial parameter  $\theta$ , initial velocity  $\mathbf{v}$ .

Initialize accumulation variable  $\mathbf{r} = \mathbf{0}$

**while** Stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ .

    Compute interim update:  $\theta \leftarrow \theta + \alpha \mathbf{v}$

    Set  $\mathbf{g} = \mathbf{0}$

**for**  $i = 1$  to  $m$  **do**

        Compute gradient:  $\mathbf{g} \leftarrow \mathbf{g} + \nabla_{\theta} L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

**end for**

    Accumulate gradient:  $\mathbf{r} \leftarrow \rho \mathbf{r} + (1 - \rho) \mathbf{g}^2$

    Compute velocity update:  $\mathbf{v} \leftarrow \alpha \mathbf{v} - \frac{\eta}{\sqrt{\mathbf{r}}} \odot \mathbf{g}$ .   % ( $\frac{1}{\sqrt{\mathbf{r}}}$  applied element-wise)

    Apply update:  $\theta \leftarrow \theta + \mathbf{v}$

**end while**

---

# Adam (Kingma and Ba, 2014)

- As a variant on RMSprop + momentum with a few important distinctions
  - Momentum is incorporated directly as an estimate of the first order moment (with exponential weighting) of the gradient
  - Adam includes bias corrections to the estimates of both the first-order moments (the momentum term) and the (uncentered) second order moments to account for their initialization at the origin

```
model.compile(loss='categorical_crossentropy',  
              optimizer='adam',  
              metrics=['accuracy'])
```

---

## Algorithm 8.7 The Adam algorithm

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**Require:** Step-size  $\alpha$

**Require:** Decay rates  $\rho_1$  and  $\rho_2$ , constant  $\epsilon$

**Require:** Initial parameter  $\theta$

Initialize 1st and 2nd moment variables  $\mathbf{s} = \mathbf{0}$ ,  $\mathbf{r} = \mathbf{0}$ ,

Initialize timestep  $t = 0$

**while** Stopping criterion not met **do**

Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ .

Set  $\mathbf{g} = \mathbf{0}$

**for**  $i = 1$  to  $m$  **do**

Compute gradient:  $\mathbf{g} \leftarrow \mathbf{g} + \nabla_{\theta} L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

**end for**

$t \leftarrow t + 1$

Get biased first moment:  $\mathbf{s} \leftarrow \rho_1 \mathbf{s} + (1 - \rho_1) \mathbf{g}$

Get biased second moment:  $\mathbf{r} \leftarrow \rho_2 \mathbf{r} + (1 - \rho_2) \mathbf{g}^2$

Compute bias-corrected first moment:  $\hat{\mathbf{s}} \leftarrow \frac{\mathbf{s}}{1 - \rho_1^t}$

Compute bias-corrected second moment:  $\hat{\mathbf{r}} \leftarrow \frac{\mathbf{r}}{1 - \rho_2^t}$

Compute update:  $\Delta \theta = -\alpha \frac{\hat{\mathbf{s}}}{\sqrt{\hat{\mathbf{r}} + \epsilon}}$  % (operations applied element-wise)

Apply update:  $\theta \leftarrow \theta + \Delta \theta$

**end while**

---

Acc: >98%

# AdaDelta

- Another recently introduced optimization algorithm that seeks to directly address problems with AdaGrad, while incorporating some second-order gradient information

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**Algorithm 8.8** The Adadelta algorithm

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**Require:** Decay rate  $\rho$ , constant  $\epsilon$

**Require:** Initial parameter  $\theta$

Initialize accumulation variables  $\mathbf{r} = \mathbf{0}$ ,  $\mathbf{s} = \mathbf{0}$ ,

**while** Stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ .

    Set  $\mathbf{g} = \mathbf{0}$

**for**  $i = 1$  to  $m$  **do**

        Compute gradient:  $\mathbf{g} \leftarrow \mathbf{g} + \nabla_{\theta} L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

**end for**

    Accumulate gradient:  $\mathbf{r} \leftarrow \rho \mathbf{r} + (1 - \rho) \mathbf{g}^2$

