Maximum Likelihood Estimation

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Likelihood of an Estimated Probability Distribution

Estimating a Probability Distribution: Setting

- Let $p(y)$ represent a probability distribution on $\mathcal{Y}$.
- $p(y)$ is **unknown** and we want to **estimate** it.
- Assume that $p(y)$ is either a
  - probability density function on a continuous space $\mathcal{Y}$, or a
  - probability mass function on a discrete space $\mathcal{Y}$.
- Typical $\mathcal{Y}$'s:
  - $\mathcal{Y} = \mathbf{R}$; $\mathcal{Y} = \mathbf{R}^d$ [typical continuous distributions]
  - $\mathcal{Y} = \{-1, 1\}$ [e.g. binary classification]
  - $\mathcal{Y} = \{0, 1, 2, \ldots, K\}$ [e.g. multiclass problem]
  - $\mathcal{Y} = \{0, 1, 2, 3, 4 \ldots\}$ [unbounded counts]

Evaluating a Probability Distribution Estimate

- Before we talk about estimation, let's talk about evaluation.
- Somebody gives us an estimate of the probability distribution

$$\hat{p}(y).$$

- How can we evaluate how good it is?
- We want $\hat{p}(y)$ to be descriptive of **future** data.

Likelihood of a Predicted Distribution

- Suppose we have

$$\mathcal{D} = (y_1, \dots, y_n) \text{ sampled i.i.d. from true distribution } p(y).$$

- Then the **likelihood** of $\hat{p}$ for the data $\mathcal{D}$ is defined to be

$$\hat{p}(\mathcal{D}) = \prod_{i=1}^{n} \hat{p}(y_i).$$

- If $\hat{p}$ is a probability mass function, then likelihood is probability.

Parametric Families of Distributions

Parametric Models

Definition

A **parametric model** is a set of probability distributions indexed by a parameter $\theta \in \Theta$. We denote this as

$$\{p(y;\theta) \mid \theta \in \Theta\},$$

where θ is the **parameter** and Θ is the **parameter space**.

- Below we'll give some examples of common parametric models.
  - But it's worth doing research to find a parametric model most appropriate for your data.
- We'll sometimes say **family of distributions** for a probability model.

Poisson Family

- Support $\mathcal{Y} = \{0, 1, 2, 3, \ldots\}$.
- Parameter space: $\{\lambda \in \mathbf{R} \mid \lambda > 0\}$
- Probability mass function on $k \in \mathcal{Y}$:

$$p(k; \lambda) = \lambda^k e^{-\lambda} / (k!)$$

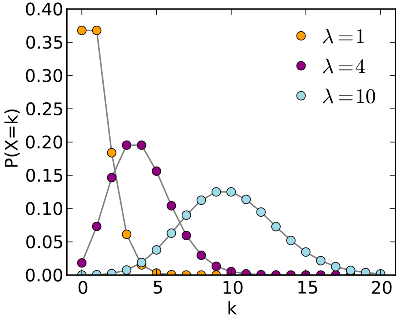

Figure is "Poisson pmf" by Skbkekas - Own work. Licensed under CC BY 3.0 via Wikimedia Commons - http://commons.wikimedia.org/wiki/File:Poisson_pmf.svg#/media/File:Poisson_pmf.svg.

Beta Family

- Support $\mathcal{Y} = (0,1)$. [The unit interval.]
- Parameter space: $\{\theta = (\alpha, \beta) \mid \alpha, \beta > 0\}$
- Probability density function on $y \in \mathcal{Y}$:

$$p(y; a, b) = \frac{y^{\alpha-1}(1-y)^{\beta-1}}{B(\alpha, \beta)}$$

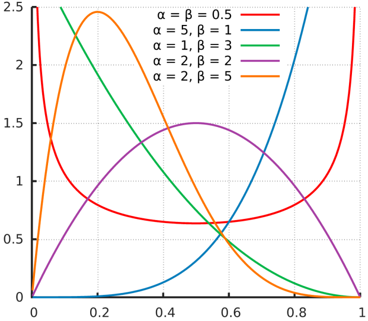

Figure by Horas based on the work of Krishnavedala (Own work) [Public domain], via Wikimedia Commons.

