

## Supervised Learning

### Naive Bayes

**Generative model:** model the prior and class-conditional distribution (each class has a particular distribution of features) by observation / assumption to use MLE on class conditional probability and Bayes decision rule (BDR) to get target probability:

$$p(y|x) = \frac{p(x,y)}{p(x)} = \frac{p(x|y) \cdot p(y)}{p(x)} = \frac{p(x|y) \cdot p(y)}{\sum_y p(x|y)} \quad (1)$$

**Naive Bayes:** assume features are independent, i.e.  $p(x = (x_1, x_2)|y) = p(x_1|y)p(x_2|y)$ .

(class) **Model**  $p(y)$ . Bernoulli distribution:  $p(y) = \pi^{\mathbb{1}(y=1)} \cdot (1 - \pi)^{\mathbb{1}(y=0)}$ .

MLE:  $\pi^* = \arg \max_{\pi} \sum_{i=1}^N \log p(y_i) \Rightarrow \pi = \frac{\#(y=1)}{\#(y=0) + \#(y=1)}$ .

(observation) **Model**  $p(x|y)$ . ① Gaussian:  $p(x|y=c) = \frac{1}{\sqrt{2\pi\sigma_c^2}} e^{(-\frac{1}{2\sigma_c^2}(x-\mu_c)^2)}$ .

MLE:  $\mu_c^* = \frac{1}{N} \sum_{i=1}^N x_i, \sigma_c^{*2} = \frac{1}{N} \sum_{i=1}^N (x_i - \mu_c^*)^2. (x_i|y=c)$

② Poisson:  $p(x|y=c) = \frac{1}{x!} e^{-\mu_c} \mu_c^x, x \in \{0, 1, 2, \dots\}, (\mu_c = \bar{x}|y=c)$ .

MLE:  $\mu_c^* = \frac{1}{N} \sum_{i=1}^N x_i. (x_i|y=c)$

Laplace smoothing (smoothed MLE):  $\pi_j = \frac{N_j + \alpha}{N + 2\alpha}$  to prevent overfitting.

### Naive Bayes Example – SMS spam

**Bag-of-Words (BoW) model:** 1. build vocabulary  $\mathcal{V}$ . 2. text  $t$  to vector  $x \in \mathbb{R}^V$  sklearn.feature\_extraction.text.

① count occurrence to vectorize: CountVectorizer(stop\_words=xx, max\_features=xx)

② Term-Frequency (TF):  $x_j = \frac{w_j}{|D|} = \frac{\# \text{word } j}{\# \text{words in document}}$ .

③ TF Inverse Document Frequency (TF-IDF):  $x_j = \frac{w_j}{|D|} \log \frac{N}{N_j}$

IDF( $j$ ) =  $\log \frac{N}{N_j} = \frac{\# \text{documents}}{\# \text{documents with word } j}$ . TfidfVectorizer

④ HashingVectorizer

**NB Gaussian**  $p(x) = \mathcal{N}(x|\mu, \Sigma) = \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} e^{-\frac{1}{2} \|x-\mu\|_\Sigma^2}$

MLE:  $\mu^* = \frac{1}{N} \sum_{i=1}^N x_i, \Sigma^* = \frac{1}{N} \sum_{i=1}^N (x_i - \mu)(x_i - \mu)^T$ .

**NB Multinomial:**  $p(x|y) = \frac{(\sum_j x_j)!}{\prod_j x_j!} \left( \prod_j \pi_{j,y}^{x_j} \right)$ , where  $x_j$  is the frequency of word  $j$  ( $\sum_j x_j = 1$ ),  $\pi_{j,y}$  is the probability of word  $w_j$  in class  $y$  ( $\sum_{j=1}^V \pi_{j,y} = 1$ ).

### $L_1$ & $L_2$

$L_1$  regularization: 1. treat all errors equally 2. encourage more sparsity 3. decision is more likely to be aligned with the coordinate axis

$L_1$  error: robust to outlier, no preference to reduce the larger errors.

## Generative → Discriminative

**Generative:** class-conditional distribution (CCD)  $\xrightarrow{\text{Bayes rule}}$  classifier  $p(y|x)$ , can be used to small dataset.

