

模式识别作业2

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1. 第三章讲义习题2

(a) $\arg \min_{\gamma_{ij}, \mu_i} \sum_{i=1}^K \sum_{j=1}^M \gamma_{ij} \|x_j - \mu_i\|^2$ means finding the value of γ_{ij}, μ_i that minimize the value

of the formula. Note that $\gamma_{ij} = 1$ if x_j is assigned to the i -th group, otherwise 0. So

$\sum_{i=1}^K \gamma_{ij} \|x_j - \mu_i\|^2 = \|x_j - \mu_c\|^2$ (given a fix j , and x_j belongs to group c). So

$\sum_{i=1}^K \sum_{j=1}^M \gamma_{ij} \|x_j - \mu_i\|^2 = \sum_{j=1}^M D_j$ (D_j means the distance between x_j and the center of the group which x_j belongs to), so the optimization means to minimize the total distance between each x and their group center, which is the goal of K-means.

(b) i. for fixed $\mu_i, J(\gamma, \mu) = \sum_{i=1}^K \sum_{j=1}^M \gamma_{ij} \|x_j - \mu_i\|^2$

for each j , exactly one of the following terms is nonzero:

$$\gamma_{1j} \|x_j - \mu_1\|^2, \gamma_{2j} \|x_j - \mu_2\|^2, \dots, \gamma_{Kj} \|x_j - \mu_K\|^2$$

Take $\gamma_{cj} = 1$ ($c = \arg \min_i \|x_j - \mu_i\|^2$), that is to assign x_j to cluster c with minimum distance

$$\|x_j - \mu_c\|^2$$

ii. For fixed γ ,

$$J(\gamma, \mu) = \sum_{i=1}^K \sum_{j=1}^M \gamma_{ij} \|x_j - \mu_i\|^2 = \sum_{i=1}^K J_c$$

$$J_c(\mu_c) = \sum \|x_i - \mu_c\|^2 \quad (i | x_i \text{ belongs to cluster } c)$$

J_c is minimized by $\mu_c = \text{mean}(\{x_i | x_i \text{ belongs to cluster } c\})$

(c) Note that the objective value never increases in an update (worst case: everything stays the same).

Consider the sequence of objective values, which are monotonously decreasing and bounded below by zero. Therefore, k-Means objective value converges to $\inf_t J_t$.

Reminder: This is convergence to a local minimum.

注：因为买的中文版教材到了，所以后面的解答都用中文

2. 第四章讲义习题2

(a) 线性回归任务即找到最优的 β ，使代价最小化，即求

$$\arg \min_{\beta} \frac{1}{n} \sum_{i=1}^n \epsilon_i^2 = \arg \min_{\beta} \frac{1}{n} \sum_{i=1}^n (y_i - x_i^T \beta)^2$$

(b)用 X 和 y 重写可以表示为, 求 $\arg \min_{\beta} \frac{1}{n}(y - X\beta)^T(y - X\beta)$

(c)

$$\begin{aligned} J(\beta) &= \frac{1}{n}(y - X\beta)^T(y - X\beta) \\ &= \frac{1}{n}(y^T - \beta^T X^T)(y - X\beta) \\ &= \frac{1}{n}(y^T y - y^T X\beta - \beta^T X^T y + \beta^T X^T X\beta) \end{aligned}$$

对上式取 β 的偏导,

$$\begin{aligned} \frac{\partial J(\beta)}{\partial \beta} &= \frac{1}{n}(2X^T X\beta - X^T y - y^T X) \\ &= \frac{1}{n}(2X^T X\beta - 2X^T y) \quad (X^T y = y^T X) \end{aligned}$$

令上式为0,

$$\beta = (X^T X)^{-1} X^T y \text{ (假设 } X^T X \text{ 可逆)}$$

(d)不可逆

(e)该正则项会对参数 β 作一个惩罚, 解决线性回归可能出现的过拟合问题以及在通过正规方法求解 β 过程中出现的 $X^T X$ 不可逆的情况。同时, 通过确定 λ 的值, 可以在方差和偏差之间达到平衡。

(f)岭回归的优化问题是求 $\arg \min_{\beta} (\frac{1}{n}(y - X\beta)^T(y - X\beta) + \lambda\beta^T \beta)$, 同样求导并令导数为0, 可得

$$\beta = (X^T X + n\lambda I)^{-1} X^T y$$

(g)岭回归在 $X^T X$ 的基础上加一个较小的 λ 扰动, 使行列式不再为0, 可求逆。

(h) $\lambda = 0$ 时, 即为普通线性回归, $\beta = (X^T X)^{-1} X^T y$. $\lambda = \infty$ 时, 欠拟合, 相当于截距回归

(i)可以。可以对于不同的 λ 值进行岭回归, 再通过交叉验证在训练集上选出最佳的 λ 值。还可以用梯度下降迭代找到最优解。

3.第四章讲义习题5

(a)

