CPEN 400D: Deep Learning

Lecture 1 (II): ML Basics & Linear Models

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Outline

- Statistical Learning Setup
- Linear Regression
  - Problem Specification
  - Model Design
  - Loss Design
  - Inference Algorithm
  - Learning/Training Algorithm (Gradient Descent)
  - Validation and Testing (Overfitting vs. Underfitting, Bias Variance Tradeoff)
- Linear Classification
  - Logistic Regression
  - Multiclass Logistic Regression

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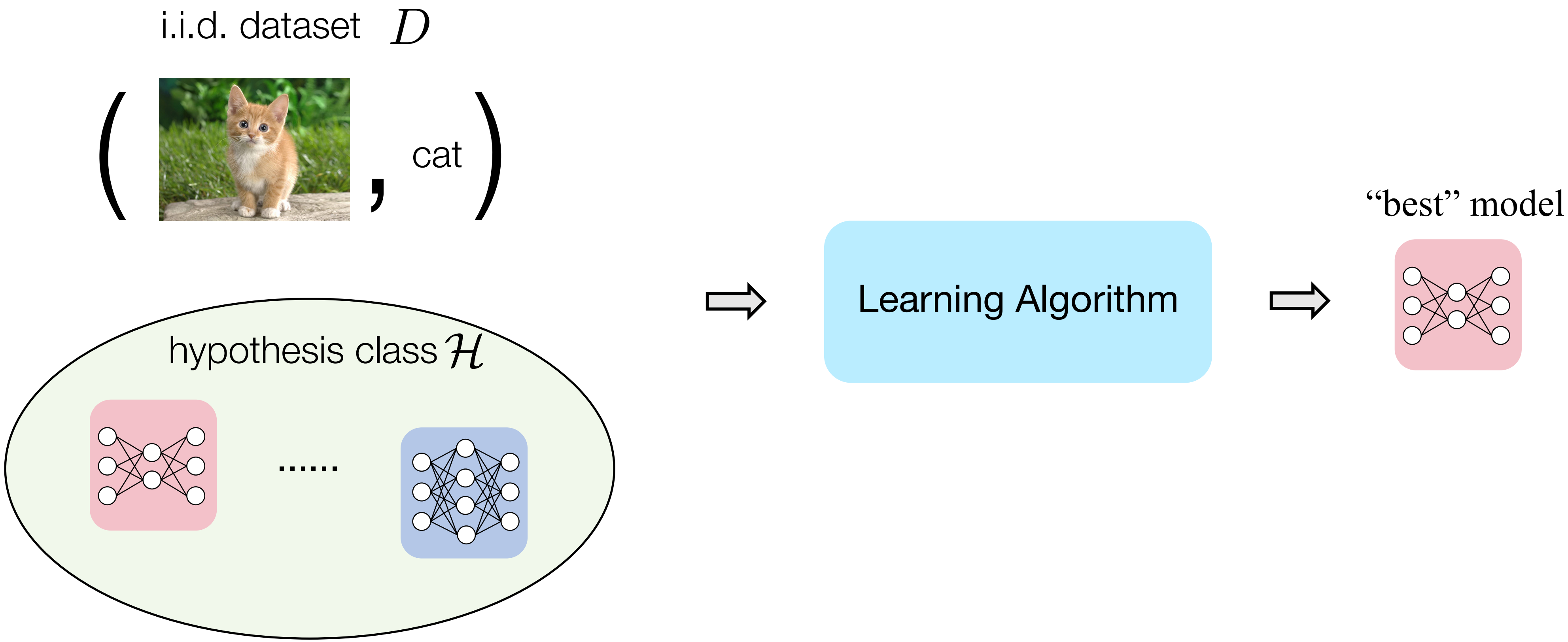
Statistical Learning Setup



Statistical Learning Setup

Let us review some key concepts and assumptions (mainly about supervised learning like classification and regression) in statistical learning theory, which was initially developed by Vladimir Vapnik, e.g., [1].

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Training data are sampled from an unknown data distribution in an i.i.d. (independent and identically distributed) fashion

$$(x_n, y_n) \overset{\text{iid}}{\sim} \mathbb{P}_{\text{data}}(x, y) \qquad n = 1, \ldots, N$$

Therefore, the training dataset

$$D = \{(x_n, y_n) | n = 1, \ldots, N\} \sim \mathbb{P}_{\text{data}}(x, y)^N$$

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Either input or output could be continuous or discrete scalars, vectors, tensors, sets, sequences, graphs, …

E.g. regression $x_n \in \mathbb{R}^2 \qquad y_n \in \mathbb{R}$

classification $x_n \in \mathbb{R}^2 \qquad y_n \in \{1, 2, \ldots, K\}$

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Loss is denoted as $\ell(y, f(x, w))$

Generalization error (a.k.a., *risk or expected loss*) is $\mathbb{E}_{\mathbb{P}_{\mathrm{data}(x,y)}} [\ell(y, f(x, w))]$

Training error (a.k.a., *empirical risk* or *training loss*) is $\frac{1}{N} \sum_{n=1}^{N} \ell(y_n, f(x_n, w))$

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Monte Carlo Estimation

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This learning framework is called *empirical risk minimization (ERM)*!

