CPEN 455: Deep Learning

Lecture 2 : 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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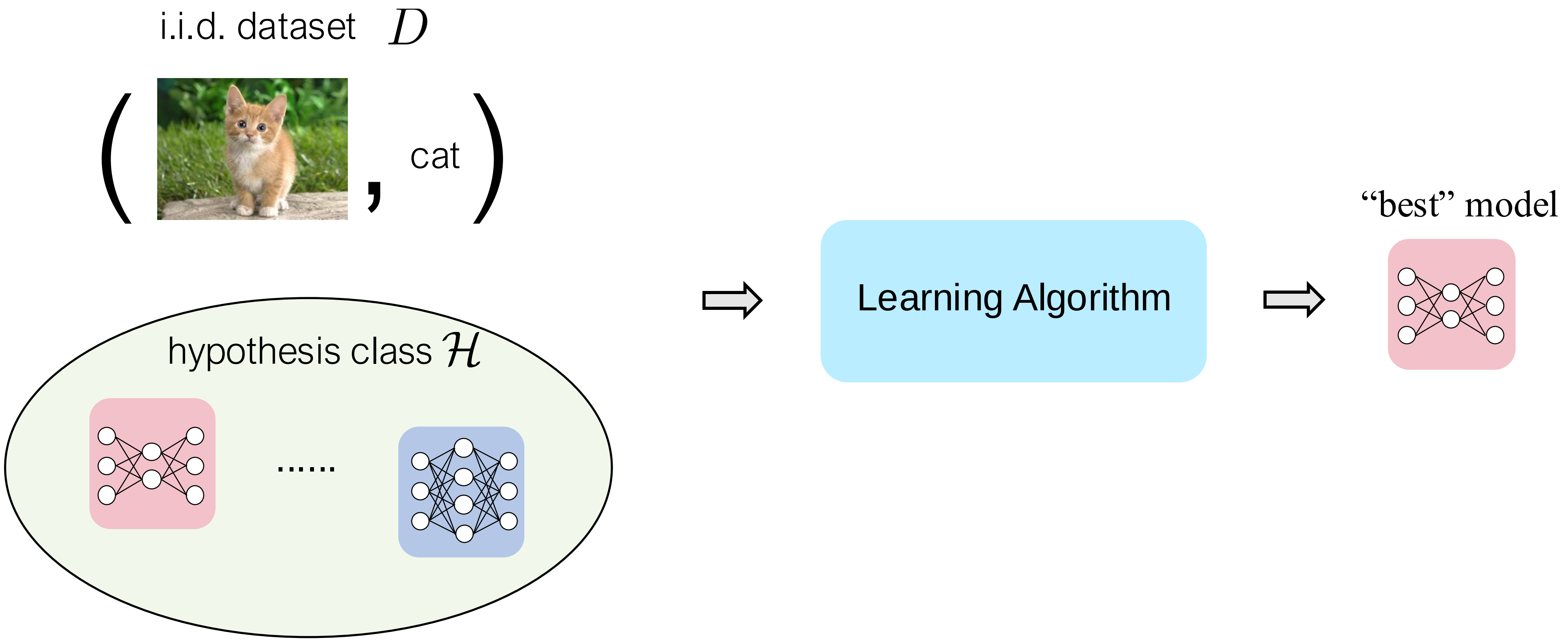
Statistical Learning Setup



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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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Ideally, we want to find a model in the hypothesis class that minimizes the risk:

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

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)

