

# Chapter 1

## Statistical Modeling

### 1.1 Statistical Models

Example 1: (Sampling inspection). A lot contains  $N$  products with defective rate  $\theta$ . Take a sample without replacement of  $n$  products and get  $x$  defective products.

What are the defective rates?

Possible outcomes: GGDGGGDD  $\dots$ , realization of outcomes.

How do we connect the sample with the population?

Modelling — think of data as a realization of a the random experiment.

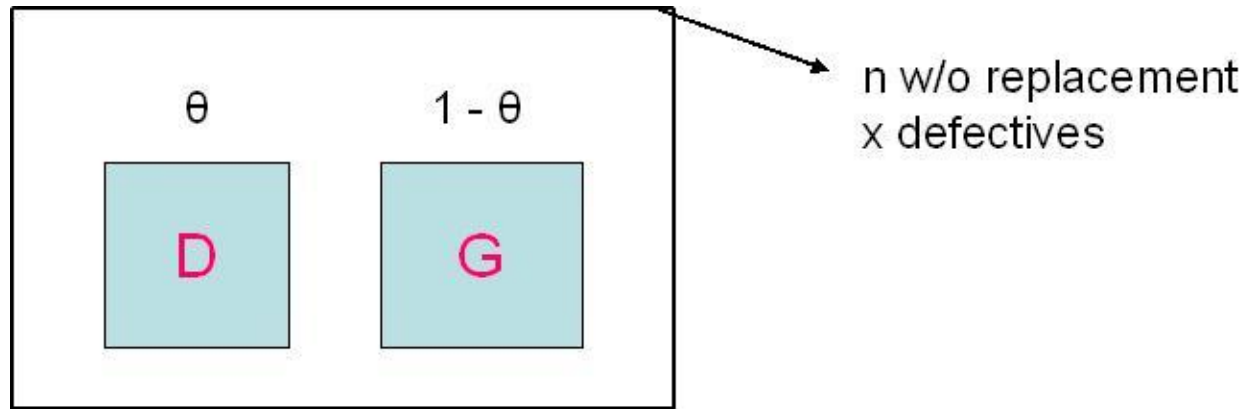


Figure 1.1: Illustration of the sampling scheme.

Observe that a "D"  $\implies \theta$  is large,

a "G"  $\implies \theta$  is small.

**Probability Law**: Under this physical experiment

$$P(X = x) = \frac{\binom{N\theta}{x} \binom{N-N\theta}{n-x}}{\binom{N}{n}},$$

for  $\max(0, n - N(1 - \theta)) \leq x \leq \min(n, N\theta)$ . Convention:  $\binom{n}{0} = 1$ ,  $\binom{n}{m} = 0$  if  $m > n$ .

For example,  $X/n \approx \theta$  and

$$\sqrt{n}(X/n - \theta) \rightarrow N(0, \theta(1 - \theta)).$$

Parameter:  $\theta$  — unknown, fixed.

**Parameter space**  $\Theta$ : the possible value of  $\theta$ :  $\Theta = \{0/N, 1/N, \dots, N/N\}$  or  $[0, 1]$ .

For this specific example, the model comes from physical experiment. Now suppose that  $N = 10,000$ ,  $n = 100$  and  $x = 2$ . Our problem becomes an inverse problem: What is the value of  $\theta$ ?

Logically, if  $\theta = 1\%$ , it is possible to get  $x = 2$ . If  $\theta = 2\%$ , it is also possible to get  $x = 2$ . If  $\theta = 3.5\%$ , it is also possible to get  $x = 2$ . So, given  $x = 2$ , we can not tell exactly which  $\theta$  it is. Our conclusion can not be drawn without uncertainty. However, we do know some are more likely than the others and the degree of uncertainty gets smaller, as  $n$  gets large, whatever  $N$  is.

### **Summary:**

— Statisticians think data as realizations from a stochastic model; this connects

the sample and parameters.

— Statistical conclusions can not be drawn without uncertainty, as we have only a finite sample.

— Probability is from a box to sample, while statistics is from a sample to a box.

**Example 2**: A measurement model (e.g. molecular weight, RNA/protein expression level, fat-free weight). An object is weighed  $n$  times, with outcomes  $x_1, \dots, x_n$ . Let  $\mu$  be the true weight. We think the observed data as realizations of random variables  $X_1, \dots, X_n$ , modeled as

$$X_i = \mu + \varepsilon_i$$

where  $\varepsilon_i$  is error of measurement noise.

## **Assumptions**

- i)  $\varepsilon_i$  is independent of  $\mu$ .
- ii)  $\varepsilon_i, i = 1, 2, \dots, n$  are independent.

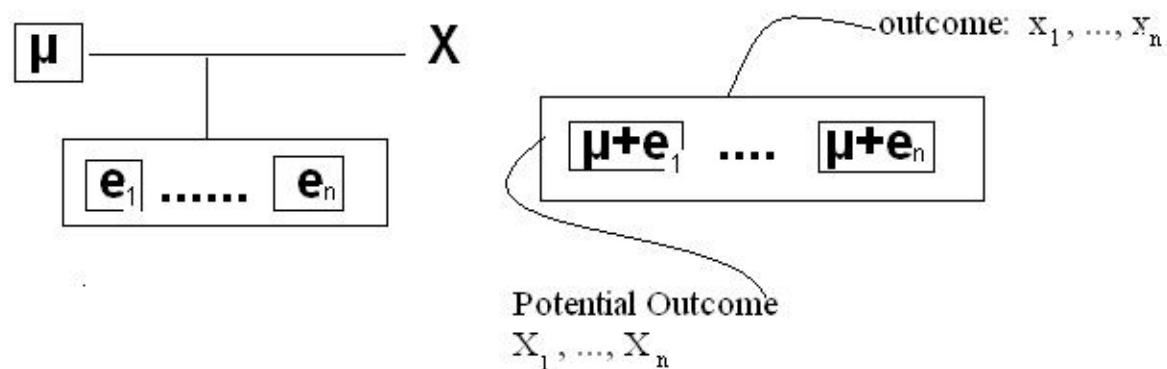


Figure 1.2: Illustration of the idea of modeling.

iii)  $\varepsilon_i, i = 1, 2, \dots, n$  are identically distributed.

iv) the distribution of  $\varepsilon$  is continuous, with  $E(\varepsilon) = 0$ ; or specifically symmetric about 0:  $f(y) = f(-y)$  for any  $y$ .

Often, we assume further that  $\varepsilon_i \sim N(0, \sigma^2)$ . Parameters in the model  $\theta = (\mu, \sigma^2)$ , where  $\sigma^2$  is a nuisance parameter.

Given a realization  $\mathbf{x} = (x_1, \dots, x_n)$  of  $\mathbf{X} = (X_1, \dots, X_n)$ , what is the value of  $\mu$ ?

Logically, if  $\mu = 100$ , it is possible to observe  $\mathbf{x}$ . If  $\mu = 1$ , it is also possible to observe  $\mathbf{x}$ . So we can not absolutely tell what value of  $\mu$  is. But from the square-root law:

$$\text{var}(\bar{X}) = E(\bar{X} - \mu)^2 = \frac{\sigma^2}{n}.$$

Thus,  $\bar{x}$  is likely close to  $\mu$  when  $n$  is large.