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A learning algorithm can be viewed as a mapping that maps a training dataset, initial parameters, and hyperparameters to "optimal" parameters:

$$w^* = \mathcal{A}(D, w^0)$$

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Linear Regression

- Problem Specification (1D-Regression)

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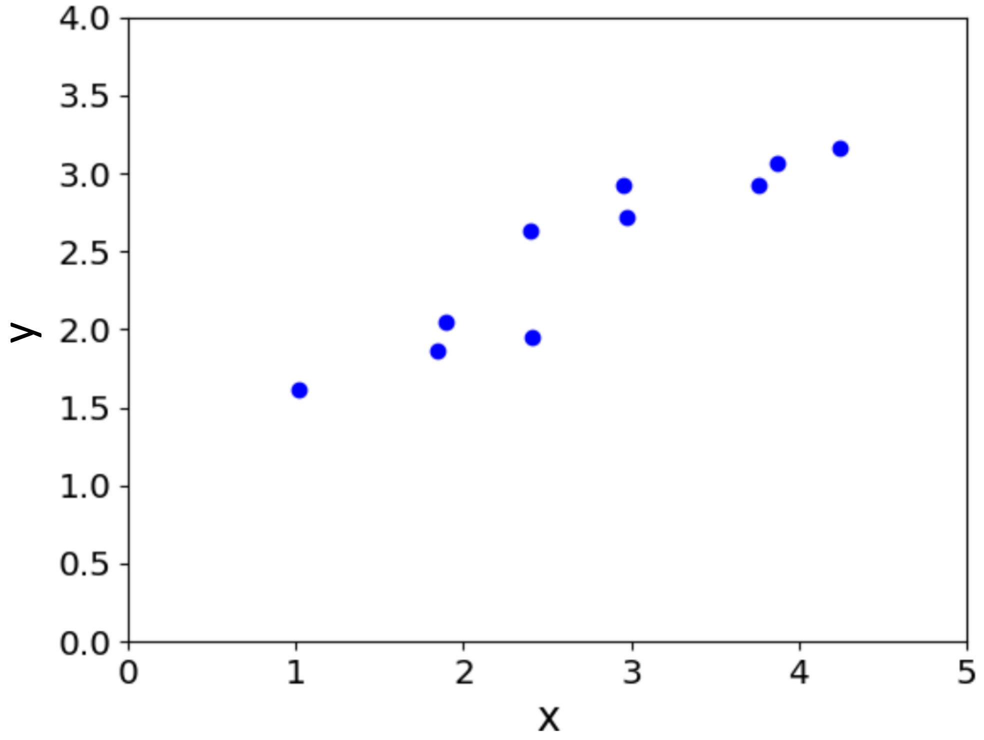

Image Credit: UofT CSC413 Lecture 1

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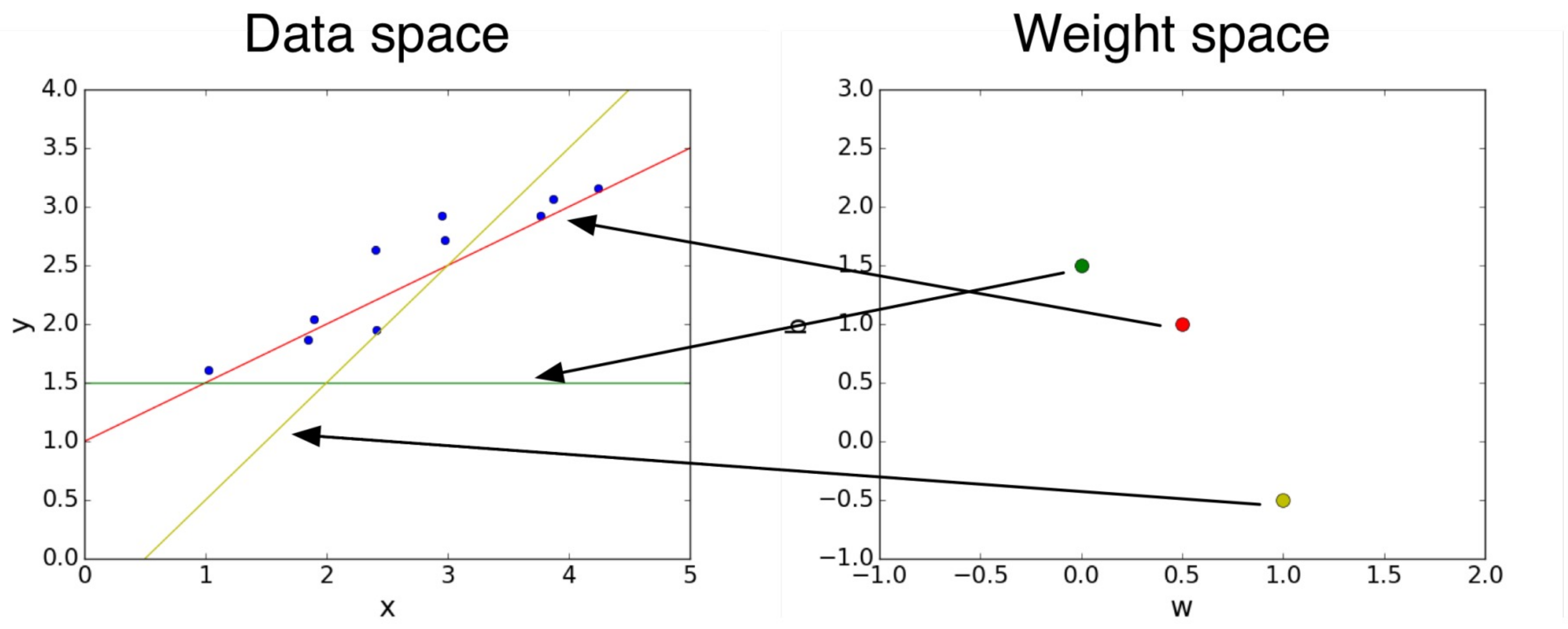

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3) Smooth L1 loss (similar to Huber loss used in robust statistics)

$$\ell(\hat{y}_n, y_n) = \begin{cases} \frac{1}{2\beta} \|\hat{y}_n - y_n\|_2^2 & \text{if } \|\hat{y}_n - y_n\|_1 < \beta \\ \|\hat{y}_n - y_n\|_1 - \frac{1}{2\beta} & \text{otherwise} \end{cases}$$