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

$$x_n \in \mathbb{R} \qquad y_n \in \mathbb{R}$$

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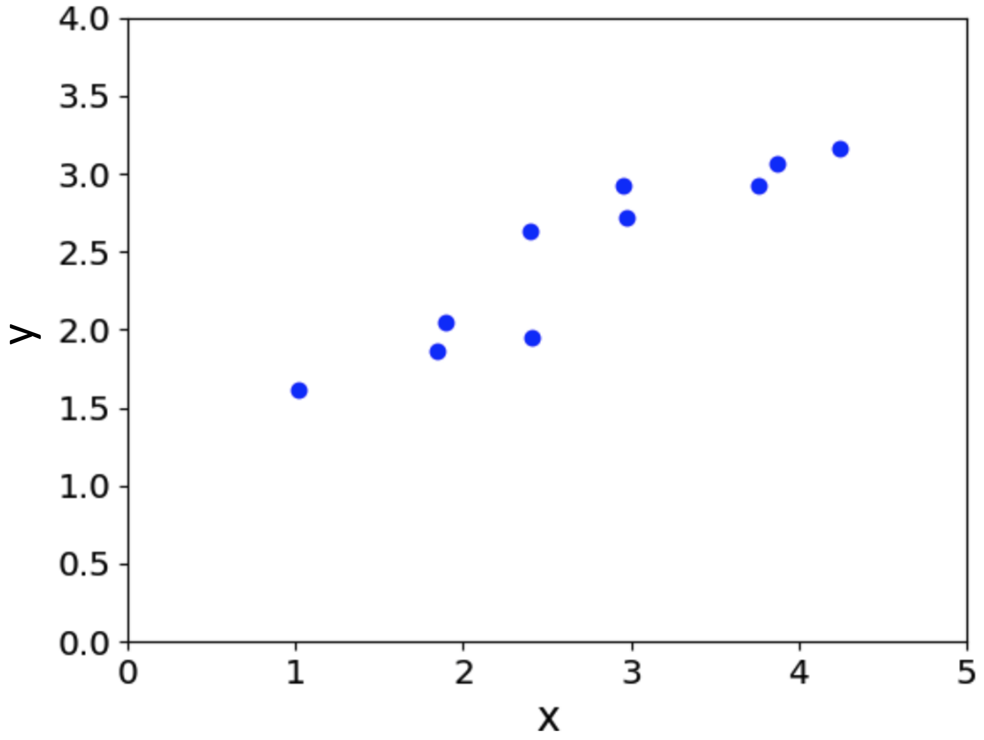

Image Credit: UofT CSC413 Lecture 1

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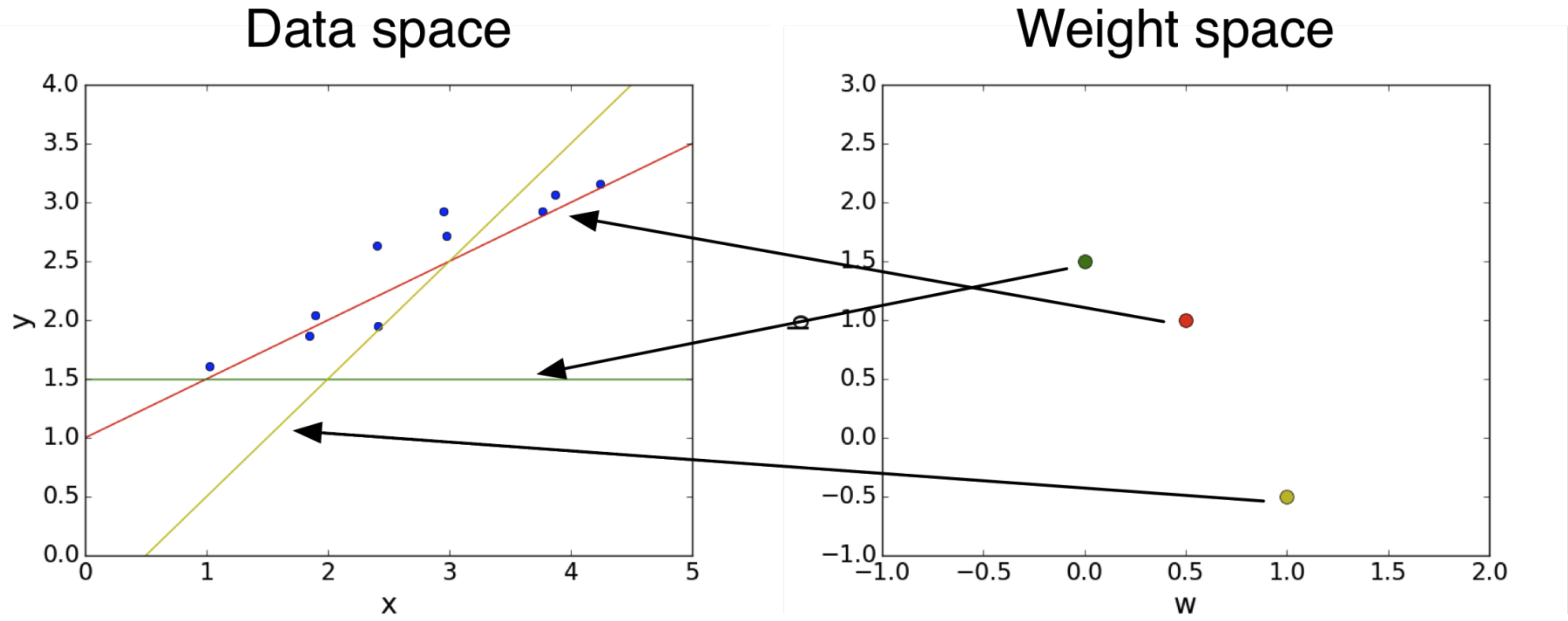

