

机器学习

- Model
+
Introduction
- linear, logistic
 - SVM (soft margin)
 - NN, CNN
 - tree
 - Bayesian
 - Clustering
 - Ensemble

Optimization:

GD: $\beta = G, Z = BX$

$$\frac{\partial L}{\partial \beta} = \frac{\partial L}{\partial G(\beta)} \cdot \frac{\partial G(\beta)}{\partial \beta} = -\sum_i \frac{y_i}{G(\beta)} - \frac{(1-y_i)}{1-G(\beta)} \cdot G(\beta) \cdot (1-G(\beta)) \cdot X_i$$

$$= -\sum_i [y_i - G(\beta)] \cdot X_i$$

Matrix: $\frac{\partial L}{\partial \beta} = X(G(X\beta) - Y)$

注意维数: $X \in \mathbb{R}^{n \times d}, Y \in \mathbb{R}^{n \times 1}$

L1 Linear

1) Model: 有时间看一眼
 $\hat{y} = w^T x + b$ PPT 非 matrix 的推导

$$\Rightarrow \hat{y} = X\hat{w}$$

$$\hat{w} = (w; b), X = (x, 1)$$

2) Loss: m 个样本, $x \in \mathbb{R}^{d \times 1}$

$$\text{MSE Loss: } \hat{y} = X\hat{w}$$

$$L = \sum_{i=1}^m (y_i - \hat{y}_i)^2$$

$$= (y - X\hat{w})^T (y - X\hat{w})$$

3) Optimization

① Closed Form **看下矩阵求导.**
 \Rightarrow 一定要检查维度.

$$\frac{\partial L}{\partial \hat{w}} = 2X^T(X\hat{w} - y) = 0$$

$$\Rightarrow \hat{w} = (X^T X)^{-1} X^T y$$

② Gradient Descent / SGD \uparrow

$$\hat{w} \leftarrow \hat{w} - \alpha \nabla_{\hat{w}} L(\hat{w}) \Rightarrow \hat{w}^T (X\hat{w} - y)$$

GD: 整个数据集 X, y 且 $(X^T - y)X$

SGD: 随机取一个样本, 直到收敛. $(X^T - y)_k X_k$

Loss 有时会 \downarrow

③ Logistic Regression **看根部解**

无 prior assumption **本质是让**

$$\hat{y} = G(w^T x + b) = \frac{1}{1+e^{-w^T x}}$$

$$G(x) = \frac{1}{1+e^{-x}}, G'(x) = G(x)(1-G(x))$$

Loss: softmax 软件 $i=1, 2, \dots, n$

由 MLE 导出: likelihood: $L(w, b) = \prod_{i=1}^n p(y_i | x_i; w, b)$

$$p(y_i | x_i; w, b) = y_i p(x_i; \hat{w}) + (1-y_i) p(x_i; \hat{w})$$

$$p(x_i; \hat{w}) = \frac{1}{1+e^{-\hat{w}^T x_i}}$$

$$p(x_i; \hat{w}) = 1 - \hat{y}_i = 1 - G(x_i)$$

$$\text{Loss: } \min_{w, b} \sum_{i=1}^m -(y_i \log p_{ii} + (1-y_i) \log p_{ii})$$

$$= \frac{1}{1+e^{-\hat{w}^T x_i}}$$

$$-\sum_{i=1}^m y_i \hat{w}^T x_i - \log(1+e^{\hat{w}^T x_i})$$

Optimization:

GD: $\beta = G, Z = BX$

$$\frac{\partial L}{\partial \beta} = \frac{\partial L}{\partial G(\beta)} \cdot \frac{\partial G(\beta)}{\partial \beta} = -\sum_i \frac{y_i}{G(\beta)} - \frac{(1-y_i)}{1-G(\beta)} \cdot G(\beta) \cdot (1-G(\beta)) \cdot X_i$$

$$= -\sum_i [y_i - G(\beta)] \cdot X_i$$

Matrix: $\frac{\partial L}{\partial \beta} = X(G(X\beta) - Y)$

注意维数: $X \in \mathbb{R}^{n \times d}, Y \in \mathbb{R}^{n \times 1}$

到 SVM 上: $(x_i - x_j) \cdot \|w\|$

$$\text{Margin: } \frac{2}{\|w\|} \Rightarrow (1-b+1+b) \cdot \frac{1}{\|w\|}$$

① Model: $w^T x + b = \begin{cases} 0 & \rightarrow \text{超平面, 分类} \\ \geq 1, \text{ 正 SV} & \rightarrow 1, \text{ 正类} \\ \leq -1, \text{ 负 SV} & \rightarrow -1, \text{ 负类} \\ (-1, 1), \text{ Margin} & \end{cases}$

② Loss: $\max_{w, b} \min_{x} \text{Hard Margin}$

$$\arg \min_{w, b} \frac{1}{2} \|w\|^2 \rightarrow \text{margin 最大}$$

$$\text{s.t. } y_i(w^T x_i + b) \geq 1 \rightarrow \text{全分对}$$

优化变量: w, b . 看 PPT 求解过程

③ Soft Margin: $\lambda \lambda \text{ slack}$

$$\min_{w, b, \xi} \frac{1}{2} \|w\|^2 + C \sum_i \xi_i \rightarrow \text{penalty}$$

$$\text{s.t. } y_i(w^T x_i + b) \geq 1 - \xi_i$$

$$\xi_i \geq 0 \quad \|w\|^2 = \sum_i \xi_i^2$$

④ Optimization **看下优化量.**

$$L(w, b, \xi, \lambda, \mu) \quad \xi \text{ 是优化量.}$$

$$= \frac{1}{2} \|w\|^2 + C \sum_i \xi_i + \lambda \sum_i (1 - \xi_i - y_i)(w^T x_i + b)$$

$$- \lambda \sum_i \xi_i$$

⑤ KKT:

$$\frac{\partial L}{\partial w} = w - \sum_i \lambda_i y_i x_i = 0 \quad \text{看详细推导}$$

$$\frac{\partial L}{\partial b} = \sum_i \lambda_i y_i = 0 \quad \text{看推导}$$

$$\text{⑥ 代入写 } g(\lambda, \mu)$$

$$g(\lambda, \mu) = \sum_i \lambda_i - \frac{1}{2} \sum_i \lambda_i y_i x_i^T x_i$$

$$\sum_i \lambda_i y_i x_i^T x_i$$

⑦ Dual Problem:

$$\min_{\lambda} -g(\lambda) \quad \Delta \rightarrow \text{hard different}$$

$$\text{s.t. } C \geq \lambda_i \geq 0 \quad \checkmark$$

$$\sum_i \lambda_i y_i = 0 \quad \checkmark$$

$$\lambda_i + \mu_i = C \quad \checkmark$$

解出 λ 用任意 SV 代入

出 b . 求解 SMO 不等式

由互补松弛性 (Sparsity)

$\lambda_i (y_i(w^T x_i + b) - 1 + \xi_i) = 0$

$\Rightarrow w = \sum_i \lambda_i y_i x_i$ P. 与

$= 1 - \xi_i$ 的 \sim SV 有关 \Rightarrow Hard 也是

kernel function
⇒ 解决线性不可分数据
⇒ 以内积形式 $K(x_i, x_j) = \phi(x_i)^T \phi(x_j) + b$, kernel function
核矩阵 $K_{ij} = K(x_i, x_j)$, kernel function 的线性组合.

⇒ Linear: $K(x_i, x_j) = x_i^T x_j$
⇒ Polynomial: $K(x_i, x_j) = (x_i^T x_j + c)^n$

二次: ⇒ 转出式

$$K(x, z) = (x^T z + c)^2$$

$$= (\underbrace{z_1 x_1}_{\text{将 } x, z \text{ 分离}}, \underbrace{z_2 x_2}_{\text{将 } x, z \text{ 分离}}, \dots, \underbrace{z_n x_n}_{\text{将 } x, z \text{ 分离}} + 2c z_i x_i + c^2)$$

$$\Rightarrow \text{构造 } \underline{a}(a) = [a_1^2, a_1 a_2, a_1 a_3, \dots, a_n^2, \sqrt{2} a_1, \dots, \sqrt{2} a_n, c]$$

Back Propagation. × MLP (CNN, Linear Layer).
⇒ 本质是快速求导, 存下先算的, 加速后算的.

