

机器学习导论

综合能力测试

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1 [40pts] Exponential Families

指数分布族 (Exponential Families) 是一类在机器学习和统计中非常常见的分布族, 具有良好的性质。在后文不引起歧义的情况下, 简称为指数族。

指数分布族是一组具有如下形式概率密度函数的分布族群:

$$f_X(x|\theta) = h(x) \exp(\eta(\theta) \cdot T(x) - A(\theta)) \quad (1.1)$$

其中, $\eta(\theta)$, $A(\theta)$ 以及函数 $T(\cdot)$, $h(\cdot)$ 都是已知的。

- (1) [10pts] 试证明多项分布 (Multinomial distribution) 属于指数分布族。
- (2) [10pts] 试证明多元高斯分布 (Multivariate Gaussian distribution) 属于指数分布族。
- (3) [20pts] 考虑样本集 $\mathcal{D} = \{x_1, \dots, x_n\}$ 是从某个已知的指数族分布中独立同分布地 (i.i.d.) 采样得到, 即对于 $\forall i \in [1, n]$, 我们有 $f(x_i|\theta) = h(x_i) \exp(\theta^T T(x_i) - A(\theta))$ 。

对参数 θ , 假设其服从如下先验分布:

$$p_\pi(\theta|\chi, \nu) = f(\chi, \nu) \exp(\theta^T \chi - \nu A(\theta)) \quad (1.2)$$

其中, χ 和 ν 是 θ 生成模型的参数。请计算其后验, 并证明后验与先验具有相同的形式。

(Hint: 上述又称为“共轭”(Conjugacy), 在贝叶斯建模中经常用到)

Solution. 1. Suppose the parameters are p_1, \dots, p_k , and $\sum_{i=1}^k p_i = 1$. Let

$$h(X) = \frac{n!}{\prod_{i=1}^k x_i!},$$

$$\eta(\theta) = [\log p_1, \dots, \log p_k],$$

$$T(X) = X,$$

$$A(\theta) = 0,$$

and the resulting distribution is multinomial distribution.

2. Suppose the parameters are $\theta = [\boldsymbol{\mu}, \boldsymbol{\Sigma}]$, and the dimension of the variable is k . Let

$$\begin{aligned} h(X) &= (2\pi)^{-\frac{k}{2}}, \\ \eta(\boldsymbol{\theta}) &= [\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}, -\frac{1}{2}\boldsymbol{\Sigma}^{-1}], \\ T(X) &= [X, XX^T], \\ A(\boldsymbol{\theta}) &= \frac{1}{2}\boldsymbol{\mu}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} + \frac{1}{2}\log|\boldsymbol{\Sigma}|, \end{aligned}$$

and the resulting distribution is multivariate Gaussian distribution.

3. Let $X = \{x_1, \dots, x_n\}$, and $g(\boldsymbol{\theta}) = \exp(-A(\boldsymbol{\theta}))$,

$$\begin{aligned} p(\boldsymbol{\theta}|X, \boldsymbol{\chi}, \nu) &\propto p(X|\boldsymbol{\theta}, \boldsymbol{\chi}, \nu)p(\boldsymbol{\theta}|\boldsymbol{\chi}, \nu) \\ &= \left(\prod_{i=1}^n h(x_i)\right) \exp\left(\boldsymbol{\theta} \cdot \sum_{i=1}^n T(x_i) - nA(\boldsymbol{\theta})\right) f(\boldsymbol{\chi}, \nu) \exp(\boldsymbol{\theta}\boldsymbol{\chi} - \nu A(\boldsymbol{\theta})) \\ &= \left(\prod_{i=1}^n h(x_i)\right) f(\boldsymbol{\chi}, \nu) g(\boldsymbol{\theta})^{(\nu+n)} \exp\left(\boldsymbol{\theta} \cdot \left(\sum_{i=1}^n T(x_i) + \boldsymbol{\chi}\right)\right) \\ &\propto g(\boldsymbol{\theta})^{(\nu+n)} \exp\left(\boldsymbol{\theta} \cdot \left(\sum_{i=1}^n T(x_i) + \boldsymbol{\chi}\right)\right) \\ &= \exp\left(\boldsymbol{\theta} \cdot \left(\sum_{i=1}^n T(x_i) + \boldsymbol{\chi}\right) - (\nu + n)A(\boldsymbol{\theta})\right). \end{aligned}$$

