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Mathematics for Machine Learning

by

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DEPARTMENT OF MATHEMATICS
IIT Kharagpur

Module 8.1

Lecture 36: MLE for Discrete Probability Distribution

Concepts Covered

Maximum Likelihood Estimation for some discrete probability distributions

MLE for Binomial distribution parameter

$$Bin(k|n,\theta) = \binom{n}{k}\theta^k(1-\theta)^{n-k}$$

Suppose that the random variables $X = \{X_1, X_2, \ldots, X_n\}$ form a *i.i.d.* random sample from a population of Binomial distribution $Bin(k|n,\theta)$. We would like to find $\boldsymbol{\theta_{MLE}}$ for θ.

if X is discrete random variable, $f(x|\theta)$ is point mass function, then for every observed random sample $x_1, x_2, \cdots, x_n$, we define joint probability or the **Likelihood Function**

$$f(x_1, x_2, \cdots, x_n|\theta) = f(x_1|\theta)\cdots f(x_n|\theta)$$

The likelihood function is

$$\boldsymbol{L(\theta) = f(x_1, x_2, \cdots, x_n|\theta) = \prod_{i=1}^{n}\binom{n}{x_i}\theta^{x_i}(1-\theta)^{(n-x_i)}}$$

MLE for Binomial distribution parameter

Suppose that the random variables $X = \{X_1, X_2, \ldots, X_n\}$ form a *i.i.d.* random sample from a population of Binomial distribution $Bin(k|n, \theta)$. We would like to find $\boldsymbol{\theta_{MLE}}$ for θ.

The likelihood function is

$$\boldsymbol{L(\theta) = f(x_1, x_2, \cdots, x_n|\theta) = \prod_{i=1}^{n} \binom{n}{x_i} \theta^{x_i}(1-\theta)^{(n-x_i)}}$$

The log-likelihood function is

$$\boldsymbol{log\ L(\theta) = log \prod_{i=1}^{n} \binom{n}{x_i} \theta^{x_i}(1-\theta)^{(n-x_i)}}$$

$$\boldsymbol{= log \sum_{i=1}^{n} \left(log \binom{n}{x_i} + x_i\ log\ \theta + (1-x_i) log\ (1-\theta) \right)}$$

MLE for Binomial distribution parameter

Suppose that the random variables $X = \{X_1, X_2, \ldots, X_n\}$ form a *i.i.d.* random sample from a population of Binomial distribution $Bin(k|n, \theta)$. We would like to find $\boldsymbol{\theta_{MLE}}$ for θ.

The log-likelihood function is:

$$\boldsymbol{log \sum_{i=1}^{n} \left(log \binom{n}{x_i} + x_i \, log \, \theta + (1 - x_i) log \, (1 - \theta) \right)}$$

Taking derivative of log-likelihood function and equating to zero –

$$\boldsymbol{\frac{d \, L(\theta)}{d\theta} = \sum_{i=1}^{n} \left(\frac{x_i}{\theta} - \frac{1 - x_i}{1 - \theta} \right) = 0}$$

$$\boldsymbol{\theta_{MLE} = \frac{1}{n} \sum_{i=1}^{n} x_i}$$

MLE for Poisson distribution parameter

$$\text{Poisson}(k|\lambda) = \frac{\lambda^k e^{-\lambda}}{k!}, \quad \lambda > 0$$

Suppose that the random variables $X = \{X_1, X_2, \ldots, X_n\}$ form a *i.i.d.* random sample from a population of Poisson distribution $\text{Poisson}(k|\lambda)$. We would like to find $\boldsymbol{\lambda_{MLE}}$ for λ.

if X is discrete random variable, $f(x|\lambda)$ is point mass function, then for every observed random sample $x_1, x_2, \cdots, x_n$, we define joint probability or the **Likelihood Function**

$$f(x_1, x_2, \cdots, x_n|\lambda) = f(x_1|\lambda) \cdots f(x_n|\lambda)$$

The likelihood function is

$$\boldsymbol{L(\lambda) = f(x_1, x_2, \cdots, x_n|\lambda) = \prod_{i=1}^{n} \frac{\lambda^{x_i} e^{-\lambda}}{x_i!}}$$

MLE for Poisson distribution parameter

Suppose that the random variables $X = \{X_1, X_2, \ldots, X_n\}$ form a *i.i.d.* random sample from a population of Binomial distribution $Bin(k|n, \theta)$. We would like to find $\boldsymbol{\theta_{MLE}}$ for θ.

The likelihood function is

$$\boldsymbol{L(\lambda) = f(x_1, x_2, \cdots, x_n|\lambda) = \prod_{i=1}^{n} \frac{\lambda^{x_i} e^{-\lambda}}{x_i!} = \frac{e^{-n\lambda} \lambda^{\sum_{i=1}^{n} x_i}}{\prod_{i=1}^{n} x_i!}}$$

The log-likelihood function is

$$\boldsymbol{log\ L(\lambda) = log \frac{e^{-n\lambda} \lambda^{\sum_{i=1}^{n} x_i}}{\prod_{i=1}^{n} x_i!}}$$

$$\boldsymbol{= -n\lambda + log\ \lambda \sum_{i=1}^{n} x_i - \sum_{i=1}^{n} log\ x_i!}$$

MLE for Binomial distribution parameter

Suppose that the random variables $X = \{X_1, X_2, \ldots, X_n\}$ form a *i.i.d.* random sample from a population of Binomial distribution $Bin(k|n, \theta)$. We would like to find $\boldsymbol{\theta_{MLE}}$ for θ.

The log-likelihood function is:

$$-n\lambda + log\ \lambda \sum_{i=1}^{n} x_i - \sum_{i=1}^{n} log\ x_i!$$

Taking derivative of log-likelihood function and equating to zero –

$$\frac{d\ L(\lambda)}{d\lambda} = -n + \frac{1}{\lambda}\sum_{i=1}^{n} x_i = 0$$

$$\lambda_{MLE} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

Example: Let a population has been considered with the following probability distribution

$$f(x|\theta) = \begin{cases} \frac{1}{4} & if\ x = 0 \\ \frac{1+2\theta}{4} & if\ x = 1 \\ \frac{1}{4} & if\ x = 2 \\ \frac{1-2\theta}{4} & if\ x = 3 \end{cases}$$

A sample with 10 observations has been considered, which is as follows:

$$(3, 0, 2, 1, 3, 2, 1, 0, 2, 1\ )$$

Find $\boldsymbol{\theta_{MLE}}$ for $\boldsymbol{\theta}$.

Example: Let a population has been considered with the following probability distribution

$$f(x|\theta) = \begin{cases} \frac{1}{4} & if\ x = 0 \\ \frac{1+2\theta}{4} & if\ x = 1 \\ \frac{1}{4} & if\ x = 2 \\ \frac{1-2\theta}{4} & if\ x = 3 \end{cases}$$

Sample: (3, 0, 2, 1, 3, 2, 1, 0, 2, 1)

The likelihood function is

$$L(\theta) = P(x=3)\ P(x=0)P(x=2)P(x=1)P(x=3)P(x=2)P(x=1)P(x=0)$$
$$P(x=2)P(x=1)$$

$$= \left(\frac{1}{4}\right)^2 \left(\frac{1+2\theta}{4}\right)^3 \left(\frac{1}{4}\right)^3 \left(\frac{1-2\theta}{4}\right)^2$$

The log-likelihood function is:

$$Log\ L(\theta) = \{2\ log\ 1 - 2log\ 4\} + \{3\ log\ (1+2\theta) - 3log\ 4\} + \{3\ log\ 1 - 3log\ 4\} +$$
$$\{2\ log\ (1-2\theta) - 2log\ 4\}$$

Example: Let a population has been considered with the following probability distribution

$$f(x|\theta) = \begin{cases} \frac{1}{4} & if\ x = 0 \\ \frac{1+2\theta}{4} & if\ x = 1 \\ \frac{1}{4} & if\ x = 2 \\ \frac{1-2\theta}{4} & if\ x = 3 \end{cases}$$

Sample: (3, 0, 2, 1, 3, 2, 1, 0, 2, 1)

The log-likelihood function is:

$$\boldsymbol{Log\ L(\theta)}$$
$$= \{2\ log\ 1 - 2log\ 4\} + \{3\ log\ (1+2\theta) - 3log\ 4\} + \{3\ log\ 1 - 3log\ 4\} + \{2\ log\ (1-2\theta) - 2log\ 4\}$$

Taking derivative of log-likelihood function and equating to zero –

$$\frac{\boldsymbol{d\ L(\theta)}}{\boldsymbol{d\theta}} = \frac{\boldsymbol{6}}{\boldsymbol{1+2\theta}} - \frac{\boldsymbol{4}}{\boldsymbol{1-2\theta}} = \boldsymbol{0}$$

$$\boldsymbol{\theta_{MLE} = .1}$$

Example: Let a population has been considered with the following probability distribution

$$f(x|\theta) = \begin{cases} \frac{1+2\theta}{4} & if\ x = 0 \\ \frac{1-\theta}{4} & if\ x = 1 \\ \frac{1+\theta}{4} & if\ x = 2 \\ \frac{1-2\theta}{4} & if\ x = 3 \end{cases}$$

A sample with 10 observations has been considered, which is as follows:

$$(3, 0, 2, 1, 3, 2, 1, 0, 2, 1\ )$$

Find $\boldsymbol{\theta_{MLE}}$ for $\boldsymbol{\theta}$.