⇒ forward ⇒ 算 output

↓
backward ⇒ 从输出向输入层算, 首作业 (PPT).
↓
update

2) 方法: 基于链式法则.

上一层 x_{in} → 上一层的 gradient: $\frac{\partial L}{\partial x_{out}}$

$\boxed{f(x_{in}, w)} \rightarrow \text{对这一层: } \frac{\partial L}{\partial w_L} = g_{out} \times \frac{\partial x_{out}}{\partial w_L}$

上一层 x_{out} → 给下一层 gradient: $\frac{\partial L}{\partial x_{in}} = \frac{\partial L}{\partial x_{out}} \times \frac{\partial x_{out}}{\partial x_{in}} = g_{out} \cdot w$

$f(x_{in}, w_L) = w_L x_{in}$

看题实操. 更新: $w_L^{t+1} = w_L^t - \eta \cdot \frac{\partial L}{\partial w_L}$

⇒ 小心 激活函数导数.

⇒ 用的是对单项求导, 不是整体求导.

⇒ 一步一步来, 不怕多写.

L9 CNN

⇒ 记住规则, 实操算一下 {Conv
↓ copy
⇒ in-channel → 一个 in Feature → 一个 2D kernel
out-channel → 一个 out Feature → 一个 3D kernel.
padding → 单边设大小, $2p = k_w / H - 1$
stride → 步幅.
kernel size.

大小: $H/W - K + 2P + S$

计算: 元素对应相乘再求和, + 偏置
参数要训练. △ 别忘.

⇒ Pooling 通道不变, 无须训练.
⇒ padding
stride
kernel size.
here.

L11 Decision Tree ⇒ {非线性
可解释
易使用.

⇒ model 条件决策, 从根节点 → 叶节点
重合结论, 看么下一个节点测试

建树算法: 选择划分特征

↓ 定义: 取此处大多数
每个特征一个节点

有: 连续划分.

是: 所有 C 同一 Label ⇒ leaf node

所有特征值相同 ⇒ leaf node 大多数.

⇒ Optimization 看题目.

用 Information Gain 来 Feature Select: increase purity

Information Entropy:

$$Ent(D) = - \sum_{k=1}^K P_k \log_2 P_k$$

label class种类
proportion of class k.

⇒ 俗的话 purity 高.

⇒ 全为一类/定时为 0, 平均分时最高: $\log_2 1$.

步 feature (最小)
feature (最大) ↑

$$Gain(D, a) = Ent(D) - \frac{V}{|D|} \sum_{v=1}^V \frac{|D_v|}{|D|} Ent(D_v)$$

⇒ Gain > 0 说明 purity ↑.

选 Gain 最大的 Feature a.

*一定要看题手算(浅显).

Pruning: { pre-prunning

↓ post-prunning ⇒ 控制模型复杂度, 防止过拟合

① pre-prunning:

⇒ 通过 validation set 看效果

②尝试 pruning:

判断当前划分能否让 val acc ↑ {能: splitting

⇒ 简单但效果不好.

③ post-prunning:

⇒ 在已训练好的树上剪枝(底向上) ⇒ 查每个结点(非叶).

⇒ 用多数类结点 label 替代子树 ↑ 剪枝

⇒ Wallace ↓ 复原.

⇒ 算法复杂稍大, 但泛化好.

Lecture 12 Bayesian Classifier.

