# Winter 2019 Math 106
# Topics in Applied Mathematics
## Data-driven Uncertainty Quantification

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## Lecture 4: Parametric Inference

# 4.1 Statistical Inference

**Statistical inference** or **learning** is the process of using data to infer the distribution that generated the data.

Therefore, we can estimate statical functionals of the unknown distribution

Note that any map of a distribution is called a *statistical functional* of the distribution

$$F = F(P).$$

For example, for a distribution $P(x)$ and its corresponding density $p(x)$

- $E[X] = \int xp(x)dx$
- median $= P^{-1}(1/2)$

For a sample of two random variables $X$ and $Y$ with a joint density $p(x, y)$

- $E[Y|X = x] = \int yp(x, y)/p(x)dy$

# 4.1 Statistical Inference

**Example.** Let $X_1, X_2, ..., X_n$ is a sample from a density $p(x)$. Infer $p(x)$ using the sample.

1. If we assume that $p(x)$ is a Gaussian, we need to estimate only the mean and variance using the sample mean and variance

$$\hat{m} = \frac{1}{n} \sum_i X_i$$

   and

$$\hat{\sigma}^2 = \frac{1}{n-1} \sum_i (X_i - \hat{m})^2$$

2. Without assuming any form for $p(x)$, we estimate the $p(x)$ using a histogram

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Example 1 is an example of *parametric inference* (where the unknown parameters are the mean and the variance). Example is an example of *nonparametric inference*.

# 4.1 Statistical Inference

Broadly speaking, inferential problems fall into one of the three types

1. Point estimation
2. Confidence set (interval for 1D)
3. Hypothesis testing

## 4.1.1 Point Estimation

Let $F$ be a statistical functional of an unknown distribution $P$ and $\{X_i\}$ be a independent and identically distributed sample of $P$.

Point estimation provide a single best guess of $F$, often denoted by

$$\hat{F} = g(X_1, X_2, ..., X_n),$$

which is a function of the sample.

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which is a function of the sample.
This means that if we have a different sample $\hat{F}$ changes. To be more precise, $\hat{F}$ **is a random variable**.

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which is a function of the sample.
The distribution of $\hat{F}$ is called the **sampling distribution** and its standard deviation is called the **standard error**, denoted by **se**.

$$\mathbf{se} = \sqrt{Var(\hat{F})}$$

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which is a function of the sample.

- If the expected value of the point estimator is equal to the true value $F_{true}$, then the estimator is called **unbiased**.
- If the estimator converges in probability to the true value as the sample size, $n$, increases, the estimator is called **consistent**.
- The estimator is asymptotically Normal if the estimator converges in distribution to a normal as the sample size increases.

# 4.1.1 Point Estimation

The **mean squared error (MSE)** defined as

$$E[(\hat{\theta} - \theta)^2]$$

can be written as

$$\text{MSE} = \text{bias}(\hat{\theta})^2 + Var(\hat{\theta}).$$

# 4.1.1 Point Estimation

**Example.** Let $X_1, X_2, ..., X_n$ is a sample of a Bernoulli($p$). The estimator of $p$ is given by

$$\hat{p} = \frac{1}{n} \sum X_i.$$

- $\hat{p}$ is unbiased.
- From the law of large numbers, it is also consistent.
- From the central limit theorem, it is asymptotically normal.
- The standard error **se**$= \sqrt{Var(\hat{p})} = \sqrt{\frac{p(1-p)}{n}}$.
- The estimated **se** uses the estimated $\hat{p}$ for the standard error

$$\hat{\mathbf{se}} = \sqrt{\frac{\hat{p}(1-\hat{p})}{n}}.$$

## 4.1.2 Confidence Sets

Let $\{X_i\}$ be an independent, identically distributed sample.
A $1-\alpha$ **confidence set** is a set $C$, which is a function of the sample, such that

$$\mu(F \in C) = 1 - \alpha.$$

That is, the probability that $C$ traps the true value $F$ is $1-\alpha$.
**Example.** Let $F$ is a scalar value. If an estimator $\hat{F}$ is asymptotically normal and the sample size $n$ is large, the $1-\alpha$ confidence interval $C_n$ is given by

$$(\hat{F} - z_{\alpha/2}\hat{\mathbf{se}}, \hat{F} + z_{\alpha/2}\hat{\mathbf{se}})$$

where $z = \Phi^{-1}(1-(\alpha/2))$ for the standard normal distribution $\Phi$.