    Compute update:  $\Delta \theta = -\frac{\sqrt{\mathbf{s} + \epsilon}}{\sqrt{\mathbf{r} + \epsilon}} \mathbf{g}$    % (operations applied element-wise)

    Accumulate update:  $\mathbf{s} \leftarrow \rho \mathbf{s} + (1 - \rho) [\Delta \theta]^2$

    Apply update:  $\theta \leftarrow \theta + \Delta \theta$

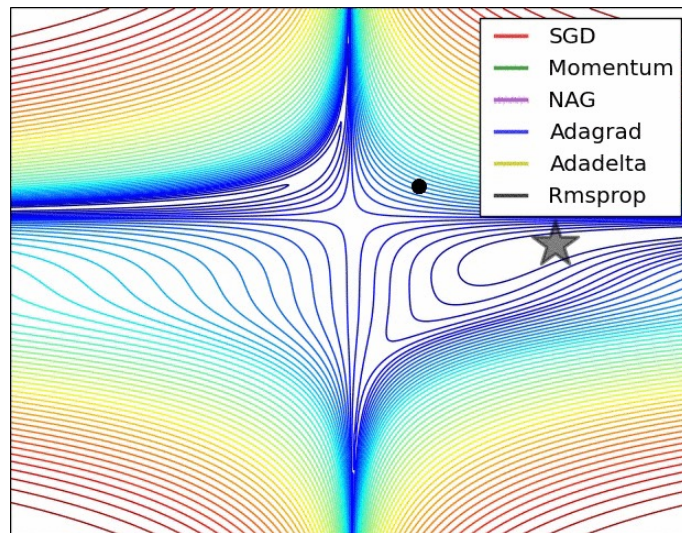
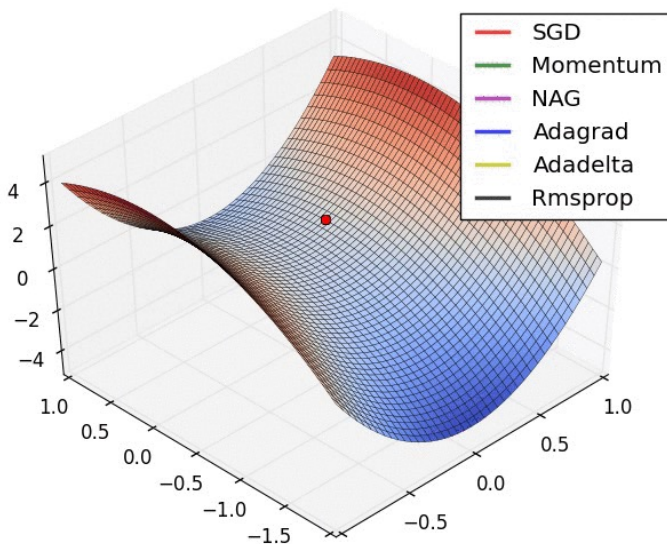
**end while**

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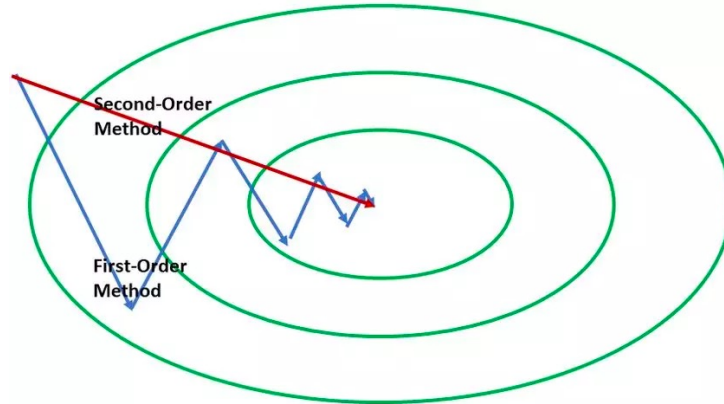
# Which algorithm should one choose?