Example: Let's assume our observed data points are: $x = [1,3,2,4,5,2,1,3,2,4]$ from a Poisson distribution.

The likelihood function for the Poisson distribution is:

$$L(\lambda) = \prod_{i=1}^{N} \frac{e^{-\lambda}\lambda^{x_i}}{x_i!}$$

Taking the logarithm of the likelihood function, we get the log-likelihood function:

$$\log L(\lambda) = -N\lambda + \sum_{i=1}^{N} x_i \log \lambda - \sum_{i=1}^{N} \log(x_i!)$$

To find the maximum likelihood estimate for λ, we differentiate the log-likelihood function with respect to λ, set it equal to zero, and solve for λ:

$$\frac{d}{d\lambda} \log L(\lambda) = -N + \frac{1}{\lambda} \sum_{i=1}^{N} x_i = 0$$

$$\Rightarrow \quad \lambda = \frac{1}{N} \sum_{i=1}^{N} x_i$$

Now, let's calculate the MLE of using our sample data:

$$\boldsymbol{\lambda_{MLE}} = \frac{1}{10} \sum_{i=1}^{10} x_i = \frac{1}{10}(1+3+2+4+5+2+1+3+2+4) = \frac{27}{10} = 2.7$$

- ✓ **Many practical problems we examine appropriate conditions and select the probability distribution**

- ✓ **A range of discrete probability distributions are considered here**

Different continuous probability distributions are in the next…..

References

- ✓ Linear Algebra and Learning from Data (2019), Gilbert Strang, Wellesley Cambridge Press
- ✓ Machine Learning: A Probabilistic Perspective, Kevin P. Murphy (MIT Press), 2021 edition
- ✓ Deisenroth MP, Faisal AA, Ong CS. Mathematics for machine learning. Cambridge University Press; 2020 Apr 23.


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Mathematics for Machine Learning

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DEPARTMENT OF MATHEMATICS
IIT Kharagpur

Module 8.2

Lecture 37: MLE for Continuous Probability Distribution

Concepts Covered

Maximum Likelihood Estimation for some continuous probability distributions

MLE for Exponential distribution parameter

Maximum likelihood estimation can be applied to a vector valued parameter. For a simple random sample of n exponential random variables, we would like to find $\boldsymbol{\lambda_{MLE}}$ for λ.

$$\mathbf{f}(\boldsymbol{x};\boldsymbol{\lambda}) = \begin{cases} \boldsymbol{\lambda e^{-\lambda x}} & \boldsymbol{x \geq 0} \\ \mathbf{0} & \boldsymbol{otherwise} \end{cases}$$

if X is continuous random variable, $f(x|\lambda)$ is probability density function, then for every observed random sample $x_1, x_2, \cdots, x_n$, we define joint probability or the **Likelihood Function**

$$f(x_1, x_2, \cdots, x_n|\lambda) = f(x_1|\lambda) \cdots f(x_n|\lambda)$$

$\lambda_{MLE} = \underset{\lambda}{\text{argmax}}\ L(\lambda)$

$= \underset{\lambda}{\text{argmax}}\ \log L(\lambda)$

The likelihood function is

$$\boldsymbol{L(\lambda) = f(x_1, x_2, \cdots, x_n|\hat{\theta}) = \prod_{i=1}^{n} \lambda e^{-\lambda x_i}}$$

MLE for Exponential distribution parameter

Maximum likelihood estimation can be applied to a vector valued parameter. For a simple random sample of n exponential random variables, we would like to find $\boldsymbol{\lambda_{MLE}}$ for λ.

$$\mathbf{f}(x;\boldsymbol{\lambda}) = \begin{cases} \boldsymbol{\lambda e^{-\lambda x}} & \boldsymbol{x \geq 0} \\ \mathbf{0} & \boldsymbol{otherwise} \end{cases}$$

The likelihood function is

$$\boldsymbol{L(\lambda) = f(x_1, x_2, \cdots, x_n|\lambda)} = \prod_{i=1}^{n} \lambda e^{-\lambda x_i}$$

The log-likelihood function is

$$\boldsymbol{\log L(\lambda) = n \log \lambda - \lambda \sum_{i=1}^{n} x_i}$$

MLE for Exponential distribution parameter

Maximum likelihood estimation can be applied to a vector valued parameter. For a simple random sample of n exponential random variables, we would like to find λ_{MLE} for λ.

$$f(x;\lambda) = \begin{cases} \lambda e^{-\lambda x} & x \geq 0 \\ 0 & otherwise \end{cases}$$

The log-likelihood function is

$$log\ L(\lambda) = n\ log\ \lambda - \lambda \sum_{i=1}^{n} x_i$$

Taking derivative of log-likelihood function w.r.t. μ and equating to zero –

$$\frac{dlog\ L(\lambda)}{d\lambda} = \frac{n}{\lambda} - \sum_{i=1}^{n} x_i = 0 \qquad \frac{n}{\lambda} = \sum_{i=1}^{n} x_i$$

$$\lambda = \frac{1}{\bar{x}} \quad \bar{x} = \text{sample}$$

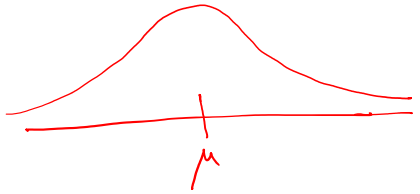
$$\lambda_{MLE} = \frac{1}{\frac{1}{n}\sum_{i=1}^{n} x_i} = \frac{1}{\bar{x}}$$

MLE for Normal distribution parameters

Maximum likelihood estimation can be applied to a vector valued parameter. For a simple random sample of n normal random variables We would like to find $\boldsymbol{\mu_{MLE}}$ for μ and $\boldsymbol{\sigma_{MLE}}$ for σ.

$$\boldsymbol{f(x;\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2}}$$

where $-\infty < x, \mu < \infty, \sigma > 0$



if X is continuous random variable, $f(x|\mu,\sigma)$ is probability density function, then for every observed random sample $x_1, x_2, \cdots, x_n$, we define joint probability or the **Likelihood Function**

$$f(x_1, x_2, \cdots, x_n|\mu,\sigma) = f(x_1|\mu,\sigma) \cdots f(x_n|\mu,\sigma)$$

$\mu_{MLE} = \underset{\mu}{\operatorname{argmax}}\, L(\mu,\sigma)$

σ^2_{MLE}

The likelihood function is

$$\boldsymbol{L(\theta) = f(x_1, x_2, \cdots, x_n|\mu,\sigma) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x_i-\mu)^2/2\sigma^2}}$$

MLE for Normal distribution parameters

Maximum likelihood estimation can be applied to a vector valued parameter. For a simple random sample of n normal random variables We would like to find $\boldsymbol{\mu_{MLE}}$ for μ and $\boldsymbol{\sigma_{MLE}}$ for σ.

$$f(x;\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2}$$

where $-\infty < x, \mu < \infty, \sigma > 0$

The likelihood function is

$$L(\mu,\sigma) = f(x_1, x_2, \cdots, x_n|\mu,\sigma) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x_i-\mu)^2/2\sigma^2}$$

The log-likelihood function is

$$log\ L(\mu,\sigma) = -\frac{n}{2} log\ 2\pi\sigma^2 - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i-\mu)^2$$

MLE for Normal distribution parameters

Maximum likelihood estimation can be applied to a vector valued parameter. For a simple random sample of n normal random variables We would like to find $\boldsymbol{\mu_{MLE}}$ for μ and $\boldsymbol{\sigma_{MLE}}$ for σ.