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3) Smooth L1 loss (similar to Huber loss used in robust statistics)

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

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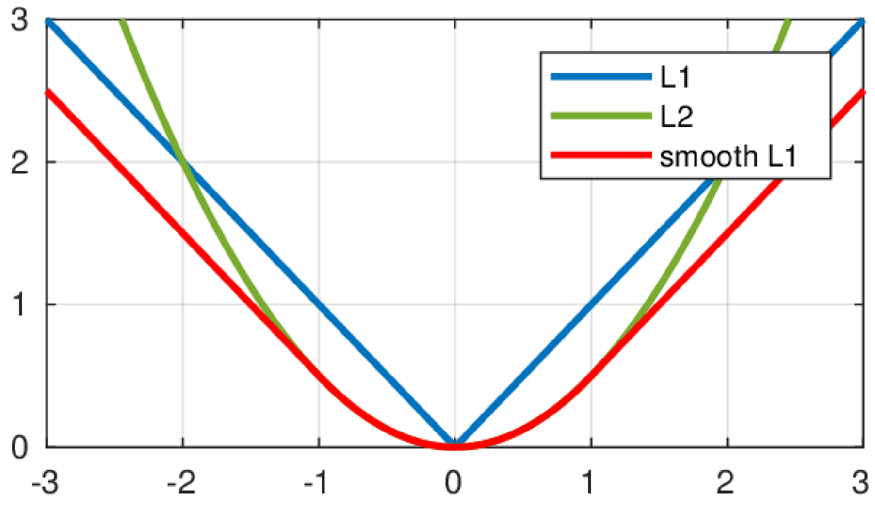

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For our linear models, inference is just: $\hat{y} = w^\top x + b$

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

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$$\min_{f \in \mathcal{H}} \quad \frac{1}{N} \sum_{n=1}^{N} \ell(f(x_n), y_n)$$

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

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

Write in a compact vector form:

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

Linear Regression

- Learning Algorithm

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

$$\frac{\partial L(w,b)}{\partial w[i]} = \sum_{n=1}^{N} \frac{\partial L(w,b)}{\partial l_n}\frac{\partial l_n}{\partial w[i]}$$

$$= \sum_{n=1}^{N} \frac{\partial \frac{1}{2N}\sum_{n=1}^{N} l_n^2}{\partial l_n}\frac{\partial l_n}{\partial w[i]}$$

$$= \frac{1}{2N}\sum_{n=1}^{N} 2l_n \frac{\partial l_n}{\partial w[i]}$$

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

$$= \boxed{\frac{1}{N}\sum_{n=1}^{N} l_n x_n[i]}$$

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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Similarly, we can obtain the partial derivative $\frac{\partial L(w,b)}{\partial b}$ (do it by yourself)

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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.