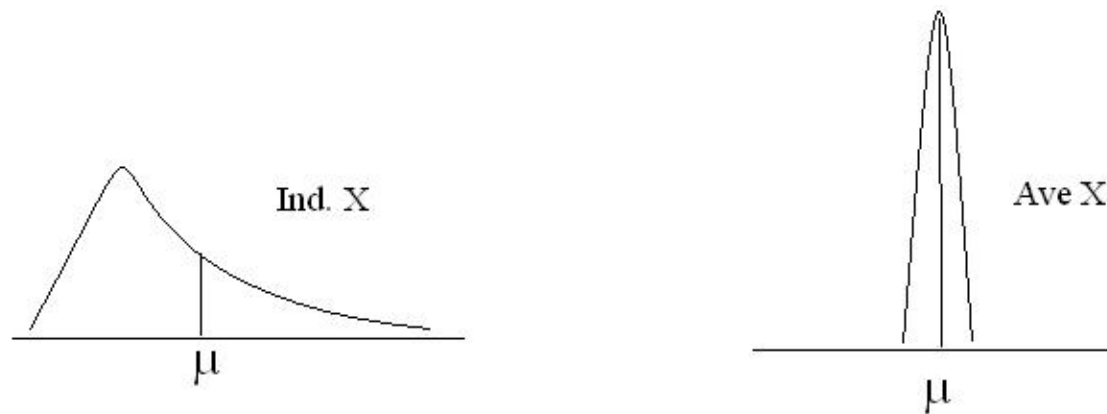


Figure 1.3: Distributions of individual observation versus that of average

**Example 3:** Drug evaluation (Hypertension drug)

Drug A  $\rightarrow$  m patients      Drug B  $\rightarrow$  n patients

Measurement: blood pressure.

To eliminate confounding factors, use randomized controlled experiment. Here are the hypothetical outcomes:

Drug A					Drug B					
150	110	160	187	153	120	140	160	180	133	136
$x_1$	$x_2$	$x_3$	$x_4$	$x_5$	$y_1$	$y_2$	$y_3$	$y_4$	$y_5$	$y_6$

To model the outcomes, a possible idealization is the following box-model.

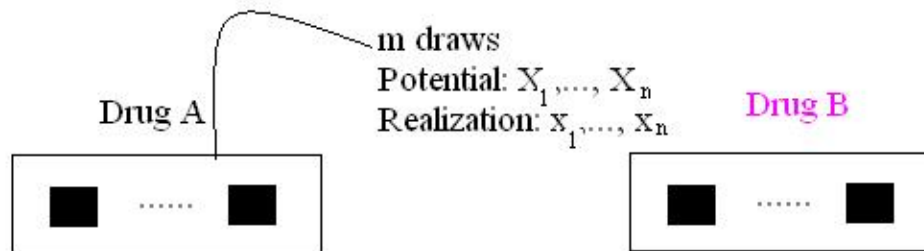


Figure 1.4: Illustration of a two-sample problem

	Drug A	Drug B
random outcomes	$X_1, \dots, X_m$	$Y_1, \dots, Y_n$
realizations	$x_1, \dots, x_m$	$y_1, \dots, y_n$

Further, we might assume that

$$X_1, \dots, X_m \stackrel{i.i.d.}{\sim} N(\mu_A, \sigma_A^2) \quad Y_1, \dots, Y_n \stackrel{i.i.d.}{\sim} N(\mu_B, \sigma_B^2).$$

We sometimes assume further  $\sigma_A = \sigma_B = \sigma$ .

Parameters in the model:  $\theta = (\mu_A, \mu_B, \sigma_A, \sigma_B)$ .

Parameters of interest:  $\mu = \mu_A - \mu_B$  and possibly  $\sigma$ .

Connection sample with population: data are realizations from a population, whose distribution depends on  $\theta$ .

**Model diagnostics**: Statistical models are idealizations, postulated by statisticians — needed to be verified. For example, the data histograms should look like theoretical distributions. Two sample variances are about the same, etc.

### General formulation

**Data**:  $\mathbf{x} = (x_1, \dots, x_n)$  are thought of the realization of a random vector  $\mathbf{X} = (X_1, \dots, X_n)$ .



**Model:** The distribution of  $\mathbf{X}$  is assumed in  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ ,  $\Theta$  is the parametric space.

**Objectives:** Inferences about  $\theta$ .

— In Example 1:

$$P_\theta(\mathbf{x}) = \frac{\binom{N\theta}{x} \binom{N-N\theta}{n-x}}{\binom{N}{n}},$$

where  $\Theta = \{0, 1/N, \dots, N/N\}$  or  $[0, 1]$ .

— In Example 2:

$$P_\theta(\mathbf{x}) = \prod_{i=1}^n \sigma^{-1} \varphi\left(\frac{x_i - \mu}{\sigma}\right)$$

where  $\varphi(\cdot)$  is the normal density,  $\Theta = \{(\mu, \sigma), \mu > 0, \sigma > 0\}$ .

— In Example 3:

$$P_\theta(\mathbf{x}) = \prod_{i=1}^m \sigma_A^{-1} \varphi\left(\frac{x_i - \mu_A}{\sigma_A}\right) \prod_{i=1}^n \sigma_B^{-1} \varphi\left(\frac{y_i - \mu_B}{\sigma_B}\right),$$

where  $\varphi(\cdot)$  is the normal density,  $\Theta = \{(\mu_A, \mu_B, \sigma_A, \sigma_B) : \mu_A, \mu_B, \sigma_A, \sigma_B > 0\}$ .

— Data  $\mathbf{x}$  or its random variable  $\mathbf{X}$  can include both  $x$ - and  $y$ -component.

The parameter  $\theta$  doesn't have to be in  $\mathbb{R}^k$ . In Example 2, without the normality assumption,

$$P_{\theta}(\mathbf{x}) = \prod_{i=1}^n f(x_i - \mu),$$

assuming that  $\{\varepsilon_i, i = 1, \dots, n\}$  are i.i.d random variables with density  $f$ . Then,

$$\Theta = \{(\mu, f) : \mu > 0, f \text{ is symmetric}\}.$$

Since no form of  $f$  has been imposed, i.e.  $f$  has not been parameterized, the parameter space  $\Theta$  is called nonparametric or semiparametric.

**Basic assumption**: Throughout this class, we will assume that

- (i) Continuous variables: All  $P_{\theta}$  are continuous with densities  $p(\mathbf{x}, \theta)$  or
- (ii) Discrete variable: All  $P_{\theta}$  are discrete with frequency functions  $p(x, \theta)$ . Further, there exists a set  $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \}$  such that

$$\sum_{i=1}^{\infty} p(\mathbf{x}_i, \theta) = 1, \text{ where } x_i \text{ is independent of } \theta.$$

For convenience, we will call  $p(\mathbf{x}, \theta)$  as density in both cases.

**Identifiability of parameters**: There are sometimes more than one way of parameterization. In Example 3: write

$$X_1, \dots, X_m \stackrel{i.i.d}{\sim} N(\mu + \alpha_1, \sigma^2) \quad Y_1, \dots, Y_n \stackrel{i.i.d}{\sim} N(\mu + \alpha_2, \sigma^2).$$

$\theta = (\mu, \alpha_1, \alpha_2, \sigma)$ . Hence,

$$p_{\theta}(\mathbf{x}, \mathbf{y}, \theta) = \prod_{i=1}^m \sigma^{-1} \varphi\left(\frac{x_i - \mu - \alpha_1}{\sigma}\right) \prod_{i=1}^n \sigma^{-1} \varphi\left(\frac{y_i - \mu - \alpha_2}{\sigma}\right),$$

If  $\theta_1 = (0, 1, 2, 1)$  and  $\theta_2 = (0.5, 0.5, 1.5, 1)$ , then  $P_{\theta_1} = P_{\theta_2}$ . Thus, the parameters  $\theta$  are not identifiable.