- Unfortunately, there is currently no consensus
- Depend on the users familiarity with the algorithm (for ease of hyperparameter tuning)



# Approximate Second-Order Methods

- Newton's Method
- Conjugate Gradients
- BFGS (Broyden – Fletcher – Goldfarb – Shanno)
  - L-BFGS (Limited Memory BFGS)



# Optimization Strategies

- Batch Normalization
- Initialization Strategies
- Supervised Pretraining
- Designing Models to Aid Optimization

# Optimization Strategies

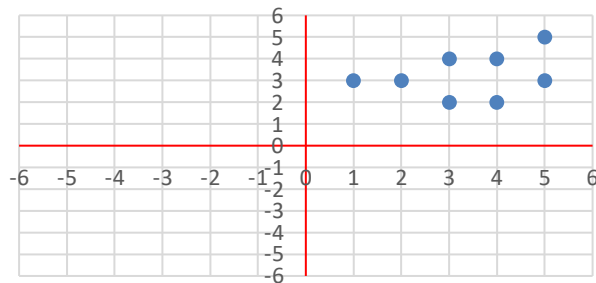
- Batch Normalization
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# Batch Normalization

- Sergey Ioffe, Christian Szegedy. Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift. International Conference on Machine Learning (ICML). 2015.
- One of the most exciting recent innovations in optimizing deep neural networks
  - Faster training
  - Better generalization

# Preprocess (Normalization)

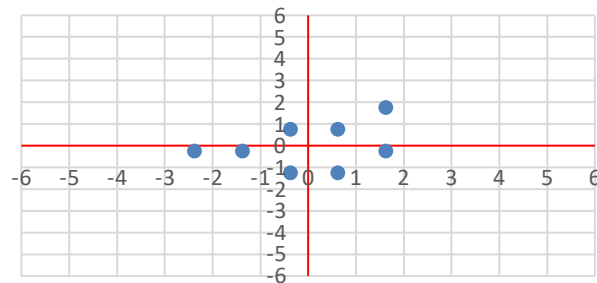
original



$$x' = x - E[x]$$

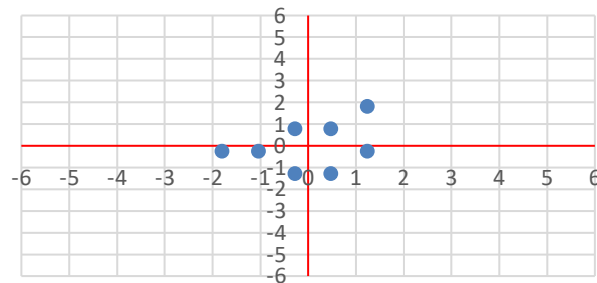


$x - E[x]$



$$x' = \frac{x - E[x]}{\sqrt{\text{Var}[x]}}$$

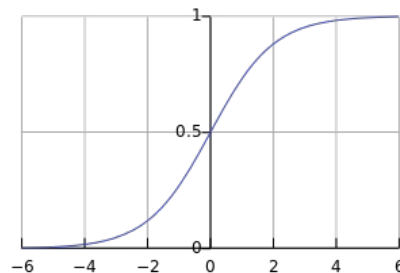
z-score



# Fixed Distribution

$$z = g(Wu + b)$$

$$g(x) = \frac{1}{1 + \exp(-x)} \quad x = Wu + b$$



- As  $|x|$  increase,  $g'(x)$  tends to zero
- Changes to those parameters  $W$  and  $b$  during training will likely move **many dimensions** of  $x$  into the **saturated regime** of the nonlinearity and **slow down the convergence**
- Solution: ReLU activation function
- Other: Ensure that the distribution of nonlinearity inputs **remains more stable**