## 4.1.2 Confidence Sets

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**A frequently asked question for a data scientist position.** The interpretation, "the probability of the true value $F$ is in the set $C$ is $1-\alpha$" is an incorrect statement.
When we construct a confidence set $C$ using a sample $\{X_i\}$, $C$ is a random variable while the true value $F$ is fixed. Thus, the definition of the confidence set

$$\mu(F \in C) = 1 - \alpha.$$

is about a probability of the random variable $C$, not $F$.

## 4.1.3 Hypothesis Testing

Hypothesis testing starts with a null hypothesis and check if the sample provide sufficient evidence to reject the theory. Check one of your favorite statistics books for details.

# 4.2 Parameteric Inference

Let $\{X_i\}$ be an IID sample of a distribution $P$. In the parametric inference, we assume that the form of the unknown distribution is parameterized by a set of parameters $\theta = (\theta_1, ..., \theta_m)$

$$P(x) = P(x; \theta).$$

If we have an estimate of the parameter, say $\hat{\theta}$, the estimator provides an estimate of the distribution $P(x; \hat{\theta})$.

**Example.**

- If we assume that the sample is from a Gaussian distribution with a mean $m$ and a variance $\sigma^2$, the parameter is a pair $(m, \sigma^2)$.
- If we assume that the sample is from a Bernoulli($p$), the parameter is the mean $p$.

# 4.2 Parameteric Inference

We will consider two methods for parametric inference

- Method of Moments
- Max Likelihood Estimator (MLE)

# 4.2.1 Method of Moments

For a sample $X_1, X_2, ..., X_n$, the $j$-th moment is

$$\alpha_j(\theta) = E[X^j] = \int x^j p(x;\theta)dx, \quad \text{i.e., a function of } \theta,$$

where $p(x;\theta)$ is the parametrized density of the parametrized distribution $P(x;\theta)$. The $j$-th sample moment, $\hat{\alpha}_j$, is

$$\hat{\alpha}_j = \frac{1}{n}\sum_i X_i^j$$

If the size of the parameter $\theta$ is $m$, the **method of moments estimator** $\hat{\theta}$ is defined to be the value $\theta$ such that

$$\alpha_j(\hat{\theta}) = \hat{\alpha}_j, \quad j = 1, 2, ..., k.$$

## 4.2.1 Method of Moments

**Example.** Let $X_1, X_2, ..., X_n$ be an IID sample of Bernoulli(p).

- The size of parameter $\theta = p$ is 1.
- The first moment $\alpha_1(\theta) = \alpha_1(p) = p$ and the first sample moment $\hat{\alpha}_1$ is
$$\hat{\alpha}_1 = \frac{1}{n} \sum X_i.$$
- By setting $\alpha_1(\theta) = \hat{\alpha}_1$, we have
$$\hat{\theta} = \hat{p} = \frac{1}{n} \sum X_i.$$

## 4.2.1 Method of Moments

**Example.** Let $X_1, X_2, ..., X_n$ be an IID sample of Normal$(m, \sigma^2)$.

- The size of parameter $\theta = (m, \sigma^2)$ is 2.
- The first and the second moments are

$$\alpha_1(m, \sigma^2) = \mu, \quad \alpha_2(m, \sigma^2) = m^2 + \sigma^2$$

- The sample first and the sample second moments are

$$\hat{\alpha}_1 = \frac{1}{n}\sum X_i, \quad \hat{\alpha}_2 = \frac{1}{n}\sum X_i^2$$

- Solving the system of equations gives

$$\hat{m}u = \frac{1}{n}\sum X_i, \quad \hat{\sigma}^2 = \frac{1}{n}\sum (X_i - \hat{u})^2.$$

Note that $\sigma^2$ is biased (but consistent).