**Identifiability**: The model  $\{P_{\theta}, \theta \in \Theta\}$  is identifiable if  $\theta_1 \neq \theta_2$  implies  $P_{\theta_1} \neq P_{\theta_2}$ .

**Example 4**: (Regression Problem). Suppose a sample of data

$\{(x_{i1}, \dots, x_{ip}, y_i)\}_{i=1}^n$  are collected e.g.

$y$  = salary,  $x_1$  = age,  $x_2$  = year of experience,

$x_3$  = job grade,  $x_4$  = gender,  $x_5$  = PC job.

We wish to study the association between  $Y$  and  $X_1, \dots, X_p$ . How to predict  $Y$  based on  $\mathbf{X}$ ? Any gender discrimination? (Note: the data  $\mathbf{x}$  in the general formulation now include all  $\{(x_{i1}, \dots, x_{ip}, y_i)\}_{i=1}^n$ ).

— Model I: linear model

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_5 X_5 + \varepsilon, \quad \varepsilon \sim G,$$

where  $\varepsilon$  is the part that can not be explained by  $\mathbf{X}$ . Thus the parameter space is  $\Theta = \{(\beta_0, \beta_1, \dots, \beta_5, G)\}$ .

— Model II: semiparametric model

$$Y = \mu(X_1, X_2, X_3) + \beta_4 X_4 + \beta_5 X_5 + \varepsilon.$$

The parameter space is  $\Theta = \{(\mu(\cdot), \beta_4, \beta_5, G)\}$ .

— Model III: nonparametric model

$$Y = \mu(X_1, \dots, X_5) + \varepsilon.$$

The parameter space is  $\Theta = \{(\mu(\cdot), G)\}$ .

**Modeling:** Data are thought of a realization from  $(Y, X_1, \dots, X_5)$  with the relationship between  $\mathbf{X}$  and  $Y$  described above.

From this example, the model is a convenient assumption made by data analysts. Indeed, statistical models are frequently useful fictions. There are trade-offs among the choice of statistical models:

larger model  $\Rightarrow$  reducing model biases

$\Rightarrow$  increasing estimation variance.

The decision depends also available sample size  $n$ .

**Statistics:** a function of data only, e.g.

$$\bar{X} = \frac{X_1 + \dots + X_n}{n}, \quad X_1, \quad X_1^2 + \sqrt{X_2^2 + X_3^2 + 3},$$

but

$$X_1 + \sigma, \quad \bar{X} + \mu$$

are not.

**Estimator**: an estimating procedure for certain parameters, e.g.  $\bar{X}$  for  $\mu$ .

**Estimate**: numerical value of an estimator when data are observed, e.g.

$$n = 3, \bar{x} = \frac{2 + 6 + 4}{3} = 3.$$

Estimator — for all potential realizations, estimate — for a realized result.

**Note**: An estimator is an estimating procedure. The performance criteria for a method is based on estimator, while statistical decisions are based on estimate in real applications.

## 1.2 Bayesian Models

**Probability**: Two view points:

$$\left\{ \begin{array}{l} \text{long run relative frequency — Frequentist} \\ \text{prior knowledge w/brief — Bayesian} \end{array} \right.$$

So far, we have assumed no information about  $\theta$  beyond that provided by data. Often, we can have some (vague) knowledge about  $\theta$ . For example,

— defective rate is 1%

— the distribution of DNA nucleotides is uniform,

— the intensity of an image is locally corrected.

**Example 1.** (Continued) Based on past records, one can construct a distribution of defective rate  $\pi(\theta)$ :

$$P(\theta = i/N) = \pi_i, \quad i = 1, 2, \dots, N.$$

This provides as a prior distribution. The defective rate  $\theta_0$  of the current lot is thought of as a realization from  $\pi(\theta)$ . Given  $\theta_0$ ,

$$P(X = x | \theta_0) = \frac{\binom{N\theta_0}{x} \binom{N-N\theta_0}{n-x}}{\binom{N}{n}},$$

**Basic element of Bayesian models**

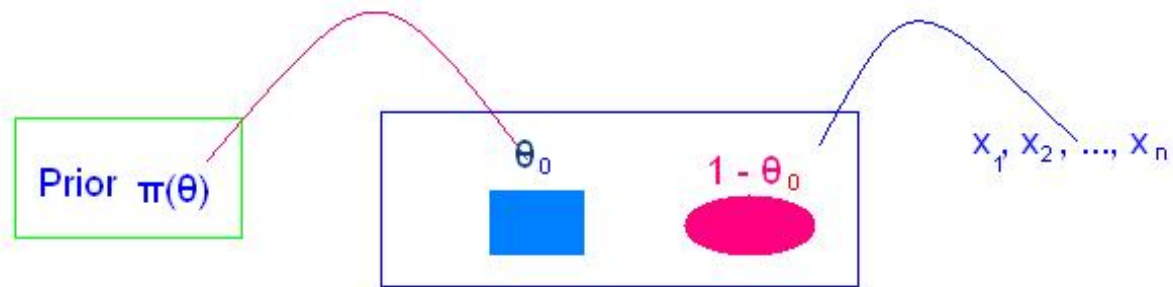


Figure 1.5: Bayesian Framework

- (i) The knowledge about  $\theta$  is summarized by  $\pi(\theta)$  — prior dist.
- (ii) A realization  $\theta$  from  $\pi(\theta)$  serves as the parameter of  $\mathbf{X}$ .
- (iii) Given  $\theta$ , the observed data  $\mathbf{x}$  are a realization of  $p_\theta$ . The joint density of  $(\theta, \mathbf{X})$  is  $\pi(\theta)p(\mathbf{x}|\theta)$ .
- (iv) The goal of the Bayesian analysis is to modify the prior of  $\theta$  after observing  $\mathbf{x}$ :

$$\pi(\theta|\mathbf{X} = \mathbf{x}) = \begin{cases} \frac{\pi(\theta)p(\mathbf{x}|\theta)}{\int \pi(\theta)p(\mathbf{x}|\theta) d\theta}, & \theta \text{ continuous,} \\ \frac{\pi(\theta)p(\mathbf{x}|\theta)}{\sum_{\theta} \pi(\theta)p(\mathbf{x}|\theta)}, & \theta \text{ discrete} \end{cases}$$

e.g. summarizing the distribution by posterior mean, median and SD, etc.