# Batch Normalization

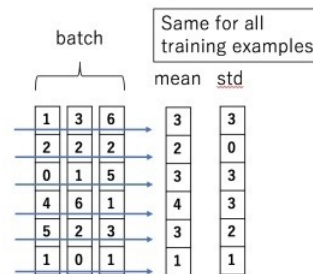
- $x^{(k)}$  represent a dimension of input
- **Simply normalizing** each input of a layer may change what the layer can represent
- $\gamma^{(k)}, \beta^{(k)}$  are learned along with the original model parameters, and **restore the representation power of the network**.

$$\hat{x}^{(k)} = \frac{x^{(k)} - E[x^{(k)}]}{\sqrt{\text{Var}[x^{(k)}]}}$$

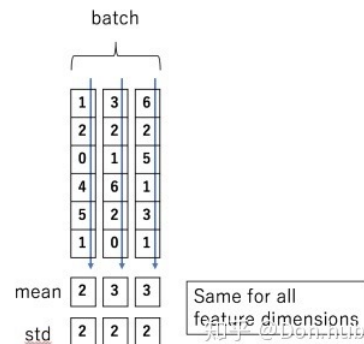
$$y^{(k)} = \gamma^{(k)} \hat{x}^{(k)} + \beta^{(k)}.$$

How to use BN at test time?

Batch Normalization



Layer Normalization





# Advantages

- Batch Normalization enables higher learning rates
- Batch Normalization makes training more resilient to the parameter scale
- Batch Normalization regularizes the model

```
model = keras.Sequential()  
# model.add(keras.layers.Dense(512, activation='relu', input_shape=(784,)))  
model.add(keras.layers.Dense(512, input_shape=(784,)))  
model.add(keras.layers.BatchNormalization())  
model.add(keras.layers.Activation('relu'))  
model.add(keras.layers.Dense(num_classes, activation='softmax'))
```

# Optimization Strategies

- Batch Normalization
- Initialization Strategies
- Supervised Pretraining
- Designing Models to Aid Optimization

# Initialization Strategies

- Most algorithms are strongly affected by the choice of initialization
- “break symmetry” → random initialization
- Too large or too small are both bad

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

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

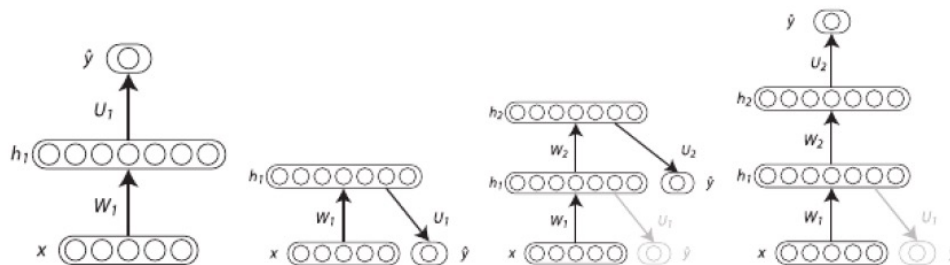
$$b^{[l]} = 0$$

Xavier initialization

# Optimization Strategies

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# Supervised Pretraining (Greedy Pretraining)



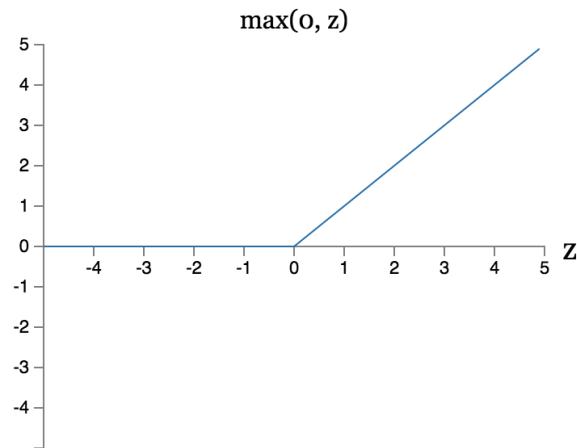
- Some related work
  - Transfer learning
  - *FitNets* (Romero *et al.* 2015)