$$f(x;\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2}$$

where $-\infty < x, \mu < \infty, \sigma > 0$

The log-likelihood function is

$$log\ L(\mu,\sigma) = -\frac{n}{2} log\ 2\pi\sigma^2 - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i-\mu)^2$$

Taking derivative of log-likelihood function w.r.t. μ and equating to zero –

$$\frac{\delta log\ L(\mu,\sigma)}{\delta\mu} = \frac{1}{\sigma^2}\sum_{i=1}^{n}(x_i-\mu) = 0$$

$$\sum_{i=1}^{n}(x_i-\mu) = 0$$

$$\sum x_i - n\mu = 0$$

$$\mu_{MLE} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

MLE for Normal distribution parameters

Maximum likelihood estimation can be applied to a vector valued parameter. For a simple random sample of n normal random variables We would like to find $\boldsymbol{\mu_{MLE}}$ for μ and $\boldsymbol{\sigma_{MLE}}$ for σ.

$$f(x;\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2}$$

where $-\infty < x, \mu < \infty, \sigma > 0$

The log-likelihood function is

$$log\ L(\mu,\sigma) = -\frac{n}{2} log\ 2\pi\sigma^2 - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i-\mu)^2$$

partial

Taking derivative of log-likelihood function w.r.t. σ^2 and equating to zero –

$$\frac{\delta log\ L(\mu,\sigma)}{\delta\sigma^2} = -\frac{n}{\sigma^2} + \frac{1}{(\sigma^2)^2}\sum_{i=1}^{n}(x_i-\mu)^2 = \frac{n}{(\sigma^2)^2}\left(-\sigma^2 + \frac{1}{n}\sum_{i=1}^{n}(x_i-\mu)^2\right) = 0$$

$$\sigma^2_{MLE} = \frac{1}{n}\sum_{i=1}^{n}(x_i-\bar{x})^2$$

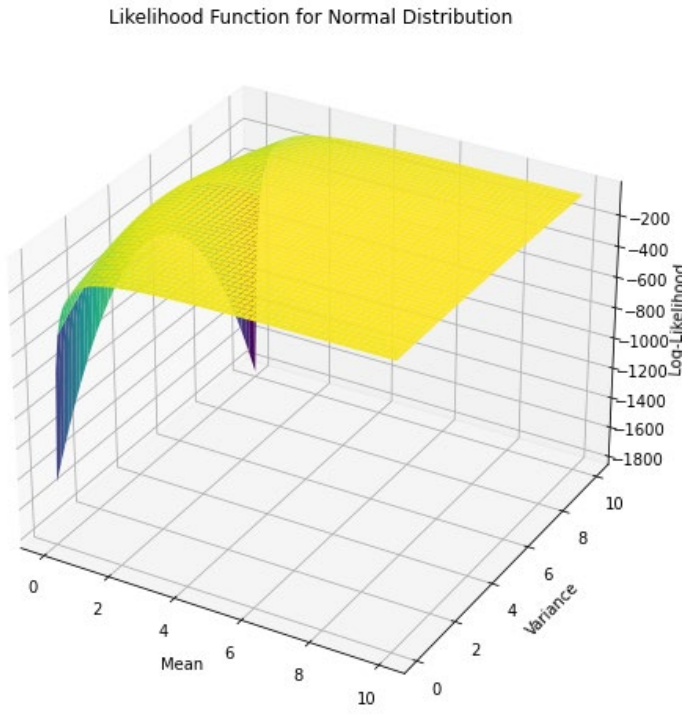
Example: Now, let's take a numerical example with some sample data. Suppose we have the following 10 observations drawn from a Normal distribution: X={2.5, 3.1, 4.0, 2.8, 3.7,8.9, 4.3,10.3,1.1,5.6}. Find MLE of μ and σ^2.

$$\sigma^2_{MLE} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

$$\mu_{MLE} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

The log-likelihood function is

$$log\ L(\mu, \sigma) = -\frac{10}{2} log\ 2\pi\sigma^2 - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i - \mu)^2$$



μ_{MLE} = 4.63.

σ^2_{MLE} = 7.54.

Example: Now, let's take a numerical example with some sample data. Suppose we have the following 10 observations drawn from the following distribution: X={2.5, 3.1, 4.0, 2.8, 3.7,8.9, 4.3,10.3,1.1,5.6}. Find MLE of θ. Find Mean and standard deviation also.

$$f(x|\theta) = (1-2\theta) + 4\theta x, \qquad 0 < x < 1, \qquad -1 < \theta < 1$$

$$E(x) = \int_0^1 x f(x)\, dx.$$

$$= \int_0^1 \{(1-2\theta)x + 4\theta x^2\}\, dx.$$

$$= \frac{(1-2\theta)x^2}{2}\Big|_0^1 + \frac{4\theta x^3}{3}\Big|_0^1$$

$$= \frac{1}{2} - \theta + \frac{4}{3}\theta = \left(\frac{1}{2} + \frac{\theta}{3}\right)$$

$$\int_0^1 f(x)\, dx = \int_0^1 \{(1-2\theta)x + 4\theta x\}\, dx$$

$$= (1-2\theta)x\Big|_0^1 + 2\theta x^2\Big|_0^1$$

$$= 1 - 2\theta + 2\theta = 1$$

$$Var(x) = \int_0^1 \{(x - E(x)\}^2 f(x)\, dx.$$

Example: Now, let's take a numerical example with some sample data. Suppose we have the following 10 observations drawn from the following distribution: X={2.5, 3.1, 4.0, 2.8, 3.7,8.9, 4.3,10.3,1.1,5.6}. Find MLE of θ. Find Mean and standard deviation also.

$$f(x|\theta) = (1-2\theta) + 4\theta x, \qquad 0 < x < 1, \qquad -1 < \theta < 1$$

$$Var(X) = \int_0^1 \left\{x - \left(\frac{1}{2}+\frac{\theta}{3}\right)\right\}^2 \left\{(1-2\theta) + 4\theta x\right\} dx.$$

$$= \int_0^1 \left[x^2 + \left(\frac{1}{2}+\frac{\theta}{3}\right)^2 - 2x\left(\frac{1}{2}+\frac{\theta}{3}\right)\right]\left[(1-2\theta) + 4\theta x\right] dx$$

$$\log L(\theta) = \log \prod_{i=1}^{10} f(x_i|\theta) = \log \prod_{i=1}^{10} \left\{(1-2\theta) + 4\theta x_i\right\}$$

$$= \log g(\theta)$$

$$\frac{d \log L(\theta)}{d\theta} = 0, \qquad \theta_{MLE} = ?$$

Example: Now, let's take a numerical example with some sample data. Suppose we have the following 10 observations drawn from the following distribution: X={2.5, 3.1, 4.0, 2.8, 3.7,8.9, 4.3,10.3,1.1,5.6}. Find MLE of θ.

$$f(x|\theta) = \frac{\theta}{x^{\theta+1}},$$

$$L(\theta) = \prod_{i=1}^{10} \frac{\theta}{x_i^{\theta+1}}, \quad \log L(\theta) = 10 \log \theta - (\theta+1) \sum_{i=1}^{10} \log x_i$$

$x_i \in X$

$$\frac{d \log L(\theta)}{d\theta} = \frac{10}{\theta} - \sum \log x_i = 0$$

$$\theta_{MLE} = \theta_{MLE} = \frac{10}{\sum_{i=1}^{10} \log x_i}$$

Example: Now, let's take a numerical example with some sample data. Suppose we have the following 10 observations drawn from the following distribution: X={2.5, 3.1, 4.0, 2.8, 3.7,8.9, 4.3,10.3,1.1,5.6}. Find MLE of θ.

$$f(x|\theta) = \frac{\theta}{x^{\theta+1}},$$

```python
import math

def MLE_theta(sample_points):
    # This code computes the MLE estimate of alpha
    log_sum = 0
    for x in sample_points:
        log_sum += math.log(x)
    n = len(sample_points)
    return n / log_sum

def main():
    sample_points = [2.5, 3.1, 4.0, 2.8, 3.7,8.9, 4.3,10.3,1.1,5.6]
    theta = MLE_theta(sample_points)
    print(theta)

if __name__ == '__main__':
    main()
```