Thus,

$$p(\boldsymbol{\theta}|X, \boldsymbol{\chi}, \nu) = p_\pi(\boldsymbol{\theta}|\boldsymbol{\chi} + \sum_{i=1}^n T(x_i), \nu + n).$$

2 [40pts] Decision Boundary

考虑二分类问题, 特征空间 $X \in \mathcal{X} = \mathbb{R}^d$, 标记 $Y \in \mathcal{Y} = \{0, 1\}$. 我们对模型做如下生成式假设:

- Attribute conditional independence assumption: 对已知类别, 假设所有属性相互独立, 即每个属性特征独立地对分类结果发生影响;
- Bernoulli prior on label: 假设标记满足 Bernoulli 分布先验, 并记 $\Pr(Y = 1) = \pi$.

(1) [20pts] 假设 $P(X_i|Y)$ 服从指数族分布, 即

$$\Pr(X_i = x_i|Y = y) = h_i(x_i) \exp(\theta_{iy} \cdot T_i(x_i) - A_i(\theta_{iy}))$$

请计算后验概率分布 $\Pr(Y|X)$ 以及分类边界 $\{x \in \mathcal{X} : P(Y = 1|X = x) = P(Y = 0|X = x)\}$. (**Hint:** 你可以使用 sigmoid 函数 $\mathcal{S}(x) = 1/(1 + e^{-x})$ 进行化简最终的结果).

(2) [20pts] 假设 $P(X_i|Y = y)$ 服从高斯分布, 且记均值为 μ_{iy} 以及方差为 σ_i^2 (注意, 这里的方差与标记 Y 是独立的), 请证明分类边界与特征 X 是成线性的。

Solution. 1.

$$\begin{aligned} \frac{P(Y = 1|X)}{P(Y = 0|X)} &= \frac{P(X|Y = 1)P(Y = 1)}{P(X|Y = 0)P(Y = 0)} \\ &= \frac{\pi}{1 - \pi} \exp \left(\sum_{i=1}^d ((\theta_{i1} - \theta_{i0}) \cdot T_i(x_i) - (A_i(\theta_{i1}) - A_i(\theta_{i0}))) \right). \end{aligned}$$

Thus,

$$P(Y = 0|X) = \mathcal{S} \left(-\log \frac{\pi}{1 - \pi} + \sum_{i=1}^d ((\theta_{i0} - \theta_{i1}) \cdot T_i(x_i) - (A_i(\theta_{i0}) - A_i(\theta_{i1}))) \right).$$

Let $P(Y = 0|X) = \frac{1}{2}$, we have

$$\log \frac{\pi}{1 - \pi} = \sum_{i=1}^d ((\theta_{i0} - \theta_{i1}) \cdot T_i(x_i) - A_i(\theta_{i0}) + A_i(\theta_{i1})),$$

which is the classification boundary.

2. Substitute the parameters in 1.(2) into the above classification boundary, and we have

$$\log \frac{\pi}{1 - \pi} = \sum_{i=1}^d \left(\frac{x_i - \mu_{i1}}{2\sigma^2} \right)^2 - \sum_{i=1}^d \left(\frac{x_i - \mu_{i0}}{2\sigma^2} \right)^2.$$

Simplify the above equation, and we have

$$\log \frac{\pi}{1 - \pi} = \sum_{i=1}^d \left(\frac{2(\mu_{i0} - \mu_{i1})x_i + \mu_{i1}^2 - \mu_{i0}^2}{2\sigma^2} \right),$$

which is linear in X .

3 [70pts] Theoretical Analysis of k -means Algorithm

给定样本集 $\mathcal{D} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$, k -means 聚类算法希望获得簇划分 $\mathcal{C} = \{C_1, C_2, \dots, C_k\}$, 使得最小化欧式距离

$$J(\gamma, \mu_1, \dots, \mu_k) = \sum_{i=1}^n \sum_{j=1}^k \gamma_{ij} \|\mathbf{x}_i - \mu_j\|^2 \quad (3.1)$$

其中, μ_1, \dots, μ_k 为 k 个簇的中心 (means), $\gamma \in \mathbb{R}^{n \times k}$ 为指示矩阵 (indicator matrix) 定义如下: 若 \mathbf{x}_i 属于第 j 个簇, 则 $\gamma_{ij} = 1$, 否则为 0.