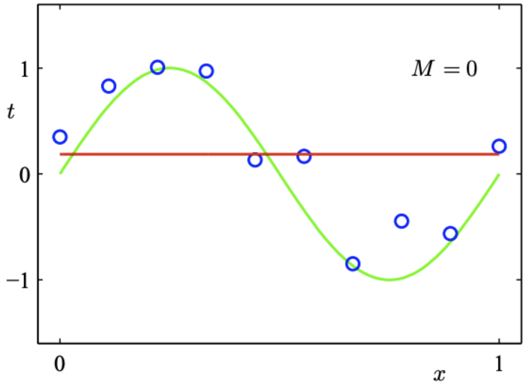
Linear Regression

- Validation and Testing: Overfitting vs. Underfitting

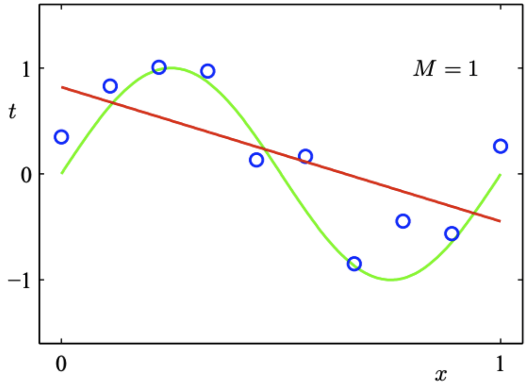
Linear Regression

- Validation and Testing: Overfitting vs. Underfitting

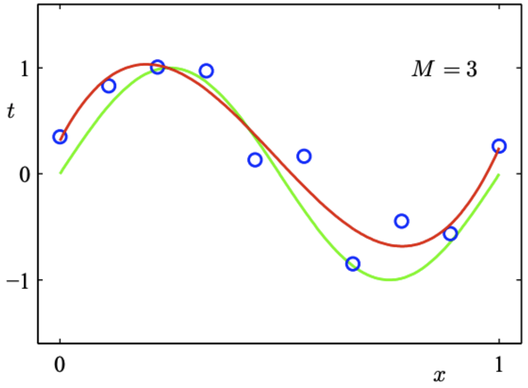
$$y = w_0$$



$$y = w_0 + w_1 x$$



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



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

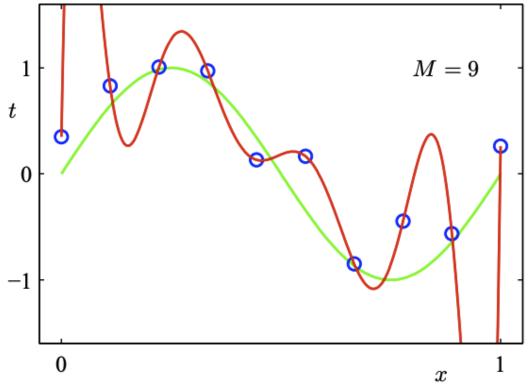


Image Credit: [2]

Linear Regression

- Validation and Testing: Overfitting vs. Underfitting

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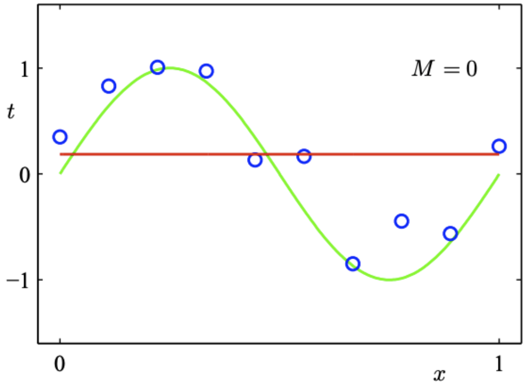

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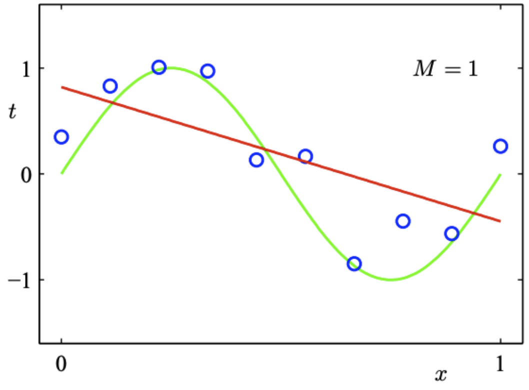

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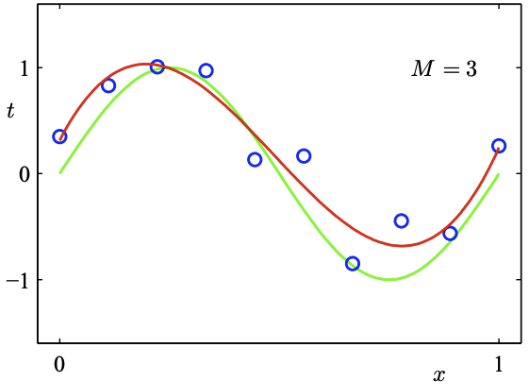