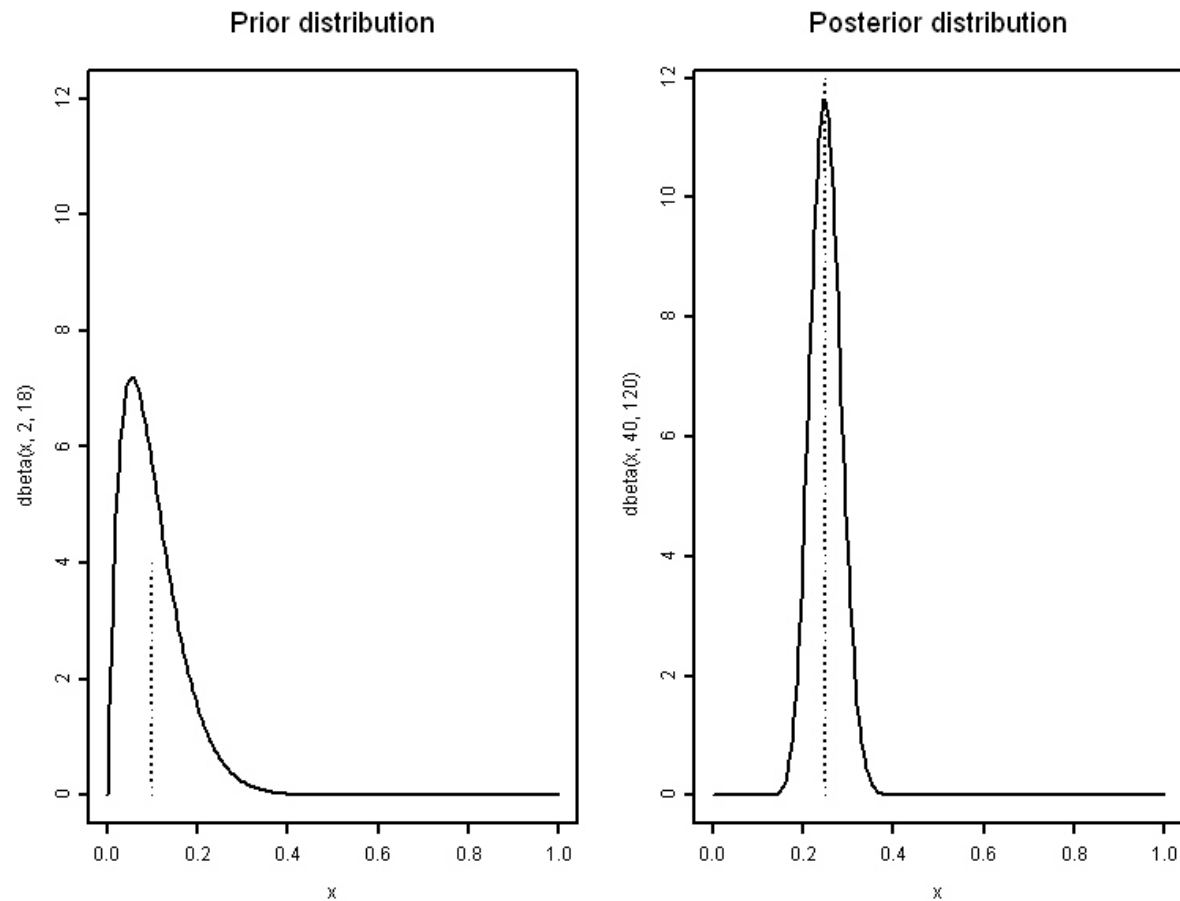


Figure 1.6: Prior versus Posterior distributions

**Example 5** (Quality inspection) Suppose that from the past experience, the defective rate is about 10%. Suppose that a lot consists of 100 products, whose quality is independent of each other.

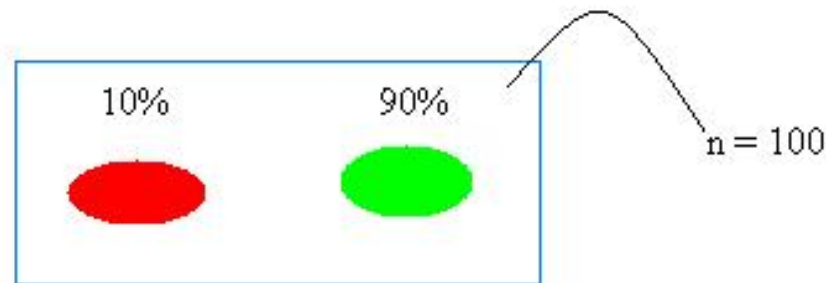


Figure 1.7: Prior knowledge of the defects

The prior distribution about the lot's defective rate is

$$\pi(\theta_i) = P(\theta = \theta_i) = \binom{100}{i} 0.1^i 0.9^{100-i}, \quad \theta_i = \frac{i}{100}.$$

Prior mean and variance are

$$E\theta = E\frac{X}{100} = 0.1$$

$$\text{var}(\theta) = \frac{1}{100^2} \text{var}(X) = \frac{100 \times 0.9 \times 0.1}{100^2},$$

$$SD(\theta) = 0.03.$$

Now suppose that  $n = 19$  products are sampled and  $x = 10$  are defective. Then

$$\pi(\theta_i | X = 10) = \frac{P(\theta = \theta_i, X = 10)}{P(X = 10)} = \frac{\pi(\theta_i)P(X = 10 | \theta = \theta_i)}{\sum_j \pi(\theta_j)P(X = 10 | \theta = \theta_j)}.$$

e.g.

$$\begin{aligned} P(\theta \geq 0.2 | X = 10) &= P(100\theta - X \geq 10 | X = 10) \\ &\approx 1 - \Phi\left(\frac{10 - 81 \times 0.1}{\sqrt{81 \times 0.9 \times 0.1}}\right) \\ &\approx 30\%. \end{aligned}$$

( $100\theta - X$  is the number of defective left after 19 draws, having distribution Bernoulli(81, 0.1)). Compared with the prior probability

$$\begin{aligned} P(\theta \geq 0.2) &= P(100\theta \geq 20) \\ &= 1 - \Phi\left(\frac{20 - 100 \times 0.1}{\sqrt{100 \times 0.9 \times 0.1}}\right) \\ &\approx 0.1\%, \end{aligned}$$

where  $100\theta \sim \text{Bernoulli}(100, 0.1)$ .

**Example 6.** Suppose that  $X_1, \dots, X_n$  are i.i.d. random variables with Bernoulli( $\theta$ ) and  $\theta$  has a prior distribution  $\pi(\theta)$ . Then

$$\pi(\theta | \mathbf{x}) = \frac{\pi(\theta)\theta^{\sum_{i=1}^n x_i}(1 - \theta)^{n - \sum_{i=1}^n x_i}}{\int_0^1 \pi(t)t^{\sum_{i=1}^n x_i}(1 - t)^{n - \sum_{i=1}^n x_i} dt}.$$