则最经典的 k -means 聚类算法流程如算法1中所示 (与课本中描述稍有差别, 但实际上是等价的)。

Algorithm 1: k -means Algorithm

1 Initialize μ_1, \dots, μ_k .

2 repeat

3 **Step 1:** Decide the class memberships of $\{\mathbf{x}_i\}_{i=1}^n$ by assigning each of them to its nearest cluster center.

$$\gamma_{ij} = \begin{cases} 1, & \|\mathbf{x}_i - \mu_j\|^2 \leq \|\mathbf{x}_i - \mu_{j'}\|^2, \forall j' \\ 0, & \text{otherwise} \end{cases}$$

4 **Step 2:** For each $j \in \{1, \dots, k\}$, recompute μ_j using the updated γ to be the center of mass of all points in C_j :

$$\mu_j = \frac{\sum_{i=1}^n \gamma_{ij} \mathbf{x}_i}{\sum_{i=1}^n \gamma_{ij}}$$

5 until the objective function J no longer changes;

- (1) [10pts] 试证明, 在算法1中, **Step 1** 和 **Step 2** 都会使目标函数 J 的值降低。
- (2) [10pts] 试证明, 算法1会在有限步内停止。
- (3) [10pts] 试证明, 目标函数 J 的最小值是关于 k 的非增函数, 其中 k 是聚类簇的数目。
- (4) [20pts] 记 $\hat{\mathbf{x}}$ 为 n 个样本的中心点, 定义如下变量,

total deviation	$T(X) = \sum_{i=1}^n \ \mathbf{x}_i - \hat{\mathbf{x}}\ ^2 / n$
intra-cluster deviation	$W_j(X) = \sum_{i=1}^n \gamma_{ij} \ \mathbf{x}_i - \mu_j\ ^2 / \sum_{i=1}^n \gamma_{ij}$
inter-cluster deviation	$B(X) = \sum_{j=1}^k \frac{\sum_{i=1}^n \gamma_{ij}}{n} \ \mu_j - \hat{\mathbf{x}}\ ^2$

试探究以上三个变量之间有什么样的等式关系? 基于此, 请证明, k -means 聚类算法可以认为是在最小化 intra-cluster deviation 的加权平均, 同时近似最大化 inter-cluster deviation.

- (5) [20pts] 在公式(3.1)中, 我们使用 ℓ_2 -范数来度量距离 (即欧式距离), 下面我们考虑使用 ℓ_1 -范数来度量距离

$$J'(\gamma, \mu_1, \dots, \mu_k) = \sum_{i=1}^n \sum_{j=1}^k \gamma_{ij} \|\mathbf{x}_i - \mu_j\|_1 \quad (3.2)$$

- [10pts] 请仿效算法1(k -means- ℓ_2 算法), 给出新的算法 (命名为 k -means- ℓ_1 算法) 以优化公式3.2中的目标函数 J' .
- [10pts] 当样本集中存在少量异常点 (outliers) 时, 上述的 k -means- ℓ_2 和 k -means- ℓ_1 算法, 我们应该采用哪种算法? 即, 哪个算法具有更好的鲁棒性? 请说明理由。

Solution. (1) **Step 1:** Let $J_i = \sum_{j=1}^k \gamma_{ij} \|\mathbf{x}_i - \mu_j\|^2$, then $J = \sum_{i=1}^n J_i$. If an instance \mathbf{x}_i is not assigned to a new cluster, the contribution of \mathbf{x}_i , i.e., J_i is not changed. Suppose \mathbf{x} was assigned to j' but reassigned to j during **Step 1**. The contribution J_i is decreased from $\|\mathbf{x}_i - \mu_{j'}\|^2$ to $\|\mathbf{x}_i - \mu_j\|^2$.

Step 2: From elementary geometry we know that the center of a point set minimizes the sum of the distances between it and the points in the set. **Step 2** minimizes the contribution of each cluster to the function J , thus it decreases J .