1) Model

Bayes theorem:

$$P(c|x) = \frac{P(c) \cdot P(x|c)}{P(x)}$$

$$= \frac{P(c) \cdot \prod_{i=1}^d P(x_i|c)}{P(x)}$$

discriminative model: 直接求 $P(c|x)$

generative model: $P(x,c) \rightarrow P(c|x)$

特征间独立 \Rightarrow Naive Bayes.
假设

2) Loss:

$\lambda_{ij|l}$ action

引入分类错误损失: $x_{ij} \rightarrow$ 真值为 j , 错分为 i 的 risk.

条件风险
 $\Rightarrow R_{ci|x} = \sum_{j=1}^N \lambda_{ij} \cdot P(c_j|x) \rightarrow$ 对一个 sample x , 分为 c_i 的 risk
conditional risk
action 分类结果

Total risk: $h(x) \rightarrow$ 分类器

$$R(h) = E_x [R(h(x))|x]$$

Optimal:

$$h^* = \underset{c \in \mathcal{Y}}{\operatorname{argmin}} R(c|x) \rightarrow$$
 找到使每个 x loss 最小的 label c

Bayes optimal $R(h^*) \Rightarrow$ Bayes Risk

classifier \Rightarrow 机器学习理论最优

3) Optimization \Rightarrow 概率模型的训练过程
就是概率计算 / 参数估计.

① Naive Bayes (求 $P(c), P(x|c)$)

\Rightarrow prior assumption: $P(c_i) = \frac{1}{D_C}$
特征属性间独立 $P(x_i|c) = \frac{1}{D_{x_i|c}}$, 连续时

$$\Rightarrow P(c|x) = \frac{P(c) \cdot P(x|c)}{P(x)} = \frac{P(c)}{P(x)} \cdot \prod_{i=1}^d P(x_i|c) \text{ Gaussian } m_{ci}, \sigma_{ci}$$

$$\Rightarrow h(x) = \underset{c \in \mathcal{Y}}{\operatorname{argmax}} P(c|x) \text{ 后验 P 最大的.}$$

NB 是线性分类器.

TIPS:

Laplace Smoothing:

\Rightarrow 当某一特征从未在此 label 上出现时,

$P(x_i|c) = 0$, 其它特征也被忽略. $P(c|x) = 0$.

\Rightarrow 做一个平滑:

$$\hat{P}(c) = \frac{1}{D_C + N} \rightarrow c$$
 类别数.

$$\hat{P}(x_i|c) = \frac{1}{D_C + N_i} \rightarrow c$$
 中 x_i 数 \Rightarrow 注意
是整个训练集中的都
要, 此集中未出现的
种类数.

4) Application

multinomial distribution:

关于有放回抽样.

$$P(X_1=x_1 \dots X_k=x_k) = \frac{n!}{x_1! \dots x_k!} \cdot p_1^{x_1} \dots p_k^{x_k} \quad (n = \sum_i x_i)$$

是一个分布
可代入数据求.

抽一次球
到 k 种 Prob

Text classification: 看 PPT 例题.

\Rightarrow Feature: 单词出现频率. / $C \rightarrow$ 文档类型

$$C_{iB} = \underset{c \in \mathcal{Y}}{\operatorname{argmax}} \log P(c) + \sum_{i=1}^m \log P(w_i|c)$$

+ 加权
逃最大
后验

Lecture 13 Ensemble Learning

\Rightarrow 集成 "好而不同" 的弱学习器, 最终产生超强性能
有定 acc 多样性 \Rightarrow Ensemble 核心是和弱 train 出

"好而不同" learner.

\Rightarrow 串行, learner 间有依赖 \Rightarrow boost

并行, 可同时生成 \Rightarrow bagging

1) Bagging \Rightarrow Bootstrap AGGREGATING (多分类, 回归可用)

未被选中训练集中有放回采样 m 个
采样的 m 个样本 \downarrow 重量
可当 val 集. \Rightarrow 用 m 个采样集训 m 个 base learner
和 dataset 一样大.

② 结合 (voting / avg) \Rightarrow 选最多学习器认可的

$$H(x) = \underset{c \in \mathcal{Y}}{\operatorname{argmax}} \sum_{t=1}^m I(h_t = c)$$

回归:
bias 没降
variance 下降.

