AI2611 CheatSheet

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Preface

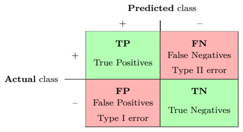
Introduction

- My Machine Learning Lecture Notes (更丰富、更全面的版本，适合学习这门课):
- LaTeX code of the CheatSheet is available at:
- CheatSheet 为 2022 版（非常少也很草率，当然有部分超纲，不适合用于学习）。

Ackonwledgement

- CS229, Stanford University. (Foundation, Kernel Method, GMM)
- CS231n, Stanford University. (Deep Learning)
- CS189, UC Berkeley. (Random Forest)
- Understanding Machine Learning, Cambridge University. (Linear Regression, KNN, SVM, K-means, PCA)
- AI2611, Shanghai Jiao Tong University. (中文部分, Spectral, Dimensionality Reduction)

§ Foundation



监督学习、无监督学习（聚类、降维）
独立同分布
最小化范化误差

Metric	Formula	Interpretation
准确率 (Accuracy)	$\frac{TP+TN}{TP+TN+FP+FN}$	Overall performance of model
查准率 (Precision)	$\frac{TP}{TP+FP}$	How accurate the positive predictions are
通过率，查全率 (Recall Sensitivity)	$\frac{TP}{TP+FN}$	Coverage of actual positive sample
假阳率 (FPR)	$\frac{FP}{TN+FP}$	
F1 score	$\frac{2TP}{\text{样例总数}+TP-TN}$	Hybrid metric useful for unbalanced classes
F_β score	$\frac{(1+\beta^2)\times Pre\times Rec}{\beta^2\times Pre+Rec}$	Precision and Recall

在不同的阈值下可以得到不同的 TPR 和 FPR 值，将它们在图中绘制出来，并依次连接起来就得到了 ROC 曲线，阈值取值越多，ROC 曲线越平滑。AUC: ROC 曲线下的面积

模型选择： 留出法（hold-out，保持数据分布的一致性，多次重复划分取平均值）、交叉验证法（留一法，10-fold，更接近期望评估的模型，但计算量巨大；测试集只包含一个数据，无法分层采样，测试误差率区别较大；）、自助法（bootstrap，有放回采样，训练集中数据存在重复，适合小规模数据集）

误差-方差分解

$E(f;D) = \text{bias}^2 + \text{variance} + \text{error}^2$

$$= (\bar{f}(x) - y)^2 + \mathbb{E}_D[f(x;D) - \bar{f}(x)] + \mathbb{E}_D[(y_D - y)^2]$$

§ Linear Regression

Loss function: $\mathcal{L}_S(h) = \frac{1}{m}\sum_{i=1}^m (h(\boldsymbol{x}) - \boldsymbol{y})^2, \forall h \in \mathcal{H}_{reg}$. We need to solve $A\boldsymbol{w} = \boldsymbol{b}$ where $A \overset{def}{=} \sum \boldsymbol{x}_i \boldsymbol{x}_i^T = XX^T$ and $\boldsymbol{b} \overset{def}{=} \sum y_i \boldsymbol{x}_i = X^T\boldsymbol{y}$.

Theorem 1 $\omega = (X^TX)^{-1}X^T\boldsymbol{y}$. 优点：single-shot 算法，易于实现；缺点：伪逆计算量大没可能导致数值不稳定（奇异矩阵）。

Theorem 2 Using A's eigenvalue decomposition,we could write A as VD^+V^T where D is a diagnonal matrix and V is an orthonormal matrix. Define D^+ to be the diagonal matrix such that $D^+_{i,i} = 0$ if $D_{i,i} = 0$ otherwise $D^+_{i,i} = 1/D_{i,i}$. Then, $A\hat{\boldsymbol{w}} = \boldsymbol{b}$ where $\hat{\boldsymbol{w}} = VD^+V^T\boldsymbol{b}$.

Remark 1 Use the **Gradient Descent** method. 优点：收敛快，易于实现；缺点：批量更新，可伸缩性问题。

$\mathcal{H}^n_{poly} = \{x \mapsto p(x)\}$ where $\psi(x) = (1, x, x^2, \cdots, x^n)$ and $p(\psi(x)) = a_0 + a_1x + a_2x^2 + \cdots + a_nx^n$. 概率解释: $y|x;\theta \sim \mathcal{N}(0, \sigma)$. Loss function 为最大似然的结果，分类器为 $E[y|x]$。

Ridge（岭）Regression

$R_{\text{egularization}}(w) = \lambda\|w\|^2$ and $\boldsymbol{w} = (2\lambda mI + A)^{-1}$. λ 适当增大可以减少方差，但会提高误差。