- (2) There are only k^n possible assignments of points. For each assignment, **Step 2** guarantees that at the end of each loop, J is minimum with respect to the current assignment. Thus, at the end of each loop, J takes finitely many possible values. From (1), we know J is non-increasing, so after finitely many loops, J will no longer change, and the algorithm terminates.
- (3) Suppose for $k = k_0 \geq 1$, the minimum of J is achieved with γ and $\mu_j, j \in \{1, \dots, k_0\}$. For $k = k_0 + 1$, Let $\gamma' = \gamma$, $\mu'_j = \mu_j, j \in \{1, \dots, k_0\}$, and $\mu'_k = \mu_0$. It is obvious that with these assignments $J(k_0 + 1) = \min J(k_0)$. Thus we have $J(k_0 + 1) \leq J(k_0)$.
- (4) Let $n_j = \sum_{i=1}^n \gamma_{ij}$. We have

$$\begin{aligned} n_j W_j(X) + n_j \|\mu_j - \hat{\mathbf{x}}\|^2 &= \sum_{i=1}^n \gamma_{ij} \|\mathbf{x}_i - \mu_j\|^2 + n_j \|\mu_j - \hat{\mathbf{x}}\|^2 \\ &= \sum_{i=1}^n \gamma_{ij} (\|\mathbf{x}_i - \mu_j\|^2 + \|\mu_j - \hat{\mathbf{x}}\|^2) \\ &= \sum_{i=1}^n \gamma_{ij} \|\mathbf{x}_i - \hat{\mathbf{x}}\|^2 \end{aligned}$$

Sum the above equation for all j , and we have

$$\frac{\sum_{j=1}^k n_j W_j(X)}{n} + B(X) = T(X).$$

As $T(X)$ is a constant, and $\frac{\sum_{j=1}^k n_j W_j(X)}{n}$ is $\frac{J}{n}$, we are minimizing the weighted average of intra-cluster deviation and maximizing inter-cluster deviation.

- (5) We need to revise both **Step 1** and **Step 2**. **Step 1** should consider ℓ_1 distance. Similarly, **Step 2** should update each cluster center to the point that minimizes the sum of ℓ_1 distances.

Algorithm 2: k -means Algorithm with ℓ_1 Distance

1 Initialize μ_1, \dots, μ_k .

2 **repeat**

3 **Step 1:** Decide the class memberships of $\{\mathbf{x}_i\}_{i=1}^n$ by assigning each of them to its nearest cluster center.

$$\gamma_{ij} = \begin{cases} 1, & \|\mathbf{x}_i - \mu_j\|_1 \leq \|\mathbf{x}_i - \mu_{j'}\|_1, \forall j' \\ 0, & \text{otherwise} \end{cases}$$

4 **Step 2:** For each $j \in \{1, \dots, k\}$, recompute μ_j using the updated γ to be the center of mass of all points in C_j :

$$\mathbf{c}_p = \text{sort}([\mathbf{x}_{ip} \text{ if } \gamma_{ij}])$$

$$\mu_{jp} = c_p[\frac{\text{len}(c_p)}{2} + 1]$$

5 **until** the objective function J no longer changes;

We should use the k -means- ℓ_1 algorithm if outliers are present. The influence of outliers is more significant under ℓ_2 distance than under ℓ_1 distance. Thus, k -means- ℓ_1 is more robust.

4 [50pts] Kernel, Optimization and Learning

给定样本集 $\mathcal{D} = \{(x_1, y_1), (x_2, y_2), \dots, (x_m, y_m)\}$, $\mathcal{F} = \{\Phi_1 \dots, \Phi_d\}$ 为非线性映射族。考虑如下的优化问题

$$\min_{\mathbf{w}, \mu \in \Delta_q} \frac{1}{2} \sum_{k=1}^d \frac{1}{\mu_k} \|\mathbf{w}_k\|^2 + C \sum_{i=1}^m \max \left\{ 0, 1 - y_i \left(\sum_{k=1}^d \mathbf{w}_k \cdot \Phi_k(x_i) \right) \right\} \quad (4.1)$$

其中, $\Delta_q = \{\mu : \mu \geq 0, \|\mu\|_q = 1\}$.