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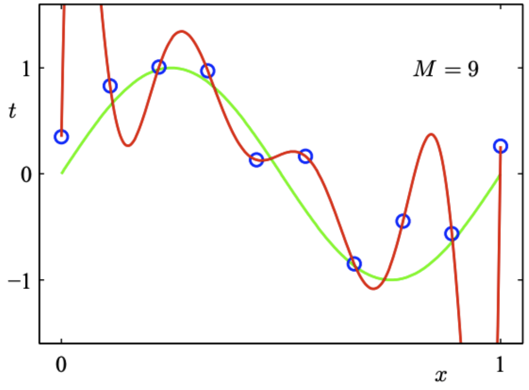

Underfitting:

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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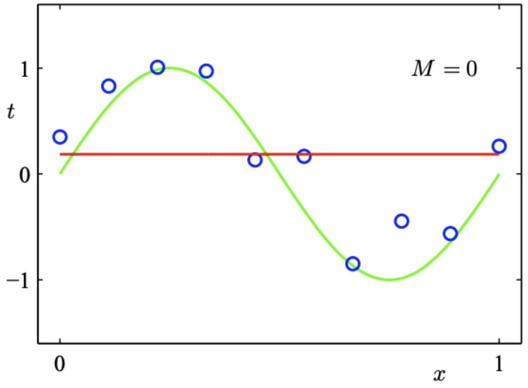

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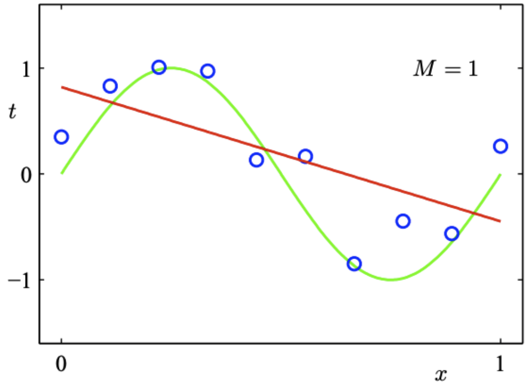

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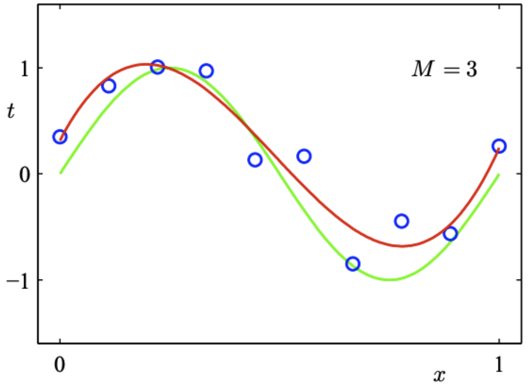

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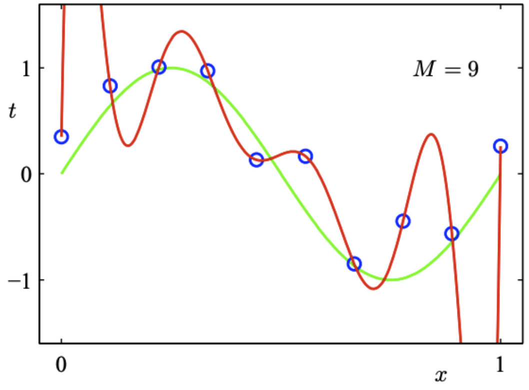

Underfitting:

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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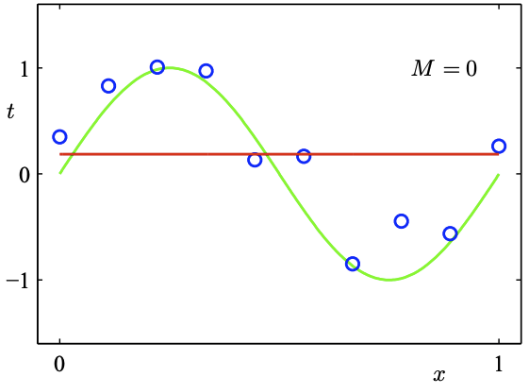

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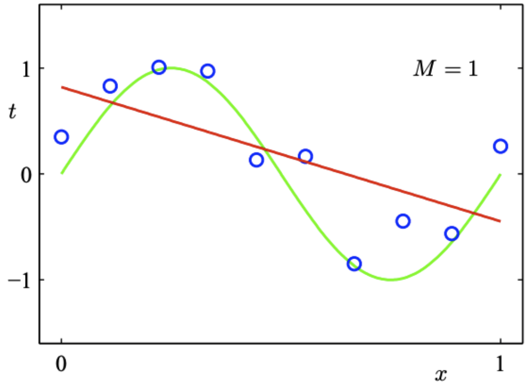