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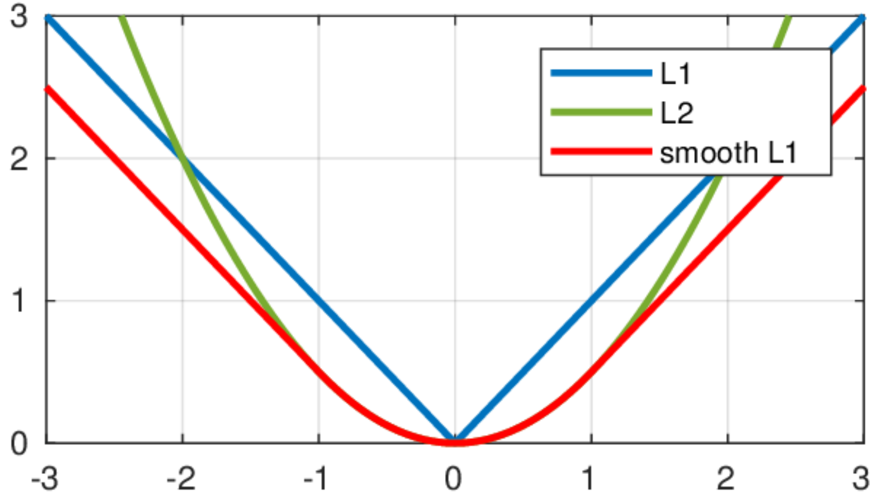

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  1) “*Inference*” in DL and many ML areas:

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For our linear models, inference is just: $\hat{y} = w^\top x + b$

For other models in DL/ML, e.g., deep energy based models, one may need both of first two!

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- Learning Algorithm

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Since learning is an optimization problem, a learning algorithm is just an optimization algorithm.

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2) Gradient-free learning algorithms:

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1) Gradient-based learning algorithms:
   - 1st order gradient method, e.g., stochastic gradient descent (SGD)
   - 2nd order gradient method, e.g., Newton's method

   ……
2) Gradient-free learning algorithms:
   - Genetic algorithms
   - Random search, e.g., simulated annealing

   ……

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In linear regression, we have

$$f(x, w, b) = \hat{y} = w^\top x + b$$

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In linear regression, we have $f(x, w, b) = \hat{y} = w^\top x + b$

Therefore, with MSE loss, the learning problem is

$$\min_{w,b} \quad L(w, b) = \frac{1}{N} \sum_{n=1}^{N} \ell(f(x_n, w, b), y_n) = \frac{1}{N} \sum_{n=1}^{N} \|w^\top x_n + b - y_n\|_2^2$$

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We can equivalently (why?) rewrite it as

$$\min_{w,b} \quad L(w, b) = \frac{1}{2N} \sum_{n=1}^{N} \|w^\top x_n + b - y_n\|_2^2$$

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What is a gradient?

Loss is typically a scalar, parameters can be viewed as a vector, the gradient is defined as

$$\frac{\partial L}{\partial w[i]} = \lim_{\epsilon \to 0} \frac{L(w + \epsilon e_i, b) - L(w,b)}{\epsilon}$$

where $w[i]$ is the i-th element (scalar) of weight and e_i is a zero vector except that the i-th element is 1.

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This definition (central difference version) is useful for checking the correctness of gradient implementation!

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We learn from calculus about how to derive gradient via basic derivatives and their rules:

$$L(w,b) = \frac{1}{2N}\sum_{n=1}^{N} \| \underbrace{w^\top x_n + b - y_n}_{l_n} \|_2^2$$

$$= \frac{1}{2N}\sum_{n=1}^{N} \left(\sum_{d=1}^{D} w[d]x_n[d] + b - y_n \right)^2$$

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&= \sum_{n=1}^{N} \frac{\partial \frac{1}{2N}\sum_{n=1}^{N} l_n^2}{\partial l_n}\frac{\partial l_n}{\partial w[i]} \\
&= \frac{1}{2N}\sum_{n=1}^{N} 2l_n \frac{\partial l_n}{\partial w[i]} \\
&= \frac{1}{N}\sum_{n=1}^{N} l_n \frac{\partial \left(\sum_{d=1}^{D} w[d]x_n[d] + b - y_n\right)}{\partial w[i]} \\
&= \frac{1}{N}\sum_{n=1}^{N} l_n x_n[i]
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\end{aligned}$$

Write in a compact vector form:

$$\frac{\partial L(w,b)}{\partial w} = \begin{bmatrix} \frac{\partial L(w,b)}{\partial w[1]} \\ \vdots \\ \frac{\partial L(w,b)}{\partial w[D]} \end{bmatrix}$$

$$= \frac{1}{N}\sum_{n=1}^{N} l_n x_n$$

Linear Regression

- Learning Algorithm

$$L(w,b) = \frac{1}{2N}\sum_{n=1}^{N} \| \underbrace{w^\top x_n + b - y_n}_{l_n} \|_2^2 = \frac{1}{2N}\sum_{n=1}^{N}\left(\sum_{d=1}^{D} w[d]x_n[d] + b - y_n\right)^2$$

$$\begin{aligned}
\frac{\partial L(w,b)}{\partial w[i]} &= \sum_{n=1}^{N} \frac{\partial L(w,b)}{\partial l_n}\frac{\partial l_n}{\partial w[i]} \\
&= \sum_{n=1}^{N} \frac{\partial \frac{1}{2N}\sum_{n=1}^{N} l_n^2}{\partial l_n}\frac{\partial l_n}{\partial w[i]} \\
&= \frac{1}{2N}\sum_{n=1}^{N} 2l_n \frac{\partial l_n}{\partial w[i]} \\
&= \frac{1}{N}\sum_{n=1}^{N} l_n \frac{\partial \left(\sum_{d=1}^{D} w[d]x_n[d] + b - y_n\right)}{\partial w[i]} \\
&= \boxed{\frac{1}{N}\sum_{n=1}^{N} l_n x_n[i]}
\end{aligned}$$

Write in a compact vector form:

$$\frac{\partial L(w,b)}{\partial w} = \begin{bmatrix} \frac{\partial L(w,b)}{\partial w[1]} \\ \vdots \\ \frac{\partial L(w,b)}{\partial w[D]} \end{bmatrix} = \frac{1}{N}\sum_{n=1}^{N} l_n x_n$$

If N is too large, we can randomly sample a smaller subset (a.k.a. mini-batch) to compute the gradient.