下标	类别标记	得分	查准率	查全率	AUC-PR	AP
0			1.0000	0.0000	-	-
1	1	1.0	1.0000	0.2000	0.2000	0.2000
2	2	0.9	0.5000	0.2000	0.0000	0.0000
3	1	0.8	0.6667	0.4000	0.1167	0.1333
4	1	0.7	0.7500	0.6000	0.1417	0.1500
5	2	0.6	0.6000	0.6000	0.0000	0.0000
6	1	0.5	0.6667	0.8000	0.1267	0.1333
7	2	0.4	0.5714	0.8000	0.0000	0.0000
8	2	0.3	0.5000	0.8000	0.0000	0.0000
9	1/2	0.2	0.5556/0.4444	0.8000	0.1056/0.0000	0.1111/0.0000
10	2/1	0.1	0.5000	1.0000	0.0000/0.0944	0.0000/0.1000
					0.6907/0.6795	0.7277/0.7166

(b)它们的值应该相差不大，但AUC-PR将面积近似为梯形，更为精确一些。因为在通常情况下，曲线是有斜率的。

(c)见上表最后几行斜杠后的数据

(d)代码如下

```

1  import numpy as np
2  #input the array [class, point]
3  data = np.array([[1,1.0],[2,0.9],[1,0.8],[1,0.7],[2,0.6],[1,0.5],[2,0.4],
4  [2,0.3],[1,0.2],[2,0.1]])
5  #calculate precision and recall
6  precision = [0]*11
7  recall=[0]*11
8  for i in range(1,11):
9      predict_class = [0]*11
10     TP=0
11     for j in range(1,11):
12         predict_class[j]=1 if data[j-1][1]>= data[i-1][1] else 2
13         if predict_class[j]==1 and data[j-1][0]==1:
14             TP+=1
15     precision[i]=TP/predict_class.count(1)
16     recall[i]=TP/5
17 precision[0]=1.0
18 recall[0]=0.0
19 #calculate AUC-PR and AP
20 auc=[0]*11
21 pr=[0]*11
22 for i in range(1,11):
23     auc[i]=(recall[i]-recall[i-1])*(precision[i]+precision[i-1])/2
24     pr[i]=(recall[i]-recall[i-1])*precision[i]

```

```

24 print(auc)
25 print(sum(auc))
26 print(pr)
27 print(sum(pr))

```

输出结果如下,和手算结果一致 (可能有一点点精度的差别)

```

/usr/local/bin/python3 /Users/zhangyiyang/workspace/python_practice/AUCPR
[0, 0.2, 0.0, 0.11666666666666665, 0.14166666666666666, 0.0, 0.12666666666666667, 0.0, 0.0, 0.10555555555555554, 0.0]
0.6905555555555555
[0, 0.2, 0.0, 0.13333333333333333, 0.14999999999999997, 0.0, 0.13333333333333336, 0.0, 0.0, 0.11111111111111109, 0.0]
0.7277777777777777

Process finished with exit code 0

```

修改第九个和第十个的类别标记后结果如下, 仍然和手算基本一致 (有一点精度差别)

```

/usr/local/bin/python3 /Users/zhangyiyang/workspace/python_practice/AUCPR
[0, 0.2, 0.0, 0.11666666666666665, 0.14166666666666666, 0.0, 0.12666666666666667, 0.0, 0.0, 0.0, 0.09444444444444441]
0.6794444444444444
[0, 0.2, 0.0, 0.13333333333333333, 0.14999999999999997, 0.0, 0.13333333333333336, 0.0, 0.0, 0.0, 0.09999999999999998]
0.7166666666666667

Process finished with exit code 0

```

4.第四章讲义习题6

(a)

$$\begin{aligned}
 E[(y - f(x; D))^2] &= E_D[(F(x) - f(x; D) + \epsilon)^2] \\
 &= E_D[(F(x) - f(x; D))^2 + \epsilon^2 + 2\epsilon(F(x) - f(x; D))] \\
 &= E_D[(F(x) - f(x; D))^2] + E[\epsilon^2] + 2E_D[\epsilon(F(x) - f(x; D))] \\
 &\quad \times E[\epsilon^2] = (E[\epsilon])^2 + \text{Var}(\epsilon) = \sigma^2 \\
 E_D[\epsilon(F(x) - f(x; D))] &= E_D[F(x) - f(x; D)]E[\epsilon] = 0 \\
 \text{so } E[(y - f(x; D))^2] &= E_D[(F(x) - f(x; D))^2] + \sigma^2 \\
 &= (E_D[F(x) - f(x; D)])^2 + \text{Var}(F(x) - f(x; D)) + \sigma^2 \\
 &\quad \text{because } E_D[F(x) - f(x; D)] = F(x) - E_D[f(x; D)] \\
 \text{and } \text{Var}(F(x) - f(x; D)) &= \text{Var}(f(x; D)) = E_D[(f(x; D) - E_D[f(x; D)])^2] \\
 \text{so } E[(y - f(x; D))^2] &= (F(x) - E_D[f(x; D)])^2 + E_D[(f(x; D) - E_D[f(x; D)])^2] + \sigma^2 \\
 &= \text{bias}^2 + \text{variance} + \text{noise}
 \end{aligned}$$