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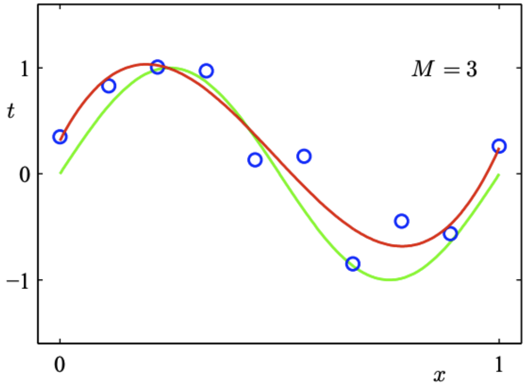

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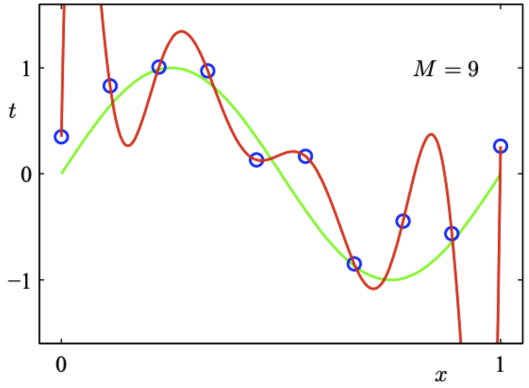

As the degree (complexity) increases, the variance of the model tends to increase, and the bias tends to decrease!

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

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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!

Linear Regression

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Let us decompose it

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

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

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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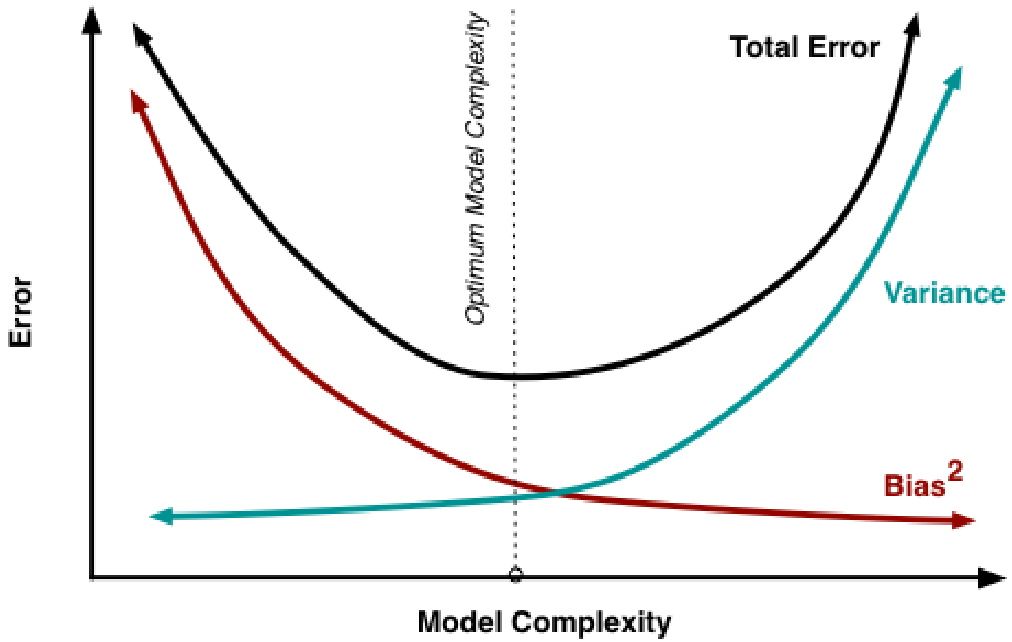