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Then we can perform the gradient descent algorithms

Algorithm 1 GD Learning Algorithm

1: **Input**: GD step T, learning Rate η, initial (w^0, b^0)
2: **For** $t=1,\cdots,T$
3: $\quad w^t=w^{t-1}-\eta\frac{\partial L(w^{t-1},b^{t-1})}{\partial w}$
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learning rate / step size

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learning rate / step size

- If we use full training dataset to compute the gradient per step, then it is called *(batch) gradient descent*
- If we use random mini-batch data to compute the gradient per step, then it is called *stochastic gradient descent*

Linear Regression

- Learning Algorithm

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Is the model at the last step necessarily the best?

Outline

- Statistical Learning Setup
- Linear Regression
  - Problem Specification
  - Model Design
  - Loss Design
  - Inference Algorithm
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  - **Validation and Testing** (**Overfitting vs. Underfitting**, Bias Variance Tradeoff)
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Linear Regression

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If your dataset is of a small size, then you can use k-fold cross-validation.

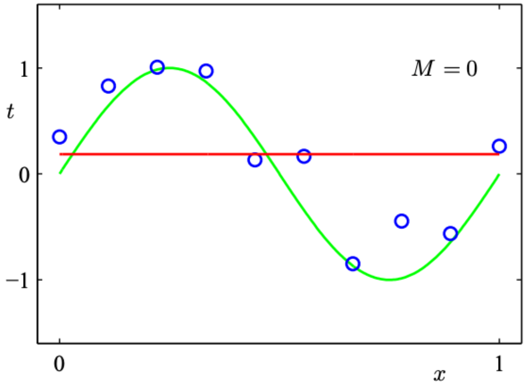
Linear Regression

- Validation and Testing: Overfitting vs. Underfitting

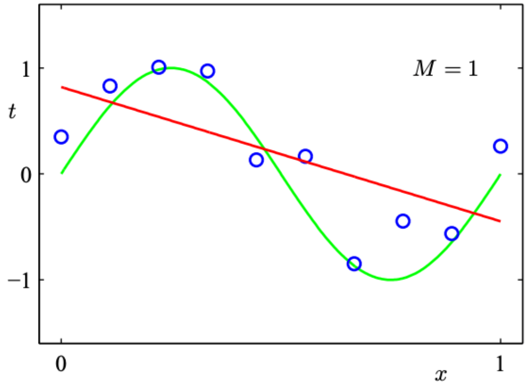
Linear Regression

- Validation and Testing: Overfitting vs. Underfitting

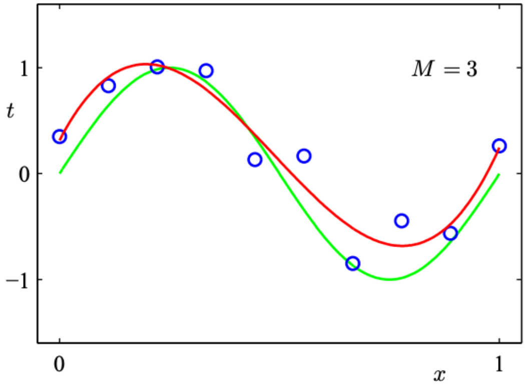
$$y = w_0$$



$$y = w_0 + w_1 x$$



$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$



$$y = w_0 + w_1 x + \cdots + w_9 x^9$$

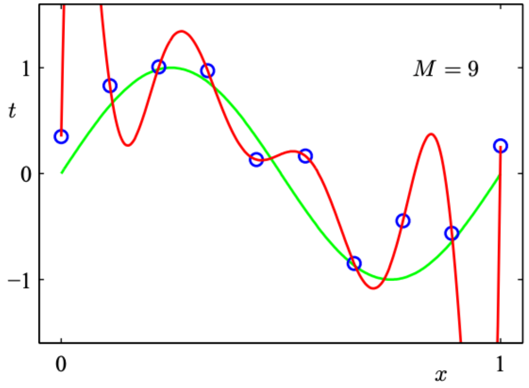


Image Credit: [2]

Linear Regression

- Validation and Testing: Overfitting vs. Underfitting

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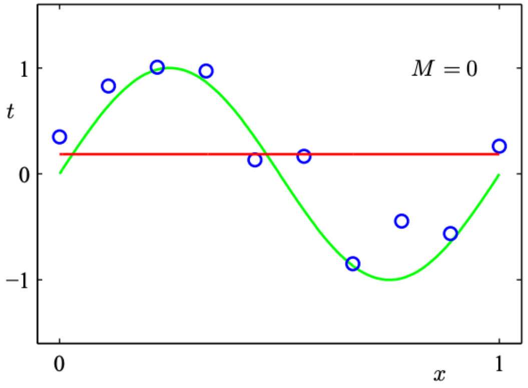

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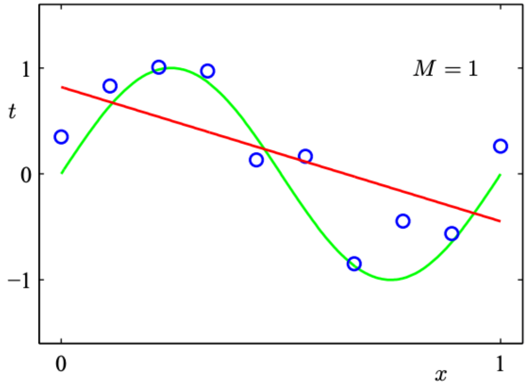

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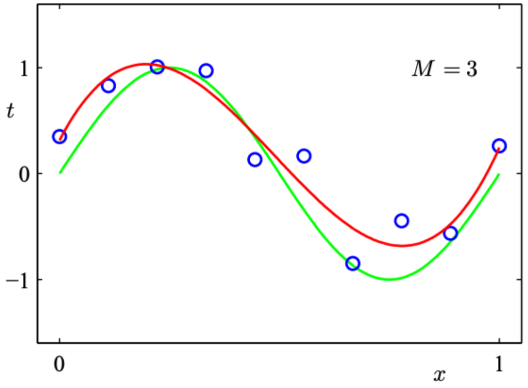

