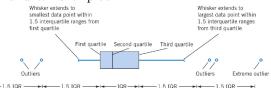
## 16. PCA

#### 18. Descriptive statistics

Box-and-Whisker plot:



Probability plot:  $x_i(j-0.5)/n/CDF(x_i)$ 

## 19. Sample mean and variance

sample **mean**:  $E(\bar{X}) = \mu$ 

sample variance:  $V(\bar{X}) = \sigma^2/n$ 

sample std/standard error (SE):  $\sigma/\sqrt{n}$ 

central limit theorem: the limiting form of the distribution of large n is the standard normal distribution: Z = $(X-\mu)/(\sigma/\sqrt{n})$ 

Two populations: the sampling distribution of  $\bar{X}_1 - \bar{X}_2$  with mean  $\mu_{\bar{X}_1-\bar{X}_2}=\mu_1-\mu_2$  and variance  $\sigma^2_{\bar{X}_1-\bar{X}_2}=\sigma^2_1/n_1+\sigma^2_2/n_2$  Sampling distribution of a **difference** in sample means: Z= $((\bar{X}_1 - \bar{X}_2) - (\mu_1 - \mu_2)) / \sqrt{\sigma_1^2 / n_1 + \sigma_2^2 / n_2}$ 

#### 20. point estimator

Unbiased point estimator:  $E(\hat{\Theta}) = \Theta$ 

Bias:  $E(\hat{\Theta}) - \Theta$ 

Mean Squared Error:  $MSE(\hat{\Theta}) = E(\hat{\Theta} - \Theta)^2 = V(\hat{\Theta}) + (\hat{\Theta})^2 = V(\hat{\Theta})^2 = V(\hat{\Theta})$ 

Methods of moment: kth moment of random variable is  $E(X^k)$ .

First moment:  $\mu = \int x f(x) dx$ ; second moment:  $\mu^2 + \sigma^2 =$  $\int x^2 f(x) dx \to E(X^2) = Var(X) + E(X)^2.$ 

Moment estimators:  $X_1, ..., X_n$  with m unknown parameters. They are found by equating first m population moments to first m sample moments.

To estimate exponential distribution, 1st moment,  $E(X) = \bar{x} =$  $1/\lambda$ ; higher moment,  $E(X^p) = p!/\lambda^p$ 

**Maximum likelihood**:  $L(\theta) = f(x_1, \theta)...f(x_2, \theta)...f(x_n, \theta).$ Maximum likelihood estimator (MLE) of  $\theta$  is the value of  $\theta$ that maximize  $L(\theta)$ . Use logarithm:  $I(\theta) = lnL(\theta)$ 

**Exponential MLE**:  $dlnL(\lambda)/d\lambda = n/\lambda - \sum x_i = 0 \rightarrow \lambda =$  $n/\sum x_i = 1/\bar{X}$ 

Bernoulli MLE:  $\hat{p} = \sum x_i/n$ 

Normal MLE for  $\mu$ :  $dlnL(\mu)/d\mu = \sum (x_i - \mu)/\sigma^2 = 0 \rightarrow$ 

MLE for poisson distribution:  $dln f(x_1,..,x_n|\lambda)/d\lambda =$ 

 $-n + \sum x_i/\hat{\lambda} = 0 \to \lambda = \sum x_i/n$ Sample variance:  $s^2 = \sum (x_i - \bar{x})^2/(n-1)$ . If mean  $\mu$  is known, use n.  $s^2 = \sum (x_i - \mu)^2/n$ 

#### 21. Confidence intervals:

two-sided:  $Prob(L < \mu < R) = 1 - \alpha \rightarrow P(\bar{X} - Z_{\alpha/2}\sigma/\sqrt{n} < R)$  $\mu < \bar{X} + Z_{\alpha/2}\sigma/\sqrt{n}) = 1 - \alpha;$ one-sided:  $Prob(\mu > R) = \alpha \rightarrow P(\bar{X} - \mu/\sigma\sqrt{n} < Z_{\alpha}) \rightarrow \mu > 0$  $\bar{X} - Z_{\alpha} \sigma / \sqrt{n}$ 

If sample is small and population variance is not **known**, use sample variance  $s^2 = \sum (x_i - \bar{x})^2/n - 1$  and use t-distribution instead of normal distribution.

t-distribution:  $f(t) = (1 + \frac{t^2}{n-1})^{-n/2}$ , n is dof.