**Discriminative:** classifier  $p(y|x)$  directly

$$\frac{p(y=1|x)}{p(y=2|x)} > 1 \Leftrightarrow \log \frac{p(y=1|x)}{p(y=2|x)} \stackrel{\text{Bayes}}{=} \log \frac{p(x|y=1)p(y=1)}{p(x|y=2)p(y=2)} > 0 \quad (1)$$

$$\text{sharing } \sigma^2: \log \frac{p(x|y=1)}{p(x|y=2)} = \log \frac{\prod_{i=1}^D \mathcal{N}(x_i|\mu_i, \sigma^2)}{\prod_{i=1}^D \mathcal{N}(x_i|\nu_i, \sigma^2)} = \frac{1}{2\sigma^2} \sum_{i=1}^D [2(\mu_i - \nu_i)x_i - \mu_i^2 + \nu_i^2]$$

$$\frac{p(y=1|x)}{p(y=2|x)} > 1 \Leftrightarrow \underbrace{\sum_{i=1}^D \frac{1}{\sigma^2} (\mu_i - \nu_i) x_i}_{w_i} + \underbrace{\frac{1}{2\sigma^2} \sum_{i=1}^D (\nu_i^2 - \mu_i^2)}_b + \log \frac{\pi_1}{\pi_2} > 0 \quad (2)$$

## Linear (Binary) Classifier

$$f(x) = w^\top x + b. f(x) > 0 \rightarrow \text{class 1} (y=1), f(x) < 0 \rightarrow \text{class 2} (y=-1)$$

## Logistic Regression (Binary) Classifier

$$f(x) = w^\top x + b, \sigma(z) = \frac{1}{1+e^{-z}}, p(y|x) = \sigma(y \cdot f(x)):$$

$$p(y=+1|x) = \sigma(f(x)), \quad p(y=-1|x) = 1 - \sigma(f(x)) = \sigma(-f(x)) \quad (3)$$

$$\text{MLE: } (w^*, b^*) = \arg \max_{w,b} \sum_{i=1}^N \log p(y_i|x_i) = \arg \min_{w,b} \sum_{i=1}^N \log(1 + e^{-y_i f(x_i)})$$

$z_i \triangleq y_i f(x_i) > 0 \Rightarrow \text{classified correctly}, z_i < 0 \Rightarrow \text{wrongly}, z_i = 0 \Rightarrow \text{boundary}$   
Logistic regression only forms a linear decision surface.

Logistic loss function:  $L(z_i) = \log(1 + \exp(-z_i))$ . convex  $\rightarrow$  one optimum

$$\text{Regularization: } (w^*, b^*) = \arg \max_{w,b} \left[ \log p(w) + \sum_{i=1}^N \log p(y_i|x_i) \right].$$

① Gaussian:  $p(w) = \mathcal{N}(0, \frac{C}{2} I) \Rightarrow \log p(w) = -\frac{1}{2} w^\top w + \text{constant}$

$$\Rightarrow (w^*, b^*) = \arg \max_{w,b} \frac{1}{C} w^\top w + \sum_{i=1}^N \log(1 + \exp(-y_i f(x_i))), : w^\top w = \sum_{j=1}^d w_j^2.$$

Large  $C \rightarrow$  big  $w \Leftrightarrow$  Small  $C \rightarrow$  small  $w$ . Equal to  $L_1$  regularization.

## Multiclass logistic regression

$$p(y=c|x) = \text{softmax}(f(x)) = \frac{e^{f_c(x)}}{e^{f_1(x)} + \dots + e^{f_K(x)}}, f_c(x) = w_c^\top x. \quad (4)$$

MLE: ① likelihood:  $p(y|x) = \prod_{j=1}^K p(y=j|x)^{y_j}$ . ② log-likelihood:  $\log p(y|x)$ .

③ (min) cross-entropy loss:  $-\log p(y|x) = -\sum_{j=1}^K y_j \log p(y=j|x)$

$$\max_{\{w_j\}} \sum_{i=1}^N \log p(y_i|x_i) = \max_{\{w_j\}} \sum_{i=1}^N \sum_{j=1}^K y_{ij} \log p(y=j|x_i) \quad (5)$$

where  $y = [y_1, \dots, y_K]$  is one-hot vector.