$\sum_{i=1}^{n} \log x_i$

$$\theta_{MLE} = 0.7370920578760686$$

$$\theta_{MLE} = \frac{10}{\sum_{i=1}^{n} \log x_i}$$

```python
import math
import numpy as np
import matplotlib.pyplot as plt

def MLE_theta(sample_points):
    # This code computes the MLE estimate of theta
    log_sum = 0
    for x in sample_points:
        log_sum += math.log(x)
    n = len(sample_points)
    return n / log_sum

def show_pdf(x, theta):
    # distribution PDF
    return theta  / x**(theta + 1)

def main():
    sample_points = [2.5, 3.1, 4.0, 2.8, 3.7, 8.9, 4.3, 10.3, 1.1, 5.6]
    theta = MLE_theta(sample_points)
    print(theta)


    # Plot the histogram of the sample data
    plt.hist(sample_points, bins=20, density=True,
             color='lightblue', label='Sample Data')

    # Generate points for the fitted distribution
    x_values = np.linspace(min(sample_points), max(sample_points), 1000)
    y_values = [show_pdf(x, theta) for x in x_values]

    # Plot the fitted distribution
    plt.plot(x_values, y_values, color='red', label='Distribution Fit')

    plt.xlabel('Value')
    plt.ylabel('Probability Density')
    plt.title('Distribution Fit to Sample Data')
    plt.legend()
    plt.show()

if __name__ == '__main__':
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```

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import numpy as np
import matplotlib.pyplot as plt

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    n = len(sample_points)
    return n / log_sum

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def main():
    sample_points = [2.5, 3.1, 4.0, 2.8, 3.7, 8.9, 4.3, 10.3, 1.1, 5.6]
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    print(theta)


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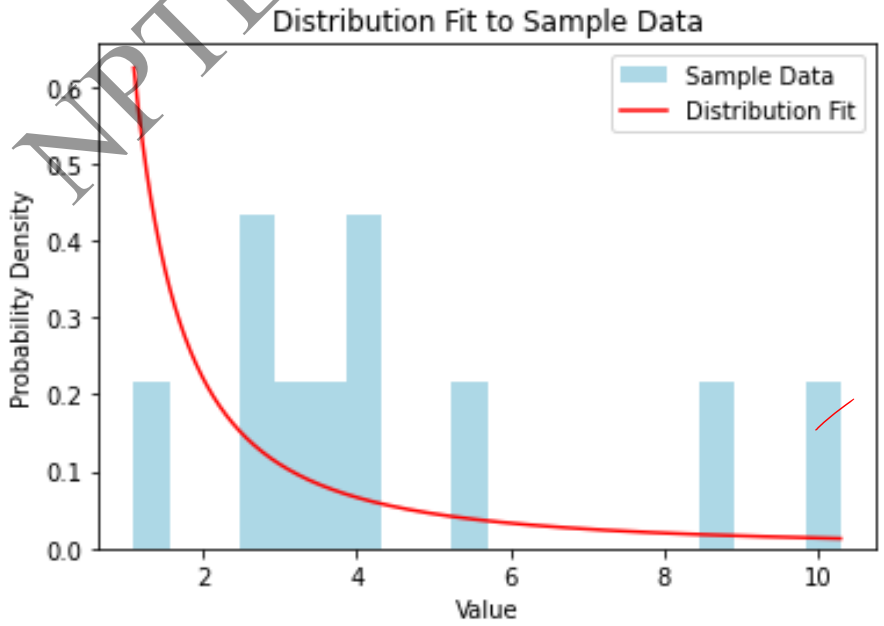
if __name__ == '__main__':
    main()
```



EXAMPLE:

Let us consider a random variable X$\sim N(\mu, \sigma^2)$. If we consider a i.i.d. sample of size 3 and consider these two estimators for μ

Estimator 1: $\hat{\theta}_1 = x_1 + x_2 - x_3$

Estimator 2: $\hat{\theta}_2 = x_1 + x_2 - 2x_3$

$\mu_{MLE} = \bar{x} = \frac{x_1 + x_2 + x_3}{3}$

Estimator 1: $E(\hat{\theta}_1) = E[x_1 + x_2 - x_3] = \mu$

Estimator 2: $E(\hat{\theta}_2) = E(x_1 + x_2 - 2x_3) = \mu$

But,

Estimator 1: $var(\hat{\theta}_1) = var[x_1 + x_2 - x_3] = 3\sigma^2$,

Estimator 2: $var(\hat{\theta}_2) = var(x_1 + x_2 - 2x_3) = 6\sigma^2$

What about MSE?

Conclusion

- ✓ **MLE for some continuous probability distributions**

To do: Properties of MLE

References

- ✓ Linear Algebra and Learning from Data (2019), Gilbert Strang, Wellesley Cambridge Press
- ✓ Machine Learning: A Probabilistic Perspective, Kevin P. Murphy (MIT Press), 2021 edition
- ✓ Deisenroth MP, Faisal AA, Ong CS. Mathematics for machine learning. Cambridge University Press; 2020 Apr 23.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by

Prof. Debjani Chakraborty

DEPARTMENT OF MATHEMATICS
IIT Kharagpur

Module 8.3

Lecture 38: Properties of Estimators

Concepts Covered

1. Unbiased Estimator
2. Consistent Estimators
3. Minimum Variance Estimators
4. Bias vs Variance

Estimators: $\widehat{\theta} = f(X_1, X_2 \cdots X_n)$

Estimate: Value of the Estimator

Bias: Expected difference between the value of the Estimator and True value of Estimator

$$Bias = E\left(\widehat{\theta} - \theta\right) = E_{X_1, X_2 \cdots X_n}[argmax_\theta\, f(X_1, X_2 \cdots X_n) - \theta]$$

- Even the sample is large, due to bias estimator does not converge to true estimator
- That is, it is not expressive enough to approximate the true value arbitrarily well
- If Bias is zero it is called unbiased Estimator
- To converge, how many sample points we need!!!!!

Estimators: $\widehat{\theta} = f(X_1, X_2 \cdots X_n)$

Estimate: Value of the Estimator

Variance: Expected difference between the value of the Estimator and True value of Estimator

$$\boldsymbol{Variance} = E\left(\left(\widehat{\theta} - E(\widehat{\theta})\right)^2\right)$$

$$= E_{X_1, X_2 \cdots X_n}\left((argmax_\theta f(X_1, X_2 \cdots X_n) - E(argmax_\theta f(X_1, X_2 \cdots X_n)))^2\right)$$

- If more training examples are taken then variance decreases
- If variance of an estimator is minimum compared to any other estimator of the same parameter and it is unbiased then it is called **Minimum Variance Unbiased Estimator (MVUE)**

Sample Mean is unbiased estimator of population Mean for $N(\mu, \sigma^2)$

$$\bar{X} = \frac{1}{n}(X_1 + X_2 + \cdots + X_n)$$

$$E(\bar{X}) = E\left(\frac{1}{n}\sum_{i=1}^{n} x_i\right) = \frac{1}{n}\sum_{i=1}^{n} E(x_i) = \frac{1}{n} \cdot n\mu = \mu$$

$\bar{X}$

$$\text{Bias}(\bar{X}) = E(\bar{X} - \mu) = 0$$

$$\text{Var}(\bar{X}) = \text{Var}\left(\frac{1}{n}\sum_{i=1}^{n} x_i\right)$$

$$= \frac{1}{n^2}\text{Var}\left(\sum_{i=1}^{n} x_i\right)$$

$$= \frac{1}{n^2} \cdot \sum_{i=1}^{n} \text{Var}(x_i)$$

$$= \frac{1}{n^2} \cdot n\sigma^2 = \frac{\sigma^2}{n}$$

$$variance(\overline{X}) = \frac{\sigma^2}{n}$$

Sample Variance is not unbiased estimator of population Variance for $N(\mu, \sigma^2)$

$$\sum_{i=1}^{n}(x_i-\mu)^2 = \sum_{i=1}^{n}(x_i-\bar{x}+\bar{x}-\mu)^2$$

$$= \sum_{i=1}^{n}(x_i-\bar{x})^2 + \sum_{i=1}^{n}(\bar{x}-\mu)^2 + 2\sum_{i=1}^{n}(x_i-\bar{x})(\bar{x}-\mu)$$

$$\frac{1}{n}\sum_{i=1}^{n}(x_i-\bar{x})^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i-\mu)^2 - \frac{1}{n}\sum_{i=1}^{n}(\bar{x}-\mu)^2$$

$$E\left(S^1_{Var}\right) = \frac{1}{n}\sum_{i=1}^{n}E(x_i-\mu)^2 - \frac{1}{n}\sum_{i=1}^{n}E(\bar{x}-\mu)^2$$

$$= \frac{1}{n}\sum_{i=1}^{n}Var(x_i) - Var(\bar{x})$$

$$= \sigma^2 - \frac{\sigma^2}{n} = \frac{n-1}{n}\sigma^2$$

$$\times S^1_{Var} = \frac{1}{n}\left(\sum_{i=1}^{n}(x_i-\bar{x})^2\right)$$

$$\checkmark S^2_{Var} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i-\bar{x})^2$$

