AI2611 CheatSheet

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Preface

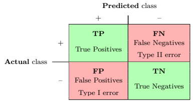
Introduction

- My Machine Learning Lecture Notes (更丰富的版本，适合学习这门课): Self-Learning/CS229/MyNotes/ML.pdf
- LaTeX code of the CheatSheet is available at: SJTU-Course-Stack/AI2611/CheatSheet
- CheatSheet 为 2022 版（非常少较草率，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: $\mathcal{L}_S(h) = \frac{1}{m}\sum_{i=1}^m (h(\boldsymbol{x}) - \boldsymbol{y})^2$. 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 $\omega = (X^T X)^{-1} X^T \boldsymbol{y}$. 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 Eigenvalue decomposition: $A = VD^+V^T$ where D is a diagnonal matrix and V is an orthonormal matrix. Define D^+ to be the diagonal matrix: $D^+_{i,i} = 0$ if $D_{i,i} = 0$ otherwise $D^+_{i,i} = 1\big/D_{i,i}$. Then, $A\hat{\boldsymbol{w}} = \boldsymbol{b}$ where $\hat{\boldsymbol{w}} = VD^+V^T\boldsymbol{b}$.

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

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: $G(Y) = 1 - \sum_k \Pr^2(Y = k)$

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 $d_j = \sum_{i \in C_j} \left|w^T x_i - w^T \mu_j\right|$
从而 $d_w = d_1^2 + d_2^2 = w^T \Sigma w$.
Solve: $\max\left(d^2\big/d_w\right) = \max\left(w^T S_b w\big/w^T S_w w\right) \triangleq \lambda(w)$.

Theorem 3 $S_w^{-1} S_b w = \lambda w$，$w$ 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

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

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

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

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

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

Soft-SVM and Norm Regularization

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

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

Output: w, b

Definition 3 (hinge loss)

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

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 $s(i) = \frac{b - a}{\max[a, b]}$.

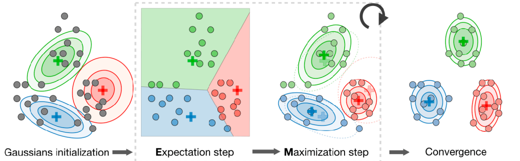
缺点：样本数据发生很小的扰动，那么样本的分类结果容易发生明显的改变。

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** Pr: $Q_i(z^i) = P(z^i|x^i; \theta)$.
- M-step: Use the posterior Pr $Qi(z^i)$ 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: $W_{ij} = s(x_i, x_j) = \exp\left(-\left\|x_i - x_j\right\|^2\big/2\sigma^2\right)$

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
$\text{cut}(A, \bar{A}) = x^T Lx$ and $\text{cut}(A_1, \cdots, A_k) = \text{trace}(X^T LX)$
Proof: LHS $= \sum_{i \in A} d_i - \sum_{i,j \in A} W_{ij}$.

Theorem 5 Relaxation: $x \in \{0, 1\}^{|V|} \to \mathbb{R}^{|V|}$.
$\min \text{cut}(A, \bar{A}) \iff \min x^T Lx = (x^T Lx)/(x^T x) \iff x$ 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 $U^T U = I$ and $W = U^T$. (The columns of U are orthonormal.)

By the fact that

$$\left\|x - UU^T x\right\|^2 = \|x\|^2 - \text{trace}(U^T xx^T U)$$

We could rewrite the Equation as follows:

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

Theorem 6 Let $x_1, \cdots, x_m$ be arbitrary vectors in $\mathbb{R}^d$, let $A = \sum_{i=1}^m x_i x_i^T$, 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 $B = V^T U$. We have

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

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

Nota Bene: $B^T B = I$ 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 Trivial.

CNN

$$N = \frac{W - F + 2P}{S} + 1.$$

RNN

$$h_{t+1} = \text{Tanh}(W_h h_t + W_x x_{t+1}).$$

Attention

$$y = \text{SoftMax}\left(\frac{QK^T}{\sqrt{D}}\right)V.$$

Weight Initialization

$$w \leftarrow \sqrt{2/n} \times \text{Rand}\mathcal{N}(0, 1)$$

Activate Function

$$\text{Sigmoid}(z) = \frac{1}{1 + \exp(-z)} \quad \text{and} \quad \text{Tanh}(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

Batch Normalization (BP for BN is challenging)
Update:

$$\mu = \alpha\mu + (1 - \alpha)\hat{\mu} \quad \text{and} \quad \sigma^2 = \alpha\sigma^2 + (1 - \alpha)\hat{\sigma}^2.$$

Forward and Eval:

$$x_i \leftarrow \gamma\frac{x_i - \mu}{\sqrt{\sigma^2 + \varepsilon}} + \beta$$

Momentum

$$v \leftarrow \mu v - \alpha dx \quad \text{and} \quad x \leftarrow x + v$$

Adam

$$m \leftarrow \beta_1 m + (1 - \beta_1)dx \quad \text{and} \quad m_t \leftarrow m\big/(1 - \beta_1^t)$$

$$v \leftarrow \beta_2 v + (1 - \beta_2)dx^2 \quad \text{and} \quad v_t \leftarrow v\big/(1 - \beta_2^t)$$

$$x \leftarrow x - \frac{\alpha m_t}{\sqrt{v_t + \varepsilon}}$$