

2.5 Maximum entropy principle

5. Maximum entropy principle.

Setting:

Given n data points $x^{(1)}, \dots, x^{(n)}$.

A feature function $\phi: \mathcal{X} \rightarrow \mathbb{R}^d$.

Define the empirical moments: $\hat{\mu} := \frac{1}{n} \sum_{i=1}^n \phi(x^{(i)})$

Define $Q := \{q \in \Delta_{|\mathcal{X}|} : E_q[\phi(x)] = \hat{\mu}\}$, where $E_q[\phi(x)] := \sum q(x) \phi(x)$

Note: $|\mathcal{X}|$ can be large but q only have d constraints.

[Definition 2] maximum entropy principle.

Choose the distribution \hat{q} with the highest entropy:

$$\hat{q} := \arg \max_{q \in Q} H(q)$$

where $H(q) := E_q[-\log q(x)]$

We will show that Maximum Likelihood is equivalent to Maximum Entropy, in the following theorem.

[Theorem 1] maximum entropy duality:

Assume Q is non-empty, then

$$\arg \max_{q \in Q} H(q) = \arg \max_{p \in P} \sum_{i=1}^n \log p(x^{(i)})$$

Pf: Straightforward application of Lagrangian duality.

$$\max_{q \in Q} H(q) = \max_{q \in \Delta_{|\mathcal{X}|}} \min_{\theta \in \mathbb{R}^d} H(q) - \theta \cdot (\hat{\mu} - E_q[\phi(x)]) \quad (i)$$

Since Q is non-empty (Slater's condition), we can switch the min & max.

$$\min_{\theta \in \mathbb{R}^d} \max_{q \in \Delta_{|\mathcal{X}|}} - \sum_{x \in \mathcal{X}} q(x) \log q(x) - \theta \cdot (\hat{\mu} - \sum_{x \in \mathcal{X}} q(x) \phi(x)) \quad (ii)$$

Next, differentiate w.r.t. γ and set it to some constant c :

$$-(1 + \log q(x)) + \theta \cdot \phi(x) = c, \quad \text{for each } x \in \mathcal{X}.$$

(Since $\sum q(x) = 1$)

Solving for q (rewrite as q_θ), then $q_\theta(x) \propto \exp(\theta \cdot \phi(x))$.

By (ii), we have

$$\begin{aligned} & \min_{\theta \in \mathbb{R}^d} -(\theta \cdot \underbrace{E_\theta[\phi(x)]} - A(\theta)) - \theta \cdot (\hat{\mu} - \underbrace{E_\theta[\phi(x)]}) \\ \Leftrightarrow & \max_{\theta \in \mathbb{R}^d} \theta \cdot \hat{\mu} - A(\theta), \quad \text{which is the maximum likelihood objective.} \end{aligned}$$

Using the fact $\Delta A(\theta) = E_\theta[\phi(x)]$, we have

$$0 = \hat{\mu} - \Delta A(\theta) = \hat{\mu} - E_\theta[\phi(x)].$$

which means $q_\theta \in \mathcal{Q}$

□