Sample Variance is not unbiased estimator of population Variance for $N(\mu, \sigma^2)$

$$E\left(S'_{var}\right) = \frac{n-1}{n}\sigma^2$$

$$S^2_{var} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})$$

$$Bias\left(S'_{var}\right) = \frac{n-1}{n}\sigma^2 - \sigma^2 = -\frac{\sigma^2}{n}$$

$$= -var(\bar{x})$$

$$E\left(\frac{n}{n-1}S'_{var}\right) = \frac{n}{n-1}\cdot\frac{n-1}{n}\sigma^2 = \sigma^2$$

S^2_{var}

$$E\left(\frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2\right) = \sigma^2$$

Consistent Estimators

If $\hat{\boldsymbol{\theta}}_{\boldsymbol{n}}$ is estimator of θ for $f(\boldsymbol{X_1}, \boldsymbol{X_2} \cdots \boldsymbol{X_n}|\boldsymbol{\theta})$ based on a sample of size n, if $\hat{\boldsymbol{\theta}}_{\boldsymbol{n}} \rightarrow \boldsymbol{\theta}$ in probability when $\boldsymbol{n} \rightarrow \infty$ then $\hat{\boldsymbol{\theta}}_{\boldsymbol{n}}$ is **consistent** estimator of $\boldsymbol{\theta}$.

$$P\left\{|\hat{\theta}_n - \theta| \rightarrow 0\right\} \rightarrow 1 \quad \text{as } n \rightarrow \infty$$

Efficient Estimators

If $\hat{\boldsymbol{\theta}}_{\boldsymbol{1}}$ and $\hat{\boldsymbol{\theta}}_{\boldsymbol{2}}$ are two unbiased estimators of $\boldsymbol{\theta}$ for $f(\boldsymbol{X_1}, \boldsymbol{X_2} \cdots \boldsymbol{X_n}|\boldsymbol{\theta})$ based on same sample of size n, then $\hat{\boldsymbol{\theta}}_{\boldsymbol{1}}$ is more efficient than $\hat{\boldsymbol{\theta}}_{\boldsymbol{2}}$ when $\boldsymbol{var}(\hat{\boldsymbol{\theta}}_{\boldsymbol{1}}) < \boldsymbol{var}(\hat{\boldsymbol{\theta}}_{\boldsymbol{2}})$.

Let $X_1, X_2 \cdots X_n$ be a random sample from $X \sim Exponential(\lambda)$. Consider the following estimators $\widehat{\theta_1} = \frac{1}{n}\sum_{i=1}^{n} X_i$ and $\widehat{\theta_2} = \frac{1}{n+1}\sum_{i=1}^{n} X_i$ of the population mean.

1. Are these unbiased estimators?
2. Find the Mean Square Errors.
3. Which estimator is better and why?

$E(\hat{\theta}_1) = \frac{1}{n}\sum E(X_i)$ $\quad \theta = \frac{1}{\lambda}$

$= \frac{\theta}{n} \cdot n = \theta$

$E(\hat{\theta}_1) - \theta = 0$ ✓

$E(\hat{\theta}_2) - \theta = \frac{1}{n+1}\sum_{i=1}^{n} E(X_i) - \theta = \frac{\theta \cdot n}{n+1} - \theta = -\frac{\theta}{n+1}$ ✓

$Var(\hat{\theta}_1) = Var\left(\frac{1}{n}\sum_{i=1}^{n} X_i\right) = \frac{1}{n^2} \cdot \frac{n}{\lambda^2} = \frac{\theta^2}{n}$

$\widehat{\theta_1} = \frac{1}{n}\sum_{i=1}^{n} X_i$ and $\widehat{\theta_2} = \frac{1}{n+1}\sum_{i=1}^{n} X_i$

1. Are these unbiased estimators?
2. Find the Mean Square Errors.
3. Which estimator is better and why?

$$Var(\hat{\theta}_2) = \frac{1}{(n+1)^2}\sum_{i=1}^{n} Var(X_i) = \frac{n}{(n+1)^2}\cdot\frac{1}{\lambda^2} = \frac{n\theta}{(n+1)^2}$$

$$Var(\hat{\theta}_1) = \frac{\theta^2}{n}$$

$$MSE(\hat{\theta}_1) = Bias^2 + Variance = 0 + \frac{\theta^2}{n} = \frac{\theta^2}{n}$$

$$MSE(\hat{\theta}_2) = \left(\frac{\theta}{n+1}\right)^2 + \frac{n\theta}{(n+1)^2} = \frac{\theta^2 + n\theta}{(n+1)^2} = \frac{\theta}{n+1}$$

$$Bias(\hat{\theta}_1) < Bias(\hat{\theta}_2)$$

$$MSE(\hat{\theta}_1) > MSE(\hat{\theta}_2)$$

$$\widehat{\theta_1} = \frac{1}{n}\sum_{i=1}^{n} X_i \quad \text{and} \quad \widehat{\theta_2} = \frac{1}{n+1}\sum_{i=1}^{n} X_i$$

1. Are these unbiased estimators?
2. Find the Mean Square Errors.
3. Which estimator is better and why?

Conclusion

- ✓ **Criteria to check efficiency of different estimators**

References

- ✓ Linear Algebra and Learning from Data (2019), Gilbert Strang, Wellesley Cambridge Press
- ✓ Machine Learning: A Probabilistic Perspective, Kevin P. Murphy (MIT Press), 2021 edition
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Module 8.4

Lecture 39: MLE for Linear and Logistic Regression

Concepts covered

- ✓ **MLE for Linear Regression**
- ✓ **MLE for logistic Regression**

The Method of Maximum Likelihood Estimation

If n random samples $X_1, X_2, .., X_n$ are drawn from a population with probability function $f(X|\theta)$, then joint probability function L of $X_1, X_2, .., X_n$ is,

$$\boldsymbol{L(\theta) = f(x_1|\theta) f(x_2|\theta) \cdots f(x_n|\theta) = \prod_{i=1}^{n} f(x_i|\theta)}$$

***L*: Likelihood function.**

Since, $X_1, X_2, .., X_n$ are independently and identically distributed.

Objective: To find θ, such that Likelihood function is maximum

i.e. $\hat{\theta} = \underset{\theta}{argmax}\ L(\theta)$

Linear Regression (Parameter Fitting with Maximum Likelihood)

- $X =$ arbitrary distribution
- If $X =$ x then $Y = w_0 + w_1 x + \beta$, for some constants w_0, w_1, and some random noise variable β.
- $\beta \sim N(0, \sigma^2)$ which is independent of X.
- Here, we are assuming noise variable β has particular Gaussian distribution.

Conditional probability density function of Y, $p(y|X = x; w_0, w_1, \sigma^2)$ for each x.

$\beta = Y - w_0 - w_1 x \sim N(0, \sigma^2)$

Training Data

x_i	y_i	Prob.
x_1	y_1	p_1
x_2	y_2	p_2
...	...	...
x_n	y_n	p_n

The probability density under the model for the given data:

$$\prod_{i=1}^{n} p(y_i|x_i; w_0, w_1, \sigma^2) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(y_1-(w_0+w_1x_i))^2/2\sigma^2}$$

$\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$

Linear Regression (Parameter Fitting with Maximum Likelihood)

When we visualize data, we don't known the true parameters, consider $(\theta_0, \theta_1, s^2)$ gives the probability density:

$$\prod_{i=1}^{n} p(y_i|x_i;\theta_0,\theta_1,s^2) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi s^2}} e^{-\left(y_1-(\theta_0+\theta_1 x_i)\right)^2 / 2s^2}$$

The above equation is the likelihood, a function of the parameter values.