# Optimization Strategies

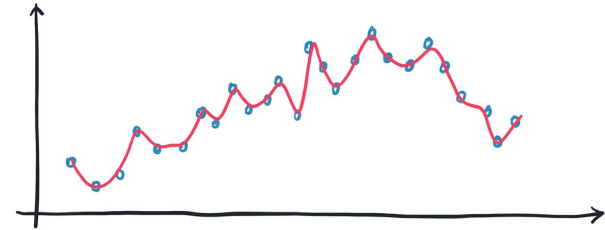
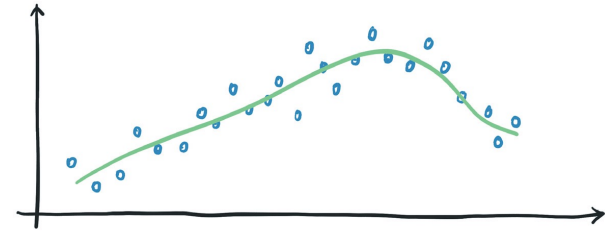
- Batch Normalization
- Initialization Strategies
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# Designing Models to Aid Optimization

- Designing models to be easier to optimize, rather than improve the optimization algorithm
- For example
  - LSTM, rectified linear units ( $\max(0, z)$ )
  - Linear paths or skip connections between layers (Srivastava *et al.* 2015)



# Regularization

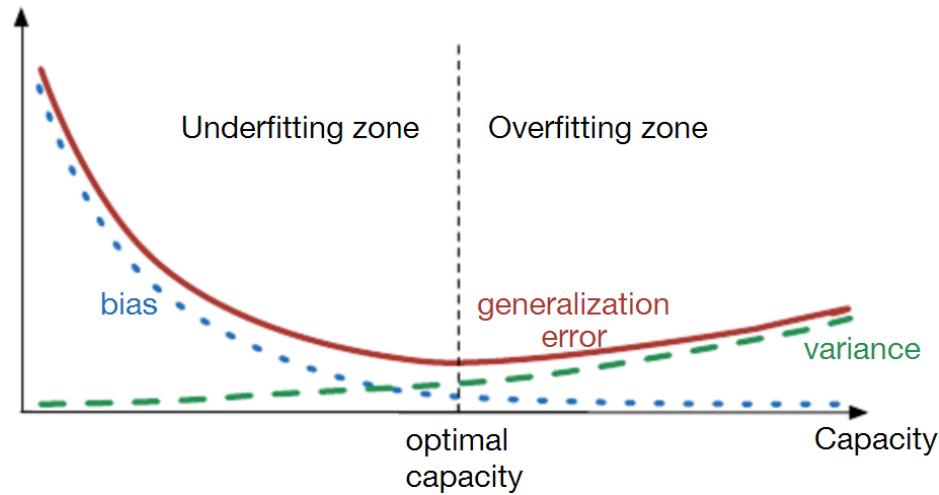




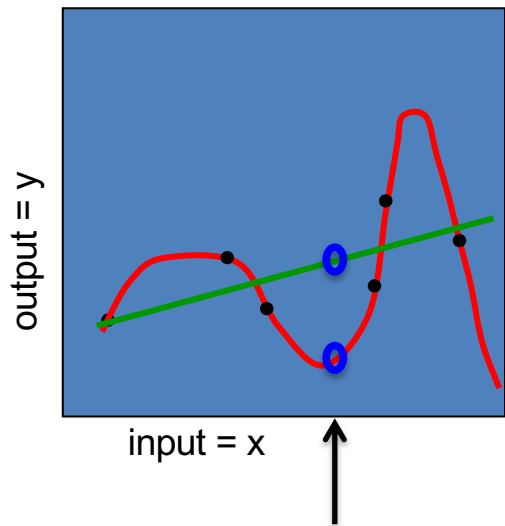
# General Purpose of Regularization

- Make machine learning algorithm not only perform well on training data, but also on new inputs. [**minimizing generalization error**]
- Regularization
  - strategies to **reduce test error**, possibly at expense of increase training error.
- Functions of regularization
  - encode specified knowledge
  - express a generic preference of simple model
  - (ensemble method) combine multiple hypotheses

# Generalization Error in Term of: Fitting Data Generation Process



# A Simple Example of Overfitting



Which output value should you predict for this test input?