(1) [30pts] 请证明, 下面的问题4.2是优化问题4.1的对偶问题。

$$\begin{aligned} \max_{\alpha} \quad & 2\alpha^T \mathbf{1} - \left\| \begin{array}{c} \alpha^T \mathbf{Y}^T \mathbf{K}_1 \mathbf{Y} \alpha \\ \vdots \\ \alpha^T \mathbf{Y}^T \mathbf{K}_d \mathbf{Y} \alpha \end{array} \right\|_p \\ \text{s.t.} \quad & \mathbf{0} \leq \alpha \leq \mathbf{C} \end{aligned} \quad (4.2)$$

其中, p 和 q 满足共轭关系, 即 $\frac{1}{p} + \frac{1}{q} = 1$. 同时, \mathbf{K}_k 是由 Φ_k 定义的核函数 (kernel).

(2) [20pts] 考虑在优化问题4.2中, 当 $p = 1$ 时, 试化简该问题。

Solution. (1) Rewrite the optimization problem:

$$\begin{aligned} \min_{\mathbf{w}, \mu \in \Delta_q} \quad & \frac{1}{2} \sum_{k=1}^d \frac{1}{\mu_k} \|\mathbf{w}_k\|^2 + C \sum_{i=1}^m \xi_i \\ \text{s.t.} \quad & y_i \left(\sum_{k=1}^d \mathbf{w}_k \cdot \Phi_k(x_i) \right) \geq 1 - \xi_i \\ & \xi_i \geq 0 \\ & \mu_i \geq 0 \\ & \|\mu\|_q = 1 \end{aligned} \quad (4.3)$$

The Lagrangian form of 4.3 is

$$\begin{aligned} L(\mathbf{w}, \xi, \mu, \alpha, \beta, \gamma, \delta) = & \frac{1}{2} \sum_{k=1}^d \frac{1}{\mu_k} \|\mathbf{w}_k\|^2 + C \sum_{i=1}^m \xi_i \\ & + \sum_{i=1}^m \alpha_i \left(1 - \xi_i - y_i \left(\sum_{k=1}^d \mathbf{w}_k \cdot \Phi_k(x_i) \right) \right) \\ & - \sum_{i=1}^m \beta_i \xi_i - \sum_{k=1}^d \gamma_k \mu_k + \delta (\|\mu\|_q - 1). \end{aligned} \quad (4.4)$$

Take the partial derivatives of \mathbf{w} , μ , and ξ , and let them equal to 0:

$$\begin{aligned} \frac{\mathbf{w}_k}{\mu_k} &= \sum_{i=1}^m \alpha_i y_i \Phi_k(x_i), \\ \frac{1}{2} \frac{\|\mathbf{w}_k\|^2}{\mu_k^2} + \gamma_k &= \delta \left(\frac{\mu_k}{\|\mu\|_q} \right)^{q-1}, \\ \alpha_i + \beta_i &= C. \end{aligned} \quad (4.5)$$

We first eliminate β and ξ with 4.5,

$$L(\mathbf{w}, \boldsymbol{\mu}, \boldsymbol{\alpha}, \gamma, \delta) = -\frac{1}{2} \sum_{k=1}^d \frac{1}{\mu_k} \|\mathbf{w}_k\|^2 + \sum_{i=1}^m \alpha_i - \sum_{i=1}^d \gamma_i \mu_i + \delta(\|\boldsymbol{\mu}\|_q - 1). \quad (4.6)$$

Then eliminate γ with 4.5.

$$\begin{aligned} L(\mathbf{w}, \boldsymbol{\mu}, \boldsymbol{\alpha}, \delta) &= -\frac{1}{2} \sum_{k=1}^d \frac{1}{\mu_k} \|\mathbf{w}_k\|^2 + \sum_{i=1}^m \alpha_i \\ &\quad + -\frac{1}{2} \sum_{k=1}^d \frac{1}{\mu_k} \|\mathbf{w}_k\|^2 - \delta \sum_{k=1}^d \frac{\mu_k^q}{\|\boldsymbol{\mu}\|_q^{q-1}} + \delta \|\boldsymbol{\mu}\|_q - \delta \\ &= \sum_{i=1}^m \alpha_i + \delta \frac{(\sum_{k=1}^d \mu_k^q) - \|\boldsymbol{\mu}\|_q^q}{\|\boldsymbol{\mu}\|_q^{q-1}} - \delta \\ &= \sum_{i=1}^m \alpha_i - \delta. \end{aligned} \quad (4.7)$$