Then the t confidence interval on  $\mu$  is  $\bar{x} - t_{\alpha/2, n-1} s / \sqrt{n} < \mu < 1$  $\bar{x} + t_{\alpha/2,n-1} s / \sqrt{n}$ 

 $\frac{(n-1)s^2}{\chi^2_{\alpha/2,n-1}} < \sigma^2 <$  24. Regression analysis Confidence interval on the variance:

 $(n-1)s^2$ 

Large sample confidence interval for a population proportion:

**16. PCA** PCA diagonalize 
$$p \times p$$
 corr coefficient matrix  $r_{ij} = \sigma_{ij}/\sigma_i\sigma_j$ .  $\hat{p} - z_{\alpha/2}\sqrt{\frac{\hat{p}(1-\hat{p})}{n}} \le p \le \hat{p} + z_{\alpha/2}\sqrt{\frac{\hat{p}(1-\hat{p})}{n}}$ 

## 22. Hypothesis Test

|             | decide $H_0$   | decide $H_1$        |
|-------------|----------------|---------------------|
|             | Correct action | Type I error        |
| probability | $1-\alpha$     | α                   |
| true $H_1$  | Type II error  | Correct action      |
| probability | β              | $power = 1 - \beta$ |
|             |                |                     |

 $\alpha = P(\text{type I error}) = P(\text{reject } H_0 \text{ when } H_0 \text{ is true})$ 

If  $H_1$  is **two-sided** hypothesis, P-value is  $2(1 - \Phi(|Z|))$ , where  $Z=((X)-\mu_0)/(s/\sqrt{n})$ . If  $\alpha$  is given, bounds are  $\mu_0 \mp z_{\alpha/2} * s$ to reject null hypothesis.

For one-sided  $\mu_1 > \mu_0$ , it's  $1 - \Phi(Z)$ ; for  $\mu_1 < \mu_0$ , it's  $\Phi(Z)$ . If sample size n is small, use t-distribution with n-1 DOF for two-sided P-value:  $2(1 - CDF_{Tdist}(|T|))$  where  $T = \bar{X}$  $\mu_0/s\sqrt{n}$ . Use  $\mu_0 \mp t_{\alpha/2,n-1}T$  to reject null hypothesis.

Type II error and choice of sample size,  $n = z_{\alpha/2} + z_{\beta}^2 \sigma^2 / \delta^2$ , where  $\delta = \mu - \mu_0$ 

m independent null hypothesis, at least one is false at significant threshold  $\alpha_1$ : Family-Wise Error Rate=1 -  $(1 - \alpha_1)^m$ ; to get FWER ;  $\alpha$ ,  $\alpha_1 = \alpha/m$ 

Hypothesis test for a **difference** in means:

$$H_0: \mu_1 - \mu_2 = \Delta_0 = 0$$
, test statistic:  $Z_0 = \frac{\bar{X}_1 - \bar{X}_2 - \Delta_0}{\sqrt{\sigma_1^2/n_1 + \sigma_2^2/n_2}}$ 

| Alternative Hypotheses                | P-Value   | Rejection Criterion For<br>for Fixed-Level Tests |
|---------------------------------------|---|--|
| $H_1$ : $\mu_1 - \mu_2 \neq \Delta_0$ | Probability above $ z_0 $ and probability below $- z_0 $ , $P = 2[1 - \Phi( z_0 )]$ | $z_0 > z_{\alpha/2}$ or $z_0 < -z_{\alpha/2}$    |
| $H_1$ : $\mu_1 - \mu_2 > \Delta_0$    | Probability above $z_0$ ,<br>$P = 1 - \Phi(z_0)$                                    | $z_0 > z_\alpha$                                 |
| $H_1$ : $\mu_1 - \mu_2 < \Delta_0$    | Probability below $z_0$ ,<br>$P = \Phi(z_0)$  | $z_0 < -z_\alpha$                                |

