Deep Learning Crash Course

Hui Xue

Fall 2021

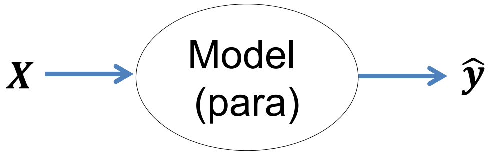
www.deeplearningcrashcourse.org

Outline

- **Loss function for classification**
- Gradient descent
- Bias and variance

How do we know a model is good?

Given a model and its parameters, how do we know this model gives correct prediction?



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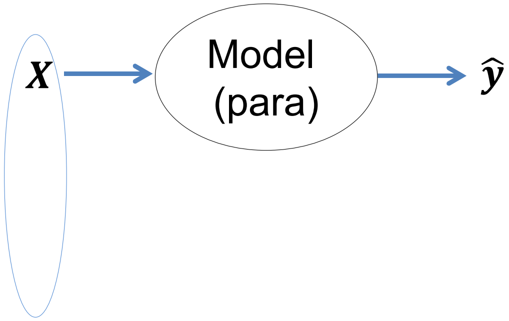

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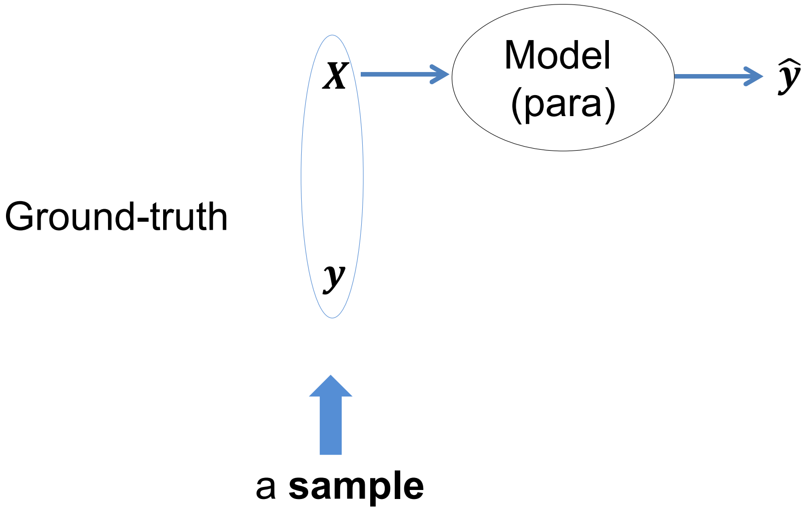

$\{\boldsymbol{X}^{(i)}, \boldsymbol{y}^{(i)}\}$

the i-th sample

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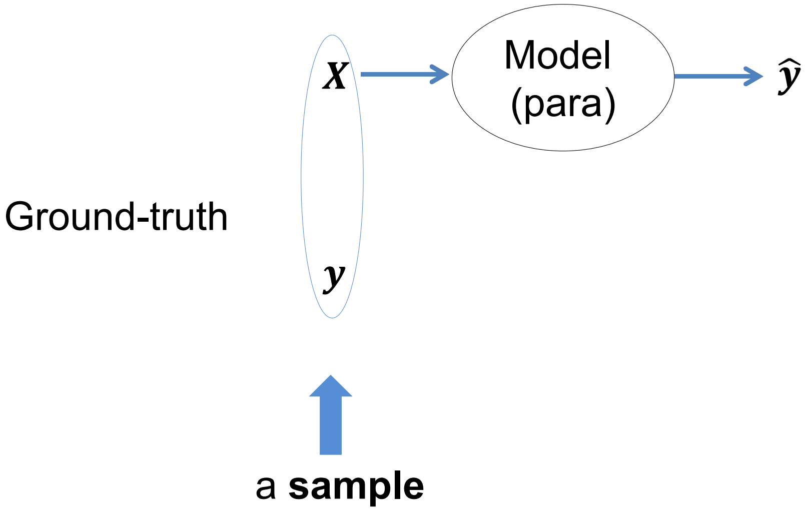

$\boldsymbol{X}$ → Model (para) → $\hat{\boldsymbol{y}}$

Ground-truth

$\boldsymbol{y}$

a **sample**

$\{\boldsymbol{X}^{(i)}, \boldsymbol{y}^{(i)}\}$

the i-th sample

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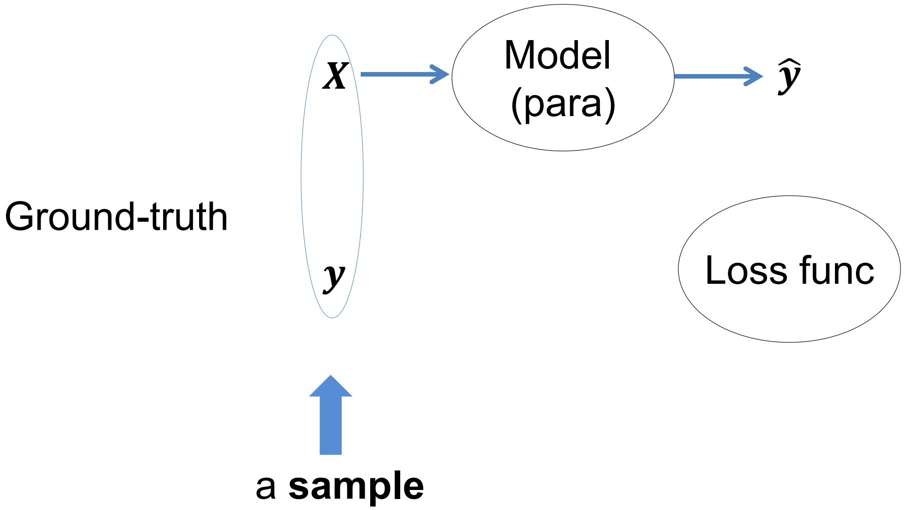

Ground-truth

$\boldsymbol{X}$

$\boldsymbol{y}$

Model (para)

$\hat{\boldsymbol{y}}$

Loss func

a **sample**

$\{\boldsymbol{X}^{(i)}, \boldsymbol{y}^{(i)}\}$

the i-th sample

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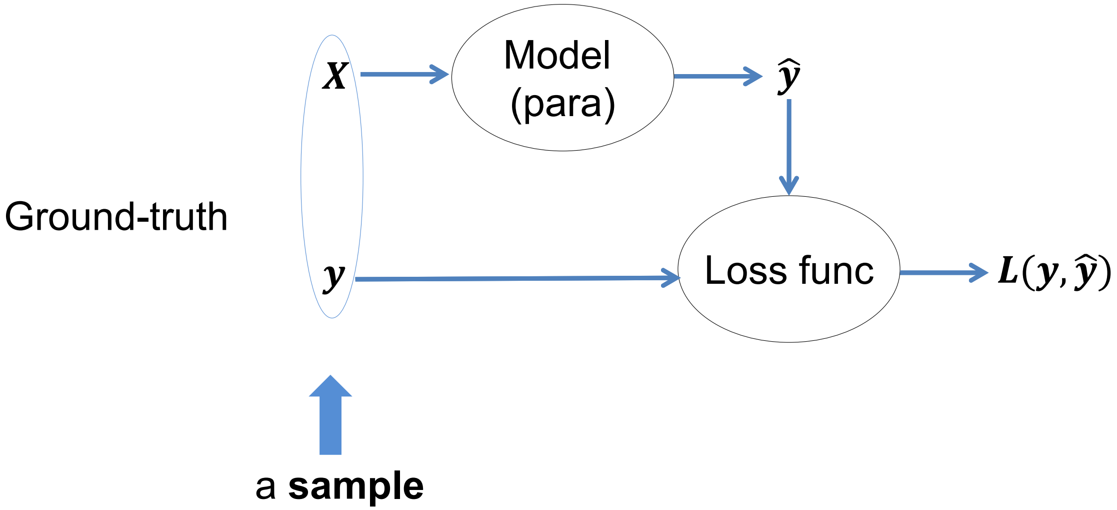


$\{\boldsymbol{X}^{(i)}, \boldsymbol{y}^{(i)}\}$

the i-th sample

Cross-entropy

Given two probability distribution p and q, p is the target distribution and p is the model predicted distribution:

$$\boldsymbol{H(p,q) = -\sum_{for\ all\ possible\ x} p(x) log[q(x;\theta)]}$$

- Measure how close two distributions are (not 100% rigorous)
- Minimized if p=q

$$\boldsymbol{H(p,q) = H(p) + D_{KL}(p \parallel q)}$$

$\boldsymbol{D_{KL}(p \parallel q)}$ is the KL divergence of p and q.

$$\boldsymbol{D_{KL}(p \parallel q) \geq 0}$$

$\boldsymbol{D_{KL}(p \parallel q) = 0}$ if and only if p=q

$\boldsymbol{H(p)}$ is the entropy of distribution p

$$\boldsymbol{H(p,q) \neq H(q,p)}$$

$$\begin{aligned}
\boldsymbol{H(p,q)} &= -\sum_{\boldsymbol{x}} \boldsymbol{p(x)} \log[\boldsymbol{q(x)}] \\
&= -\sum_{\boldsymbol{x}} \boldsymbol{p(x)} \log\left[\frac{\boldsymbol{p(x)}}{\boldsymbol{p(x)}}\boldsymbol{q(x)}\right] \\
&= -\sum_{\boldsymbol{x}} \boldsymbol{p(x)} \left\{\log[\boldsymbol{p(x)}] + \log\left[\frac{\boldsymbol{q(x)}}{\boldsymbol{p(x)}}\right]\right\} \\
&= -\sum_{\boldsymbol{x}} \boldsymbol{p(x)} \log[\boldsymbol{p(x)}] - \sum_{\boldsymbol{x}} \boldsymbol{p(x)} \log\left[\frac{\boldsymbol{q(x)}}{\boldsymbol{p(x)}}\right] \\
&= \underbrace{-\sum_{\boldsymbol{x}} \boldsymbol{p(x)} \log[\boldsymbol{p(x)}]}_{\boldsymbol{H(p)}} + \underbrace{\sum_{\boldsymbol{x}} \boldsymbol{p(x)} \log\left[\frac{\boldsymbol{p(x)}}{\boldsymbol{q(x)}}\right]}_{\boldsymbol{D_{KL}(p \parallel q)}}
\end{aligned}$$

Entropy of distribution p

Binary Cross-entropy loss

For the binary classification,

$\boldsymbol{y}$ = 1 for the "Yes" class and 0 for the "No" class

$\widehat{\boldsymbol{y}}$ $\in [\mathbf{0}, \mathbf{1}]$, probability belonging to the "Yes" class
$\mathbf{1} - \widehat{\boldsymbol{y}}$ for the "No" class