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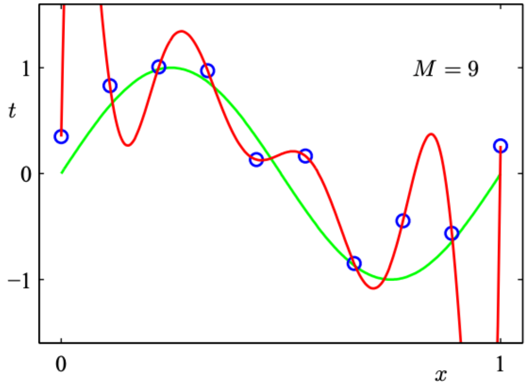

Underfitting:

Model is too simple to fit the data

Overfitting:

Model is too complicate, perfectly fits the data, but does not generalize

Image Credit: [2]

Linear Regression

- Validation and Testing: Overfitting vs. Underfitting

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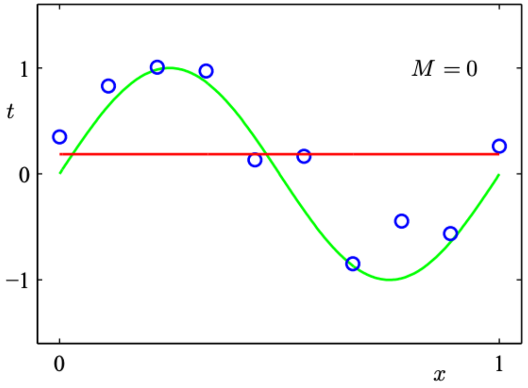

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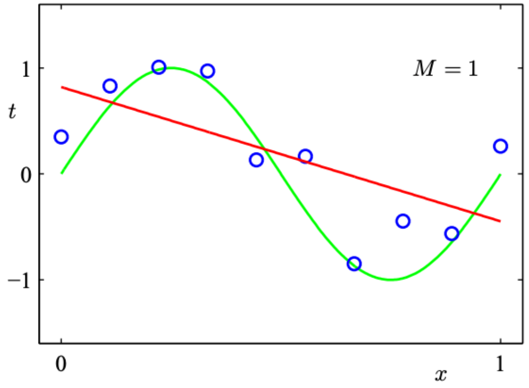

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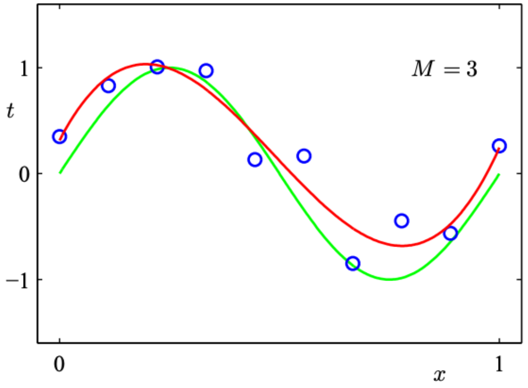

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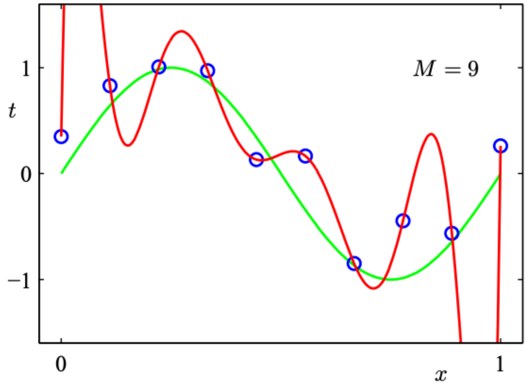

Underfitting:

Model is too simple to fit the data

Overfitting:

Model is too complicate, perfectly fits the data, but does not generalize

There exists *benign overfitting* (i.e., complicated models perfectly fit and generalize well) in deep learning (cf. [32])!

Image Credit: [2]

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Linear Regression

- Validation and Testing: Bias vs. Variance Tradeoff

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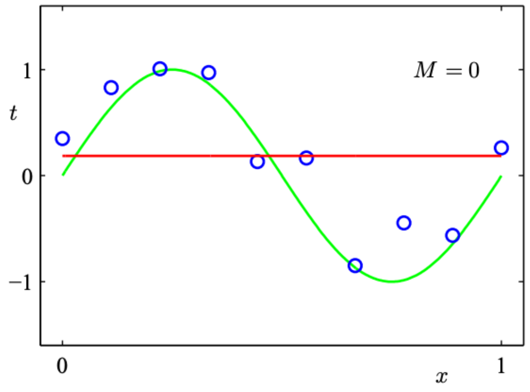

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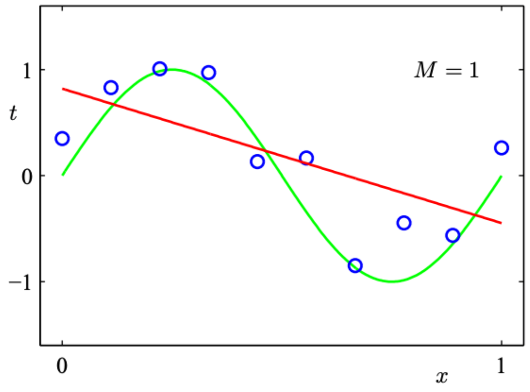

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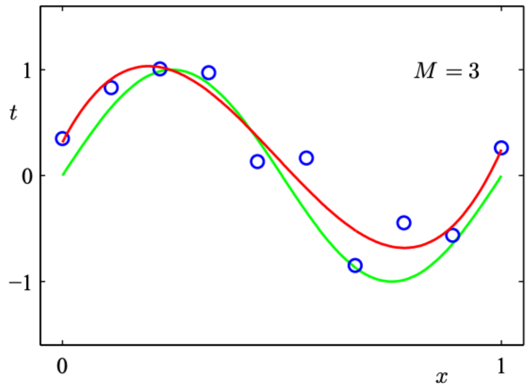

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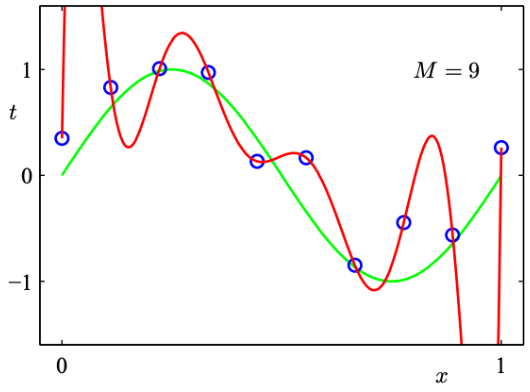

As the degree (complexity) increases, the variance of the model tends to increase, and the bias tends to decrease!