## 4.2.2 Maximum Likelihood Estimator

Let $X_1, X_2, ..., X_n$ be IID with a density $p(x; \theta)$. The joint distribution of the sample $p(x_1, x_2, ..., x_n; \theta)$ is

$$p(x_1, x_2, ..., x_n; \theta) = \Pi_i^n p(x_i; \theta) = p(x_1; \theta)p(x_2; \theta) \cdots p(x_n; \theta)$$

This joint density as a function of $\theta$ is called the **likelihood function**

$$\mathcal{L}_n(\theta) = \Pi_i^n p(x_i; \theta).$$

The likelihood is the probability (density) of the sample under the assumption of the parametric model. Note that $n$ is the sample size.

**Warning.** The likelihood function is not a density of $\theta$.

## 4.2.2 Maximum Likelihood Estimator

**Definition.** The **maximum likelihood estimator** (MLE) $\hat{\theta}$ is the value $\theta$ that maximizes the likelihood function $\mathcal{L}_n(\theta)$.

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**Example.** Let $X_1, X_2, ..., X_n$ is IID Bernoulli(p). The likelihood function is

$$\mathcal{L}_n(p) = \Pi_i^n p^{X_i}(1-p)^{1-X_i} = p^S(1-P)^{n-S}$$

where $S = \sum X_i$.
Hence,

$$\ln \mathcal{L}(p) = S \ln p + (n-S)\ln(1-p).$$

Take the derivative and set it equal to zero gives

$$\hat{p} = \frac{S}{n}.$$

## 4.2.2 Maximum Likelihood Estimator

**Definition.** The **maximum likelihood estimator** (MLE) $\hat{\theta}$ is the value $\theta$ that maximizes the likelihood function $\mathcal{L}_n(\theta)$.

**Example.** Let $X_1, X_2, ..., X_n$ is IID Normal$(m, \sigma^2)$. The likelihood function after a scaling is

$$\mathcal{L}(m,\sigma) = \Pi \frac{1}{\sigma} \exp\left(-\frac{1}{2\sigma^2}(X_i - m)^2\right) = \sigma^{-n} \exp\left(-\frac{1}{2\sigma^2}\sum_i (X_i - m)^2\right)$$

$$= \sigma^{-n} \exp\left(-\frac{nS^2}{2\sigma^2}\right) \exp\left(-\frac{n(\overline{X} - m)^2}{2\sigma^2}\right)$$

where $\overline{X} = \frac{1}{n}\sum X_i$ and $S^2 = \frac{1}{n}\sum (X_i - m)^2$. The log-likelihood is

$$l(m,\sigma) = -n \ln \sigma - \frac{nS^2}{2\sigma^2} - \frac{n(\overline{X} - m)^2}{2\sigma^2}.$$

Solving the gradient of $l(m,\sigma)$ equal to zero gives

$$\hat{m} = \overline{X} \quad \text{and} \quad \hat{\sigma} = S.$$

## 4.2.2 Maximum Likelihood Estimator

**Exercise.** Let $X_1, X_2, ..., X_n$ is IID Uniform$(0, \theta)$. Find the MLE of $\theta$.

## 4.2.3 Properties of MLE

Under certain conditions on the model, the MLE has the following properties

1. It is **consistent**. That is, $\hat{\theta}_n \to \theta_{true}$ in probability.
2. It is **equivalent**. If $\hat{\theta}_n$ is the MLE of $\theta$, then $g(\hat{\theta})$ is the MLE of $g(\theta)$.
3. It is **asymptotically normal**. $\hat{\theta}_n - \theta_{true}$ converges in distribution to $N(0, \mathbf{se}^2)$.
4. It is **asymptotically optimal**. That is, roughly speaking, among all well-behaved estimators, the MLE has the smallest variance, at least for large samples.
5. It is approximately the **Bayes estimator**.

## 4.2.3 Properties of MLE

**Idea of the proof for the consistency.**

- Maximizing $\mathcal{L}_n(\theta)$ is equivalent to maximizing

$$M_n(\theta) = \frac{1}{n} \sum \ln \frac{p(X_i;\theta)}{p(X_i;\theta_{true})}.$$

- From the law of large numbers, $M_n$ converges to the expected value

$$E\left( \ln \frac{p(X;\theta)}{p(X;\theta_{true})} \right) = \int \ln \frac{p(x;\theta)}{p(x;\theta_{true})} p(x;\theta_{true}) dx$$

$$= -D(p(x;\theta_{true}), p(x;\theta)) \leq 0$$

with equality when $\theta = \theta_{true}$.