- Which model do you trust?
  - The complicated model fits the data better.
  - But it is not economical.
- A model is convincing when it fits a lot of data surprisingly well.
  - It is not surprising that a complicated model can fit a small amount of data well.

# Examples of Regularization

General form

$$\tilde{J}(\theta) = J(\theta) + \alpha\Omega(\theta)$$

- Parameter norm penalty
  - $\tilde{J}(\theta) = J(\theta) + \alpha||w||^2$
- Entropy regularizer (Bengio 2005)
  - $\tilde{J}(\theta) = J(\theta) + \alpha H(z_i)$
- Generalized expectation (Mann and McCallum, 2008)
  - $\tilde{J}(\theta) = J(\theta) + \alpha KL(y||\hat{y})$

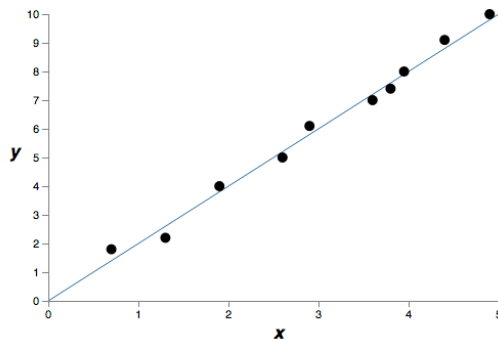
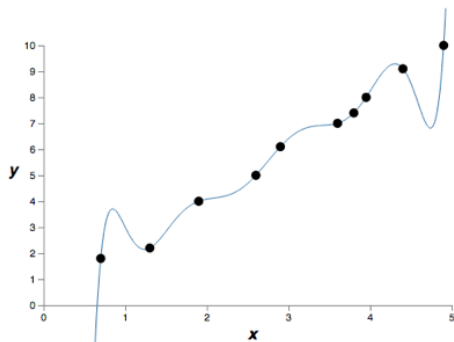
# Norm (范数) Penalty in Classical Perspective

- L2 regularizer:  $\Omega(\theta) = \frac{1}{2} \sum_i |\theta_i|^2$
- L1 regularizer:  $\Omega(\theta) = \sum_i |\theta_i|$

```
model = keras.Sequential()  
model.add(keras.layers.Dense(512, kernel_regularizer=keras.regularizers.l2(1e-4), activation='relu', input_shape=(784,)))  
model.add(keras.layers.Dense(num_classes, kernel_regularizer=keras.regularizers.l2(1e-4), activation='softmax'))
```

# Intuition 1 (on L2)

- L2 regularizer control  $\theta$  and penalize on large  $\theta$



## Intuition 2 (on L2): Single Update Step View

- gradient:

$$- \nabla_{\theta} \tilde{J}(\theta) = \nabla_{\theta} J(\theta) + \alpha \theta$$

- one gradient update

$$- \theta^{new} = \theta^{old} - \epsilon \left( \alpha \theta^{old} + \nabla_{\theta} J(\theta^{old}) \right)$$

- write it in other way

$$- \theta^{new} = (1 - \alpha\epsilon) \theta^{old} - \epsilon \nabla_{\theta} J(\theta^{old})$$