Image Credit: [2]

Linear Regression

- Validation and Testing: Bias vs. Variance Tradeoff

Recall

$$(x_n, y_n) \overset{\text{iid}}{\sim} \mathbb{P}_{\text{data}}(x, y) \qquad n = 1, \ldots, N$$

Our training dataset

$$D = \{(x_n, y_n) | n = 1, \ldots, N\} \sim \mathbb{P}_{\text{data}}(x, y)^N$$

Expected label/output

$$\bar{y}(x) = \mathbb{E}_{\mathbb{P}_{\text{data}}(y|x)}[y] = \int_y y \mathbb{P}_{\text{data}}(y|x) dy$$

Linear Regression

- Validation and Testing: Bias vs. Variance Tradeoff

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Our learned model $$f(x, w^*) = f(x, \mathcal{A}(D, w^0)) \equiv f_D(x)$$

Linear Regression

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Learning algorithm depends on training dataset, initial parameters, and hyperparameters

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Linear Regression

- Validation and Testing: Bias vs. Variance Tradeoff

Generalization error $\mathbb{E}_{\mathbb{P}_{\mathrm{data}}(x,y)}\left[(y - f_D(x))^2\right]$

Expected generalization error $\mathbb{E}_{D\sim\mathbb{P}_{\mathrm{data}}(x,y)^N,(x,y)\sim\mathbb{P}_{\mathrm{data}}(x,y)}\left[(y - f_D(x))^2\right]$

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This is what we really care in comparing different learning systems as it considers all possible training sets!

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Let us decompose it

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\begin{aligned}
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&= \mathbb{E}_{D,x,y}\left[(f_D(x) - \bar{f}(x) + \bar{f}(x) - y)^2\right] \\
&= \mathbb{E}_{D,x,y}\left[(f_D(x) - \bar{f}(x))^2\right] + 2\mathbb{E}_{D,x,y}\left[(f_D(x) - \bar{f}(x))(\bar{f}(x) - y)\right] + \mathbb{E}_{D,x,y}\left[(\bar{f}(x) - y)^2\right] \\
&= \mathbb{E}_{D,x}\left[(f_D(x) - \bar{f}(x))^2\right] + 2\mathbb{E}_{D,x,y}\left[(f_D(x) - \bar{f}(x))(\bar{f}(x) - y)\right] + \mathbb{E}_{x,y}\left[(\bar{f}(x) - y)^2\right]
\end{aligned}
$$

Linear Regression

- Validation and Testing: Bias vs. Variance Tradeoff

Decomposition of expected generalization error:

$$\mathbb{E}_{D,x,y}\left[(y - f_D(x))^2\right] = \mathbb{E}_{D,x}\left[(f_D(x) - \bar{f}(x))^2\right] + 2\mathbb{E}_{D,x,y}\left[(f_D(x) - \bar{f}(x))(\bar{f}(x) - y)\right] + \mathbb{E}_{x,y}\left[(\bar{f}(x) - y)^2\right]$$

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$$\begin{aligned}
\mathbb{E}_{D,x,y}\left[(f_D(x) - \bar{f}(x))(\bar{f}(x) - y)\right] &= \mathbb{E}_{x,y}\left[\mathbb{E}_D\left[(f_D(x) - \bar{f}(x))(\bar{f}(x) - y)\right]\right] \\
&= \mathbb{E}_{x,y}\left[\mathbb{E}_D\left[(f_D(x) - \bar{f}(x))\right](\bar{f}(x) - y)\right] \\
&= \mathbb{E}_{x,y}\left[(\mathbb{E}_D\left[f_D(x)\right] - \bar{f}(x))(\bar{f}(x) - y)\right] \\
&= \mathbb{E}_{x,y}\left[(\bar{f}(x) - \bar{f}(x))(\bar{f}(x) - y)\right] \\
&= 0
\end{aligned}$$

Linear Regression

- Validation and Testing: Bias vs. Variance Tradeoff

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Linear Regression

- Validation and Testing: Bias vs. Variance Tradeoff

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Variance: Captures how much your classifier changes if you train on a different training set. How "over-specialized" is your classifier to a particular training set (overfitting)? If we have the best possible model for our training data, how far off are we from the average classifier?

Bias: What is the inherent error that you obtain from your classifier even with infinite training data? This is due to your classifier being "biased" to a particular kind of solution (e.g. linear classifier). In other words, bias is inherent to your model.

Noise: How big is the data-intrinsic noise? This error measures ambiguity due to your data distribution and feature representation. You can never beat this, it is an aspect of the data.

Credit & More Info: https://www.cs.cornell.edu/courses/cs4780/2018fa/lectures/lecturenote12.html