(b)

$$\begin{aligned}
 E[f] &= E\left[\frac{1}{k} \sum_{i=1}^k y_{nn}(i)\right] = E\left[\frac{1}{k} \sum_{i=1}^k F(x_{nn}(i)) + \epsilon\right] \\
 &= E\left[\frac{1}{k} \sum_{i=1}^k F(x_{nn}(i))\right] + E[\epsilon] = \frac{1}{k} E\left[\sum_{i=1}^k F(x_{nn}(i))\right] = \frac{1}{k} \sum_{i=1}^k F(x_{nn}(i))
 \end{aligned}$$

(c)

$$\begin{aligned}
E[(y - f(x; D))^2] &= (F(x) - E[f])^2 + E[(f - E[f])^2] + \sigma^2 \\
&= (F - \frac{1}{k} \sum_{i=1}^k F(x_{nn}(i)))^2 + E[\frac{1}{k} \sum_{i=1}^k (y_{nn}(i) - F(x_{nn}(i)))^2] + \sigma^2 \\
&= (F - \frac{1}{k} \sum_{i=1}^k F(x_{nn}(i)))^2 + E[\frac{1}{k} \sum_{i=1}^k (\epsilon_{nn}(i))^2] + \sigma^2
\end{aligned}$$

(d)方差项是 $E[\frac{1}{k} \sum_{i=1}^k (\epsilon_{nn}(i))^2]$,当k减小, 方差变大; 当k增大, 方差变小

(e)偏置的平方项是 $(F - \frac{1}{k} \sum_{i=1}^k F(x_{nn}(i)))^2$, 当k变小时, 它也随着变小; 当k变大, 偏置也变大

5.第五章讲义习题5

(a)要证范数相等, 即证 $X^T X = (GX)^T (GX)$, $X^T X = (G^T X)^T (G^T X)$, 因为G是正交矩阵, 所以 $G^T G = GG^T = I$

$$\begin{aligned}
(GX)^T (GX) &= X^T G^T GX = X^T (G^T G) X = X^T I X = X^T X \\
(G^T X)^T (G^T X) &= X^T (G^T)^T G^T X = X^T GG^T X = X^T (GG^T) X = X^T I X = X^T X \text{证毕}
\end{aligned}$$

(b)

$$\begin{aligned}
\|X\|_F &= \sqrt{\text{tr}(XX^T)} \\
\|G^T XG\|_F &= \sqrt{\text{tr}(G^T XG(G^T XG)^T)} = \sqrt{\text{tr}(G^T XGG^T X^T G)} = \sqrt{\text{tr}(G^T X(GG^T)X^T G)} \\
&= \sqrt{\text{tr}(G^T XX^T G)} = \sqrt{\text{tr}(G^T X(G^T X)^T)} = \sqrt{\text{tr}((G^T X)^T G^T X)} \\
&= \sqrt{\text{tr}(X^T GG^T X)} = \sqrt{\text{tr}(X^T (GG^T) X)} = \sqrt{\text{tr}(X^T X)} \\
\text{so } \|X\|_F &= \|G^T XG\|_F
\end{aligned}$$

(c)对于实对称矩阵X, 可以分解为 $X = J^T A J$, 其中J是正交矩阵, A是对角矩阵, 且对角线上的元素是特征值。所以计算主成分就是要将X近似对角化。根据(b)的证明可以知道实矩阵的F范数是正交不变量, 因此要使X近似对角化, 就应该使对角元的平方和尽可能增大, 非对角元的平方和尽可能减小, 即 $\text{off}(X)$ 尽可能减小。所以这一基本步骤很有用。

(d)令 $J(i, j, \theta)$ 为一个Givens旋转矩阵, 因为第 (i, j) 项和第 (j, i) 项都是0, 代入得

$$\begin{aligned}
x_{ii} \sin^2 \theta - 2x_{ij} \cos \theta \sin \theta + x_{jj} \cos^2 \theta &= 0 \\
\frac{1}{2}(x_{jj} - x_{ii}) \sin 2\theta + x_{ij} \cos 2\theta &= 0
\end{aligned}$$

解得

$$\begin{aligned}
\tan 2\theta &= \frac{2x_{ij}}{x_{ii} - x_{jj}} \\
\text{if } x_{ii} &= x_{jj}, \theta = \frac{\pi}{4} \text{sign}(x_{ij})
\end{aligned}$$

所以令J为Givens旋转矩阵, 按照上述解取 θ 的值。

(e)根据F范数不变性, 变换前后 $x_{ii}^2 + x_{jj}^2 + 2x_{ij}^2$ 不变。由于旋转变化将第 (i, j) 项和第 (j, i) 项都置0, 所以对角元的模平方和最多增加 $2x_{ij}^2$, 所以一次迭代不会增加 $\text{off}(X)$ 。

(f)根据经典*Jacobi*法的迭代步骤，可以保证对角元的模平方和不断增加， $off(X)$ 广义单调减。所以总可以在有限次迭代后，使 X 成为严格对角占优阵。根据定理：若 X 为严格对角占优阵，则*Jacobi*迭代法收敛。