It is easier to work with **log-likelihood**,

$$L(\theta_0,\theta_1,s^2) = \log \prod_{i=1}^{n} p(y_i|x_i;\theta_0,\theta_1,s^2)$$

$$= \sum_{i=1}^{n} \log p(y_i|x_i;\theta_0,\theta_1,s^2) = -\frac{n}{2}\log 2\pi - n\log s - \frac{1}{2s^2}\sum_{i=1}^{n}\left(y_i-(\theta_0+\theta_1 x_i)\right)^2$$

Linear Regression (Parameter Fitting with Maximum Likelihood)

$$L(\theta_0, \theta_1, s^2) = -\frac{n}{2}\log 2\pi - n\log s - \frac{1}{2s^2}\sum_{i=1}^{n}\left(y_i - (\theta_0 + \theta_1 x_i)\right)^2 \quad \text{---------(1)}$$

To finding the parameters θ_0 and θ_1, first we will partial differentiate equation (1) with respect to θ_0,

$$\frac{\partial L}{\partial \theta_0} = 0$$

$$\frac{1}{2s^2} \times 2\sum_{i=1}^{n}\{y_i - (\theta_0 + \theta_1 x_i)\} = 0 \Rightarrow \sum_{i=1}^{n}\{y_i - (\theta_0 + \theta_1 x_i)\} = 0$$

$$\sum_{i=1}^{n} y_i - \sum_{i=1}^{n} \theta_0 - \sum_{i=1}^{n} \theta_1 x_i = 0$$

Linear Regression (Parameter Fitting with Maximum Likelihood)

$$L(\theta_0, \theta_1, s^2) = -\frac{n}{2}\log 2\pi - n\log s - \frac{1}{2s^2}\sum_{i=1}^{n}\left(y_i - (\theta_0 + \theta_1 x_i)\right)^2 \quad \text{---------(1)}$$

To finding the parameters θ_0 and θ_1, first we will partial differentiate equation (1) with respect to θ_0,

$$\frac{\partial L}{\partial \theta_0} = 0$$

$$\sum_{i=1}^{n} y_i - \sum_{i=1}^{n} \theta_0 - \sum_{i=1}^{n} \theta_1 x_i = 0$$

$$n\bar{y} - n\theta_0 - n\theta_1 \times \frac{1}{n}\sum_{i=1}^{n} x_i = 0$$

$$n\bar{y} - n\theta_0 - n\theta_1\bar{x} = 0 \implies \bar{y} - \theta_0 - \theta_1\bar{x} = 0$$

$$\boldsymbol{\theta_0^{MLE} = \bar{y} - \theta_1^{MLE}\bar{x}} \quad \text{----------(2)}$$

Linear Regression (Parameter Fitting with Maximum Likelihood)

$$L(\theta_0, \theta_1, s^2) = -\frac{n}{2}\log 2\pi - n\log s - \frac{1}{2s^2}\sum_{i=1}^{n}(y_i - (\theta_0 + \theta_1 x_i))^2 \quad \text{---------(1)}$$

$$\theta_0 = \bar{y} - \theta_1 \bar{x} \quad \text{----------(2)}$$

partial differentiate equation (1) with respect to θ_1, $\frac{\partial L}{\partial \theta_1} = 0$

$$\frac{1}{2s^2} \times 2\sum_{i=1}^{n}\{y_i - (\theta_0 + \theta_1 x_i)\}x_i = 0 \Rightarrow \sum_{i=1}^{n}\{y_i - (\theta_0 + \theta_1 x_i)\}x_i = 0$$

$$\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n}\theta_0 x_i - \sum_{i=1}^{n}\theta_1 x_i^2 = 0 \Rightarrow \sum_{i=1}^{n} x_i y_i - n \times \theta_0 \times \frac{1}{n}\sum_{i=1}^{n} x_i - \theta_1 \sum_{i=1}^{n} x_i^2 = 0$$

$$\sum_{i=1}^{n} x_i y_i - n\theta_0 \bar{x} - \theta_1 \sum_{i=1}^{n} x_i^2 = 0 \quad \text{----------(3)}$$

Linear Regression (Parameter Fitting with Maximum Likelihood)

$$L(\theta_0, \theta_1, s^2) = -\frac{n}{2}\log 2\pi - n\log s - \frac{1}{2s^2}\sum_{i=1}^{n}(y_i - (\theta_0 + \theta_1 x_i))^2 \quad \text{---------(1)}$$

$$\theta_0 = \bar{y} - \theta_1 \bar{x} \quad \text{----------(2)}$$

$\frac{\partial L}{\partial \theta_0} = 0$

$$\sum_{i=1}^{n} x_i y_i - n\theta_0 \bar{x} - \theta_1 \sum_{i=1}^{n} x_i^2 = 0 \quad \text{----------(3)}$$

$\frac{\partial L}{\partial \theta_1} = 0$

Using equation (2) in equation (3),

$$\sum_{i=1}^{n} x_i y_i - \theta_1 \sum_{i=1}^{n} x_i^2 - n(\bar{y} - \theta_1 \bar{x})\bar{x} = 0 \Rightarrow \sum_{i=1}^{n} x_i y_i - \theta_1 \sum_{i=1}^{n} x_i^2 - n\bar{x}\bar{y} + n\theta_1 \bar{x}^2 = 0$$

$$\theta_1 \left(\sum_{i=1}^{n} x_i^2 - n\bar{x}^2 \right) = \sum_{i=1}^{n} x_i y_i - n\bar{x}\bar{y}$$

$$\Rightarrow \theta_1 = \frac{\sum_{i=1}^{n} x_i y_i - n\bar{x}\bar{y}}{\sum_{i=1}^{n} x_i^2 - n\bar{x}^2}$$

Linear Regression (Parameter Fitting with Maximum Likelihood)

$$\theta_1 = \frac{\sum_{i=1}^{n} x_i y_i - n\bar{x}\bar{y}}{\sum_{i=1}^{n} x_i^2 - n\bar{x}^2}$$

$$\theta_1 = \frac{\sum_{i=1}^{n} x_i y_i - \bar{y}\sum_{i=1}^{n} x_i}{\sum_{i=1}^{n} x_i^2 - n\bar{x}^2 + n\bar{x}^2 - n\bar{x}^2} = \frac{\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \bar{y}}{\sum_{i=1}^{n} x_i^2 - 2n\bar{x}^2 + n\bar{x}^2}$$

$$\theta_1 = \frac{\sum_{i=1}^{n} x_i (y_i - \bar{y})}{\sum_{i=1}^{n} x_i^2 - \sum_{i=1}^{n} 2\,\bar{x} x_i + \sum_{i=1}^{n} \bar{x}^2} = \frac{\sum_{i=1}^{n} (x_i - \bar{x} + \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n} (x_i^2 - 2x_i\bar{x} + \bar{x}^2)}$$

$$\theta_1 = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y}) + \sum_{i=1}^{n} \bar{x}(y_i - \bar{y})}{\sum_{i=1}^{n} (x_i - \bar{x})^2} = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y}) + n\bar{x}\bar{y} - n\bar{x}\bar{y}}{\sum_{i=1}^{n} (x_i - \bar{x})^2}$$

$$\boldsymbol{\theta_1 = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n} (x_i - \bar{x})^2}}$$

Linear Regression (Parameter Fitting with Maximum Likelihood)

In the maximum likelihood method, the following estimators we will obtain:

$$w_1^{MLE} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

$$w_0^{MLE} = \bar{y} - w_1^{MLE}\bar{x}$$

$$\sigma_{MLE}^2 = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \left(w_0^{MLE} + w_1^{MLE}x_i\right)\right)^2$$

- The above estimators for the slope and intercept is exactly similar to the least square estimators.
- This is the crucial property of considering independent Gaussian noise.

Linear Regression (Parameter Fitting with Maximum Likelihood)

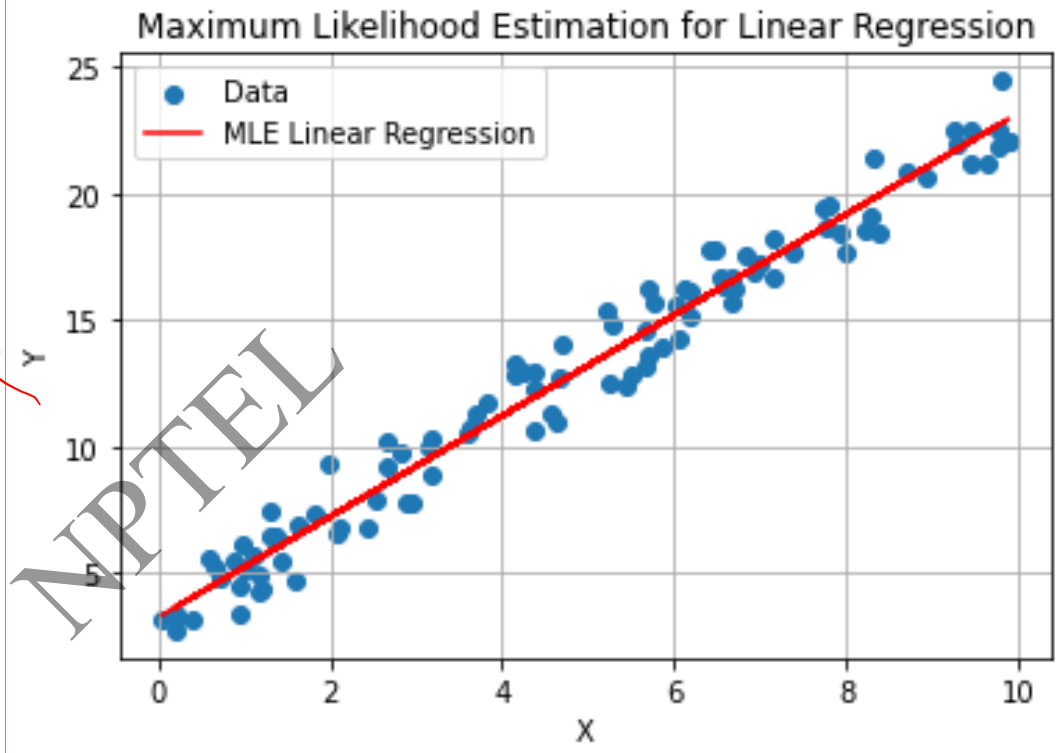
In the maximum likelihood method, the following estimators we will obtain:

$$w_1^{MLE} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

$$w_0^{MLE} = \bar{y} - w_1^{MLE}\bar{x}$$

$$\sigma_{MLE}^2 = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \left(w_0^{MLE} + w_1^{MLE}x_i\right)\right)^2$$

- The above estimators for the slope and intercept is exactly similar to the least square estimators.
- This is the crucial property of considering independent Gaussian noise.

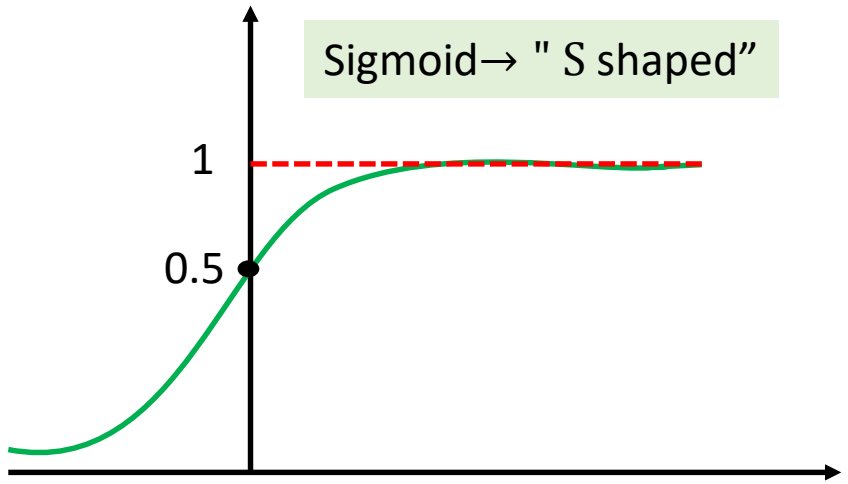


Logistic Regression (Parameter Fitting with Maximum Likelihood)

$$\sigma(x) = h_\theta(x) = \frac{1}{1+e^{-\theta^T x}} = \frac{1}{1+e^{-(\theta_0+\theta_1 x)}}$$

Where $0 \leq \sigma(x) \leq 1$ is the sigmoid function used in logistic regression.

$\sigma(x)$= Gives the probability



$$P(y=1|x=x_i) = p(x_i) = \sigma(x_i) = \frac{1}{1+e^{-(\theta_0+\theta_1 x_i)}}$$

Rearrange: $z = \theta_0 + \theta_1 x_i = \ln\left[\frac{p(x_i)}{1-p(x_i)}\right]$

$$1 - p(x_i) = 1 - \frac{1}{1+e^{-(\theta_0+\theta_1 x_i)}}$$

$$= \frac{e^{-(\theta_0+\theta_1 x_i)}}{1+e^{-(\theta_0+\theta_1 x_i)}}$$

Logistic Regression (Parameter Fitting with Maximum Likelihood)

Probability for being in category 1,

$$p(y = 1|x = x_i) = p(x_i) = \sigma(x_i) = \frac{1}{1+e^{-(\theta_0+\theta_1 x_i)}} \quad \text{---------- (1)}$$

Probability for being in category 0,

$$p(y = 0|x = x_i) = 1 - p(x_i) \quad \text{---------- (2)}$$

By equation (1) and (2),

$$P(y = y_i|x = x_i) = p(x_i)^{y_i}[1 - p(x_i)]^{1-y_i} \text{ where } y_i \in \{0,1\}$$

when $y_i = 1,\ p(y = y_i|x = x_i) = p(x_i)$ ---------- (3)

when $y_i = 0,\ p(y = y_i|x = x_i) = 1 - p(x_i)$ ---------- (4)

Fitting using maximum likelihood,

$$p(x_i) = \frac{1}{1 + e^{-(\theta_0+\theta_1 x_i)}}$$

$$P(y = y_i|x = x_i) = p(x_i)^{y_i}[1 - p(x_i)]^{1-y_i}$$

$y_i = 0$

$y_i = 1$

Logistic Regression (Parameter Fitting with Maximum Likelihood)

For n independent training example, we can write

$$= P_1 \times P_2 \times \cdots \times P_n$$

$$= \prod_{i=1}^{n} p(x_i)^{y_i} [1 - p(x_i)]^{1-y_i}$$

For n data points the likelihood function.

Find θ_0 and $\theta_i, i = 1,2 \ldots n$ that maximize L or $\log(L)$.

$$\sigma(x) = \frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2+\cdots+\theta_n x_n)}}$$

$$\log\left[\frac{p(x_i)}{1-p(x_i)}\right] = \theta_0 + \theta_1 x_1 + \cdots + \theta_n x_n$$

$$\log(L) = \sum_{i=1}^{n} y^{(i)} \log p(x_i) + \left(1 - y^{(i)}\right) \log\left(1 - p(x_i)\right)$$

It does not have a closed- form solution so we cannot write down a simple expression of the estimator

Training Data

x_i	y_i (1 or 0)	Prob.
x_1	y_1	P_1
x_2	y_2	P_2
...	...	...
x_n	y_n	P_n

Logistic Regression (Parameter Fitting with Maximum Likelihood)

To find the parameters maximize $\log(L)$ equivalently we can minimize $\log(likelihood)$ (NLL) to maintain uniformity with other algorithm:

$$J(w) = -\log(L) = -\sum_{i=1}^{n} \{y^{(i)} \log p(x_i) + (1 - y^{(i)}) \log(1 - p(x_i)\}$$

$$= -\sum_{i=1}^{n} \{y^{(i)} \log \hat{y}^{(i)} + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)}\}$$

References

- ✓ Linear Algebra and Learning from Data (2019), Gilbert Strang, Wellesley Cambridge Press
- ✓ Machine Learning: A Probabilistic Perspective, Kevin P. Murphy (MIT Press), 2021 edition
- ✓ Deisenroth MP, Faisal AA, Ong CS. Mathematics for machine learning. Cambridge University Press; 2020 Apr 23.

SWAYAM & NPTEL COURSE ON

Mathematics for Machine Learning

by

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DEPARTMENT OF MATHEMATICS
IIT Kharagpur

Module 8.5

Lecture 40: MLE for Naïve Bayes Model

Concepts covered

- ✓ **MLE for Naïve Bayes Model**

The Method of Maximum Likelihood Estimation

If k random samples $X_1, X_2, .., X_k$ are drawn from a population with probability function $f(X|\theta)$, then joint probability function L of $X_1, X_2, .., X_k$ is,

$$\boldsymbol{L(\theta) = f(x_1|\theta) f(x_2|\theta) \cdots f(x_k|\theta) = \prod_{i=1}^{k} f(x_I|\theta)}$$

***L*: Likelihood function.**

Since, $X_1, X_2, .., X_k$ are independently and identically distributed.

Objective: To find θ, such that Likelihood function is maximum

i.e. $\hat{\theta} = \underset{\theta}{argmax}\ L(\theta)$

Assume,

1. we have some prior knowledge $p(x)$
2. a random variable y, assumes value from random sample
3. We can update the knowledge $p(x)$ after observing y, $P(x/y)$

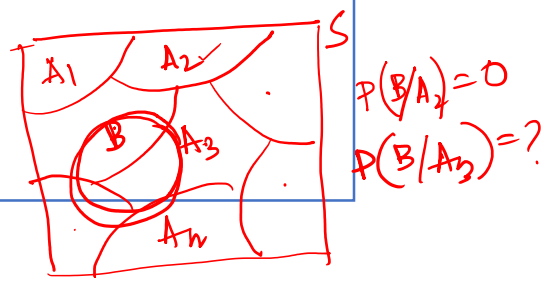
$$\underbrace{P(x/y)}_{\text{posterior}} = \frac{\overbrace{P(y/x)}^{\text{likelihood}}\overbrace{P(x)}^{\text{prior}}}{\underbrace{P(y)}_{\text{evidence}}}$$

Bayes Rule :

Hypothesis: (Equal division of ignorance): If nothing is known about the prior probabilities $P(A_1) \cdots P(A_n)$ then they are all equal.

