

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

(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 \rightarrow 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

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

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

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

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

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

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

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

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

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

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

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

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

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)

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

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

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

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

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

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

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

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

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

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

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

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.

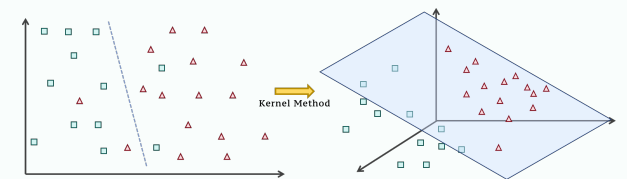


Figure 1: Kernel trick

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 $\mathbf{X} = [\mathbf{x}_1 \cdots \mathbf{x}_N]$ is the data matrix, $\mathbf{y} = [y_1, \dots, y_N]$.

$\Rightarrow \min_{\mathbf{w}} \mathbf{y}^\top \mathbf{y} - 2\mathbf{y}^\top \mathbf{X}^\top \mathbf{w} + \mathbf{w}^\top \mathbf{X} \mathbf{X}^\top \mathbf{w} \Rightarrow \mathbf{w}^* = (\mathbf{X} \mathbf{X}^\top)^{-1} \mathbf{X} \mathbf{y}$, 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 $\|\mathbf{w}\|_0 = \#$ 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: $j = \arg \max_j |r^T \mathbf{x}_j|$, 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 ϵ , loss function $L = \sum l(\mathbf{x}, y)$
- 2: Classify all data as inlier or outlier by calculating the prediction errors l and comparing to the threshold ϵ . (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 $\Phi = [\phi(\mathbf{x}_1), \dots, \phi(\mathbf{x}_N)]^\top \in \mathbb{R}^{N \times d}$, $\mathbf{w} \in \mathbb{R}^d \Rightarrow \mathbf{w} = (\Phi^\top \Phi + \lambda \mathbf{I})^{-1} \Phi^\top \mathbf{y} \Rightarrow \hat{y} = \hat{\mathbf{k}}^\top (K + \lambda \mathbf{I})^{-1} \mathbf{y}$, where $K = [k(\mathbf{x}_i, \mathbf{x}_j)] \in \mathbb{R}^{N \times N}$, $\hat{\mathbf{k}} = [k(\mathbf{x}_1, \hat{\mathbf{x}}), \dots, k(\mathbf{x}_N, \hat{\mathbf{x}})]^\top \in \mathbb{R}^N$.

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. $f_1, \dots, f_N | x_1, \dots, x_N \sim \mathcal{N}(0, K)$, where K is the kernel matrix.

GPR: ① observation noise: $y = f + \epsilon, \epsilon \sim \mathcal{N}(0, \sigma^2)$, $p(y|f) = \mathcal{N}(y|f, \sigma^2 \mathbf{I})$
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: $p(f_*|\mathbf{x}_*, X, y) = \mathcal{N}(f_*|\mu_*, \sigma_*^2)$, $\mu_* = \mathbf{k}_*^T (\mathbf{K} + \sigma^2 \mathbf{I})^{-1} \mathbf{y}$, $\sigma_*^2 = k_{**} - \mathbf{k}_*^T (\mathbf{K} + \sigma^2 \mathbf{I})^{-1} \mathbf{k}_*$, where $k_{**} = k(\mathbf{x}_*, \mathbf{x}_*)$.

Support Vector Regression (SVR). ① objective: $\min_{w, b} \sum_{i=1}^N |y_i - (w^\top \mathbf{x}_i + b)|_\epsilon$
 $+ \frac{1}{C} \|\mathbf{w}\|^2$, 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: $h_t(\mathbf{x}) \approx \frac{dL}{d\hat{f}}, f_t(\mathbf{x}) = f_{t-1}(\mathbf{x}) - \alpha_t h_t(\mathbf{x}) \approx f_{t-1}(\mathbf{x}) - \alpha_t \frac{dL}{d\hat{f}_{t-1}}$.
XGBoost / AdaBoost can run in parallel.

Tricks

Improve accuracy: more features + complex features + complex model

Neural Network

Neural Network

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

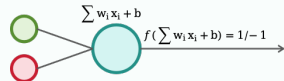


Figure 1: One perceptron

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 $p(y = j|x) = f_j(\mathbf{x}) = s_j(\mathbf{g}(\mathbf{x})) = \frac{\exp(g_j(\mathbf{x}))}{\sum_{k=1}^C \exp(g_k(\mathbf{x}))}$, $g_j(\mathbf{x}) = \mathbf{w}_j^T \mathbf{x}$, for $j \in \{1, \dots, C\}$.

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

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

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. $\mathbf{h} = f(\mathbf{W}^T \mathbf{x})$, 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.