Image Credit: http://scott.fortmann-roe.com/docs/BiasVariance.html

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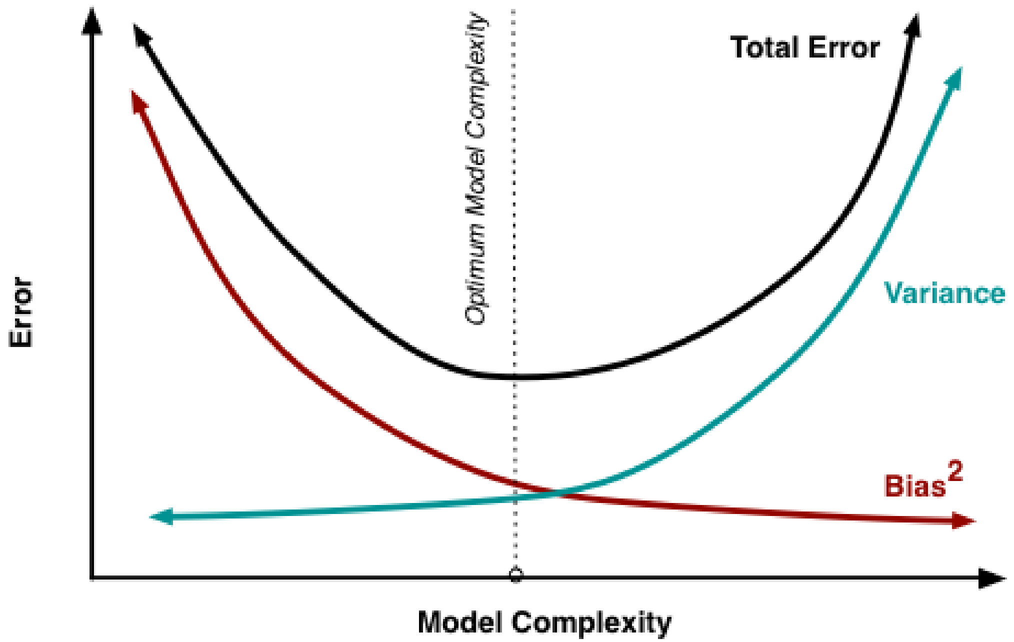

This classic bias-variance tradeoff can not explain deep learning as the model complexity measure is hard to find, e.g., #parameters is clearly not the right one!

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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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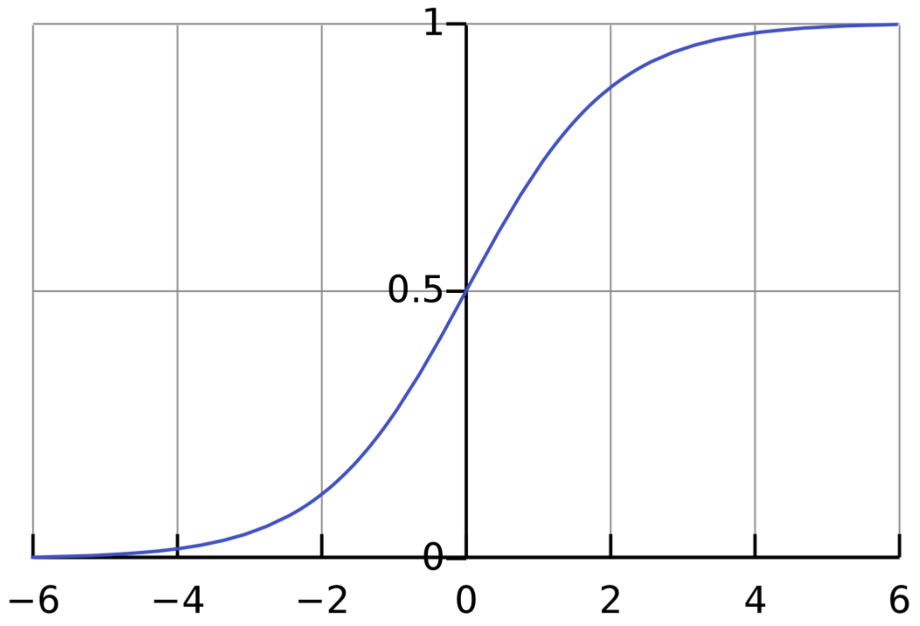