↓

1.1) Random Forest

\Rightarrow 除了样本扰动再加上属性扰动

\Rightarrow 对 base learner 每个结点, 先在所有可选 feature 中随机选 k 个,
再从这 k 个中选最好的

与 bagging 比:
① 训练效率高, 只
算子集 feature
② 开始精度低,
learner 少时差。
(由于子集, 学习器弱)
但之后泛化强.

Lecture 14 Clustering

K-means (过)

Hierarchical clustering 层次聚类

1) AGNES (bottom up):

- ① 初始时每个样本视为一个簇 cluster
 - ② 每一轮将最近的簇融合成一个 距离度量
 - ③ 直到剩下预定的 k 个簇.
- ↓
观察.

Implementation:

Distance Matrix

$$\begin{array}{|c|cccc|} \hline & a & b & c & d \\ \hline a & 0 & d_{ab} & & \\ b & d_{ba} & 0 & \cdots & \\ c & \cdots & 0 & & \\ d & 0 & & & 0 \\ \hline \end{array} \quad \Rightarrow \quad \begin{array}{|c|cc|} \hline & (a,b) & c,d \\ \hline (a,b) & 0 & \cdots \\ c,d & \vdots & 0 \\ \hline \end{array}$$

* 更新只修改有变化的行列.

其余不变.

变化的行列的值由之前的推.

Ex:

$$\Rightarrow \min (a, b, c)$$

$$= \min (d_{ac}, d_{bc})$$

维数

$$dist(x_i, x_j) = \left(\sum_{u=1}^n |x_{iu} - x_{ju}|^r \right)^{\frac{1}{r}}$$

P342. Euclidean.

$$\left\{ \begin{array}{l} \text{minimum: } d = \min_{x \in C_i, y \in C_j} dist(x, y) \quad [\text{single linkage}] \\ \text{maximum: } d = \max_{x \in C_i, y \in C_j} dist(x, y) \quad [\text{complete linkage}] \\ \text{average: } d = \frac{1}{|C_i| + |C_j|} \sum_{x \in C_i, y \in C_j} dist(x, y) \quad [\text{average linkage}] \end{array} \right.$$

不同策略适合不同数据分布, 效果不同.

* K-means

Derivative:

$$\textcircled{1} \quad \frac{\partial x^T A x}{\partial x} = (A + A^T) x$$

$$\textcircled{2} \quad \frac{\partial x^T a}{\partial a x} = \frac{\partial a^T x}{\partial x} = a.$$

$$\textcircled{3} \quad \frac{\partial a^T x b}{\partial x} = a \cdot b^T$$

$$\textcircled{4} \quad \frac{\partial a^T x^T b}{\partial x} = b a^T$$

* 考虑分类讨论,

$$\begin{cases} c > 0 & \dots \\ c < 0 & \dots \end{cases}$$

Gaussian: $x \sim N(\mu, \sigma^2)$

$$\therefore f(x) = \frac{1}{2\pi\sigma^2} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

SUM Kernel:

① 先写判别函数: $f(x) = \Sigma \lambda_i y_i x \cdot x + b$.

② 观察. 二次核 \Rightarrow 单圆 / 双曲线

高斯 \Rightarrow 圆.

$$\downarrow \\ \text{Ex: } \exp(-r(x_i - x_j)^2) \Rightarrow r \text{ 越大, 当 } x_i \neq x_j \text{ 差的大时结果相近} \Rightarrow \text{SV多.}$$

$$\Rightarrow \text{kernel matrix} = \begin{bmatrix} K(x_1, x_1) & \dots \\ \vdots & \ddots \\ K(x_n, x_n) \end{bmatrix}$$

半正定, 则可当核函数.

Bayesian Decision

$$PCH|X) = \frac{P(CH) \cdot P(X|CH)}{P(X)}$$

直接判断.