Then, the cross entropy (in this case, the BCE loss) is:

$$\boldsymbol{L_{BCE\_loss}}(\boldsymbol{y}, \widehat{\boldsymbol{y}}) = -[\boldsymbol{y} \cdot \boldsymbol{log}(\widehat{\boldsymbol{y}}) + (\mathbf{1} - \boldsymbol{y}) \cdot \boldsymbol{log}(\mathbf{1} - \widehat{\boldsymbol{y}})]$$

To minimize the BCE loss,

if $\boldsymbol{y} = \mathbf{0}$, $\widehat{\boldsymbol{y}} = \mathbf{0}$ will reach minimum of log(1)=0

if $\boldsymbol{y}$ =1, $\widehat{\boldsymbol{y}} = \mathbf{1}$ will reach minimum of log(1)=0

For all other cases, $\boldsymbol{L_{BCE\_loss}}$ > 0

Cross-entropy loss for multi-class

For the multi-class classification,

$$\boldsymbol{y} = \left\{ \begin{array}{llllll} \boldsymbol{CH3}, & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \boldsymbol{CH2}, & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \boldsymbol{CH4}, & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \boldsymbol{SAX}, & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} & \mathbf{0} \\ \boldsymbol{Other}, & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{1} \end{array} \right.$$

y is one-hot encoding for the correct class

$$y_k = \begin{cases} CH3, 0 \\ CH2, 1 \\ CH4, 2 \\ SAX, 3 \\ Other, 4 \end{cases}$$

y_k is the index of correct class for sample $\boldsymbol{y}$

$\hat{\boldsymbol{y}}$ is a [K,1] vector for the probability of X belonging to each lass

$\hat{\boldsymbol{y}}[0]$ is a scalar to predict X being CH3
$\hat{\boldsymbol{y}}[1]$ is a scalar to predict X being CH2
$\hat{\boldsymbol{y}}[2]$ is a scalar to predict X being CH4
… …

$\hat{\boldsymbol{y}}[y_k]$ is a scalar to predict X being class y_k

Cross-entropy loss

For the multi-class classification,

$$\boldsymbol{L_{CE\_loss}}(\boldsymbol{y},\hat{\boldsymbol{y}}) = -\sum_{\boldsymbol{k=0}}^{\boldsymbol{4}} \boldsymbol{y}[k]\,\boldsymbol{log}(\hat{\boldsymbol{y}}[k])$$

$\hat{\boldsymbol{y}}$ is a [K,1] vector for the probability of X being each lass

$\hat{\boldsymbol{y}}[y_k]$ is a scalar to predict X being class y_k

y_k is the index of correct class for sample $\boldsymbol{y}$

y is one-hot encoding for the correct class

$$\boldsymbol{L_{CE\_loss}}(\boldsymbol{y},\hat{\boldsymbol{y}}) = -\boldsymbol{log}(\hat{\boldsymbol{y}}[y_k])$$

Only one term left!

To minimize the cross-entropy loss,

We need $\hat{\boldsymbol{y}}[y_k] = \mathbf{1}$; for all other cases, $\boldsymbol{L_{CE\_loss}} > 0$

Cross-entropy loss

	$\boldsymbol{y}$	$\hat{\boldsymbol{y}}$
CH2	0	0.2
CH3	0	0.3
CH4	1	0.1
SAX	0	0.15
Other	0	0.25

$$\boldsymbol{L_{CE\_loss}}(\boldsymbol{y}, \hat{\boldsymbol{y}}) = -\sum_{\boldsymbol{k=0}}^{\boldsymbol{4}} \boldsymbol{y}[k]\, \boldsymbol{log}(\hat{\boldsymbol{y}}[k])$$
$$= -[0 \times \log(0.2)$$
$$+0 \times \log(0.3)$$
$$+1 \times \log(0.1)$$
$$+0 \times \log(0.15)$$
$$+0 \times \log(0.25)]$$
$$= -\log(0.1) = 2.3$$

Cross-entropy loss

	$\boldsymbol{y}$	$\boldsymbol{\hat{y}}$
CH2	0	0.02
CH3	0	0.1
CH4	1	0.8
SAX	0	0.05
Other	0	0.03

$$\boldsymbol{L_{CE\_loss}}(\boldsymbol{y}, \boldsymbol{\hat{y}}) = -\sum_{\boldsymbol{k=0}}^{\boldsymbol{4}} \boldsymbol{y}[k]\, \boldsymbol{log}(\boldsymbol{\hat{y}}[k])$$

$$= -[0 \times \log(0.02)$$

$$+0 \times \log(0.1)$$

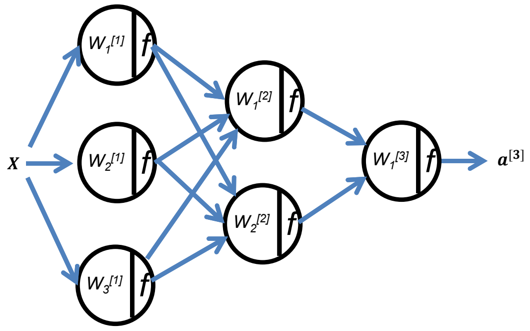
$$+1 \times \log(0.8)$$

$$+0 \times \log(0.05)$$

$$+0 \times \log(0.03)]$$

$$= -\log(0.8) = 0.22$$

Where we are



$$\boldsymbol{Z}^{[1]} = \boldsymbol{W}^{[1]}\boldsymbol{X} + \boldsymbol{b}^{[1]}$$

$$\boldsymbol{a}^{[1]} = \boldsymbol{f}(\boldsymbol{Z}^{[1]})$$

$$\boldsymbol{Z}^{[2]} = \boldsymbol{W}^{[2]}\boldsymbol{a}^{[1]} + \boldsymbol{b}^{[2]}$$

$$\boldsymbol{a}^{[2]} = \boldsymbol{f}(\boldsymbol{Z}^{[2]})$$

$$\boldsymbol{Z}^{[3]} = \boldsymbol{W}^{[3]}\boldsymbol{a}^{[2]} + \boldsymbol{b}^{[3]}$$

$$\hat{\boldsymbol{y}} = \boldsymbol{a}^{[3]} = \boldsymbol{f}(\boldsymbol{Z}^{[3]})$$

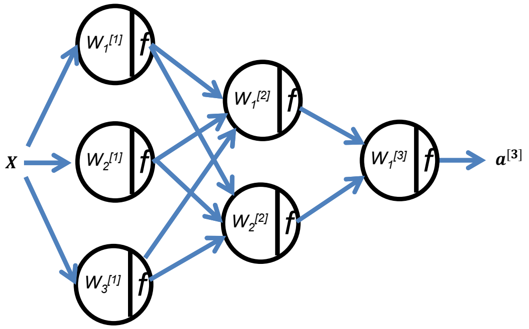
$$\boldsymbol{L}_{\boldsymbol{BCE\_loss}}(\boldsymbol{y}, \hat{\boldsymbol{y}})$$

$$\boldsymbol{L}_{\boldsymbol{CE\_loss}}(\boldsymbol{y}, \hat{\boldsymbol{y}})$$

Model : map input to output

Loss : measure how good the output is, compared to the label

How do we determine the model parameters?

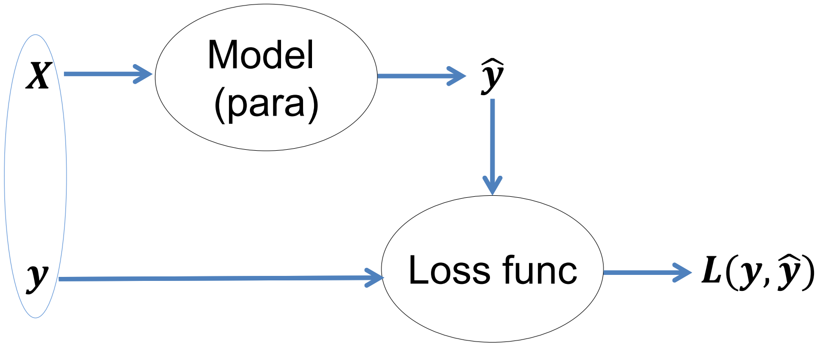


$\boldsymbol{W}^{[1]}, \boldsymbol{b}^{[1]}$

$\boldsymbol{W}^{[2]}, \boldsymbol{b}^{[2]}$

$\boldsymbol{W}^{[3]}, \boldsymbol{b}^{[3]}$

Model : map input to output



$\boldsymbol{X}$

Model (para)

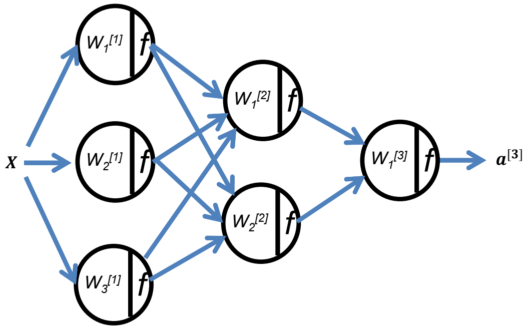
$\hat{\boldsymbol{y}}$

$\boldsymbol{y}$

Loss func

$\boldsymbol{L}(\boldsymbol{y}, \hat{\boldsymbol{y}})$

How do we determine the model parameters?

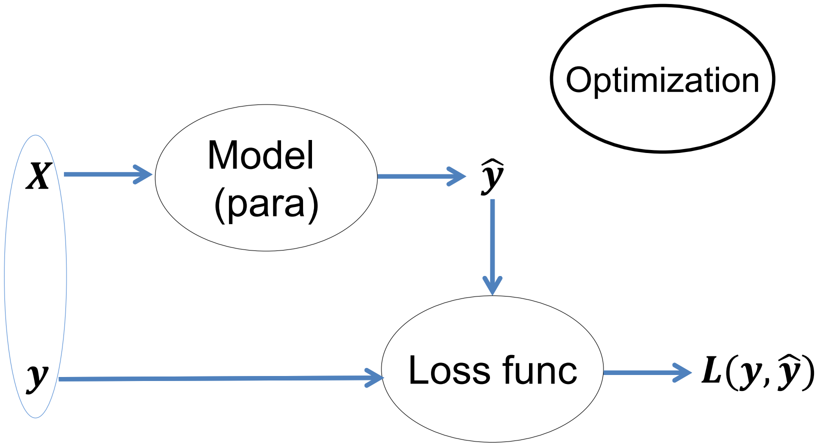


$\boldsymbol{W}^{[1]}, \boldsymbol{b}^{[1]}$

$\boldsymbol{W}^{[2]}, \boldsymbol{b}^{[2]}$

$\boldsymbol{W}^{[3]}, \boldsymbol{b}^{[3]}$

Model : map input to output



Optimization

$\boldsymbol{X}$

Model (para)

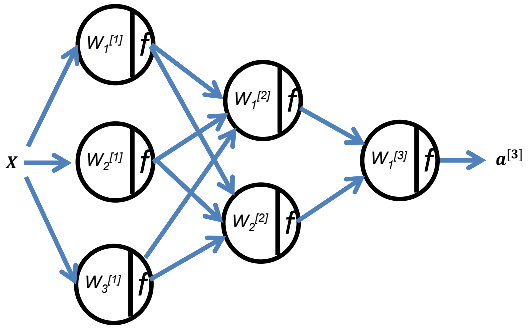
$\hat{\boldsymbol{y}}$

$\boldsymbol{y}$

Loss func

$\boldsymbol{L}(\boldsymbol{y}, \hat{\boldsymbol{y}})$

How do we determine the model parameters?

