Data-Driven Sampling (Lecture 4)
Monte Carlo algorithm, Maximum likelihood estimator, Stochastic search

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Law of large number (LLN)

Theorem

Let $X, X_1, ..., X_n$ *are independent identical distributed random variables and* g *be a function.* $\mathbb{E}[|g(X)|] < \infty$, *then we have*

$$\lim_{n\to\infty} \frac{g(X_1) + ... + g(X_n)}{n} = \mathbb{E}[g(X)], \quad \textit{with probability } 1.$$

If X *has a pdf* $f(x)$, *then*

$$\mathbb{E}[g(X)] = \int_{\mathbb{R}^d} g(x) f(x) dx.$$

Computation of Gamma function

Let us consider the following Gamma function:

$$\Gamma(\lambda) = \int_0^\infty x^{\lambda-1} e^{-x} dx$$

where $\lambda \geq 0$.

- When $\lambda = 0, 1, 2, ...$, we can compute $\Gamma(\lambda)$ by hand (Assignment 1).
- When λ is not an integer, we can not get an exact value.
- Now we use LLN to obtain an approximate number as the following:
  - Sample i.i.d. random variables $X_1, ..., X_n \sim Exp(1)$, and take $g(x) = x^{\lambda-1}$;
  - Compute $\frac{g(X_1)+...+g(X_n)}{n}$ for large n.

Python code for the computation of Gamma function

```
import numpy as np
lam,size=2.5,1000
X=np.random.exponential(1,size)
Y=sum(X**(lam-1))/size
print(Y)
```

Monte Carlo method

Monte Carlo is a casino city in Monaco. The Monte Carlo method is to sample n i.i.d. random variables with probability density f

$$X_1, X_2, ..., X_n$$

and use the following average:

$$\frac{g(X_1) + ... + g(X_n)}{n}$$

to compute the integral

$$\int_{\mathbb{R}^d} g(x)f(x)dx.$$

Example

Compute

$$\Phi(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{-\frac{t^2}{2}} dt.$$

- One can't get an explicit formula for $\Phi(x)$.
- We can use Monte Carlo method to compute its value: define $h(t) = 1_{(-\infty,x]}(t)$ and $f(t) = \frac{1}{\sqrt{2\pi}} e^{-\frac{t^2}{2}}$, we have

$$\frac{h(X_1) + ... + h(X_n)}{n}$$

is very close to $\Phi(x)$ when n is large, where $X_1, ..., X_n \sim N(0,1)$ are i.i.d.

Python code for the example

```
import numpy as np
x,size=0.78,10000
Y=0
X=np.random.normal(0,1,size)
for i in range(size):
 if X[i] <= x:
  Y=Y+1
Phi=Y/size
print(Phi)
```

Assignment

Assignment 2: Create a python program to compute the following integral:

$$\int_0^{2\pi} [\sin(100x) + \cos(50x)]^2 dx$$

Importance sampling

Let us consider the following integral problem

$$\int_{\mathbb{R}^d} h(x)f(x)dx$$

where f is the pdf of a probability distribution.

- It often happens that the distribution with the pdf f is hard to be sampled.
- One way is to choose another distribution with the pdf g which can be easily sampled and consider

$$\int_{\mathbb{R}^d} \left[h(x)\frac{f(x)}{g(x)} \right] g(x)dx$$

- We sample $X_1, ..., X_n$ with pdf g and compute $\frac{1}{n}\sum_{i=1}^{n} h(X_i)\frac{f(X_i)}{g(X_i)}$.

Idea of maximum likelihood estimator

- Aim: There exists a probability distribution $p(x, \theta)$ with θ being some important parameter not known. We need to learn this θ.
- Method: Take n samples $X_1, X_2, ..., X_n$ (which are usually observed data in practice) and consider the **likelihood** of these n samples as the following

$$L_n(\theta) := p(X_1, \theta)...p(X_n, \theta).$$

- Maximization: Consider the following maximization problem:

$$\hat{\theta}_n = argmax_\theta L_n(\theta),$$

where $\hat{\theta}_n$ is a function of $X_1, ..., X_n$. $\hat{\theta}_n$ is called maximum likelihood estimator based on the samples of $X_1, ..., X_n$.