## Support Vector Machine (SVM)

Margin distance:  $\gamma = \min_i d_i = \min_i \frac{|f(x_i)|}{\|w\|} = \min_i \frac{|w^\top x_i + b|}{\|w\|}$

Support vector: points on  $y = w^\top x + b$ .

Normalization:  $\frac{|aw^\top x_i + ab|}{\|aw\|} = \frac{|w^\top x_i + b|}{\|w\|} \Rightarrow$  just let  $f(x_i) = w^\top x_i + b = 1$ .

Maximize margin:  $(\hat{w}, b) = \arg \max_{w,b} \frac{1}{\|w\|} \text{ s.t. } \min_i |f(x_i)| = 1$

$\Leftrightarrow (\hat{w}, b) = \arg \min_{w,b} \frac{1}{2} \|w\|^2 = \frac{1}{2} w^\top w \text{ s.t. } y_i f(x_i) \geq 1, \forall i. \text{ (for binary class)}$

Lagrangian:  $L(x, \lambda) = f(x) - \lambda g(x)$

$\Rightarrow$  SVM dual:  $\min L(w, \alpha) = \frac{1}{2} w^\top w - \sum_i \alpha_i [y_i(w^\top x_i + b) - 1], w = \sum_{i=1}^N \alpha_i y_i x_i$

$$\arg \max_{\alpha} \sum_i \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j x_i^\top x_j \text{ s.t. } \sum_{i=1}^N \alpha_i y_i = 0, \quad \alpha_i \geq 0 \quad (1)$$

non-separable data:  $(\hat{w}, b) = \arg \min_{w,b} \frac{1}{2} w^\top w, \text{ s.t. } y_i f(x_i) \geq 1 - \xi_i, \xi_i \geq 0, \forall i$

soft-SVM:  $(\hat{w}, b) = \arg \min_{w,b} \frac{1}{2} w^\top w + \sum_{i=1}^N C \xi_i, \text{ s.t. } y_i f(x_i) \geq 1 - \xi_i, \xi_i \geq 0, \forall i$

objective function:  $\arg \min_{w,b} \frac{1}{C} w^\top w + \sum_{i=1}^N \max(0, 1 - y_i f(x_i))$   
hinge loss

prediction: need training data to calculate similarity  $f(x) = \sum_i \alpha_i y_i k(x_i, x) + b$ .

## Tricks

① Normalization for Logistic regression and SVM, due to their sensitivity to absolute value. ② Apply weights to loss of unbiased data. ③ Bigger weights to loss of more important class. ④ Change threshold to one class.

## Kernel SVM

idea: learn linear classifier in high-dim space  $\phi(x) \in \mathbb{R}^D$  rather than  $x \in \mathbb{R}^d$   
kernel function:  $k(x_i, x_j) = \phi(x_i)^\top \phi(x_j)$ , which is  $x_i^\top x_j$  in dual SVM

example: ① polynomial kernel:  $k(x, x') = (x^\top x')^p = (\sum_{i=1}^d x_i x'_i)^p$

② RBF(radial basis function):  $k(x, x') = e^{-\gamma \|x-x'\|^2}$ .  $\gamma \uparrow$ : smooth function.

③ Laplacian kernel:  $k(x, x') = \exp(-\alpha \|x-x'\|)$

kernel SVM:  $\hat{y} = \text{sign}(\sum_{i=1}^N \alpha_i y_i k(x_i, x) + b)$ , where

$$\alpha = \arg \max_{\alpha} \sum_i \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j k(x_i, x_j) \text{ s.t. } \sum_{i=1}^N \alpha_i y_i = 0, \quad \alpha_i \geq 0 \quad (2)$$

Kernel matrix:  $K = [k(x_i, x_j)]_{i,j}$ , where  $k(x_i, x_j) = \phi(x_i)^\top \phi(x_j)$ .

$K$  is a positive semi-definite matrix, i.e.  $z^\top K z \geq 0, \forall z$ .

Kernel computation for high dimension is of high cost. Memory usage is based on the number of support vectors kept.