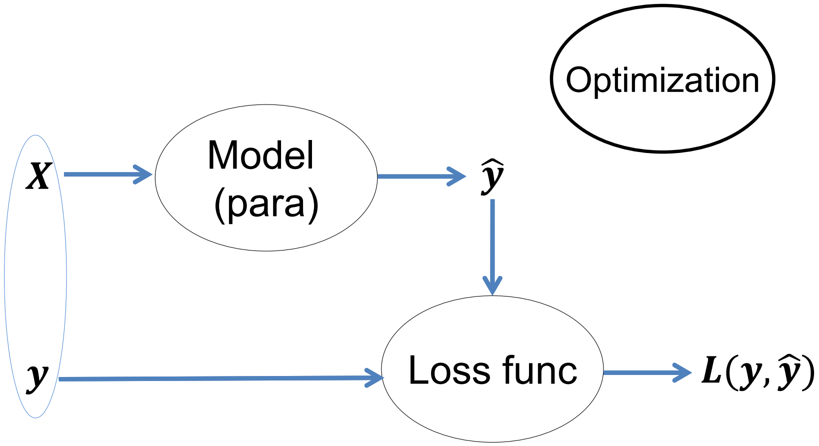


$\boldsymbol{W}^{[1]}, \boldsymbol{b}^{[1]}$

$\boldsymbol{W}^{[2]}, \boldsymbol{b}^{[2]}$

$\boldsymbol{W}^{[3]}, \boldsymbol{b}^{[3]}$

Model : map input to output



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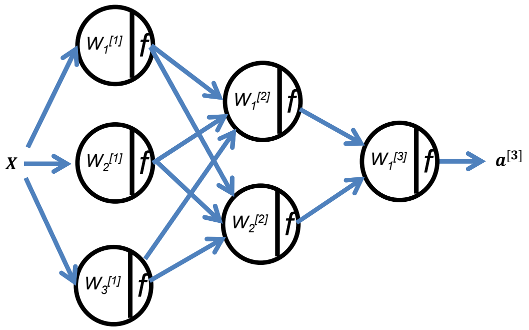
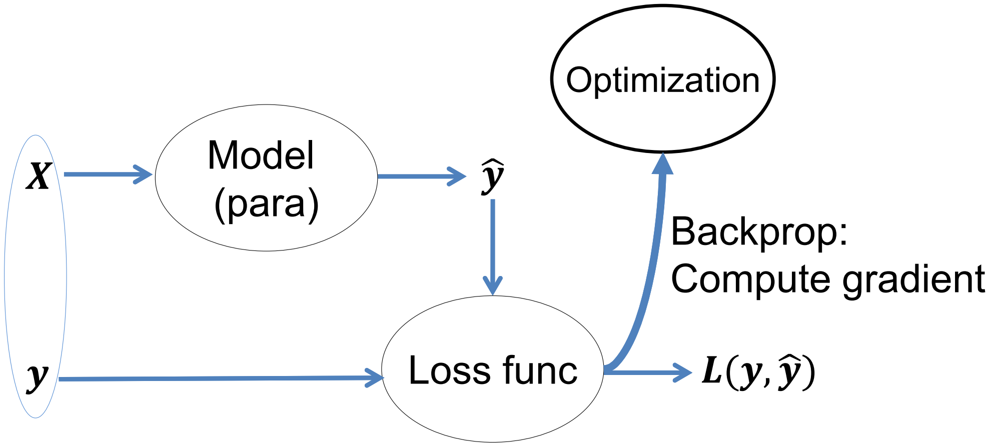


$\boldsymbol{W}^{[1]}, \boldsymbol{b}^{[1]}$

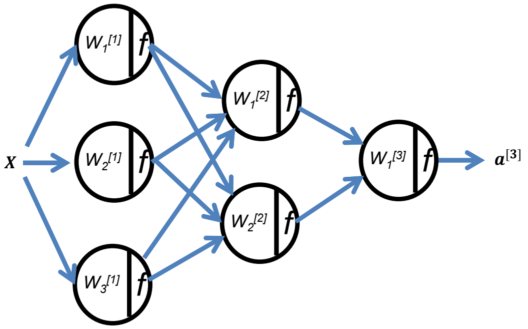
$\boldsymbol{W}^{[2]}, \boldsymbol{b}^{[2]}$

$\boldsymbol{W}^{[3]}, \boldsymbol{b}^{[3]}$



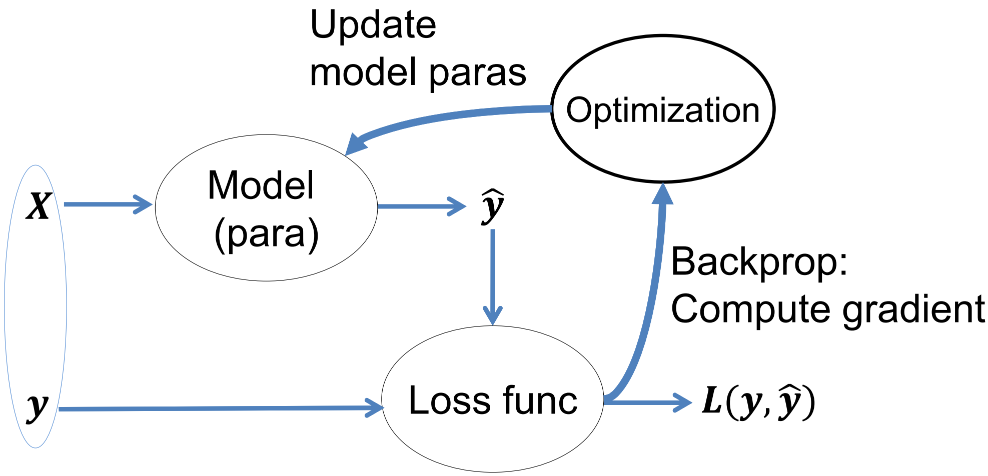
Model : map input to output

How do we determine the model parameters?

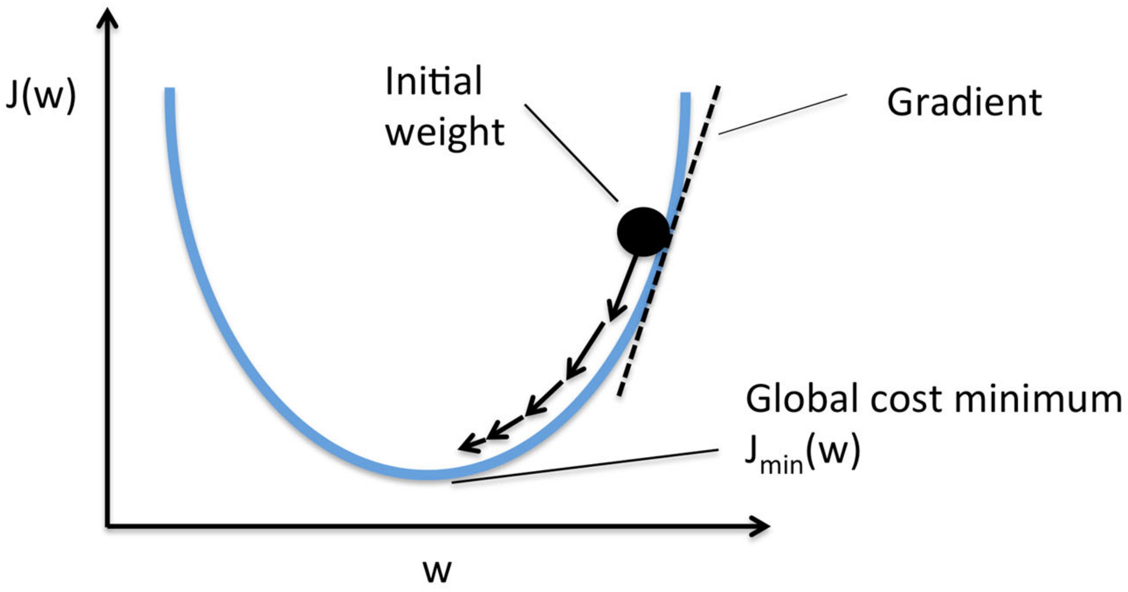


$$\boldsymbol{W}^{[1]}, \boldsymbol{b}^{[1]}$$
$$\boldsymbol{W}^{[2]}, \boldsymbol{b}^{[2]}$$
$$\boldsymbol{W}^{[3]}, \boldsymbol{b}^{[3]}$$

Model : map input to output



Gradient descent



To fine minimal point of a function

- Start from an initial point
- Follow the negative gradient direction

https://www.quora.com/Whats-the-difference-between-gradient-descent-and-stochastic-gradient-descent

Gradient of a function

Gradient of a function indicates the steepest direction to **increase** this function in a neighborhood.
Negative gradient of a function indicates the steepest direction to **decrease** this function in a neighborhood.

f is a scalar function.