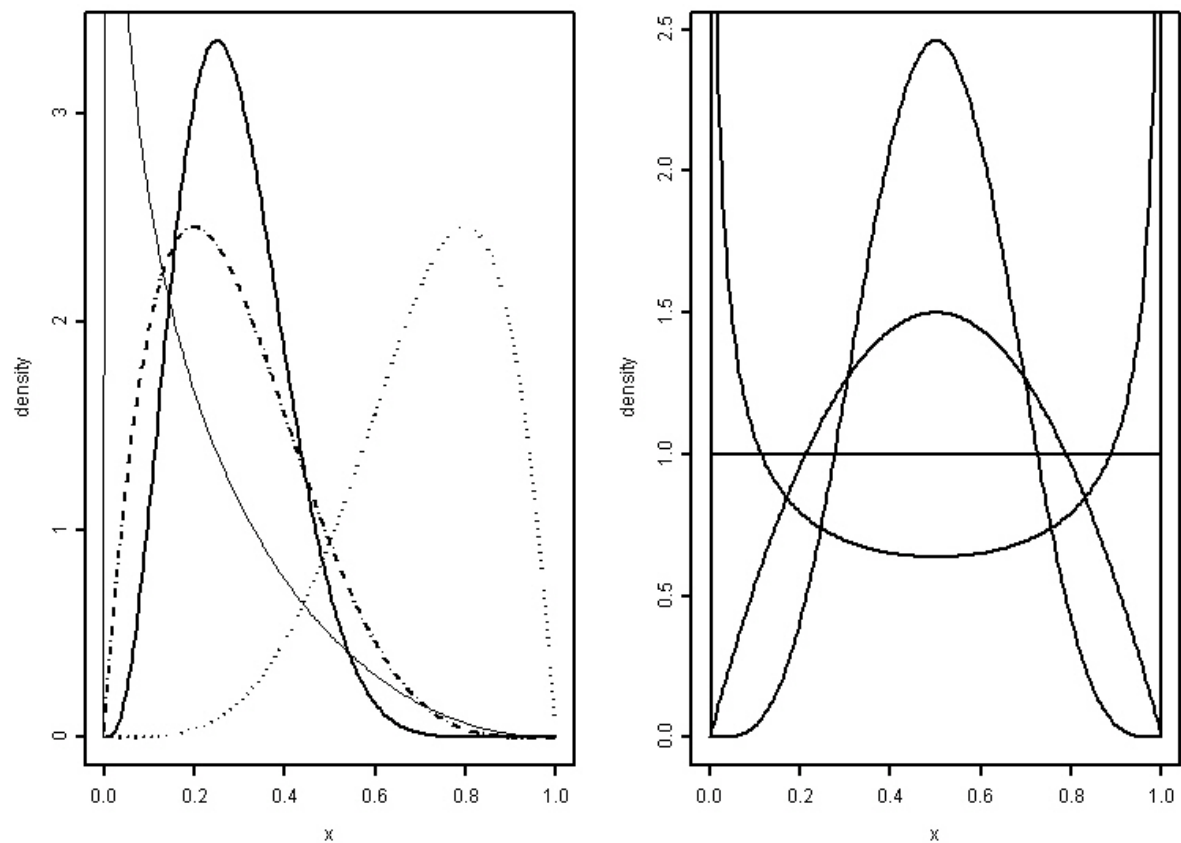


Figure 1.8: Beta distributions with shape parameters: Left panel: (4, 10), (5, 2), (2, 5), (.7, 3); right panel: (5, 5), (2, 2), (1, 1), (0.5, 0.5)

If  $\theta \sim \text{Beta}(r, s)$ , i.e.

$$\pi(\theta) = \frac{\theta^{s-1}(1-\theta)^{r-1}}{B(s, r)}, \quad E\theta = \frac{s}{r+s},$$

then

$$\pi(\theta|\mathbf{x}) \propto \theta^{s+\sum x_i-1}(1-\theta)^{n-\sum x_i+r} \sim \text{Beta}(s + \sum x_i, n - \sum x_i + r).$$

Thus,

$$E(\theta|\mathbf{x}) = \frac{s + \sum_{i=1}^n x_i}{n + s + r} = \begin{cases} \frac{\sum_{i=1}^n x_i + 1}{n+2} & s = r = 1 \\ \approx n^{-1} \sum_{i=1}^n x_i, & n \text{ is large} \end{cases}$$

**Conjugate prior**: Note that the prior and posterior in this example belong to the same family. Such a prior is called “conjugate prior”. It was introduced to facilitate the computation.

### 1.3 Sufficiency

Commonly-used principles for data reduction

$$\begin{cases} 1^\circ \text{ Sufficiency} \\ 2^\circ \text{ Invariant/equivariant} \end{cases}$$

## Purpose:

- 1 simplify probability structure, less obscure than the whole data
- 2 understand whether a loss in reduction
- 3 useful technical tools

**Example 7.** A machine produces  $n$  items in secession with probability  $\theta$  of producing defective product. Suppose that there is no dependence between the quality of products.

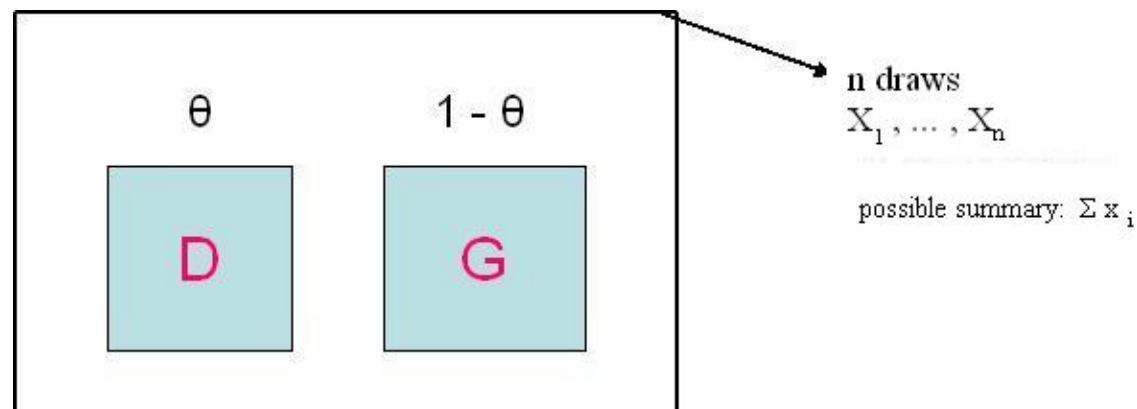


Figure 1.9: Probability model and its summary statistic.

Then, the probability model is

$$p(\mathbf{x}, \theta) = \prod_{i=1}^n \theta^{x_i} (1 - \theta)^{1-x_i} = \theta^{\sum x_i} (1 - \theta)^{1 - \sum x_i}.$$

Any loss of information by using  $\sum x_i$ ?

$$\begin{cases} \text{Yes} & \text{— can not examine the length of a run} \\ \text{No} & \text{— on inference of } \theta \end{cases}$$

**Heuristic:** Consider a vector of statistics  $T(\mathbf{X})$ , which summarizes the original data  $\mathbf{X}$ . Then

Full information, i.e. the information of  $\theta$  contained in  $X_1, X_2, \dots, X_n$   
 = The information about  $\theta$  given in  $T(\mathbf{X})$  (reduced information)  
 + Given  $T(\mathbf{X})$ , the information of  $\theta$  remained in  $X_1, X_2, \dots, X_n$  (the rest information).

**Definition.** A statistic is sufficient if given  $T(\mathbf{X})$ , the conditional distribution of  $\mathbf{X}$  is independent of  $\theta$  — introduced by R.A.Fisher 1922.

**Example 7** (continued). The conditional distribution of  $\mathbf{X}$  given  $\sum_{i=1}^n X_i$  is

$$P_{\theta}\{\mathbf{X} = \mathbf{x} \mid \sum_{i=1}^n X_i = s\} = \begin{cases} 0 & \text{if } \sum x_i \neq s, \\ \frac{P(\mathbf{X}=\mathbf{x}, \sum_{i=1}^n X_i=s)}{P(\sum_{i=1}^n X_i=s)} = \frac{\theta^s(1-\theta)^{n-s}}{\binom{n}{c}\theta^s(1-\theta)^{n-s}} & \text{otherwise} \end{cases}.$$

Obviously, this conditional distribution is independent of  $\theta$ . Thus,  $\sum_{i=1}^n X_i$  is sufficient.