Maximum likelihood estimator (MLE)

Definition

Let $p(x, \theta)$ be a probability distribution with an unknown parameter θ. Let $X_1, ..., X_n$ be n independent random variables with distribution $p(x, \theta)$. The **likelihood function** based on $X_1, ..., X_n$ is defined as

$$L_n(\theta) = \prod_{i=1}^{n} p(X_i, \theta).$$

The **maximum likelihood estimator (MLE)** of θ based on $X_1, ..., X_n$ is defined as

$$\hat{\theta}_n = argmax_{\theta \in \Theta} L_n(\theta),$$

where Θ is a set in which the parameter θ can take its values. We know $\hat{\theta}_n$ is a function of $X_1, ..., X_n$.

Maximum log likelihood estimator (log-MLE)

Definition

Let $p(x, \theta)$ be a probability distribution with an unknown parameter θ. Let $X_1, ..., X_n$ be n independent random variables with distribution $p(x, \theta)$. The **log likelihood function** based on $X_1, ..., X_n$ is defined as

$$l_n(\theta) = \log L_n(\theta) = \sum_{i=1}^{n} \log p(X_i, \theta).$$

The **maximum likelihood estimator (MLE)** of θ based on $X_1, ..., X_n$ can also be defined as

$$\hat{\theta}_n = argmax_{\theta \in \Theta} l_n(\theta).$$

An example

Suppose that we survey 20 individuals working for a large company and ask each whether they favor implementation of a new policy regarding retirement funding. If, in our sample, 6 favored the new policy, find an estimate for θ, the true but unknown proportion of employees that favor the new policy.

Solution

- Randomly choose an individual, he/she has a probability $\theta \in [0, 1]$ in favor of the new policy and a probability $1 - \theta$ not in favor. We define the random variable X such that

$$X = \begin{cases} 1, & in\ favor, \\ 0, & not\ in\ favor. \end{cases}$$

  The probability distribution of X is Bernoulli with a parameter θ, i.e. $p(1, \theta) = \theta$ and $p(0, \theta) = 1 - \theta$. We aim to estimate this θ.

- We have 20 samples $X_1, ..., X_{20}$, the likelihood function is

$$L_{20}(\theta) = \prod_{i=1}^{20} p(X_i, \theta) = \theta^6 (1 - \theta)^{14}.$$

Solution (continued)

- Maximize the $L_{20}(\theta)$. Differentiating $\log[\theta^6(1-\theta)^{14}]$ about θ, we obtain

$$\frac{6}{\theta} - \frac{14}{1-\theta} = 0.$$

Solving, we obtain

$$\theta = 6/20.$$

Cauchy distribution

A Cauchy distribution with parameter $\theta \in \mathbb{R}$ and $\gamma > 0$, denoted by Cauchy(θ, γ), has the following pdf:

$$f(x, \theta, \gamma) = \frac{1}{\pi} \frac{\gamma}{\gamma^2 + (x - \theta)^2}.$$

Assignment 4: Verify that $f(x, \theta, \gamma)$ is a pdf.

Example: MLE for Cauchy distribution

We consider maximize the likelihood of a Cauchy distribution Cauchy$(\theta, 1)$ based on sample $X_1, ..., X_n$:

$$L_n(\theta) = \prod_{i=1}^{n} \frac{1}{\pi} \frac{1}{1 + (X_i - \theta)^2}. \tag{1}$$

In order to obtain the MLE, we consider

$$\frac{dL_n(\theta)}{d\theta} = 0.$$

It is equivalent to compute

$$\frac{d[\log L_n(\theta)]}{d\theta} = 0.$$

Unfortunately, there does not exist a closed solution for the previous two equations.

MLE for Cauchy distribution

Theorem

Let $X_1, ..., X_n$ be n independent random variables with Cauchy distribution Cauchy$(\theta, 1)$. Then the MLE $\hat{\theta}_n$ of θ based on $X_1, ..., X_n$ with the form:

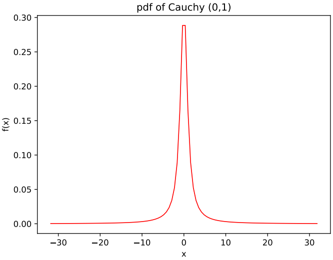
$$\hat{\theta}_n = argmin_{\theta \in \mathbb{R}} L_n(\theta),$$

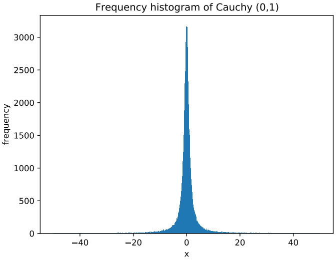
($\hat{\theta}_n$ depends on $X_1, ..., X_n$), satisfies

$$\lim_{n \to \infty} \hat{\theta}_n = \theta \quad \text{with probability 1.}$$

The proof of the theorem is out of the scope of this course, but we will show it is approximately true when $\theta = 0$ by a Python program.