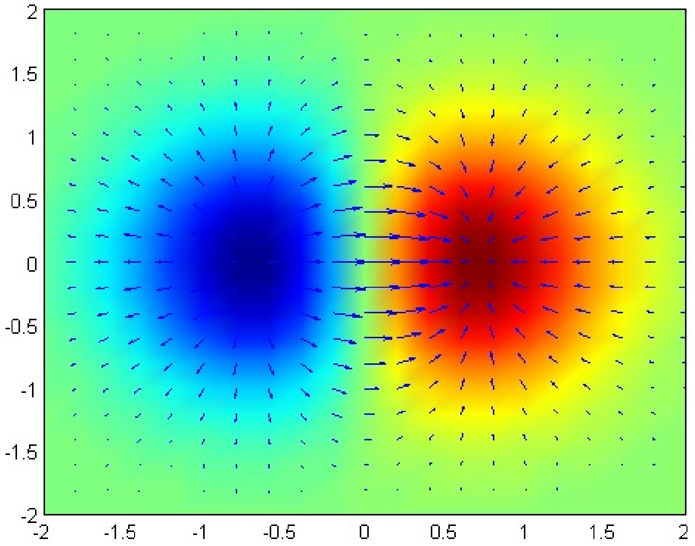
In 1-dimension, the derivative of a function:

$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

$$\nabla f(\boldsymbol{p}) = \begin{bmatrix} \frac{\partial f}{\partial x_0} \\ \frac{\partial f}{\partial x_1} \\ \cdots \\ \frac{\partial f}{\partial x_{N-1}} \end{bmatrix}$$

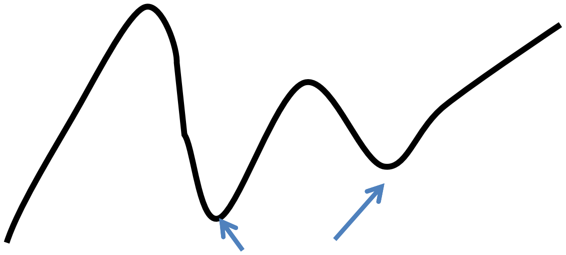
- $\boldsymbol{p} = [\boldsymbol{x_0}, \boldsymbol{x_1}, \boldsymbol{x_2}, \ldots, \boldsymbol{x_{N-1}}]^{\boldsymbol{T}}$
is a point in N-dimensional space

- $\nabla f(\boldsymbol{p})$ is the gradient at point $\boldsymbol{p}$.
- Its direction points to the steepest slope to increase the function.
- The steepness of the slope at that point is given by the $|\nabla f(\boldsymbol{p})|$



https://en.wikipedia.org/wiki/Gradient#/media/File:Gradient_of_a_Function.tif

Gradient descent



local minima

Gradient direction
is
the steepest direction to **increase** this function

We want to minimize the loss $\boldsymbol{L}(\boldsymbol{y}, \hat{\boldsymbol{y}}(\boldsymbol{W}, \boldsymbol{b}))$ by adjusting the model parameters

For every layer l :

$$\boldsymbol{W}^{[l]} = \boldsymbol{W}^{[l]} - \alpha \frac{\partial \boldsymbol{L}(\boldsymbol{y}, \hat{\boldsymbol{y}}(\boldsymbol{W}, \boldsymbol{b}))}{\partial \boldsymbol{W}^{[l]}}$$

$$\boldsymbol{b}^{[l]} = \boldsymbol{b}^{[l]} - \alpha \frac{\partial \boldsymbol{L}(\boldsymbol{y}, \hat{\boldsymbol{y}}(\boldsymbol{W}, \boldsymbol{b}))}{\partial \boldsymbol{b}^{[l]}}$$

α : **learning rate**

Guarantee to find a local minima

Gradient Descent (GD) over a set of samples

We have M samples

Empirical loss on measured data = $\frac{1}{M}\sum_{i=0}^{M-1} L(\boldsymbol{y}^{(\boldsymbol{i})}, \widehat{\boldsymbol{y}}^{(\boldsymbol{i})}(\boldsymbol{W}, \boldsymbol{b}))$

$$\frac{\partial \boldsymbol{L}(\boldsymbol{y}, \widehat{\boldsymbol{y}}(\boldsymbol{W}, \boldsymbol{b}))}{\partial \boldsymbol{W}^{[l]}} = \frac{1}{M}\sum_{i=0}^{M-1} \frac{\boldsymbol{\partial} L(\boldsymbol{y}^{(\boldsymbol{i})}, \widehat{\boldsymbol{y}}^{(\boldsymbol{i})}(\boldsymbol{W}, \boldsymbol{b}))}{\partial \boldsymbol{W}^{[l]}}$$

Find best parameters to minimize the mean loss across all training samples

$$\frac{\partial \boldsymbol{L}(\boldsymbol{y}, \widehat{\boldsymbol{y}}(\boldsymbol{W}, \boldsymbol{b}))}{\partial \boldsymbol{b}^{[l]}} = \frac{1}{M}\sum_{i=0}^{M-1} \frac{\boldsymbol{\partial} L(\boldsymbol{y}^{(\boldsymbol{i})}, \widehat{\boldsymbol{y}}^{(\boldsymbol{i})}(\boldsymbol{W}, \boldsymbol{b}))}{\partial \boldsymbol{b}^{[l]}}$$

Gradient descent

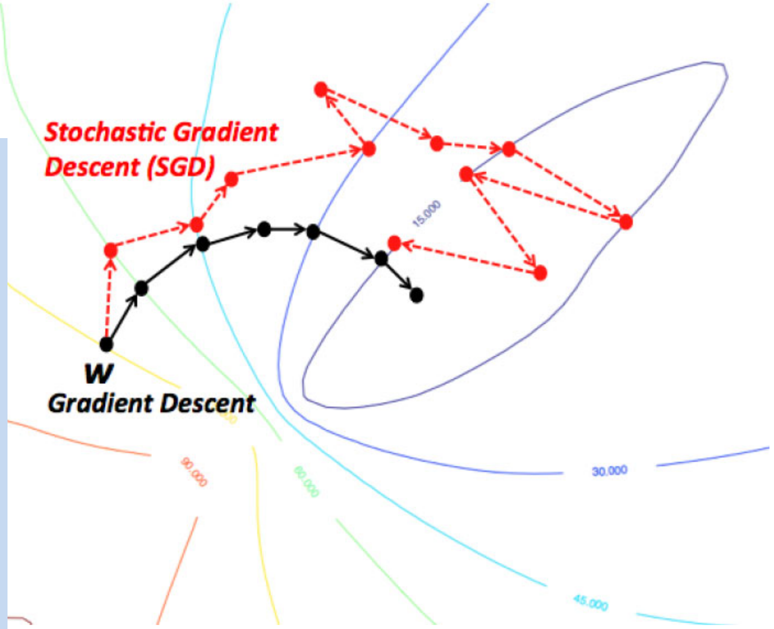
```
Initialize weights and bias

for iter in range(t):

    Evaluate loss function (forward pass) over all samples
        $L = \frac{1}{M}\sum_{i=0}^{M-1} L(\boldsymbol{y}^{(\boldsymbol{i})}, \hat{\boldsymbol{y}}^{(\boldsymbol{i})}(\boldsymbol{W}, \boldsymbol{b}))$

    Compute gradient
        $\frac{\partial L}{\partial \boldsymbol{W}^{[l]}}, \frac{\partial L}{\partial \boldsymbol{b}^{[l]}}$

    Update parameter
        $\boldsymbol{W}^{[l]} = \boldsymbol{W}^{[l]} - \alpha \frac{\partial L}{\partial \boldsymbol{W}^{[l]}}$
        $\boldsymbol{b}^{[l]} = \boldsymbol{b}^{[l]} - \alpha \frac{\partial L}{\partial \boldsymbol{b}^{[l]}}$
```

Stochastic Gradient Descent (SGD)

GD performs one parameter update step after going through entire training set

→Slow if M is large
→Gradient update may lack “exploration”

```
Initialize weights and bias
Random shuffle dataset
for epoch in range(E):
    select one sample with index $i$
    Evaluate loss function (forward pass) at this sample
        $L = L(\boldsymbol{y}^{(i)}, \hat{\boldsymbol{y}}^{(i)}(\boldsymbol{W}, \boldsymbol{b}))$
    Compute gradient $\frac{\partial L}{\partial \boldsymbol{W}^{[l]}}, \frac{\partial L}{\partial \boldsymbol{b}^{[l]}}$
    Update parameter $\boldsymbol{W}^{[l]} = \boldsymbol{W}^{[l]} - \alpha \frac{\partial L}{\partial \boldsymbol{W}^{[l]}}$, $\boldsymbol{b}^{[l]} = \boldsymbol{b}^{[l]} - \alpha \frac{\partial L}{\partial \boldsymbol{b}^{[l]}}$
```



https://data-notes.co/the-10-deep-learning-methods-ai-practitioners-need-to-apply-885259f402c1

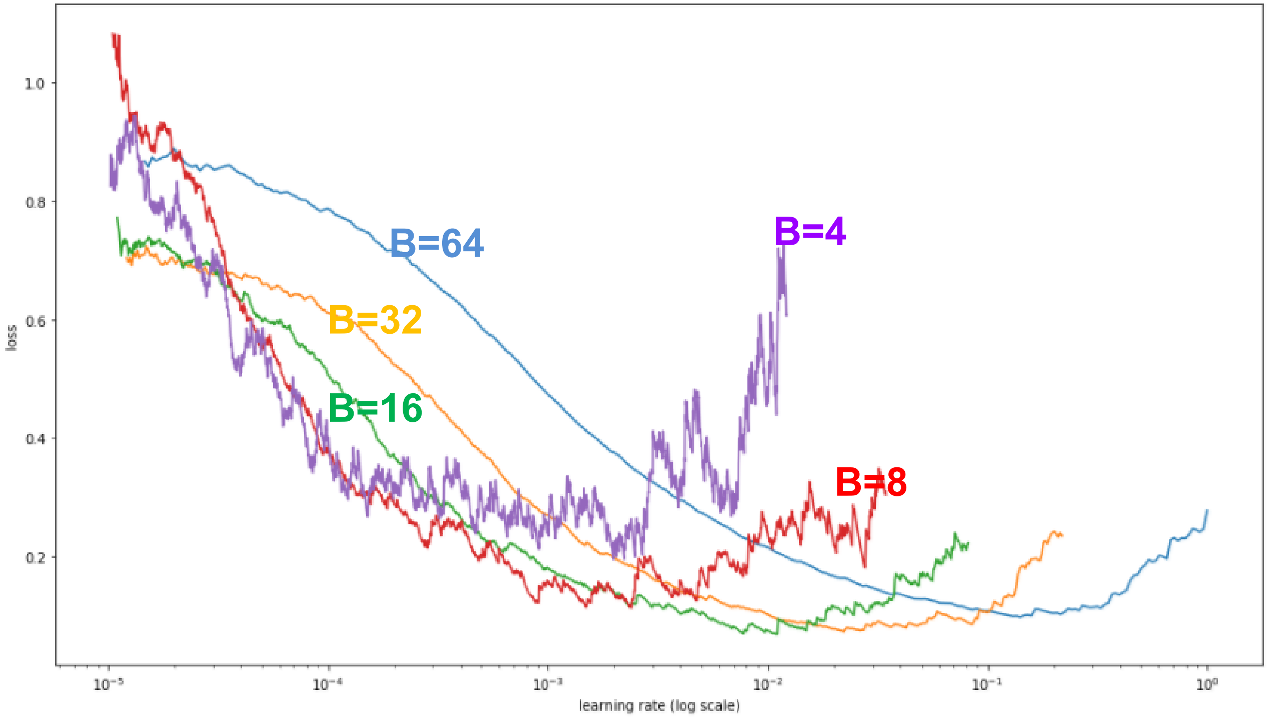
Mini-Batch SGD

SGD can have too much “noise” during convergence
Not fully utilize the computing hardware

```
Initialize weights and bias

Random shuffle dataset

BatchSize = 32

for epoch in range(E):

    select #BatchSize samples

    Evaluate loss function (forward pass) at this ~~sample~~ batch
        $L = \frac{1}{B}\sum_{i=0}^{B-1} L(\boldsymbol{y}^{(i)}, \hat{\boldsymbol{y}}^{(i)}(\boldsymbol{W}, \boldsymbol{b}))$

    Compute gradient $\frac{\partial L}{\partial \boldsymbol{W}^{[l]}}, \frac{\partial L}{\partial \boldsymbol{b}^{[l]}}$

    Update parameter $\boldsymbol{W}^{[l]} = \boldsymbol{W}^{[l]} - \alpha \frac{\partial L}{\partial \boldsymbol{W}^{[l]}}, \ \boldsymbol{b}^{[l]} = \boldsymbol{b}^{[l]} - \alpha \frac{\partial L}{\partial \boldsymbol{b}^{[l]}}$
```

- Batch size often is limited by the GPU RAM
- Different way to select a batch, e.g. sequential, random, fixed step size etc.