at each step, make  
 $\theta$  a little smaller

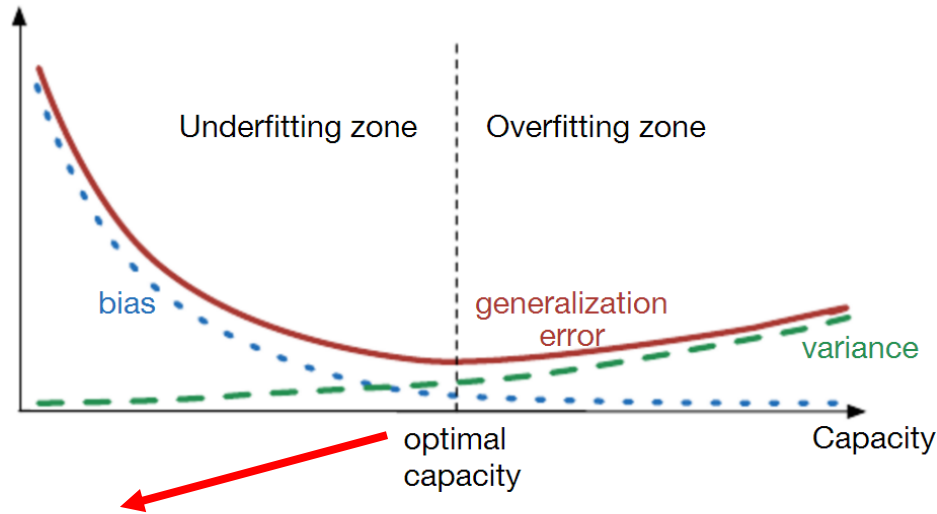
# Dataset Argument

- Improve generalization error in other way
  - feed more data
- However, lack data
- Solution1: making fake data
  - Can not distinguish between “b” and “d”
- Solution 2
  - Impose random noise to input data





# Early Stopping



Decide the best generalization error model by a validation set  
tune the hyperparameter of iteration number

# Early Stopping (cont.)

- Early stopping:
  - for iteration in max\_iteration:
    - learn model on training data
    - `valuate_score_of_current_model` = evaluate on validation data
    - if `valuate_score_of_current_model > best_validation_score`:
      - `best_validation_score = valuate_score_of_current_model`
      - save current model
      - **`patient = 0`**
    - **else: `patient += 1`**
    - **if `patient > max_patient`:**
      - **`break`**

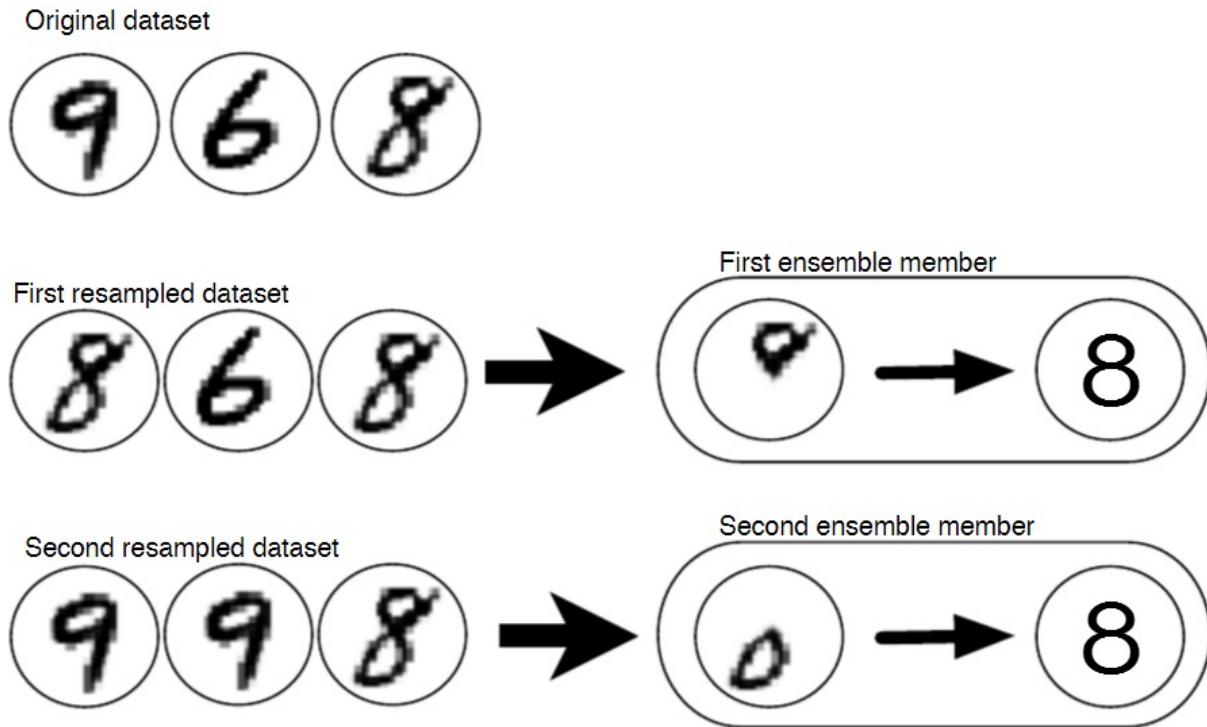
## Early Stopping (cont.)