② X, Ω, A, λ 损失.

$$\Delta R(a_i|X) = \sum_{j=1}^c \lambda(x_j|w_j) \cdot P(w_j|X)$$

\Rightarrow Bayes decision rule: 损失小的选.

$$\alpha(x) = \operatorname{argmin}_{a \in A} R(a|x).$$

分类问题中 a_i 为分类的类别.

二分类: $R(a_1|x) < R(a_2|x) \Leftrightarrow P(w_1|x) > P(w_2|x)$

$$\Leftrightarrow \frac{P(x|w_1)}{P(x|w_2)} > \frac{\lambda_{12} - \lambda_{21}}{\lambda_{11} - \lambda_{22}} \cdot \frac{P(w_2)}{P(w_1)}$$

多分类: 使用 0-1 损失时: 对 a 错.

$$k(a|x) = 1 - P(w_i|x).$$

w_i if $P(w_i|x) > P(w_j|x)$

$P(x|w_i) \sim N(\mu_i, \sigma_i^2)$

高斯分布: $X \sim N(\mu, \sigma^2)$

$$P(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2}$$

$$\mathbb{E}[x] = \int_{-\infty}^{+\infty} x \cdot p(x) = \mu$$

$$\text{Var}[x] = \int_{-\infty}^{+\infty} (x-\mu)^2 \cdot p(x) = \sigma^2$$

针对 Gaussian 的判别函数推导 (P28)

$\int g(x) = \Sigma_i \rightarrow \text{linear}$ 带入后二次项无意义(书上)

$\Sigma_i = \Sigma \rightarrow \text{quadratic}$

$$g_i(x) = \ln P(x|w_i) + \ln P(w_i)$$

$$\Leftrightarrow g_i(x) = -\frac{1}{2}(x-\mu_i)^2 + \Sigma_j^2(x-\mu_j)^2 - \frac{1}{2} \ln \Sigma_i + \ln P(w_i)$$

Parametric Estimation

Maximum Likelihood

$$\partial P(w_j) \rightarrow \text{count}.$$

$$\partial P(x|w_j) \rightarrow \text{假设服从某一分布}$$

$$\Rightarrow P(D|B) = \prod_{k=1}^n P(x_k|B)$$

$$\hat{\theta} = \operatorname{argmax}_\theta P(B|\theta).$$

求解: ① 加上 λ ② 对 θ 求导为 0 ③ 检查极值点哪个最优(代入)

应用: Gaussian {已知, 估计} μ, σ^2 P10

$$\hat{\mu} = \frac{1}{n} \sum_{k=1}^n x_k$$

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{k=1}^n (x_k - \hat{\mu})^2$$

Bayesian Estimation

$$\text{求 } P(w_j|x, D^*).$$

每个类的后验, 最大的即结果 \Rightarrow 可能求别的

$$\text{此处 } P(x|D) = P(x|w_1, D). \text{ 后验: } P(w_1|D)$$

$$\text{乘法公式+条件概率可得: } P(w_1|D) \cdot P(x|w_1, D)$$

求解: $P(w_1|D)$, 高斯情况,

$$\text{求 } P(w_1|D).$$

$$\text{模型: } P(w_1|w_j, D)$$

$$\partial P(x|D) = \int P(x|w_1) P(w_1|D) dw_1$$

$$\text{条件: } P(w_1|D) = \frac{P(w_1|D)}{\int P(w_1|D) dw_1}$$

$$\text{边缘: } P(w_1) = \sum_{i=1}^n P(w_1, b_i)$$

$$\text{条件: } P(w_1|b_i) = \frac{P(w_1, b_i)}{P(b_i)}$$

$$\text{求 } P(w_1|D).$$

$$\text{模型: } P(w_1|w_j, D)$$

$$\partial P(x|D) = \int P(x|w_1) P(w_1|D) dw_1$$

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$$\text{求 } P(w_1|D).$$

$$\text{模型: } P(w_1|w_j, D)$$

$$\partial P(x|D) = \int P(x|w_1) P(w_1|D) dw_1$$

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