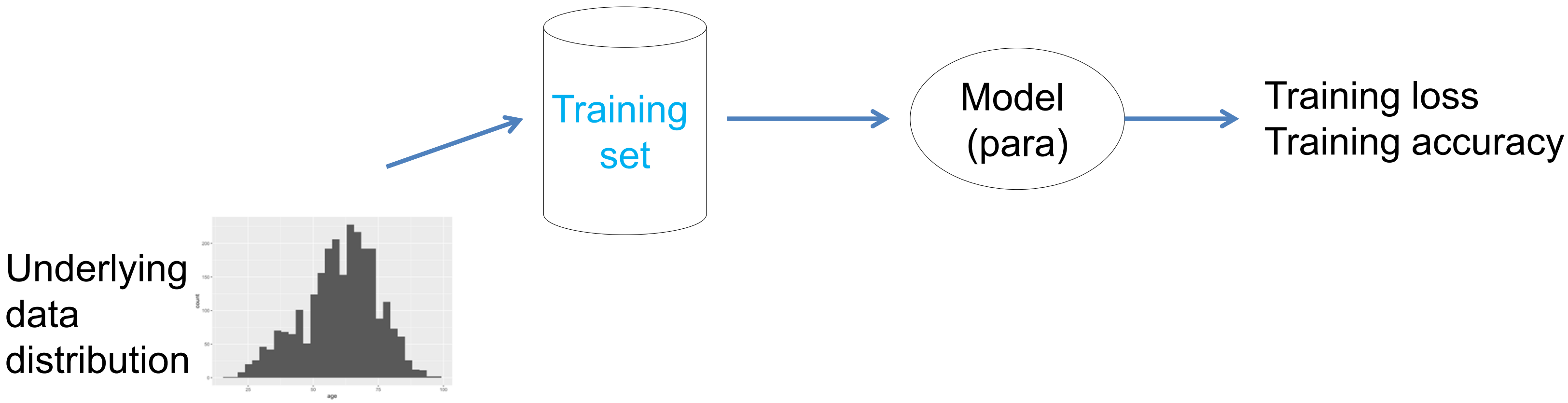
Larger batch size, higher learning rate



- Larger BatchSize, better estimation of gradient
- Larger BatchSize, less exploration
- High learning rate for small BatchSize can lead to failed convergence
- Overall, set BatchSize large, subject to the GPU RAM limit
- More on how to find good learning rate …

https://miguel-data-sc.github.io/2017-11-05-first/#:~:text=For%20the%20ones%20unaware%2C%20general,descent%20(batch%20size%201). https://arxiv.org/abs/1506.01186

Model Generalization

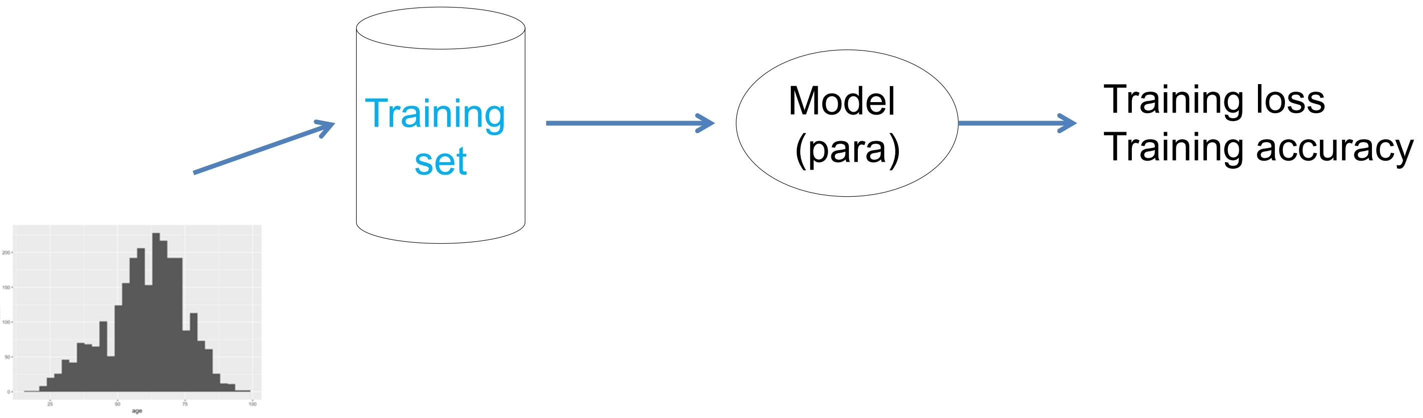


We don’t have this distribution or an effective way to compute it!

- Training and test sets are sampled from the same distribution, i.i.d. (independent and identically distributed)
- We care test/generalization performance; that is, the performance of training model on a new dataset

Model Generalization

Underlying
data
distribution



Training set

Model (para)

Training loss
Training accuracy

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distribution or an effective
way to compute it!

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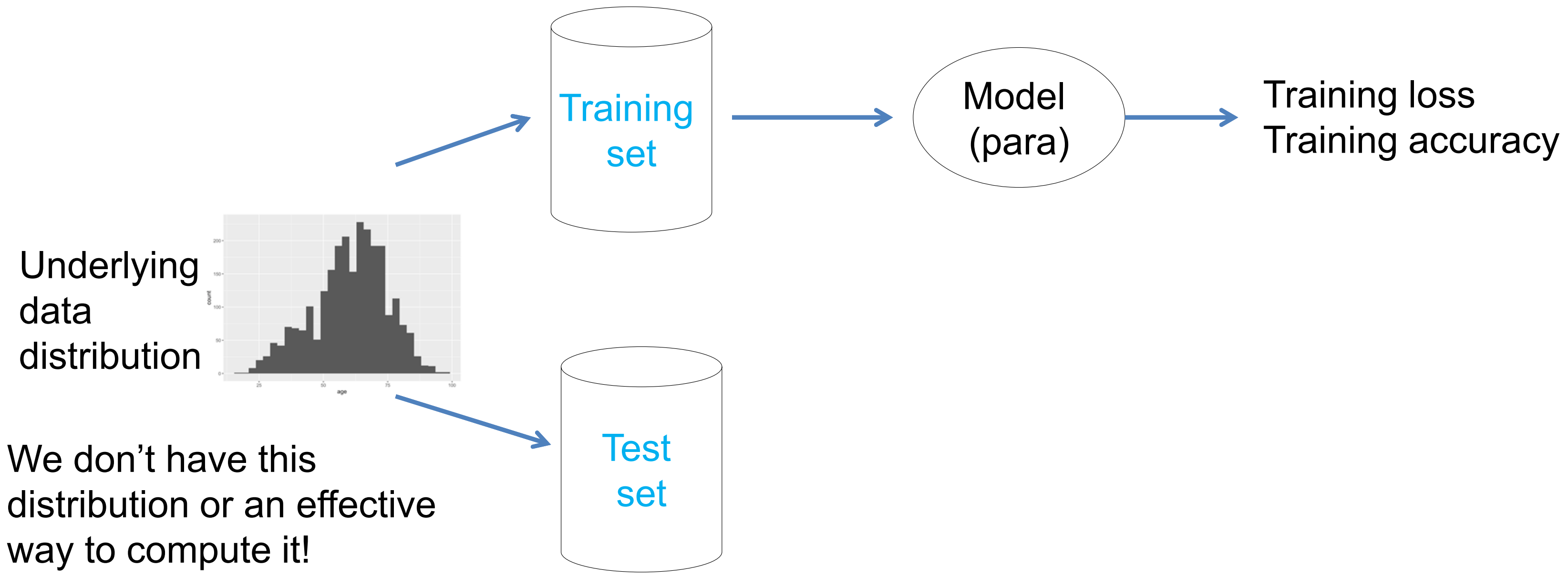
Model Generalization



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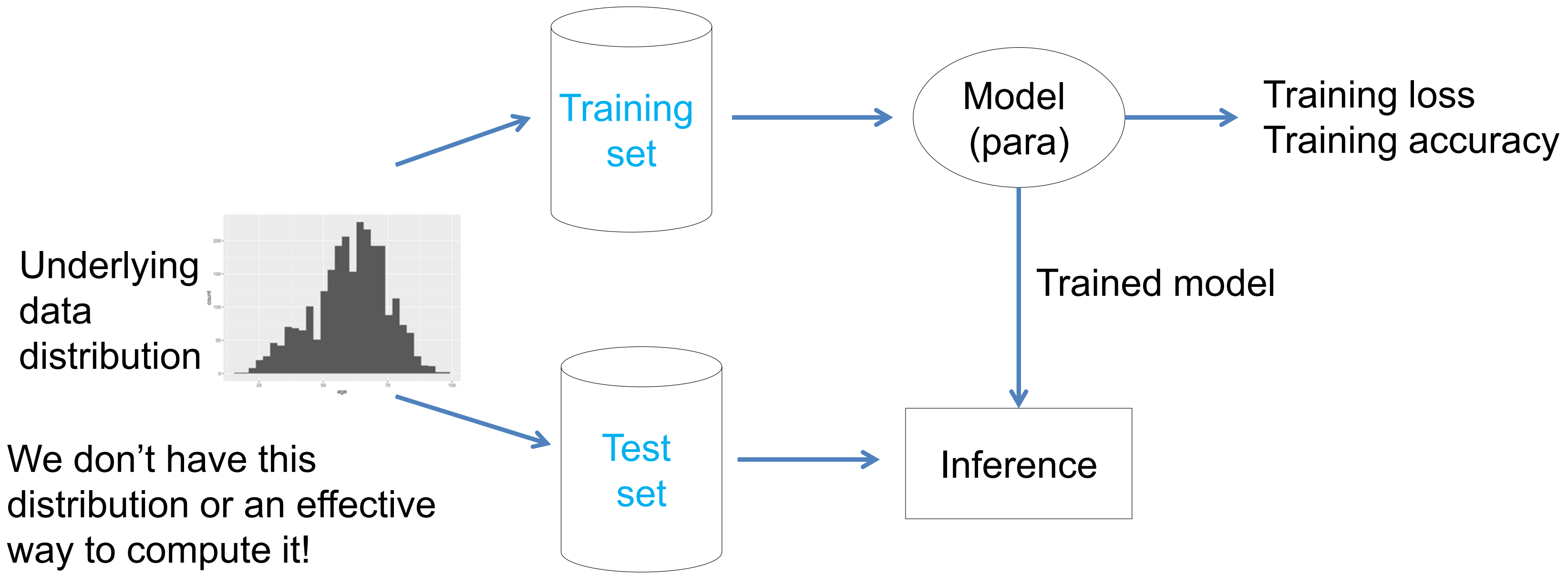
Model Generalization