- To make use of the validation set
  - Second pass training
    - tune the best iteration *BEST*
    - train on the merge of {train, validation} set with *BEST* iteration.
  - Continuous training
    - continue training on the merge of {train, validation}
    - stop when  $\mathcal{J}$  on validation set reach a small value

## Bagging in Practice (9-fold)

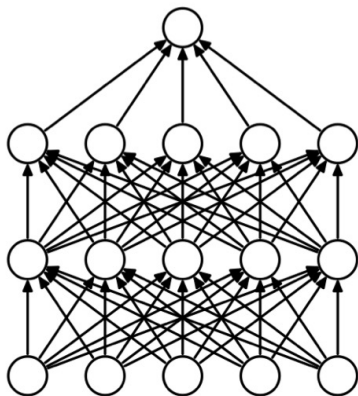
- Considering a binary classification problem on training set  $D$ .
- We randomly sample 9 subsets:  $\{D_1, D_2, \dots, D_9\}$ 
  - maybe  $|D_i| = 0.63|D|$
- Obtain 9 models on different subset:  $\{M_1, M_2, \dots, M_9\}$
- On test phase, these 9 models give 9 results:
  - if 5 or more positive, we got positive
  - otherwise, negative

# Cartoon Depiction of How Bagging Works

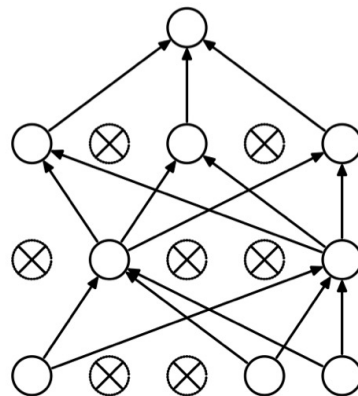


# Dropout

- Hinton et al. 2012
- Proved a powerful tool for training neural network
- Description: during learning phase, for an input  $v \in \mathbb{R}^n$ , randomly generate a vector  $d \in \mathbb{R}^n$ , where  $d_i = 0$  if  $\text{rand}() < \text{threshold}$



(a) Standard Neural Net



(b) After applying dropout.

# Dropout as Bagging

- Dropout like bagging
  - many different models are trained on different subsets of the data
- Dropout dislike bagging
  - each model is trained for only one step and all of the models share parameters

```
model = keras.Sequential()  
# model.add(keras.layers.Dense(512, activation='relu', input_shape=(784,)))  
model.add(keras.layers.Dense(512, input_shape=(784,)))  
model.add(keras.layers.BatchNormalization())  
model.add(keras.layers.Activation('relu'))  
model.add(keras.layers.Dropout(0.2))  
model.add(keras.layers.Dense(num_classes, activation='softmax'))
```

# How to Choose Hyper-parameters?

1. Reducing the size of training data and network structure to get rapid insight
2. Repeatedly tuning one of hyper-parameters to get better results
  - Learning rate
  - Regularization parameter
  - Mini-batch size
  - .....
3. More training data and complicated network structure, goto 2
  - More of an art than a science
  - Automated techniques: grid search



# Summary

- Optimization
  - SGD → Momentum → Nesterov Momentum
  - AdaGrad → RMSprop → Adam → AdaDelta
  - Other optimization strategies
- Regularization
  - L1/L2, Early stopping, Dropout