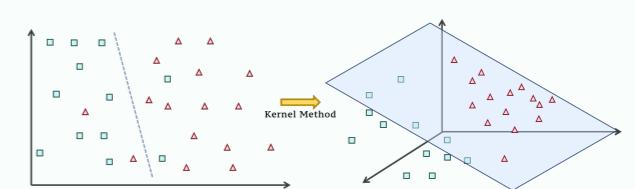


Figure 1: Kernel trick

## Regression

**Linear Regression.**  $\hat{y} = w_0 + w_1x_1 + \dots + w_dx_d = \mathbf{w}^\top \mathbf{x} = f(\mathbf{x}_i)$ , where  $\mathbf{w} = [w_0, w_1, \dots, w_d]^\top$ ,  $\mathbf{x} = [1, x_1, \dots, x_d]^\top$   
**Ordinary Least Squares (OLS).**  $\min_{\mathbf{w}} \sum_{i=1}^N (y_i - f(\mathbf{x}_i))^2 = \min_{\mathbf{w}} \|\mathbf{y} - \mathbf{X}^\top \mathbf{w}\|^2$ , where  $\mathbf{X} = [x_1 \dots x_N]$  is the data matrix,  $\mathbf{y} = [y_1, \dots, y_N]$ .  
 $\Rightarrow \min_{\mathbf{w}} \mathbf{y}^\top \mathbf{y} - 2\mathbf{y}^\top \mathbf{X}^\top \mathbf{w} + \mathbf{w}^\top \mathbf{X} \mathbf{X}^\top \mathbf{w} \Rightarrow \mathbf{w}^* = (\mathbf{X} \mathbf{X}^\top)^{-1} \mathbf{X}$ , i.e. *pseudo-inverse*

**Ridge Regression.**  $\min_{\mathbf{w}} \alpha \|\mathbf{w}\|_2^2 + \sum_{i=1}^N (y_i - f(\mathbf{x}_i))^2$ , where  $\|\mathbf{w}\|_2^2 = \sum_{j=0}^d w_j^2$   
 $\Rightarrow \mathbf{w}^* = (\mathbf{X} \mathbf{X}^\top + \alpha \mathbf{I})^{-1} \mathbf{X} \mathbf{y}$ . (In OLS,  $\mathbf{X} \mathbf{X}^\top$  may be non-invertible)

**LASSO** (*Least absolute shrinkage and selection operator*).  $\min_{\mathbf{w}} \alpha \|\mathbf{w}\|_1 + \sum_{i=1}^N (y_i - f(\mathbf{x}_i))^2$ , where  $\|\mathbf{w}\|_1 = \sum_{j=0}^d |w_j|$ . LASSO encourage more sparsity

**Sparsity Constraints.**  $\min_{\mathbf{w}} \sum_{i=1}^N (y_i - f(\mathbf{x}_i))^2$ , s.t.  $\|\mathbf{w}\|_0 \leq K$ , where  $\|\mathbf{w}\|_0 = \# \text{non-zero entries}$ . nonconvex and NP-hard v.s. Ridge and LASSO are convex

**OMP (Orthogonal Matching Pursuit).** Iteratively and greedily selects the most related feature to current residual error.

### Algorithm 1 Orthogonal Matching Pursuit (OMP)

- 1: Initialize the residual:  $\mathbf{r} = \mathbf{y}$
- 2: **for**  $t = 1$  to  $K$  **do**
- 3: Find the most correlated feature:  $j = \arg \max_j |\mathbf{r}^\top \mathbf{x}_j|$ , where  $\mathbf{x}_j$  is the  $j$ -th row of  $\mathbf{X}$  (the  $j$ -th feature).
- 4: Compute the weight:  $w_j = \arg \min_{w_j} \|\mathbf{r} - \mathbf{x}_j w_j\|^2$
- 5: Update the residual:  $\mathbf{r} = \mathbf{r} - \mathbf{x}_j w_j$
- 6: **end for**

**RANSAC (RANdom SAmple Consensus).** Split the data into inliers (good data) and outliers (bad data) and learn the model only from the inliers.

### Algorithm 2 RANSAC (Random Sample Consensus)

- 1: **Given:** training set  $D = \{\mathbf{x}_i, y_i\}$ , threshold  $\epsilon$ , loss function  $L = \sum l(x, y)$
- 2: Classify all data as inlier or outlier by calculating the prediction errors  $l$  and comparing to the threshold  $\epsilon$ . (typically set as the median absolute deviation (MAD) of  $y$ , i.e.  $\text{median}(|y_i - \text{median}(y)|)$ )
- 3: The set of inliers is called the *consensus set*.
- 4: Save the model with the highest number of inliers.
- 5: Use the largest consensus set to learn the final model.