## 4.2.3 Properties of MLE

**Idea of the proof for the asymptotically normal property.**
For $l_n(\theta) = \log \mathcal{L}_n(\theta)$

$$0 = l_n'(\hat{\theta}) \approx l_n'(\theta) + (\hat{\theta} - \theta) l_n''(\theta)$$

which yields

$$\hat{\theta} - \theta = -\frac{l_n'(\theta)}{l_n''(\theta)}$$

From the central limit theorem, $l_n'(\theta)/\sqrt{n}$ converges in distribution to $N(0, I(\theta))$ where $I(\theta)$ is the variance of $\frac{\partial}{\partial x} \ln p(x;\theta)$.
Also, from the law of large numbers, $l_n''(\theta)/n$ converges in probability to the mean of $\frac{\partial^2}{\partial x^2} \ln p(x;\theta)$, which is $I(\theta)$.
**Exercise.** Show that the mean of $\frac{\partial}{\partial x} \ln p(x;\theta)$ is 0.
**Exercise.** Show that the mean of $\frac{\partial^2}{\partial x^2} \ln p(x;\theta)$ is the variance of $\frac{\partial}{\partial x} \ln p(x;\theta)$, that is $I(\theta)$.

# 4.2.3 Properties of MLE

- The **score function** is the first derivative of the parametrized density

$$s(X;\theta) = \frac{\partial}{\partial x} \ln p(x;\theta).$$

- The variance of the sum of the score functions is called **Fisher information**

$$I_n(\theta) = Var(\sum_{i}^{n} s(X_i;\theta)).$$

That is, the Fisher information is $nI(\theta)$ where $I(\theta)$ is the variance of the score function.

# 4.2.4 The Expectation-Maximization (EM) Algorithm

**Goal:** Find a $\theta$ that maximize $\mathcal{L}_n(\theta)$, i.e., the MLE estimator.
**Algorithm:**

1. Pick an initial value $\theta^0$. For $j = 1, 2, \ldots,$, repeat steps 1 and 2
2. (The E-step): Calculate

$$J(\theta|\theta^j) = E\left(\ln \frac{\Pi p(x_i, y_i; \theta)}{\Pi p(x_i, y_i; \theta^j)} |x\right)$$

   This expectation is over the missing variable $\{y_i\}$ treating $\theta^j$ and $\{x_i\}$ are fixed.
3. Find $\theta^{j+1}$ maximizing $J(\theta|\theta^j)$.

# 4.2.4 The Expectation-Maximization (EM) Algorithm

**Idea of the proof.** We want to show that the procedure increases the likelihood, that is, $\mathcal{L}(\theta^{j+1}) \geq \mathcal{L}(\theta^j)$.
From

$$J(\theta^{j+1}|\theta^j) = E\left(\ln \frac{\Pi p(x_i, y_i; \theta^{j+1})}{\Pi p(x_i, y_i; \theta^j)} | \{x_i\}\right)$$

$$= \ln \frac{\mathcal{L}(\theta^{j+1})}{\mathcal{L}(\theta^j)} + E\left(\ln \frac{\Pi p(y_i|x_i; \theta^{j+1})}{\Pi p(y_i|x_i; \theta^j)} | \{x_i\}\right)$$

we have

$$\ln \frac{\mathcal{L}(\theta^{j+1})}{\mathcal{L}(\theta^j)} = J(\theta^{j+1}|\theta^j) - E\left(\ln \frac{\Pi p(y_i|x_i; \theta^{j+1})}{\Pi p(y_i|\{x_i\}; \theta^j)} | \{x_i\}\right)$$

$$= J(\theta^{j+1}|\theta^j) + D(f_j, f_{j+1}) \geq 0$$

where $f_j = \Pi p(y_i|x_i; \theta^j)$.

## 4.2.4 The Expectation-Maximization (EM) Algorithm

**Example.** Let $X_1, X_2, ..., X_n$ be a sample from a parametrized density

$$p(x) = \frac{1}{2}\phi(x; \mu_1, 1) + \frac{1}{2}\phi(x; \mu_0, 1)$$

where $\phi(x; \mu_i, 1)$ is a Gaussian density with a mean $\mu_i$ and a variance 1. Find the MLE.