Lasso（索套）Regression $R(w) = \lambda\|w\|_1^2$. **SPARSE**

§ **KNN** 超参数: k 和 $d(x_1, x_2)$. 计算量大，The "Curse of Dimensionality", $m \geq \left(4c\sqrt{d}/\varepsilon\right)^{d+1}$. 低维度 + 边界非线性 + 密度高时使用。

§ **贝叶斯** 先验: $\Pr\left(\omega_j\right)$, 后验: $\Pr\left(\omega_j|x\right)$, Likelihood: $\Pr\left(x|\omega_j\right)$ and Post = likely × Prior/ $\Pr(x)$ where ω_j 表示类别，x 表示数据（特征）。

最小化采取 α_i 行动的风险: $R(\alpha_i|x) = \sum_{j=1}^{j=c}\lambda(\alpha_i|\omega_j)\Pr\left(\omega_j|x\right)$，其中 λ 表示在自然状态为 ω_j 的情况下因采取行动 α_i 而产生的损失。If $R(\alpha_1|x) < R(\alpha_2|x)$, then we adopt α_1 (ω_1). Usually,

$$\lambda(\alpha_i, \omega_j) = 1 - \delta_{ij} \quad \text{and} \quad R(\alpha_i|x) = 1 - \Pr(\omega_i|x)$$

参数估计

$$\hat{\theta} = \arg\max_\theta \mathcal{L}(\theta) = \sum_{k=1}^n \log\Pr(x_k|\theta).$$

§ Random Forest

Definition 1 (Entropy)

$$H(Y) = -\sum_k \Pr(Y = k)\log\Pr(Y = k)$$

$$H(Y|X_j) = \Pr\left(X_j = 1\right)H(Y|X_j = 1) + \Pr\left(X_j = 0\right)H(Y|X_j = 0)$$

Mutual information between X_j and Y.

$$\max I(X_j; Y) \triangleq H(Y) - H(Y|X_j)$$

Gini impurity/index

$$G(Y) = \sum_k \Pr(Y = k)\sum_{j\neq k}\Pr(Y = j) = 1 - \sum_k \Pr^2(Y = k)$$

Random Forest

Ensemble method+randomized+reduce correlation

- **bagging (bootstrap aggregating)**: sample some data points uniformly with replacement, and use these as the training set.
- **feature randomization**: sample some number $k < d$ of features as candidates to be considered for this split.

§ LDA

类间 $d = \left|w^T\mu_1 - w^T\mu_2\right|$, 类内 $d_j = \sum_{i\in C_j}\left|w^Tx_i - w^T\mu_j\right|$

从而 $d_w = d_1^2 + d_2^2 = w^T\Sigma w$.

Solve: $\max\left(d^2/d_w\right) = \max\left(w^TS_bw/w^TS_ww\right) \triangleq \lambda(w)$.

Theorem 3 $S_w^{-1}S_bw = \lambda w$, w 为最大特征值所对应的特征向量。

Remark 2 多类问题最多可以降至 $M-1$ 维。

Calinski-Harabaz index:

$$S_b = \sum_{j-1}^M N_j(\mu_j - \mu)(\mu_j - \mu)^T$$

$$S_w = \sum_{j=1}^M\sum_{i\in C_j}(x_i - \mu_j)(x_i - \mu_j)^T$$

§ Kernel Method $K(x, z) \triangleq \langle\phi(x), \phi(z)\rangle$

Remark 3 **Kernel** is a corresponding to the feature map ϕ as a function that maps $\mathcal{X}\times\mathcal{X}\mapsto\mathbb{R}$.

Definition 2 (Gaussian kernel)

$$K(x, z) = \exp\left(-\frac{\|x - z\|^2}{2\sigma^2}\right).$$

The gaussian kernel is corresponding to an **infinite** dimensional feature mapping ϕ. Also, ϕ lives in Hilbert space.

§ SVM

$$\arg\max_{(w,b):\|w\|=1}\min_{i\in[m]}\left|w^Tx^i + b\right| \quad \text{s.t. } \forall i, y^i\left(w^Tx^i + b\right) \geq 1.$$

Equivalently,

$$\arg\max_{(w,b):\|w\|=1}\min_{i\in[m]} y^i\left(w^Tx^i + b\right) \tag{1}$$

$$(w_0, b_0) = \arg\min_{(w,b)}\frac{1}{2}\|w\|^2 \quad \text{s.t. } \forall i, y^i\left(w^Tx^i + b\right) \geq 1.$$