**Nonlinear Regression.**  $\hat{y} = \mathbf{w}^\top \phi(\mathbf{x})$ , where  $\mathbf{w} = [w_0, w_1, \dots, w_d]^\top$ .

**Kernel Ridge Regression.**  $\min_{\mathbf{w}} \|\mathbf{y} - \Phi \mathbf{w}\|_2^2 + \lambda \|\mathbf{w}\|_2^2$ , where  $\Phi = [\phi(\mathbf{x}_1), \dots, \phi(\mathbf{x}_N)]^\top \in \mathbb{R}^{N \times d}$ ,  $\mathbf{w} \in \mathbb{R}^d \Rightarrow \mathbf{w} = (\Phi^\top \Phi + \lambda \mathbf{I})^{-1} \Phi^\top \mathbf{y} \Rightarrow \hat{y} = \hat{k}^\top (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{y}$ , where  $\mathbf{K} = [\mathbf{k}(\mathbf{x}_i, \mathbf{x}_j)] \in \mathbb{R}^{N \times N}$ ,  $\hat{k} = [\mathbf{k}(\mathbf{x}_1, \hat{\mathbf{x}}), \dots, \mathbf{k}(\mathbf{x}_N, \hat{\mathbf{x}})]^\top \in \mathbb{R}^N$ .

**Gaussian Process Regression (GPR).** Gaussian process: an sequential random variable set whose any finite subset is joint Gaussian distributed.  $f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$  where  $f, m, k$  are value, mean and covariance function separately.  $f_1, \dots, f_N | \mathbf{x}_1, \dots, \mathbf{x}_N \sim \mathcal{N}(0, K)$ , where  $K$  is the kernel matrix.

**GPR:** ① observation noise:  $y = f + \epsilon, \epsilon \sim \mathcal{N}(0, \sigma^2)$ ,  $p(y|f) = \mathcal{N}(y|f, \sigma^2 I)$   
 ② function prior:  $f \sim \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}'))$  ③ train:  $p(f|X, y) = \frac{p(y|X, f)p(f|X)}{p(y|X)} = \frac{p(y|f)p(f)}{p(y|X)}$   
 ④ inference:  $p(\hat{f}|\hat{\mathbf{x}}, X, y) = \int p(\hat{f}|\hat{\mathbf{x}}, f)p(f|X, y)df$ . ⑤ prediction:  $p(f_*|\mathbf{x}_*, X, y) = \mathcal{N}(f_*|\mu_*, \sigma_*^2)$ ,  $\mu_* = \mathbf{k}_*^\top (\mathbf{K} + \sigma^2 I)^{-1} \mathbf{y}$ ,  $\sigma_*^2 = k_{**} - \mathbf{k}_*^\top (\mathbf{K} + \sigma^2 I)^{-1} \mathbf{k}_*$ , where  $k_{**} = \mathbf{k}(\mathbf{x}_*, \mathbf{x}_*)$ .

**Support Vector Regression (SVR).** ① objective:  $\min_{\mathbf{w}, b} \sum_{i=1}^N |y_i - (\mathbf{w}^\top \mathbf{x}_i + b)|_\epsilon$

$$+ \frac{1}{C} \|\mathbf{w}\|^2, \text{ where } |z|_\epsilon = \begin{cases} 0, & |z| \leq \epsilon \\ |z| - \epsilon, & |z| > \epsilon \end{cases}$$

## Regression – Model Ensemble

Idea: combine multiple regression model together to form a better algorithm.

① **bagging**: train multiple models from random selection of training data. ② **boosting**: train multiple models which focus on errors made by previous one.