Let $A_1, A_2 \cdots A_n$ denote a disjoint partition of a outcome set S and let B be any event. Let $P(A_i) \neq 0, i = 1,2 \cdots n$ and $P(B) \neq 0$, then for $i = 1,2 \cdots n$

$$P(A_i/B) = \frac{P(B/A_i)P(B)}{\sum_{i=1}^{n} P(B/A_i)P(B)}$$



Result: Let $A_1, A_2 \cdots A_n$ denote a disjoint partition of a outcome set S and let B be any event. Let $P(A_i) \neq 0, i = 1,2 \cdots n$ and $P(B) \neq 0$, then for $i = 1,2 \cdots n$

$$P(B) = \sum_{i=1}^{n} P(A_i)P(B/A_i)$$

Naïve Bayes Model

Example: Classifying documents using bag of words

Document classification is the problem of classifying text documents into different categories. One simple approach is to represent each document as a binary vector,

each word is present or not, so $x_{ij} = 1$ iff word j occurs in document i, otherwise $x_{ij} = 0$

Email Subject	Label
Offer: Double your income	Spam
Free gift	spam
You have been selected for Award	spam
Open for a free webinar	Not Spam
Meeting scheduled for tomorrow	Not Spam
Reminder: Review meeting agenda	Not spam

In Naive Bayes, we make a "naive" assumption that all features are conditionally independent given the class label.

Example: Classifying documents using bag of words

Email Subject	Label
Offer: Double your income	Spam
Free gift	spam
You have been selected for Award	spam
Open for a free webinar	Not Spam
Meeting scheduled for tomorrow	Not Spam
Reminder: Review meeting agenda	Not spam

$$P(Spam \mid \text{"offer"}, \text{"free"})$$

$$= \frac{P(\text{Spam}) \cdot P(\text{"offer"}|\text{Spam}) \cdot P(\text{"free"}|\text{Spam})}{P(\text{"offer"}, \text{"free"})}$$

$$P(spam) = .5, P(not\ spam) = .5$$

$$P(A/B) = \frac{P(B/A)\,P(A)}{P(B)}$$

$$P(\text{“offer”}|\text{”}spam\text{”})$$

$$= \frac{\text{number of occurrences of feature} + \alpha}{\text{total number of instances of the given class} + \alpha * Dimension\ of\ the\ data}$$

$$= \frac{3+1}{3+2} = \frac{4}{5} = .8$$

$$P(\text{“offer”}|\text{”Not }spam\text{”}) = .2$$

Naïve Bayes Model

Classifying documents using bag of words

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Open for a free webinar	Not Spam
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$$P(Spam \mid \text{"offer"}, \text{"free"})$$

$$= \frac{P(\text{Spam}) \cdot P(\text{"offer"} \mid \text{Spam}) \cdot P(\text{"free"} \mid \text{Spam})}{P(\text{"offer"}, \text{"free"})}$$

$$P(spam) = .5, P(not\ spam) = .5$$

$$P(\text{“free”} \mid \text{”}spam\text{”}) = \frac{\text{number of occurrences of feature} + \alpha}{\text{total number of instances of the given class} + \alpha * Dimension\ of\ the\ data}$$

$$= \frac{1+1}{3+2} = \frac{2}{5} = .4$$

$$P(\text{“free”} \mid \text{”Not } spam\text{”}) = .6$$

Naïve Bayes Model

Classifying documents using bag of words

Email Subject	Label
Offer: Double your income	Spam
Free gift	spam
You have been selected for Award	spam
Open for a free webinar	Not Spam
Meeting scheduled for tomorrow	Not Spam
Reminder: Review meeting agenda	Not spam

$$P(Spam \mid \text{"offer"}, \text{"free"})$$

$$= \frac{P(\text{Spam}) \cdot P(\text{"offer"} \mid \text{Spam}) \cdot P(\text{"free"} \mid \text{Spam})}{P(\text{"offer"}, \text{"free"})}$$

$$P(spam) = .5, P(not\ spam) = .5$$

$$\frac{P(\text{Spam}) \cdot P(\text{"offer"} \mid \text{Spam}) \cdot P(\text{"free"} \mid \text{Spam})}{P(\text{"offer"}, \text{"free"})}\ equivalent\ to\ .5..8..4 = .16$$

Naïve Bayes Model

Document classification is the problem of classifying text documents into different categories.
One simple approach is to represent each document as a binary vector,

each word is present or not, so $x_{ij} = 1$ iff word j occurs in document i, otherwise $x_{ij} = 0$

We can then use the following class conditional density:

$$P(Spam \mid \text{"offer"}, \text{"free"})$$

$$= \frac{P(\text{Spam}) \cdot P(\text{"offer"} \mid \text{Spam}) \cdot P(\text{"free"} \mid \text{Spam})}{P(\text{"offer"}, \text{"free"})}$$

$$P(\text{class}_i / \text{feature}_{n \in [1..N]})$$

$$= P(\text{class}_i) \prod_{n=1}^{N} P(\text{feature}_n / c_i)$$

Fitting a naive Bayes model with maximum likelihood

$$P(\text{class}_i/\text{feature}_{n\in[1..n]}) = P(\text{class}_i)\prod_{n=1}^{N} P(\text{feature}_n/c_i)$$

We use the maximum likelihood method method in finding parameters that maximize the likelihood of the observed w_n data set of size D, $\{w_n, c_i\}_{i=1..C,n=1..N}$ in class c_i

Then likelihood under a certain model with parameters $f(X|\theta_i)$ of class c_i

$$L\left(D\middle|\theta_{i\in[1..C]}, f(X|\theta_i)\right) = \prod_{d=1}^{D}\left(P(c_i)\prod_{n=1}^{N} P(w_n/c_i)\right)$$

Taking log-likelihood

$$\log L = \sum_{d=1}^{D}\sum_{i=1}^{C}\log P(c_i) + \sum_{d=1}^{D}\sum_{c=1}^{C}\sum_{n=1}^{N}\sum_{v=1}^{V}\log P(w_n|c_i),$$

Fitting a naive Bayes model with maximum likelihood

$$P(\text{class}_i/\text{feature}_{n\in[1..n]}) = P(\text{class}_i)\prod_{n=1}^{N} P(\text{feature}_n/c_i)$$

Taking log-likelihood

$$\log L = \sum_{d=1}^{D}\sum_{i=1}^{C} \log P(c_i) + \sum_{d=1}^{D}\sum_{c=1}^{C}\sum_{n=1}^{N}\sum_{v=1}^{V} \log P(w_n|c_i),$$

e.g. D: Number of emails C: Number of classes
V: Total number of words in the vocabulary
N: Number of words / features we are looking for

$$\sum_{i=1}^{C} P(c_i) = 1$$

$$\sum_{n=1}^{N}\sum_{i=1}^{C} P(w_n|c_i) = 1$$

$$P(c_i) = \frac{Total\ number\ of\ time\ we\ see\ the\ class\ c_i}{Number\ of\ data}$$

Fitting a naive Bayes model with maximum likelihood

$$P(\text{class}_i/\text{feature}_{n\in[1..n]}) = P(\text{class}_i)\prod_{n=1}^{N} P(\text{feature}_n/c_i)$$

Taking log-likelihood

$$\log L = \sum_{d=1}^{D}\sum_{i=1}^{C} \log P(c_i) + \sum_{d=1}^{D}\sum_{c=1}^{C}\sum_{n=1}^{N}\sum_{v=1}^{V} \log P(w_n|c_i)\,,$$

e.g. D: Number of emails C: Number of classes
V: Total number of words in the vocabulary
N: Number of words / features we are looking for

$$P(c_i) = \frac{Total\ number\ of\ time\ we\ see\ the\ class\ c_i}{Number\ of\ data}$$

Each c_i has its own probability of success θ_i in the probability distribution

$$\theta_i^{MLE} = \frac{\text{number of time we see the word in the class } c_i}{\text{Total number of times we see the word in all classes}}$$

Conclusion

Maximum likelihood estimation based on training data

References

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