Training set

Model (para)

Training loss
Training accuracy

Underlying data distribution

Trained model

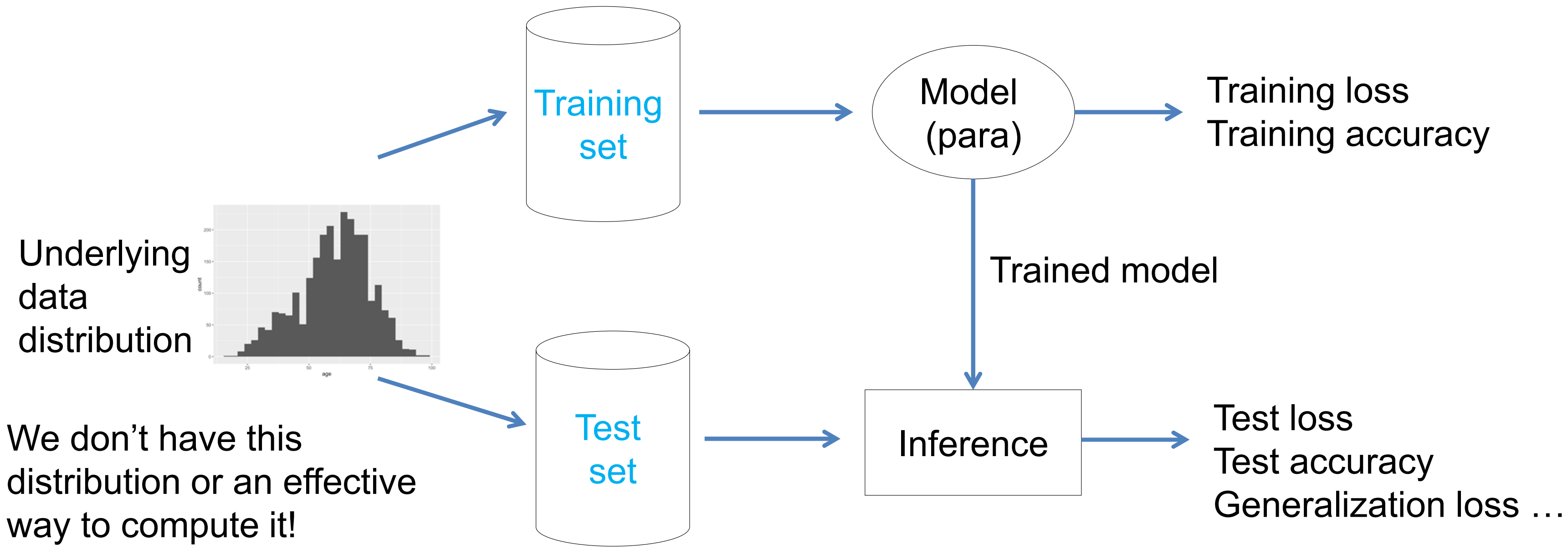
Test set

Inference

We don’t have this distribution or an effective way to compute it!

- Training and test sets are sampled from the same distribution, i.i.d. (independent and identically distributed)
- We care test/generalization performance; that is, the performance of training model on a new dataset

Model Generalization



Underlying data distribution

Training set

Model (para)

Training loss
Training accuracy

Trained model

Test set

Inference

Test loss
Test accuracy
Generalization loss …

We don’t have this distribution or an effective way to compute it!

- Training and test sets are sampled from the same distribution, i.i.d. (independent and identically distributed)
- We care test/generalization performance; that is, the performance of training model on a new dataset

Model error

Given the underlying function $f(\boldsymbol{x})$, the model $M(\boldsymbol{x};\boldsymbol{D})$ to approximate $f(x)$

$\boldsymbol{D}$ is a data set sampled from function $f(\boldsymbol{x})$. $\boldsymbol{D} = [(\boldsymbol{x_0}, \boldsymbol{y_0}), (\boldsymbol{x_1}, \boldsymbol{y_1}), \ldots, (\boldsymbol{x_{N-1}}, \boldsymbol{y_{N-1}})]$

Every sample $(\boldsymbol{x_i}, \boldsymbol{y_i})$ is contaminated by noise: $\boldsymbol{y_i} = \boldsymbol{f}(\boldsymbol{x}) + \boldsymbol{\epsilon}$, $\boldsymbol{\epsilon}$ is the random noise

We want to know the expected error of model, given the dataset D:

$$E_{\boldsymbol{D}}[(y - M(\boldsymbol{x};\boldsymbol{D}))^2]$$

This error consists of three parts:

$$E_{\boldsymbol{D}}\left[\left(y - M(\boldsymbol{x};\boldsymbol{D})\right)^2\right] = \{E_{\boldsymbol{D}}[M(\boldsymbol{x};\boldsymbol{D})] - f(\boldsymbol{x})\}^2 + E_{\boldsymbol{D}}\left[(E_{\boldsymbol{D}}\left(M(\boldsymbol{x};\boldsymbol{D})\right) - M(\boldsymbol{x};\boldsymbol{D}))^2\right] + \boldsymbol{\sigma}^2$$

http://statweb.stanford.edu/~tibs/ElemStatLearn/, section 2.9
https://en.wikipedia.org/wiki/Bias%E2%80%93variance_tradeoff

Model error

Model prediction error consists of three parts:

$$E_{\boldsymbol{D}}\left[\left(y - M(\boldsymbol{x};\boldsymbol{D})\right)^2\right] = \{E_{\boldsymbol{D}}[M(\boldsymbol{x};\boldsymbol{D})] - f(\boldsymbol{x})\}^2 + E_{\boldsymbol{D}}\left[(E_{\boldsymbol{D}}\left(M(\boldsymbol{x};\boldsymbol{D})\right) - M(\boldsymbol{x};\boldsymbol{D}))^2\right] + \boldsymbol{\sigma}^2$$

$$Bias(\boldsymbol{M},\boldsymbol{D}) = E_{\boldsymbol{D}}[M(\boldsymbol{x};\boldsymbol{D})] - f(\boldsymbol{x})$$

This is the **Bias**, for the difference between the mean model performance and ground-truth

$E_{\boldsymbol{D}}[M(\boldsymbol{x};\boldsymbol{D})]$ is the expected model performance over all possible datasets <- the best model we can get

http://statweb.stanford.edu/~tibs/ElemStatLearn/

Model error

Model prediction error consists of three parts:

$$E_{\boldsymbol{D}}\left[\left(y - M(\boldsymbol{x};\boldsymbol{D})\right)^2\right] = \{E_{\boldsymbol{D}}[M(\boldsymbol{x};\boldsymbol{D})] - f(\boldsymbol{x})\}^2 + E_{\boldsymbol{D}}\left[(E_{\boldsymbol{D'}}\left(M(\boldsymbol{x};\boldsymbol{D'})\right) - M(\boldsymbol{x};\boldsymbol{D}))^2\right] + \boldsymbol{\sigma}^2$$

$$Var(\boldsymbol{M},\boldsymbol{D}) = E_{\boldsymbol{D}}\left[(E_{\boldsymbol{D'}}\left(M(\boldsymbol{x};\boldsymbol{D'})\right) - M(\boldsymbol{x};\boldsymbol{D}))^2\right]$$

This is the **Variance,** measuring model performance fluctuation due to different datasets.

Measure how much the model prediction can change, after trained with different training sets

http://statweb.stanford.edu/~tibs/ElemStatLearn/

Model error

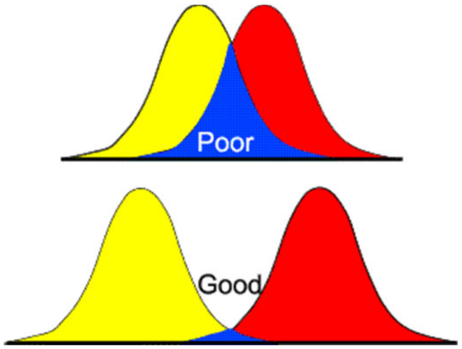
Model prediction error consists of three parts:

$$E_{\boldsymbol{D}}\left[\left(y - M(\boldsymbol{x};\boldsymbol{D})\right)^2\right] = \{E_{\boldsymbol{D}}[M(\boldsymbol{x};\boldsymbol{D})] - f(\boldsymbol{x})\}^2 + E_{\boldsymbol{D}}\left[(E_{\boldsymbol{D}'}\left(M(\boldsymbol{x};\boldsymbol{D}')\right) - M(\boldsymbol{x};\boldsymbol{D}))^2\right] + \boldsymbol{\sigma}^2$$

$\boldsymbol{\sigma}^2$ Bayes error, irreducible error

lowest possible error rate for any classifier

If one would know exactly what process/distribution generates the data, one still cannot achieve 100% accuracy, due to randomness



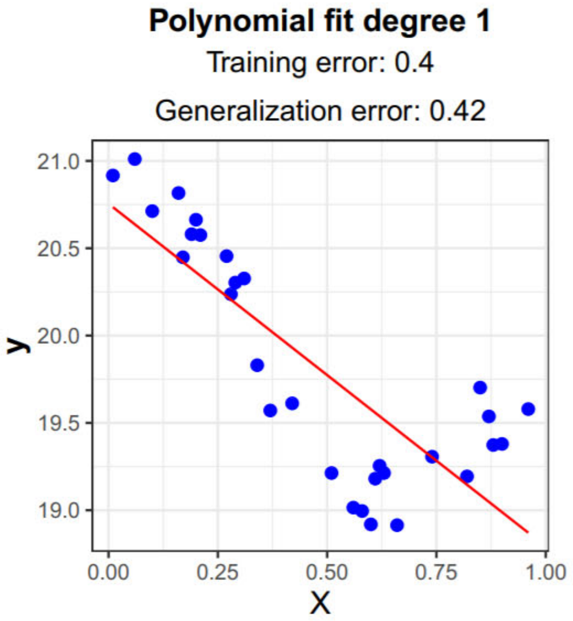
Distribution of two classes can overlap

If the test error has a lower-bound, there will be a Bias-Variance trade-off.