Linear Regression

- Validation and Testing: Bias vs. Variance Tradeoff

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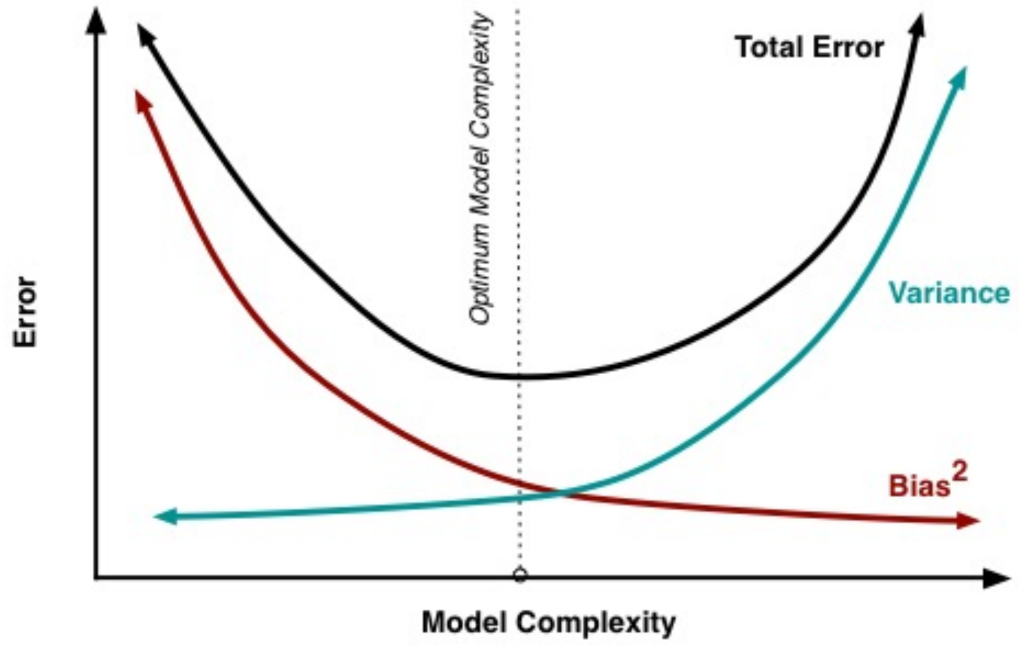

Image Credit: http://scott.fortmann-roe.com/docs/BiasVariance.html

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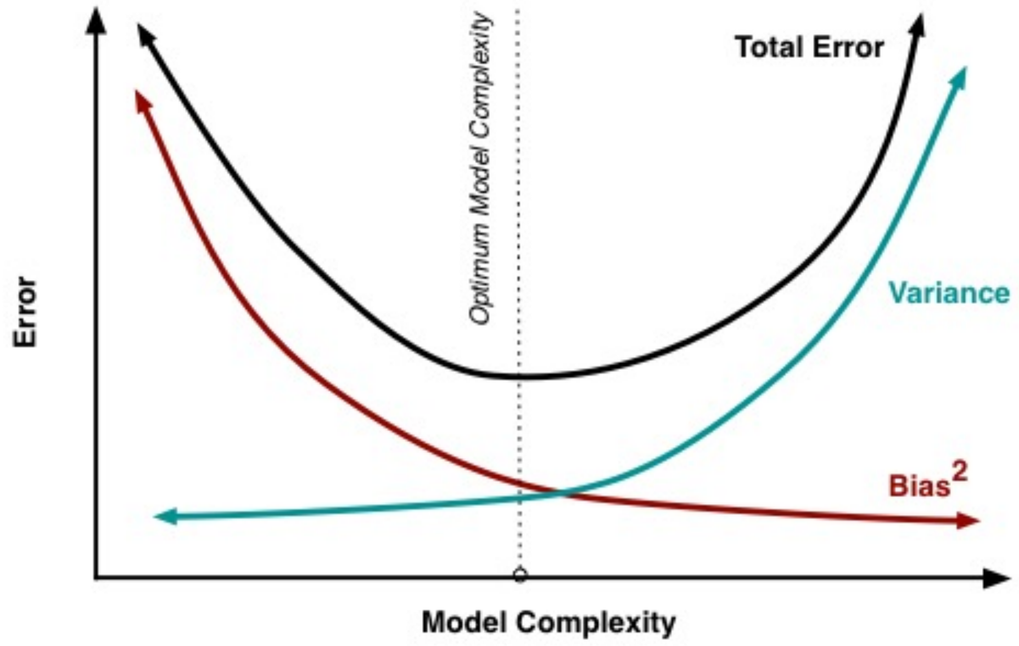

This classic bias-variance tradeoff can not explain deep learning as the model complexity measure is hard to find, e.g., #parameters is clearly not the right one!

Image Credit: http://scott.fortmann-roe.com/docs/BiasVariance.html

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Linear Models for Classification

Suppose we'd like to do a binary classification with a linear model

$$\{(x_n, y_n) | n = 1, \ldots, N\} \overset{\text{iid}}{\sim} \mathbb{P}_{\text{data}}(x, y)$$

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$$\hat{y} = \begin{cases} 1 & \text{if } f(x, w, b) > 0 \\ 0 & \text{otherwise} \end{cases}$$

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Answer: continuous approximation!

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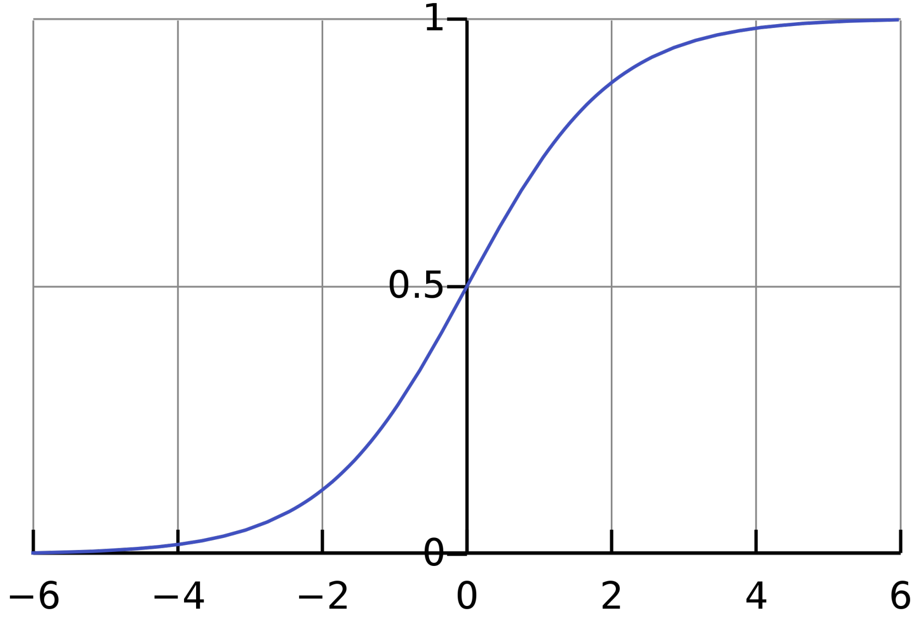