We manipulate the second equation of 4.5 to evaluate δ ,

$$\left(\frac{\|\mathbf{w}_k\|^2}{\mu_k^2} \right)^{\frac{q}{q-1}} = \left(2\delta \left(\frac{\mu_k}{\|\boldsymbol{\mu}\|_q} \right)^{q-1} - \gamma_k \right)^{\frac{q}{q-1}}.$$

We are maximizing the Lagrangian, and the Lagrangian is monotonically decreasing in δ . Therefore, we need to minimize δ . γ is dependent only on δ , and δ is monotonically increasing in γ_k . Thus we can safely set γ_k to 0. Then, the above equation simplifies into

$$\left(\frac{\|\mathbf{w}_k\|^2}{\mu_k^2} \right)^{\frac{q}{q-1}} = (2\delta)^{\frac{q}{q-1}} \left(\frac{\mu_k}{\|\boldsymbol{\mu}\|_q} \right)^q$$

Sum it over k , and take the $\frac{q-1}{q}$ -th root,

$$\left(\sum_{k=1}^d \left(\frac{\|\mathbf{w}_k\|^2}{\mu_k^2} \right)^{\frac{q}{q-1}} \right)^{\frac{q-1}{q}} = 2\delta \|\boldsymbol{\mu}\|_q^{1-q} \left(\sum_{k=1}^d \mu_k^q \right)^{\frac{q-1}{q}} = 2\delta,$$

which is equivalent to

$$\frac{1}{2} \left\| \begin{bmatrix} \frac{\|\mathbf{w}_1\|^2}{\mu_1^2} \\ \vdots \\ \frac{\|\mathbf{w}_d\|^2}{\mu_d^2} \end{bmatrix} \right\|_p = \delta. \quad (4.8)$$

Substitute the first equation of 4.5 into 4.8,

$$\frac{1}{2} \left\| \begin{bmatrix} \boldsymbol{\alpha}^T \mathbf{Y}^T \mathbf{K}_1 \mathbf{Y} \boldsymbol{\alpha} \\ \vdots \\ \boldsymbol{\alpha}^T \mathbf{Y}^T \mathbf{K}_d \mathbf{Y} \boldsymbol{\alpha} \end{bmatrix} \right\|_p = \delta. \quad (4.9)$$

With 4.5 and 4.9, the Lagrangian 4.4 is simplified into

$$\begin{aligned} \max_{\boldsymbol{\alpha}} \quad & \sum_{i=1}^m \alpha_i - \frac{1}{2} \left\| \begin{array}{c} \boldsymbol{\alpha}^T \mathbf{Y}^T \mathbf{K}_1 \mathbf{Y} \boldsymbol{\alpha} \\ \vdots \\ \boldsymbol{\alpha}^T \mathbf{Y}^T \mathbf{K}_d \mathbf{Y} \boldsymbol{\alpha} \end{array} \right\|_p \\ \text{s.t.} \quad & \mathbf{0} \leq \boldsymbol{\alpha} \leq \mathbf{C} \end{aligned} \quad (4.10)$$

which is exactly 4.2.

(2) When $p = 1$, the optimization problem degenerates to

$$\begin{aligned} \max_{\boldsymbol{\alpha}} \quad & 2\boldsymbol{\alpha}^T \mathbf{1} - \boldsymbol{\alpha}^T \mathbf{Y}^T \left(\sum_{k=1}^d \mathbf{K}_k \right) \mathbf{Y} \boldsymbol{\alpha} \\ \text{s.t.} \quad & \mathbf{0} \leq \boldsymbol{\alpha} \leq \mathbf{C} \end{aligned} \quad (4.11)$$

(3) 第一小题中, 将 γ_k 置为 0 所得到的优化问题与原问题之对偶问题等价的想法来自计科(19') 的卢以宁小姐.