http://www.alanfielding.co.uk/multivar/dawords.htm

http://statweb.stanford.edu/~tibs/ElemStatLearn/

Underfitting and overfitting



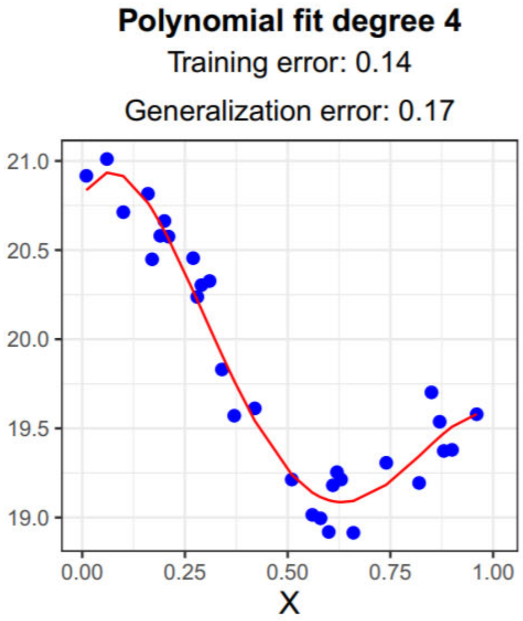
Polynomial fit degree 1

Training error: 0.4

Generalization error: 0.42

Underfit

Model cannot represent the data distribution



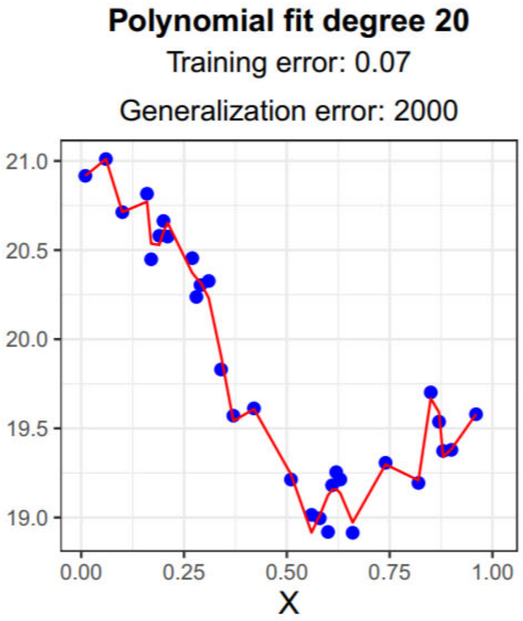
Polynomial fit degree 4

Training error: 0.14

Generalization error: 0.17

Good fit

Model well represents the data distribution, and does not capture data noise



Polynomial fit degree 20

Training error: 0.07

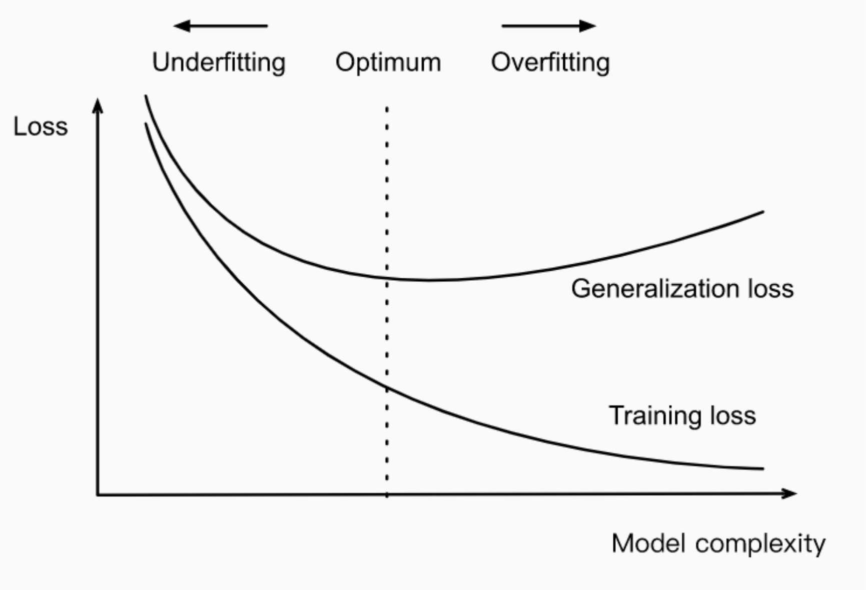
Generalization error: 2000

Overfit

Model is so flexible that it captures unwanted fluctuation due to noise

https://ascpt.onlinelibrary.wiley.com/doi/10.1002/cpt.1796

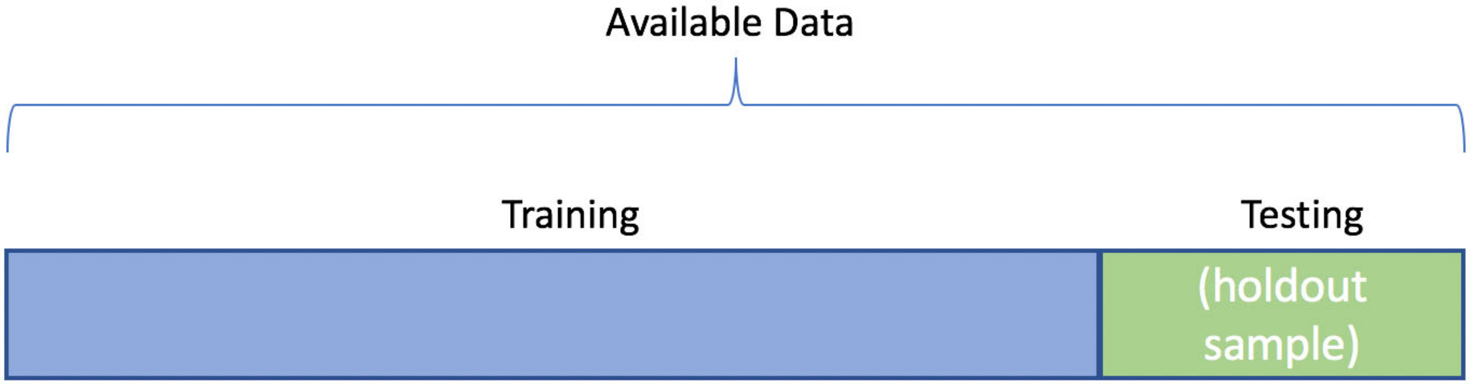
Underfitting and overfitting



- Increasing model capacity/complexity can lead to overfitting
- When applying trained model to a new dataset, e.g. test set, model performance can decrease, as a result of overfitting, indicated by the high **generalization loss**
- Model can also underfitting the data, indicated by the high **training loss**

https://ja.d2l.ai/chapter_deep-learning-basics/underfit-overfit.html

In Deep Learning set up



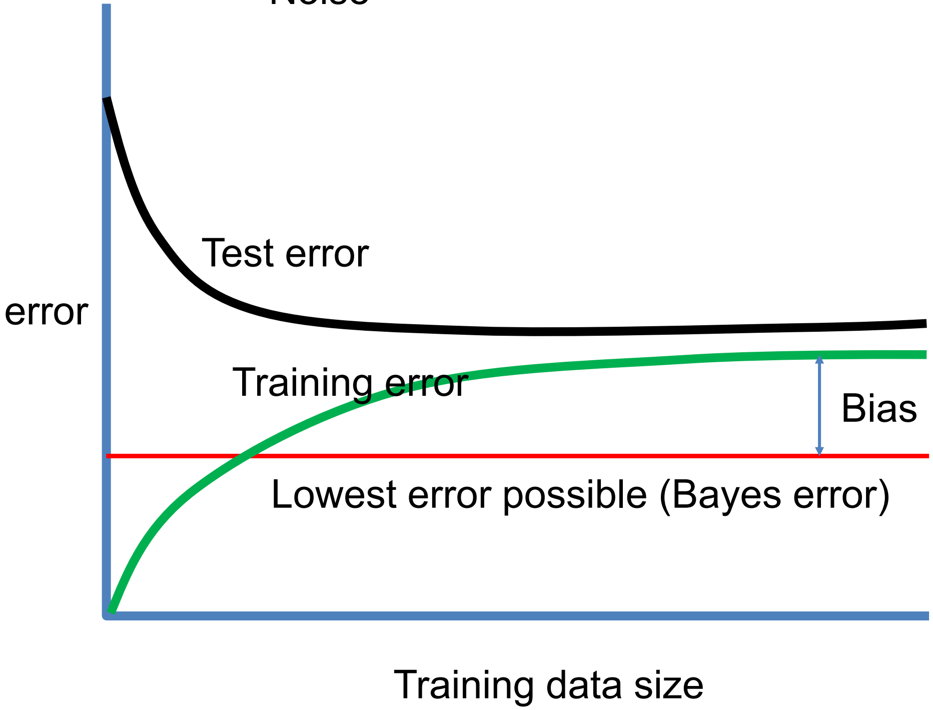
- We train on Training set and use training accuracy to estimate model performance ← **Bias.**

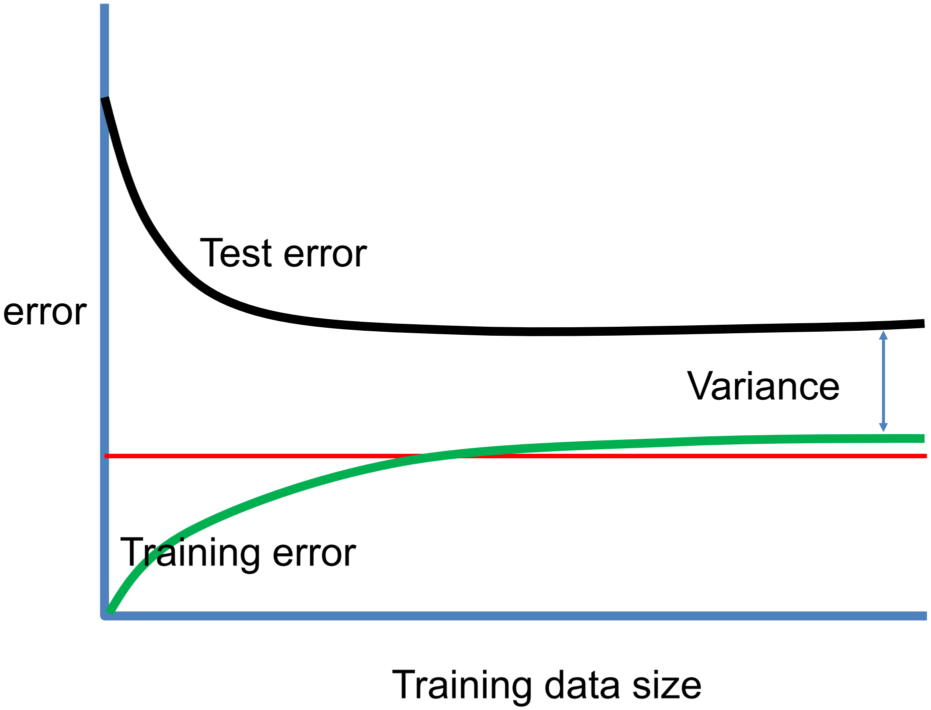
- We apply the trained model on Testing set. Performance difference between training accuracy and test accuracy gives an estimation of **Variance**.