① **Random Forest Regression**. Use **bagging** to make an ensemble of *Decision Tree Regressor*. Random subset of data is used to train different tree, whose nodes use different features. The prediction is the average value of each tree.  
**RFR is sensitive to outliers.**

② **XGBoost Regression**. (*eXtreme Gradient Boosting*) Use **boosting** to combine a set of less accurate models to create a accurate model. Weak learner fits the gradient of the loss:  $h_t(\mathbf{x}) \approx \frac{dL}{df}, f_t(\mathbf{x}) = f_{t-1}(\mathbf{x}) - \alpha_t h_t(\mathbf{x}) \approx f_{t-1}(\mathbf{x}) - \alpha_t \frac{dL}{df_{t-1}}$ .  
**XGBoost / AdaBoost can run in parallel.**

## Tricks

Improve accuracy: more features + complex features + complex model

## Neural Network

### Neural Network

**Perceptron.** Model a single neuron  $y = f(\mathbf{w}^\top \mathbf{x}) = f(\sum_{j=0}^d w_j x_j) = \begin{cases} 1 & \text{if } \mathbf{w}^\top \mathbf{x} \geq 0 \\ -1 & \text{otherwise} \end{cases}$ , loss:  $E(w) = \sum_{i=1}^N L(z_i) = \sum_{i=1}^N \max(0, -z_i)$ ,  $z_i = y_i \mathbf{w}^\top \mathbf{x}_i$ .

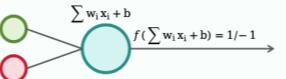


Figure 1: One perceptron

**Perceptron Alg. / SGD.**  $w \leftarrow w + \eta y_i x_i = w - \eta g_w(x_i)$ , where  $x_i$  is misclassified  
**Result (1st in ML):** 1. only converge on linearly separable data; 2. # iteration  $\sim \frac{1}{m}$ , where  $m$  is the separation (margin) between classes.

Multi-layer Perceptron now called *neural network*.

**Multi-class Logistic regression.** class labels  $y \in \{1, \dots, C\}$ , class vector  $\mathbf{y} \in \mathbb{R}^C$  is one-hot vector. Output  $p(y = j|\mathbf{x}) = f_j(\mathbf{x}) = s_j(g(\mathbf{x})) = \frac{\exp(g_j(\mathbf{x}))}{\sum_{k=1}^C \exp(g_k(\mathbf{x}))}$ ,  $g_j(\mathbf{x}) = \mathbf{w}_j^\top \mathbf{x}$ , for  $j \in \{1, \dots, C\}$ .

**MLE:**  $\log p(\mathbf{y}|\mathbf{x}) = \log \prod_{j=1}^C f_j(\mathbf{x})^{y_j} = \sum_{j=1}^C y_j \log f_j(\mathbf{x}) = \mathbf{y}^\top \log f(\mathbf{x})$

$\mathbf{W}^* = \arg \max_{\mathbf{W}} \sum_{i=1}^N \log p(y_i|\mathbf{x}_i) = \arg \max_{\mathbf{W}} \sum_{i=1}^N \mathbf{y}_i^\top \log f(\mathbf{x}_i) = \arg \min_{\mathbf{W}} \sum_{i=1}^N \{-\sum_{j=1}^C y_{ij} \log f_j(\mathbf{x}_i)\}$ .

**cross-entropy loss:**  $L(\mathbf{y}, \mathbf{f}) = -\sum_{j=1}^C y_j \log f_j(\mathbf{x})$ .

**chain rule:**  $\frac{dL}{dw_j} = \frac{dL}{dg} \frac{dg}{dw_j} = \frac{dL}{df} \frac{df}{dg} \frac{dg}{dw_j} = \mathbf{x}(f_j(\mathbf{x}) - y_j)$ .

**Multi-layer Perceptron(MLP).** Add hidden layers between inputs and outputs.  $\mathbf{h} = f(\mathbf{W}^\top \mathbf{x})$ , where  $f(\cdot)$  is the *activation function*.

**Activation function:** ① Sigmoid:  $\mathbb{R} \mapsto [0, 1], f(x) = \frac{1}{1+e^{-x}}$  ② Tanh:  $\mathbb{R} \mapsto [-1, 1], f(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$  ③ Rectifier Linear Unit (ReLU):  $f(x) = \max(0, x)$ .

**Overfitting:** the training loss decreases, but the validation loss increases.

**Early stopping:** stop training when the validation loss is stable (change below a threshold) for a number of iterations to prevent overfitting.

**Universal Approximation Theorem:** A MLP with one hidden layer and finite nodes can approximate any continuous function up to a desired error.

**Vanishing Gradient problem:** Backprop recursively multiplies gradients causing numerical values get smaller.