Output: $\hat{w} = w_0/\|w_0\|$, $\hat{b} = b_0/\|w_0\|$

Support Vector: $g(x) = \pm1$. $\gamma \sim \frac{1}{\|w\|}$

Soft-SVM and Norm Regularization

$$\min_{w,b,\xi}\left(\lambda\|w\|^2 + \frac{1}{m}\sum_{i=1}^m\xi_i\right)$$

$$\text{s.t. } \forall i,\ y^i\left(w^Tx^i + b\right) \geq 1 - \xi_i \text{ and } \xi_i \geq 0$$

Output: w, b

Definition 3 (hinge loss)

$$l^{\text{hinge}}((w, b), (x, y)) = \max\left\{0, 1 - yw^Tx + b\right\}.$$

Now we just need to optimize $\lambda\|w\|^2 + \mathcal{L}^{\text{hinge}}(w, b)$. 松弛变量几何意义：对越界数据惩罚力度。

§ **K-means** 收敛：递减 + 有下界。

前辈 将采样数据从某一分组分类到另一分组，目的是使得损失函数 $\min J = \sum_{i=1}^c J_i = \sum_{i=1}^c\sum_{x\in H_i}\|x - \mu_i\|^2$。$\hat{x}$ 从类别 i 移至 j，更新公式为: $m_j^* = m_j + \frac{\hat{x}-\mu_j}{n_j+1}$, $J_j^* = J_j + \frac{n_j}{n_j+1}\left\|\hat{x} - \mu_j\right\|^2$ and $J_i^* = J_i - \frac{n_i}{n_i-1}\|\hat{x} - \mu_i\|^2$. Transer $\hat{x}$ to H_k whose $J_k^* - J_l$ is smallest.

The Choice of k

- The Elbow Method: Calculate the Within Cluster Sum of Squared Errors for different values of k, and choose the k for which WSS becomes first starts to diminish.
- The Silhouette value: $a(i) = \frac{1}{|C_I|-1}\sum_{j\in C_I, j\neq i} d(i, j)$, $b(i) = \min_{J\neq I}\frac{1}{|C_J|}\sum_{j\in C_J} d(i, j)$ and $s(i) = \frac{b-a}{\max[a,b]}$.

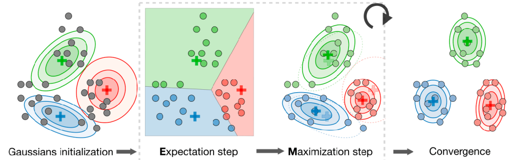
缺点：样本数据发生很小的扰动，那么样本的分类结果容易发生明显的改变。

Linkage-Based Clustering Algorithms aka **Agglomerative** Clustering which is trivial. Stopping criteria: numbers of clusters 或 current distance.

§ **GMM** $x|z \sim \mathcal{N}(\nu, \Sigma)$ where $z \sim \text{Mul}(\phi)$ is the latent variable

- E-step: Evaluate the **posterior** probability: $Q_i(z^i) = P(z^i|x^i;\theta)$.
- M-step: Use the posterior probabilities $Qi(z^i)$ as cluster specific weights on data points x^i to separately re-estimate each cluster model:

$$\theta_i = \arg\max_\theta\sum_i\int_{z^i}Q_i(z^i)\log\left(\frac{P(x^i, z^i;\theta)}{Q_i(z^i)}\right)dz^i$$



Likelihood:

$$\mathcal{L}(\phi, \mu, \Sigma) = \sum_{i=1}^n\log\sum_{z^i=1}^k\Pr\left(x^i|z^i;\mu, \Sigma\right)\Pr\left(z^i|\phi\right)$$

§ **Spectral** 对数据有很好的表征，非凸数据；但是拓展性不好。

Similarity: $W_{ij} = s(x_i, x_j) = \exp\left(-\left\|x_i - x_j\right\|^2/2\sigma^2\right)$

Graph Constructin: ε-neighborhood, fully connected and KNN.

Definition 4 Some useful definations:

$d_i = \sum_{j\in V}W_{ij}$

$\text{cut}(A, B) = \sum_{i\in A, j\in B}W_{ij}$

$\text{cut}(A_1, A_2, \cdots, A_k) = \frac{1}{2}\sum_{i=1}^k\text{cut}(A_i, \bar{A}_i)$

$\text{RatioCut}(A_1, A_2, \cdots, A_k) = \frac{1}{2}\sum_{i=1}^k\text{cut}(A_i, \bar{A}_i)/|A_i|$

$\text{Ncut}(A_1, A_2, \cdots, A_k) = \frac{1}{2}\sum_{i=1}^k\text{cut}(A_i, \bar{A}_i)/\text{vol}(A_i)$

Degree of the subgraph A: $\text{vol}(A) = d_A = \sum_{i,j\in A}W_{ij}$

Laplacian: $L = D - W$ where $W = \text{diag}_\text{i}\left(\sum_{(i,j)\in E}W_{ij}\right)$

Theorem 4

$\text{cut}(A, \bar{A}) = x^TLx$ and $\text{cut}(A_1, \cdots, A_k) = \text{trace}(X^TLX)$

Proof: LHS $= \sum_{i\in A}d_i - \sum_{i,j\in A}W_{ij}$.