Gamma Family

- Support $\mathcal{Y} = (0, \infty)$. [Positive real numbers]
- Parameter space: $\{\theta = (k, \theta) \mid k > 0, \theta > 0\}$
- Probability density function on $y \in \mathcal{Y}$:

$$p(y; k, \theta) = \frac{1}{\Gamma(k)\theta^k} x^{k-1} e^{-y/\theta}.$$

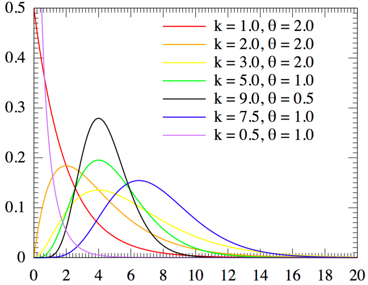

Figure from Wikipedia `https://commons.wikimedia.org/wiki/File:Gamma_distribution_pdf.svg`.

Maximum Likelihood Estimation

Likelihood in a Parametric Model

Suppose we have a parametric model $\{p(y;\theta) \mid \theta \in \Theta\}$ and a sample $\mathcal{D} = \{y_1, \dots, y_n\}$.

- The **likelihood** of parameter estimate $\hat{\theta} \in \Theta$ for sample $\mathcal{D}$ is

$$p(\mathcal{D};\hat{\theta}) = \prod_{i=1}^{n} p(y_i;\hat{\theta}).$$

- In practice, we prefer to work with the **log-likelihood**. Same maximum but

$$\log p(\mathcal{D};\hat{\theta}) = \sum_{i=1}^{n} \log p(y_i;\theta),$$

  and sums are easier to work with than products.

Definition

The **maximum likelihood estimator (MLE)** for θ in the model $\{p(y,\theta) \mid \theta \in \Theta\}$ is

$$\begin{aligned}\hat{\theta} &= \underset{\theta\in\Theta}{\arg\max} \log p(\mathcal{D},\hat{\theta}) \\ &= \underset{\theta\in\Theta}{\arg\max} \sum_{i=1}^{n} \log p(y_i;\theta).\end{aligned}$$

Maximum Likelihood Estimation

- Finding the MLE is an optimization problem.
- For some model families, calculus gives a closed form for the MLE.
- Can also use numerical methods we know (e.g. SGD).

MLE Existence

- In certain situations, the MLE may not exist.
- But there is usually a good reason for this.

- e.g. Gaussian family $\left\{\mathcal{N}(\mu, \sigma^2) \mid \mu \in \mathbf{R}, \sigma^2 > 0\right\}$
- We have a single observation y.
- Is there an MLE?

- Taking $\mu = y$ and $\sigma^2 \to 0$ drives likelihood to infinity.
- MLE doesn't exist.

Example: MLE for Poisson

- Observed counts $\mathcal{D} = (k_1, \ldots, k_n)$ for taxi cab pickups over n weeks.
  - k_i is number of pickups at Penn Station Mon, 7-8pm, for week i.
- We want to fit a Poisson distribution to this data.
- The Poisson log-likelihood for a single count is

$$\begin{aligned} \log\left[p(k;\lambda)\right] &= \log\left[\frac{\lambda^k e^{-\lambda}}{k!}\right] \\ &= k\log\lambda - \lambda - \log(k!) \end{aligned}$$

- The full log-likelihood is

$$\log p(\mathcal{D},\lambda) = \sum_{i=1}^{n}\left[k_i\log\lambda - \lambda - \log(k_i!)\right].$$

Example: MLE for Poisson

- The full log-likelihood is

$$\log p(\mathcal{D}, \lambda) = \sum_{i=1}^{n} [k_i \log \lambda - \lambda - \log (k_i!)]$$

- First order condition gives

$$\begin{aligned} 0 = \frac{\partial}{\partial \lambda} [\log p(\mathcal{D}, \lambda)] &= \sum_{i=1}^{n} \left[\frac{k_i}{\lambda} - 1 \right] \\ \implies \lambda &= \frac{1}{n} \sum_{i=1}^{n} k_i \end{aligned}$$

- So MLE $\hat{\lambda}$ is just the mean of the counts.

Test Set Log Likelihood for Penn Station, Mon-Fri 7-8pm

Method	Test Log-Likelihood
Poisson	-392.16
Negative Binomial	-188.67
Histogram (Bin width $= 7$)	$-\infty$
95% Histogram +.05 NegBin	-203.89

Estimating Distributions, Overfitting, and Hypothesis Spaces

- Just as in classification and regression, MLE can overfit!
- Example Probability Models:
  - $\mathcal{F} = \{\text{Poisson distributions}\}$.
  - $\mathcal{F} = \{\text{Negative binomial distributions}\}$.
  - $\mathcal{F} = \{\text{Histogram with 10 bins}\}$
  - $\mathcal{F} = \{\text{Histogram with bin for every } y \in \mathcal{Y}\}$ [will likely overfit for continuous data]
- How to judge which model works the best?
- Choose the model with the **highest likelihood on validation set**.