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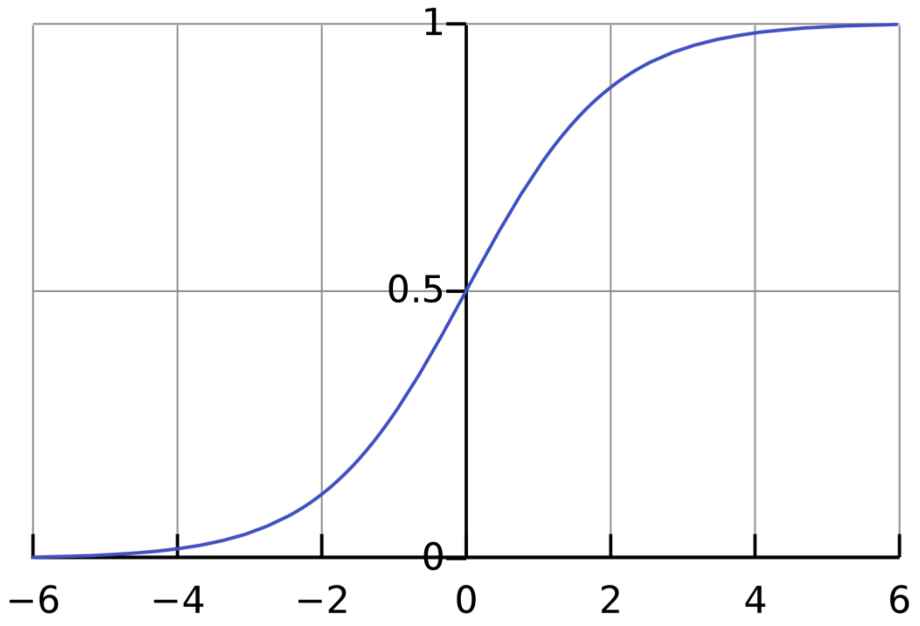

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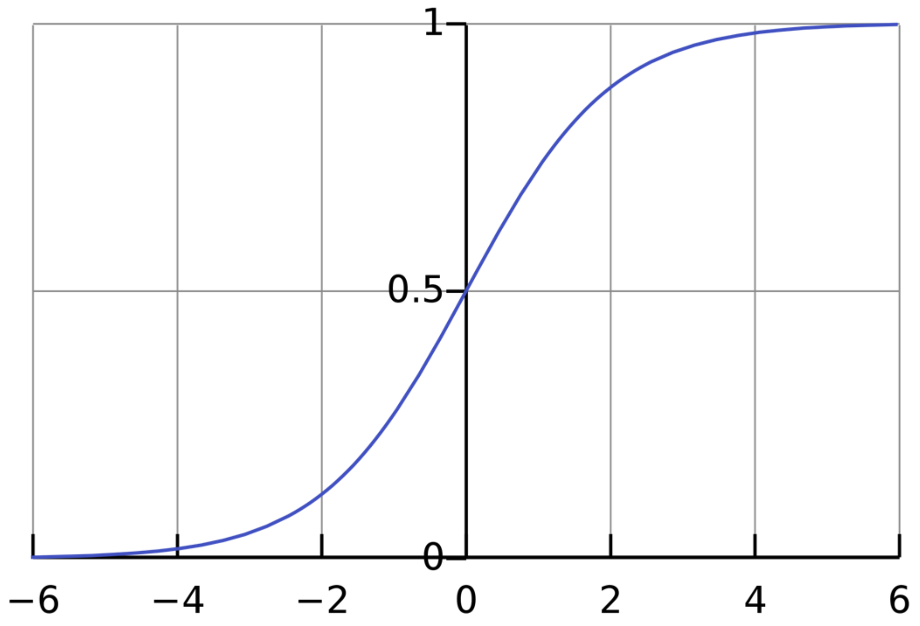
This outputs a probability!



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

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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

$$L(\{\hat{y}_n\}, \{y_n\}) = -\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K} \mathbf{1}\left[y_n = k\right] \log \hat{y}_n[k]$$

$$= -\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K} \mathbf{1}\left[y_n = k\right] \log \mathrm{softmax}(f(x_n, w, b))[k]$$

$$= -\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K} \mathbf{1}\left[y_n = k\right] \left(f(x_n, w, b)[k] - \boxed{\log \sum_{j=1}^{K} \exp}(f(x_n, w, b)[j]) \right)$$

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

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Then softmax becomes

$$\text{softmax}(x)[i] = \frac{\exp(\frac{1}{\beta}x[i])}{\sum_{k=1}^{K} \exp(\frac{1}{\beta}x[k])}$$

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Therefore, *softmax* should actually be called *softargmax*!

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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?