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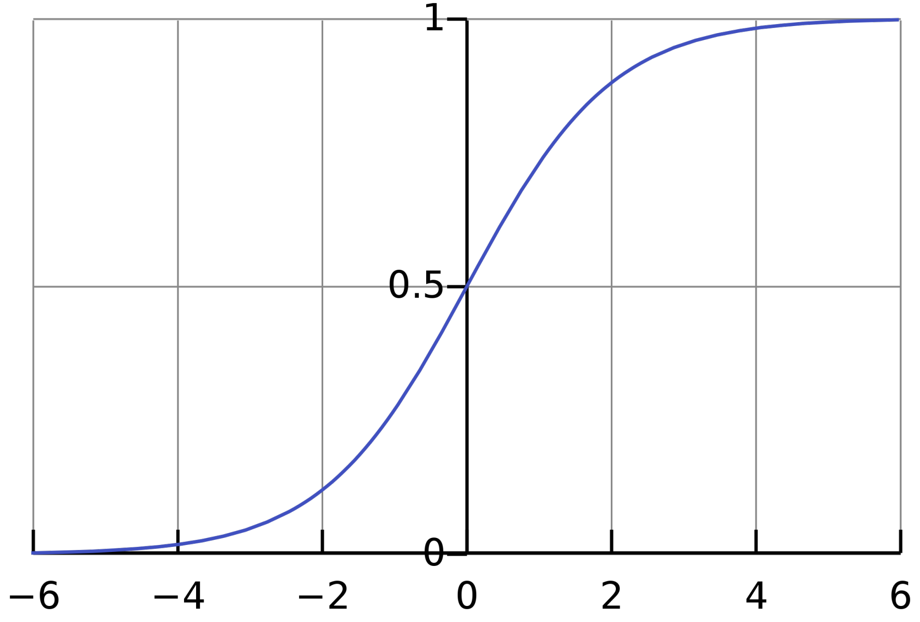

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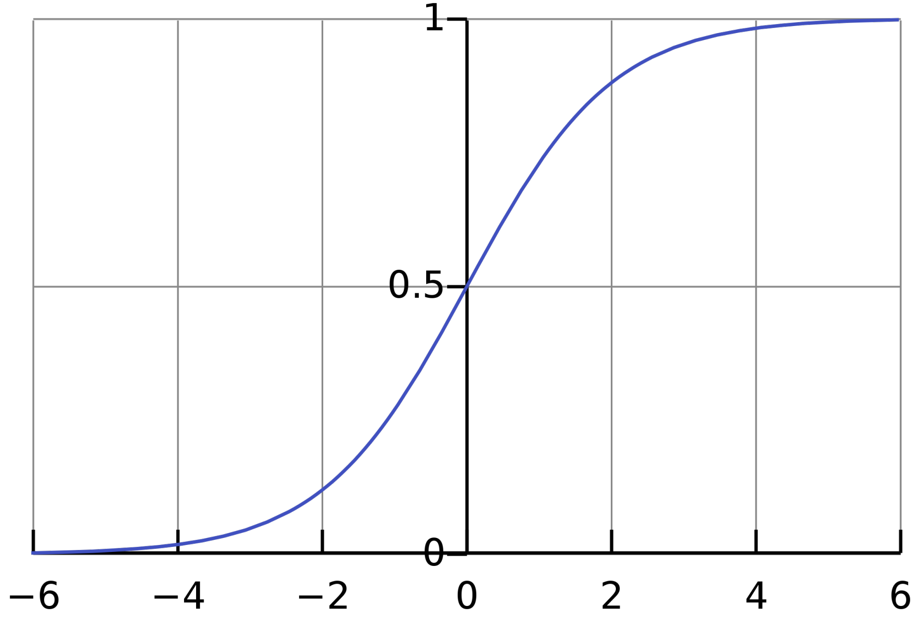
This outputs a probability!



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The non-differentiable 0-1 loss for classification is,

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It approximates *maximum* operator.

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log-sum-exp permits numerically-efficient (avoid overflow/underflow) implementation since

$$\log\sum_{i=1}^{K}\exp(x_i) = x^* - \log\exp(x^*) + \log\sum_{i=1}^{K}\exp(x_i) = x^* + \log\sum_{i=1}^{K}\exp(x_i - x^*) \qquad x^* = \max\{x_1, \ldots, x_K\}$$

Linear Models for Classification

We can write the cross-entropy as

$$
\begin{aligned}
L(\{\hat{y}_n\},\{y_n\}) &= -\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K}\mathbf{1}\left[y_n = k\right]\log \hat{y}_n[k] \\
&= -\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K}\mathbf{1}\left[y_n = k\right]\log \mathrm{softmax}(f(x_n,w,b))[k] \\
&= -\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K}\mathbf{1}\left[y_n = k\right]\left(f(x_n,w,b)[k] - \boxed{\log\sum_{j=1}^{K}\exp}(f(x_n,w,b)[j])\right)
\end{aligned}
$$

This is the *log-sum-exp* operator!
It approximates *maximum* operator.

log-sum-exp permits numerically-efficient (avoid overflow/underflow) implementation since

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\log\sum_{i=1}^{K}\exp(x_i) = x^* - \log\exp(x^*) + \log\sum_{i=1}^{K}\exp(x_i) = x^* + \log\sum_{i=1}^{K}\exp(x_i - x^*) \qquad x^* = \max\{x_1,\ldots,x_K\}
$$

In practice, the *softmax+cross-entropy* is implemented via this log-sum-exp trick!

More About Softmax

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Why?

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Why? Also,

$$\lim_{\beta \to \infty} \text{softmax}(x) = [\frac{1}{K}, \ldots, \frac{1}{K}]$$

β is often called as *temperature*.

References

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Questions?