**Theorem 1** (Factorization, Fisher-Neyman Theorem)

*In a regular model, a statistic  $T(\mathbf{X})$  is sufficient in  $\theta \iff$*

$$p(\mathbf{x}, \theta) = g(T(\mathbf{x}), \theta)h(\mathbf{x}), \forall \mathbf{x} \in \mathbb{R}^n \text{ and } \theta \in \Theta$$

*for some functions  $g(t, \theta)$  and  $h$ .*

**Proof:** For simplicity to illustrate the idea, we concentrate on discrete case.



Suppose that  $T(\mathbf{X})$  is sufficient. Then

$$\begin{aligned} p(\mathbf{x}, \theta) &= P_\theta[\mathbf{X} = \mathbf{x}, T(\mathbf{X}) = T(\mathbf{x})] \\ &= P_\theta[T(\mathbf{X}) = T(\mathbf{x})]P_\theta[\mathbf{X} = \mathbf{x}|T(\mathbf{X}) = T(\mathbf{x})] \\ &= g(T(\mathbf{x}), \theta)h(\mathbf{x}). \end{aligned}$$

Conversely,

$$\begin{aligned} &P_\theta\{\mathbf{X} = \mathbf{x}|T(\mathbf{X}) = T(\mathbf{x})\} \\ &= \frac{P_\theta\{\mathbf{X} = \mathbf{x}\}}{P_\theta\{T(\mathbf{X}) = T(\mathbf{x})\}} \\ &= \frac{g(T(\mathbf{x}), \theta)h(\mathbf{x})}{\sum_{\{y:T(\mathbf{y})=T(\mathbf{x})\}} g(T(\mathbf{y}), \theta)h(\mathbf{y})} \\ &= \frac{h(\mathbf{x})}{\sum_{\{y:T(\mathbf{y})=T(\mathbf{x})\}} h(\mathbf{y})}. \end{aligned}$$

**Example 8.** Let  $X_1, \dots, X_n$  be the inter-arrival times of  $n$  customers with arrival rate  $\theta$ .

Then, under some conditions (rare; constant rate; independence)  $X_1, X_2, \dots, X_n$

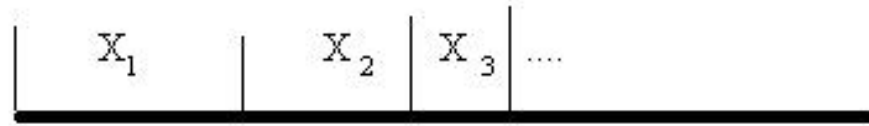


Figure 1.10: Arrival times of customer

are *i.i.d.* random variables with  $Exponential(\theta)$ , i.e.

$$p(\mathbf{X}, \theta) = \prod_{i=1}^n \theta \exp(-\theta x_i) = \theta^n \exp(-\theta \sum_{i=1}^n x_i), \forall x_i \geq 0$$

Hence, by taking  $g(t, \theta) = \theta^n \exp(-\theta t)$  and  $h(\mathbf{x}) = 1$ , we conclude that  $T(\mathbf{X}) = \sum_{i=1}^n X_i$  is sufficient.

**Example 9.**(Size of population)

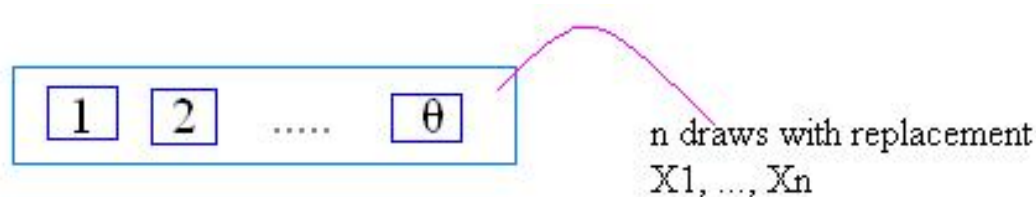


Figure 1.11: Estimation the size of population

Then,  $X_1, X_2, \dots, X_n$  are i.i.d. with

$$P(X_i = x_i) = \frac{1}{\theta} I\{1 \leq x_i \leq \theta\}.$$

Thus,

$$p(\mathbf{x}, \theta) = \frac{1}{\theta^n} \prod_{i=1}^n I\{1 \leq x_i \leq \theta\} = \theta^{-n} I\{\max\{x_i\} \leq \theta\},$$

and the largest order statistic  $X_{(n)} = \max\{X_i\}$  is sufficient.

**Note:** This is not a realistic model. More realistic one is the capture-recapture model.

**Example 10** (Linear regression model). Suppose that  $\{(X_i, Y_i)\}$  are a random sample from

$$Y_i = \alpha + \beta X_i + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2).$$

Then,

$$\begin{aligned}
 & p(\mathbf{X}, \mathbf{y}, \theta) \\
 & \propto \prod_{i=1}^n \sigma^{-1} \exp\left(-\frac{1}{2\sigma^2}(Y_i - \alpha - \beta X_i)^2\right) f(X_i) \\
 & = \prod_{i=1}^n f(X_i) \exp\left(-\log \sigma - \frac{1}{2\sigma^2} \sum_{i=1}^n [Y_i - \alpha - \beta X_i]^2\right) \\
 & \quad \times \exp\left(-\frac{1}{2\sigma^2} \left[ \sum_{i=1}^n Y_i^2 - 2\alpha \sum_{i=1}^n Y_i - 2\beta \sum_{i=1}^n X_i Y_i \right]\right)
 \end{aligned}$$

where  $f(\cdot)$  is density function of  $X$ . Thus,

$$T = \left( \sum_{i=1}^n Y_i, \sum_{i=1}^n Y_i^2, \sum_{i=1}^n X_i Y_i, \sum_{i=1}^n X_i, \sum_{i=1}^n X_i^2 \right)$$

is a sufficient statistic. This is equivalent to the fact that

$$T^* = (\bar{X}, \bar{Y}, \hat{\sigma}_X^2, \hat{\sigma}_Y^2, r)$$

is a sufficient statistic.

**Sufficiency Principle**: Suppose that  $T(\mathbf{X})$  is sufficient. For any decision rule

$\delta(\mathbf{X})$ , we can find a decision rule  $\delta^*(T(\mathbf{X}))$ , depending on  $T(\mathbf{X})$  and  $\delta(\mathbf{X})$  such that

$$R(\theta, \delta) = R(\theta, \delta^*) \text{ for all } \theta,$$

where  $R(\theta, \delta) = E_{\theta}\ell(\theta, \delta(\mathbf{X}))$  is the expected loss function — risk function. Namely, considering the class of sufficient statistic is good enough for making statistical decisions.