Bias and variance

Bayes error is the best possible error rate if we knew true data distribution. It will not be zero :

- Overlap between class distribution
- Noise





Regularization to control model complexity

Deep learning model is very powerful, that it may overfit training data → degraded generalization

IDEA: change loss function to control model complexity

$$L = \frac{1}{B}\sum_{i=0}^{B-1} L^{(\boldsymbol{i})} + \lambda R(\boldsymbol{W})$$

Data loss: how well model fits the data

Regularization loss: prevent model from fitting training data too well

L2 Regularization, weight decay

$$L = \frac{1}{B}\sum_{i=0}^{B-1} L^{(\boldsymbol{i})} + \frac{\lambda}{2}\|\boldsymbol{W}\|_2^2$$

$\|\boldsymbol{W}\|_2^2 = \sum_{k=0}^{P-1} {w_k}^2$ For all parameters in the model, flatten them and computing the element-wise L2 norm

$$\frac{\partial L}{\partial w_k} = \frac{1}{B}\sum_{i=0}^{B-1}\frac{\partial L^{(i)}}{\partial w_k} + \lambda w_k \qquad w_k = w_k - \alpha\left(\frac{1}{B}\sum_{i=0}^{B-1}\frac{\partial L^{(i)}}{\partial w_k}\right) - \underbrace{\alpha\lambda w_k}_{\text{weight decay}}$$

L1 Regularization

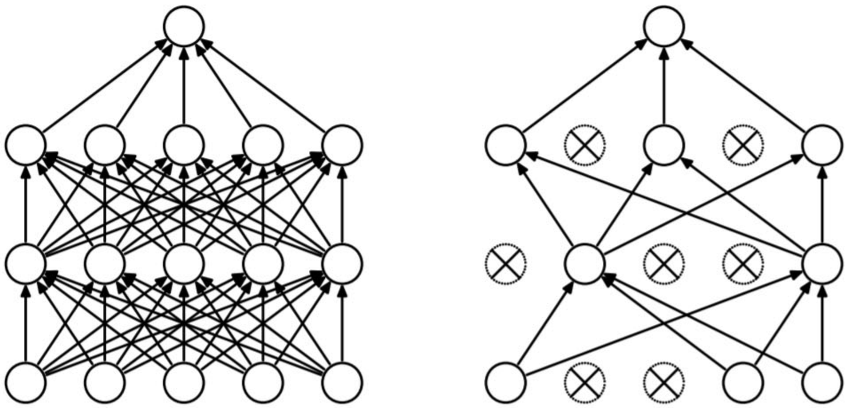
$$L = \frac{1}{B}\sum_{i=0}^{B-1} L^{(\boldsymbol{i})} + \frac{\lambda}{2}\|\boldsymbol{W}\|_{\mathbf{1}}$$

$$\|\boldsymbol{W}\|_{\mathbf{1}} = \sum_{k=0}^{P-1} |w_k|$$

For all parameters in the model, flatten them and computing the element-wise absolute value

$$\frac{\partial L}{\partial w_k} = \frac{1}{B}\sum_{i=0}^{B-1} \frac{\partial L^{(i)}}{\partial w_k} + \lambda sign(w_k) \qquad sign(w_k) = \begin{cases} 1, w_k > 0 \\ 0, w_k == 0 \\ -1, w_k < 0 \end{cases}$$

Drop Out



(a) Standard Neural Net (b) After applying dropout.

Figure 1: Dropout Neural Net Model. **Left**: A standard neural net with 2 hidden layers. **Right**: An example of a thinned net produced by applying dropout to the network on the left. Crossed units have been dropped.

- Jointly train many smaller network, randomly selected
- Implicitly combine exponentially many different neural network architectures efficiently

- Randomly drop out a set of neurons during training phase, with a probability of 1-p (e.g. p=0.5)
- It means to randomly select different rows in the W matrix, for every batch, every epoch
- During the test time, use all neurons, but scale the score by p
- Or, in training time, scale the score by 1/p ← inverse dropout
- Often used with linear layer, not for convolution
- Require more epochs to train

Nitish Srivastava, Geoffrey Hinton, Alex Krizhevsky, Ilya Sutskever, Ruslan Salakhutdinov. Dropout: a simple way to prevent neural networks from overfitting. JMLR, 15(56):1929−1958, 2014.

Other operations with regularization effects

Regularization will:

- Increase training error
- Decrease testing error
- Introduce new hyper-parameters
- Often requires experiments

Other operations to improve test error:

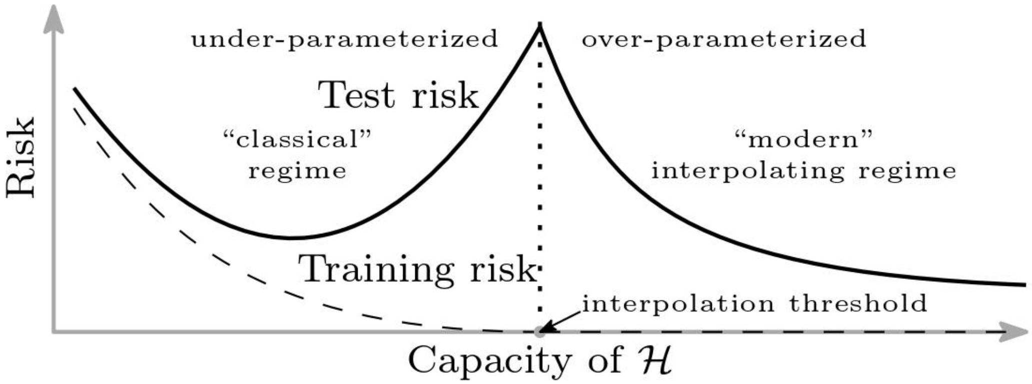
- Data augmentation
- Drop connection, random connection
- Batch/Layer/Channel normalization
- Early stopping

…

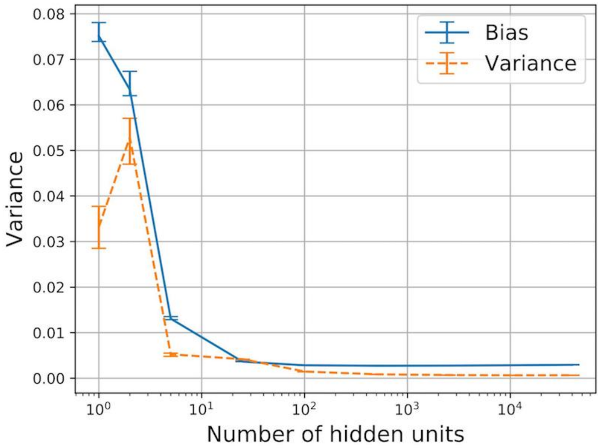
More on this topic in later lecturers

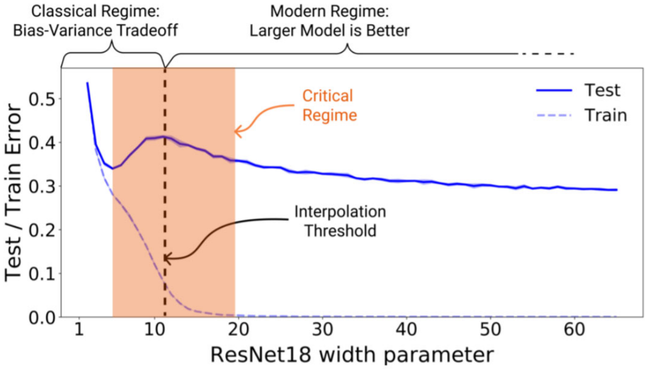
Double-descent of test error in deep models

Test error = Bias^2 + Variance + Bayes error



- Total test error can decrease with more complex model and longer training (#epochs)
- Still under research, but for deep model, Bias and variance may not act as a trade-off



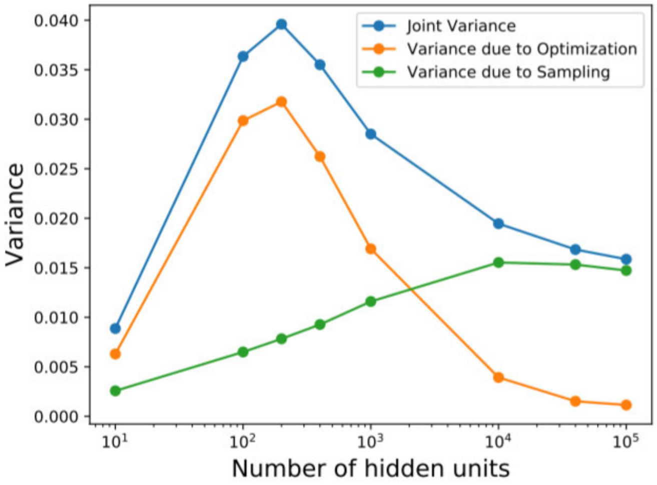


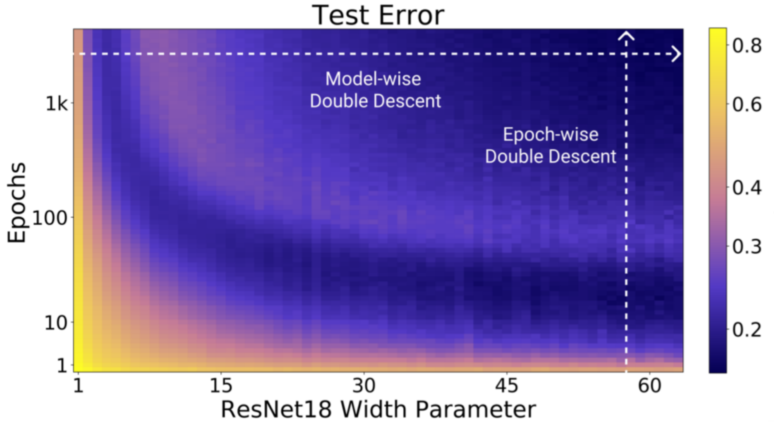
https://arxiv.org/pdf/1912.08286.pdf
https://arxiv.org/pdf/1912.02292.pdf

Double-descent of test error in deep models

Test error = Bias^2 + Variance + Bayes error

$$Var(\boldsymbol{M},\boldsymbol{D}) = E_{\boldsymbol{D}}\left[\left(E_{\boldsymbol{D}'}\left(M(\boldsymbol{x};\boldsymbol{D}')\right) - M(\boldsymbol{x};\boldsymbol{D})\right)^2\right]$$





- More complex model → reduce variance due to sampling the training set D; may help reduce variance due to optimization
- Longer training → reduce variance due to optimization

https://arxiv.org/pdf/1912.08286.pdf
https://arxiv.org/pdf/1912.02292.pdf