Standard Cauchy distribution Cauchy(0,1)





Python of MLE for Cauchy distribution

```
import numpy as np
from scipy.stats import cauchy
from scipy.optimize import minimize_scalar
import matplotlib.pyplot as plt
fig, ax = plt.subplots(1, 1)
x = np.linspace(cauchy.ppf(0.01),cauchy.ppf(0.99), 100)
ax.plot(x, cauchy.pdf(x),'r-', lw=1, alpha=1, label='cauchy pdf')
plt.title('pdf of Cauchy (0,1)')
plt.xlabel('x')
plt.ylabel('f(x)')
plt.savefig('CPDF.pdf')
plt.show()
X = np.random.standard_cauchy(100000)
X = X[(X>-50) & (X<50)]  # truncate distribution so it plots well
plt.hist(X, bins=1000)
plt.title('Frequency histogram of Cauchy (0,1)')
plt.xlabel('x')
plt.ylabel('frequency')
plt.savefig('CH.pdf')
plt.show()
def L(x):        # Define -log MLE function
    return sum(-np.log(1/(1+(X-x)**2)))
res=minimize_scalar(L)      # find minimizer
res.x
print(res.x)
```

Stochastic search for optimization problems

- Problem: In many problems in Statistics and machine learning, one needs to search the maximum of a given function h in a domain $\mathcal{D} \subset \mathbb{R}^d$, i.e., $h^* = \max_{x \in \mathcal{D}} h(x)$.
- Classical numerical method: One makes a grid $G = \{x_1, ..., x_N\}$ on $\mathcal{D}$, and compute the value of h on the grid and compute $\max\{h(x_1), ..., h(x_N)$ as an approximation of h^*.
- Stochastic search: We sample n random variables $X_1, ..., X_n$ which satisfy the uniform distribution on $\mathcal{D}$, i.e. each X_i has a distribution $\mathcal{U}_{\mathcal{D}}$, and compute

$$\max\{h(X_1), ..., h(X_n)\}$$

as an approximation of h^*.

Stochastic search for optimization problems

- The computation complexity increasing exponentially with the dimension d, and computation resources will usually be huge when $d \geq 5$.
- The advantage of stochastic search is that their computation complexity does not depend on the dimension d.

Stochastic search for MLE for Cauchy distribution

We consider maximizing the likelihood of a Cauchy distribution Cauchy$(\theta, 1)$ based on samples $X_1, ..., X_n$:

$$L_n(\theta) = \prod_{i=1}^{n} \frac{1}{\pi} \frac{1}{1 + (X_i - \theta)^2}. \tag{2}$$

- If the samples $X_1, ..., X_n$ is from Cauchy$(0, 1)$, we generate m (e.g. m=1000) random variables $\theta_1, ..., \theta_m$ from the distribution $\mathcal{U}(-5, 5)$ and find

$$\max\{L_n(\theta_1), ..., L_n(\theta_m)\}.$$

Python of stochastic search for MLE for Cauchy distribution with m=100

```
import numpy as np
from scipy.stats import cauchy
from scipy.optimize import minimize_scalar
import matplotlib.pyplot as plt
fig, ax = plt.subplots(1, 1)
x = np.linspace(cauchy.ppf(0.01),cauchy.ppf(0.99), 100)
ax.plot(x, cauchy.pdf(x),'r-', lw=1, alpha=1, label='cauchy pdf')
plt.title('pdf of Cauchy (0,1)')
plt.xlabel('x')
plt.ylabel('f(x)')
plt.savefig('CPDF.pdf')
plt.show()
X = np.random.standard_cauchy(100000)
X = X[(X>-50) & (X<50)]  # truncate distribution so it plots well
plt.hist(X, bins=1000)
plt.title('Frequency histogram of Cauchy (0,1)')
plt.xlabel('x')
plt.ylabel('frequency')
plt.savefig('CH.pdf')
plt.show()
def L(x):       # Define -log MLE function
    return sum(-np.log(1/(1+(X-x)**2)))
res=minimize_scalar(L)      # find minimizer
res.x
print(res.x)
# Stochastic Search
size=100
x=np.random.uniform(-5,5,size)
mp=x[0]
for i in range(size):
    if L(x[i])<L(mp):
        mp=x[i]
print(mp)
```