**Proof.** For better understanding, let us first assume that  $\ell(\theta, a)$  is convex in  $a$ . Then, let  $\delta^*(T) = E\{\delta(\mathbf{X})|T(\mathbf{X})\}$ . By Jensen's inequality,

$$\begin{aligned} E\ell(\theta, \delta(\mathbf{X})) &= E\{E[\ell(\theta, \delta(\mathbf{X}))|T]\} \\ &\geq E\{\ell(\theta, \delta^*)\} = R(\theta, \delta^*). \end{aligned}$$

In general, let  $\delta^*(T(\mathbf{x}))$  be drawn at random from the conditional distribution  $\delta(\mathbf{x})$  given  $T(\mathbf{X}) : \delta^* \sim L(\delta|T)$ . Then,

$$R(\theta, \delta) = E\{E[\ell(\theta, \delta)|T]\} = E\{E[\ell(\theta, \delta^*)|T]\} = R(\theta, \delta^*).$$

## Sufficiency and Equivariant estimator

**Example 11.** Suppose  $X_1, X_2, \dots, X_n \sim i.i.d.N(\mu, \sigma^2)$ , e.g. measurement of temperature.

data (in $^{\circ}C$ )	data(in $^{\circ}F$ /unnamed scale)
$x_1$	$ax_1 + b$
$x_2$	$ax_2 + b$
$\vdots$	$\vdots$
$x_n$	$ax_n + b$

$$\hat{\mu}: T(x_1, x_2, \dots, x_n) \mid T(ax_1 + b, ax_2 + b, \dots, ax_n + b)$$

$$\text{Estimate of } \mu: T(X_1, X_2, \dots, X_n) \text{ in } ^{\circ}C = aT(X_1, X_2, \dots, X_n) + b \text{ in } ^{\circ}F$$

**Hope:**  $T(ax_1 + b, ax_2 + b, \dots, ax_n + b) = aT(x_1, x_2, \dots, x_n) + b$

**Equivariance:** Such an estimator is called equivariant under linear transformation.

If we are interested in  $\sigma$ , we hope

$$T(X_1 + b, \dots, X_n + b) = T(X_1, \dots, X_n)$$

— invariant under the translation transform or more generally

$$T(aX_1 + b, \dots, aX_n + b) = aT(X_1, \dots, X_n),$$

— equivariant under scale transformation /invariant under translations.

By sufficient principle, we need only to consider the estimator of form

$$T(\bar{X}, S).$$

The equivariance for estimating  $\mu$  requires

$$T(a\bar{X} + b, aS) = aT(\bar{X}, S) + b, \quad \forall a \text{ and } b$$

Taking  $a = 1$  and  $b = -\bar{X}$ ,  $\implies T(0, S) = T(\bar{X}, S) - \bar{X}$

$$T(\bar{X}, S) = \bar{X} + T^*(S).$$

From

$$\begin{aligned} T(a\bar{X}, aS) &= a\bar{X} + T^*(aS) \\ &= a[\bar{X} + T^*(S)] \\ \implies T^*(aS) &= aT^*(S) \\ \implies T^*(S) &= ST^*(1). \end{aligned}$$

Thus, denoting by  $T^* = T^*(1)$ ,

$$T(\bar{X}, S) = \bar{X} + T^*S.$$

Among this invariant class,

$$\begin{aligned} E[T(\bar{X}, S) - \mu]^2 &= (ET^*S)^2 + \text{var}(\bar{X} + T^*S) \\ &= T^{*2}(ES)^2 + T^{*2}\text{var}(S) + \sigma^2/n \end{aligned}$$

It attains the minimum at  $T^* = 0$ , namely,  $\bar{X}$  is the best equivalent estimator.

## Sufficiency and Bayesian Model

**Theorem 2** (Kolmogorov) *If  $T(\mathbf{X})$  is sufficient for  $\theta$ , then for any prior  $\pi(\theta)$ , the conditional distribution*

$$\mathcal{L}(\theta|T(\mathbf{X})) = \mathcal{L}(\theta|\mathbf{X}) \text{ — Bayes sufficient.}$$

According to the theorem,

$$E(g(\theta)|T) = E(g(\theta)|\mathbf{X}).$$

This implies that given  $T(\mathbf{X})$ , and  $\mathbf{X}$  and  $\theta$  are independent, since

$$\begin{aligned} E[f(\theta)g(\mathbf{X})|T] &= E[E(f(\theta)g(\mathbf{X})|\mathbf{X})|T] \\ &= E[g(\mathbf{X})E(f(\theta)|T)|T] \\ &= E[g(\mathbf{X})|T]E[f(\theta)|T]. \end{aligned}$$



## 1.4 Exponential Families

Many useful distributions admit a common structure:

Normal (continuous), Poisson (counts)

Examples Binomial (categorical), Beta

Gamma (constant Coefficient of Variation)

They form the basis of GLIM (Generalized Linear Models). Such a family is called exponential families, discovered independently by Koopman, Pitman and Darmois.

It is nice to give them a unified mathematical treatment.

### The one parameter case

Example 12. Let  $P_\theta = \{N(\mu, \sigma_0^2), \sigma_0 \text{ is known}\}$ . Then its density

$$\begin{aligned} p(x, \mu) &= \frac{1}{\sqrt{2\pi}\sigma_0} \exp\left(-\frac{(x-\mu)^2}{2\sigma_0^2}\right) \\ &= \exp\left\{\frac{x\mu}{\sigma_0^2} - \frac{\mu^2}{2\sigma_0^2} - \left(\frac{x^2}{2\sigma_0^2} + \log \sqrt{2\pi}\sigma_0\right)\right\} \\ &= \exp(T(x)c(\theta) + d(\theta) + S(x)). \end{aligned}$$

**Example 13.** Let  $P_\theta = \{\text{Binomial}(n, \theta)\}$ . Then,

$$\begin{aligned} p(x, \theta) &= \binom{n}{x} \theta^x (1 - \theta)^{n-x} \\ &= \exp \left\{ x \log \frac{\theta}{1 - \theta} + n \log(1 - \theta) + \log \binom{n}{x} \right\} \\ &= \exp \{T(x)c(\theta) + d(\theta) + S(x)\}. \end{aligned}$$

**Definition:** The family of distributions of a model  $\{P_\theta : \theta \in \Theta\}$  is said to be a one-parameter exponential one if

$$p(x, \theta) = \exp\{c(\theta)T(x) + d(\theta) + S(x)\}.$$

**Example 14.** Let  $X \sim \text{Unif}(0, \theta)$ . Then

$$p(x, \theta) = \frac{1}{\theta} I_{[0, \theta]}(x) = \exp(\log I_{[0, \theta]}(x) - \log \theta),$$

not an exponential family. Another example is

$$p(x, \theta) = \frac{1}{9} I(x \in \{0.1 + \theta, \dots, 0.9 + \theta\}).$$

By setting  $c(\theta) = \eta$ , the exponential family can be written in the canonical form as

$$p(x, \eta) = \exp(\eta T(x) + d_0(\eta) + S(x)),$$

where  $d_0(\eta) = d(c^{-1}(\eta))$ , when  $c(\theta)$  is one-to-one.

$\eta$  — canonical (natural) parameter and

$c(\cdot)$  — canonical link,

**Examples** of canonical link functions:

Normal     $c(\theta) = \theta$         identity

Binomial    $c(\theta) = \log \frac{\theta}{1-\theta}$     logit

Poisson     $c(\theta) = \log \theta$         logarithm.

**Regeneration properties:**

1. Let  $X_1, \dots, X_n \sim i.i.d.P_\theta$ , belonging to an exponential family. Then, the joint density  $\prod_{i=1}^n p(x_i, \theta)$  is also in the exponential family. Further,  $\sum_{i=1}^n T(X_i)$  is a sufficient statistic.