Theorem 5 Relaxation: $x \in \{0, 1\}^{|V|} \to \mathbb{R}^{|V|}$.

$\min\text{cut}(A, \bar{A}) \iff \min x^TLx = (x^TLx)/(x^Tx) \iff x$ 为 L 的最小非零特征值所对应的特征向量 (Rayleigh quotient Theorem)。

Definition 5 **Normalized** Spectral Clustering:

- 对拉普拉斯矩阵进行标准化操作: $L \leftarrow D^{-0.5}LD^{-0.5}$
- 计算标准化操作后拉普拉斯矩阵最小的 k_1 个特征值对应的特征向量 F
- 将 F 组成的矩阵按行标准化，组成 $n\times k_1$ 的特征矩阵 P。
- 对 P 中的每一行作为一个 k_1 维的样本，用聚类方法进行聚类。

§ **PCA** Compressing matrix $W \in \mathbb{R}^{n,d}$ and recovering matrix $U \in \mathbb{R}^{d,n}$: $\arg\min_{W,U}\sum_{i=1}^n\|x_i - UWx_i\|^2$

Lemma 1 Let (U, W) be a solution of Equation above. Then $U^TU = I$ and $W = U^T$. (The columns of U are orthonormal.)

By the fact that

$$\left\|x - UU^Tx\right\|^2 = \|x\|^2 - \text{trace}(U^Txx^TU)$$

We could rewrite the Equation as follows:

$$\arg\max_{U\in\mathbb{R}^{d,n}:U^TU=I}\ \text{trace}\left[U^T\left(\sum_{i=1}^m x_ix_i^T\right)U\right]$$

Theorem 6 Let $x_1, \cdots, x_m$ be arbitrary vectors in $\mathbb{R}^d$, let $A = \sum_{i=1}^m x_ix_i^T$, and let $u1, \cdots, u_n$ be n eigenvectors of the matrix A corresponding to the largest n eigenvalues of A. Then, the solution to the PCA optimization problem given in Equation is to set U to be the matrix whose columns are $u_1, \cdots, u_n$ and to set $W = U^T$. (More Intuition: MathOverFlow)

Proof 1 Let VDV^T be the spectral decomposition of A (suppose that $D_{1,1} \geq \cdots \geq D_{d,d}$) and let $B = V^TU$. We have

$$\text{trace}\left(U^TAU\right) = \text{trace}\left(B^TDB\right) = \sum_{j=1}^d D_{j,j}\sum_{i=1}^n B_{j,i}^2$$

$$\leq \max_{\boldsymbol{\beta}\in[0,1]^d:\|\boldsymbol{\beta}\|\leq n}\sum_{j=1}^d D_{j,j}\beta_j = \sum_{j=1}^n D_{j,j}$$

Nota Bene: $B^TB = I$ which entails $\sum_{j=1}^d\sum_{i=1}^n B_{j,i}^2 = n$.

§ Dimensionality Reduction

PCA 拟合了训练数据的长轴短轴，使得映射后得到的低维度向量分布散射最大

MDS 找到映射方向使得在低维空间中高维度样本间距离不变

$$\min\sum_{i<j}\left\|\hat{x}_i - \hat{x}_j\right\| - d_{ij}$$

ISOMAP Geodesic 距离 ($d_{ij} \leftarrow$ shortest path) 能反映该数据的真正低维流形结构，保留数据集的本征几何特征。

Locally Linear Embedding 从局部的线性结构关系，恢复全局的非线性流形。假设: $\hat{x}_i = \sum_j W_{ij}x_j$ and $\sum_j W_{ij} = 1$.

$$\min\sum_i\left\|x_i - \sum_j W_{ij}x_j\right\|^2 \text{s.t.} W_{ij} = 0 \text{ if } X_j \in \mathcal{N}(X_i)$$

ISOMAP VS LLE 都保留了邻接的几何结构；都没有显式的映射函数，故使用比较麻烦；LLE 需要更多的训练数据；ISOMAP 计算效率高，实用性更高

§ Deep Learning