2. If  $X \sim P_\theta$  which is exponential family, and  $\{Q_\theta\}$  be the distribution of  $T(X)$ ,  
Then,  $\{Q_\theta\}$  is also in the exponential family.

**Theorem 3** If  $X \sim \exp\{\eta T(X) + d_0(\eta) + S(x)\}$ ,  $\eta$  is an interior of  $\mathcal{E}$ , then

$$\psi(s) = E \exp\{sT(X)\} = \exp[d_0(\eta) - d_0(s + \eta)], \text{ for } s \text{ near } 0$$

Moreover,  $ET(X) = -d'_0(\eta)$ ,  $\text{var}(T(\mathbf{x})) = -d''_0(\eta)$ . (The function  $d_0$  is concave.)

**Proof:** Note that

$$\begin{aligned} & \int_{-\infty}^{+\infty} \exp\{\eta T(x) + d_0(\eta) + S(x)\} dx = 1, \\ \implies & \int_{-\infty}^{+\infty} \exp\{\eta T(x) + S(x)\} dx = \exp(-d_0(\eta)). \end{aligned}$$

Now,

$$\begin{aligned}
 \psi(s) &= E\{\exp(sT(x))\} \\
 &= \int_{-\infty}^{+\infty} \exp\{sT(x) + \eta T(x) + d_0(\eta) + S(x)\} dx \\
 &= \exp(d_0(\eta) - d_0(\eta + s)).
 \end{aligned}$$

From the properties of the moment generating function,

$$\begin{aligned}
 \psi'(s)|_{s=0} &= E\{T(X) \exp(sT(X))|_{s=0}\} \\
 &= ET(X) \\
 &= -\exp(d_0(\eta) - d_0(\eta + s))d'_0(\eta + s)|_{s=0}.
 \end{aligned}$$

Similarly,

$$\begin{aligned}
 ET^2(X) &= \psi''(s)|_{s=0} = -d''_0(\eta) + d'_0(\eta)^2 \\
 \implies \text{var}(T(X)) &= -d''_0(\eta).
 \end{aligned}$$

**Example 15.**  $X_1, \dots, X_n \sim i.i.d.$

$$p(x, \theta) = k\theta(\theta x)^{k-1} \exp(-(\theta x)^k), \quad x > 0.$$

— Weibull distribution  $\implies$  model “failure time” with hazard risk:  $\frac{f(t)}{1-F(t)} = k\theta(\theta t)^{k-1}$

$k = 1 \implies$  exponential distribution — constant risk

$k = 2 \implies$  Raleigh distribution —  $k\theta^2 t$  (linear risk)

Then, the joint density

$$\begin{aligned} p(\mathbf{x}, \theta) &= \prod_{i=1}^n k\theta(\theta x_i)^{k-1} \exp(-\theta^k x_i^k) \\ &= \exp\left(-\theta^k \sum_{i=1}^n x_i^k - nk \log \theta + \sum_{i=1}^n \log x_i^{k-1} + n \log k\right). \end{aligned}$$

For this family of distributionm,

$$\eta = -\theta^k$$

$$d_0(\eta) = -n \log \theta^k = -n \log(-\eta).$$

Hence,

$$\sum_{i=1}^n X_i^k \text{ — natural sufficient statistic,}$$

$$E \sum_{i=1}^n X_i^k = \frac{-n}{\eta} = \frac{n}{\theta^k},$$

$$\text{var}\left(\sum_{i=1}^n X_i^k\right) = \frac{n}{\eta^2} = \frac{n}{\theta^{2k}}.$$

Direct computation of these moments are more complicated.

### The k parameter case

A family of distributions  $\{P_\theta : \theta \in \Theta\}$  is said to be  $k$  parameter exponential family if its joint density admits the form

$$\begin{aligned} p(\mathbf{x}, \theta) &= \exp\left(\sum_{i=1}^k C_i(\theta)T_i(\mathbf{x}) + d(\theta) + S(\mathbf{x})\right) \\ &= \exp\left(\sum_{i=1}^k \eta_i T_i(\mathbf{x}) + d_0(\eta)\right). \end{aligned}$$

By the factorization theorem, the vector  $T(\mathbf{x}) = (T_1(\mathbf{x}), \dots, T_k(\mathbf{x}))$  is a sufficient statistic.

Suppose that  $\mathbf{X}_1, \dots, \mathbf{X}_n$  are a random sample from  $P_\theta$ . Put  $\mathbf{X} = (\mathbf{X}_1, \dots, \mathbf{X}_n)$  which is available data.

Then, the distribution of  $\mathbf{X}$  forms a  $k$ -parametric family with

$$T(\mathbf{X}) = \left( \sum_{i=1}^n T_1(\mathbf{X}_i), \dots, \sum_{i=1}^n T_k(\mathbf{X}_i) \right)$$

Let  $\psi(\mathbf{s}) = E \exp(\mathbf{s}^T T(\mathbf{x}))$ . Then,

$$\psi(\mathbf{s}) = \exp(d_0(\eta) - d_0(\eta + \mathbf{s}))$$

$$ET(\mathbf{x}) = -d'_0(\eta) \text{— mean vector}$$

$$\text{var}(T(\mathbf{x})) = -d''_0(\eta) \text{— variance-covariance matrix}$$

**Example 16.** (Multinomial trials)

$$P(X_i = j) = p_j = \prod_{\ell=1}^k p_\ell^{I(j=\ell)}$$





Figure 1.12: Multinomial trial. Each outcome is a  $k$ -dimensional unit vector, indicating which category is observed.

$$\prod_{i=1}^n P(x_i, \mathbf{p}) = \prod_{i=1}^n \prod_{\ell=1}^k p_{\ell}^{I(x_i=\ell)} = \prod_{\ell=1}^k p_{\ell}^{n_{\ell}}.$$

$$n_{\ell} = \sum_{i=1}^n I(x_i = \ell) \text{ — \# of times observing } \ell$$

The joint density is

$$\begin{aligned} p(\mathbf{x}, \mathbf{p}) &= \exp\left\{\sum_{\ell=1}^k n_{\ell} \log p_{\ell}\right\} \\ &= \exp\left\{\sum_{\ell=1}^{k-1} n_{\ell} \log \frac{p_{\ell}}{p_k} + n \log p_k\right\}. \end{aligned}$$

Let  $\alpha_j = \log p_j - \log p_k, j = 1, \dots, k - 1$ . Then

$$p_k = 1 - p_1 - \dots - p_{k-1} = 1 - p_k \sum_{j=1}^{k-1} e^{\alpha_j}$$

$$\implies p_k = \frac{1}{1 + \sum_{j=1}^{k-1} e^{\alpha_j}}$$

Hence,

$$p(\mathbf{x}, \mathbf{p}) = \exp \left\{ \sum_{\ell=1}^{k-1} n_{\ell} \alpha_{\ell} - n \log \left( 1 + \sum_{j=1}^{k-1} e^{\alpha_j} \right) \right\}.$$

The variance and covariance matrix of  $(n_1, \dots, n_k)$  can easily be completed.

**Other Examples**: — Multivariate normal distributions

— Dirichlet distribution (multivariate  $\beta$ -distribution):

$$c x_1^{\beta_1-1} \dots x_p^{\beta_p-1} (1 - x_1 - \dots - x_p)^{\beta_{p+1}-1}.$$