If  $\sigma_1^2 \neq \sigma_2^2$ , t-distribution with **DOF**  $v = n_1 + n_2 - 2$ 

23. Goodness of fit test Pearson chi<sup>2</sup> goodness of fit test:  $\chi_0^2 = \sum_{i=1}^k (O_i - E_i)^2 / E_i$ , where  $O_i$  is observed number and  $E_i$  is expected number. P-value=P( $H_0$  is correct)= 1 - $CDF_{chi-squared}(\chi_0^2, k-1).$ 

How to test hypothesis if samples are drawn from same population: P(group1; color = green) = P(group1)P(color = green)green).

 $E_{green}(group1) = n_{tot}(group1/n_{tot})(green/n_{tot}).$  And  $\chi^2 =$  $\sum_{groups\&colors}^{n_{tot}} (O_{color}(group) - E_{color}(group))^2 / E_{color}(group),$ where DOF is (colors-1)(groups-1)

# Goodness of fit with a PDF defined by m parameters

- As before: k classes (e.g. M&M colors)
- Use parameter estimators to find the best parameters for the fit
  - Method of moments
  - MLE: method of maximum likelihood
- Use chi-squared distribution with k-1-m degrees of freedom
- As before: if  $E_i < 3$ , group it until  $E_{group} > = 3$  make k equal to the new number of bins

$$X_0^2 = \sum_{i=1}^k \frac{(O_i - E_i)^2}{E_i}$$
 (9-47)

Confidence interval for population variance:  $\chi_{n-1}^2 =$  $(n-1)S^2/\sigma^2$ .

Interval form:  $\frac{(n-1)S^2}{\chi^2_{\alpha/2,n-1}} < \sigma^2 < \frac{(n-1)S^2}{\chi^2_{1-\alpha/2,n-1}}$ 

 $Y = \beta_0 + \beta_1 X + \epsilon, \ \beta_1 = Cov(X, Y) / Var(X); \beta_0 = E(Y) -$ 

Use least squares to estimate:  $\beta_1 = \frac{\sum y_i x_i - (\sum y_i)(\sum x_i)/n}{\sum x_i^2 - (\sum x_i)^2/n}$ 

analysis of variance  $\sum (y_i - \bar{y})^2 = \sum (\hat{y}_i - \bar{y})^2 + \sum (y_i - \hat{y}_i)^2 \rightarrow$  $SS_T = SS_R + SS_E$ 

coefficient of determination:  $R^2 = SS_R/SS_T = 1 - SS_E/SS_T$ 

Estimate  $\sigma_e^2$ :  $SS_E = \sum e_i^2 = (n-2)\sigma_e^2$ 

Slope property:  $E(\hat{\beta}_1) = \beta_1; V(\hat{\beta}_1) = \sigma^2/S_{xx} = \hat{\sigma}_e^2/n\sigma_x^2$ Intercept property:  $E(\hat{\beta}_0) = \beta_0; V(\hat{\beta}_0) = \sigma^2[1/n + \bar{x}^2/S_{xx}] =$ 

 $\sigma_e^2 [1 + \mu_x^2 / \sigma_x^2] / n$ 

**Hypothesis test**: H0:  $\beta_1 = 0$ ; H1:  $\beta_1 \neq 0$ 

Use Z-test for large n:  $Z = \hat{\beta}_1/(\hat{\sigma}_e/\sigma_x\sqrt{n})$ . Reject H0 if |Z| > $Z_{\alpha/2}$ 

Use t-test for smaller n:  $Z = \hat{\beta_1}/(\hat{\sigma_e}/\sigma_x\sqrt{n})$ . Reject H0 if  $|Z| > t_{\alpha/2, n-2}$ 

### 25. Multiple linear regression

$$\mathbf{y} = \mathbf{X}\beta + \epsilon$$
, where least square is  $L = \sum e_i^2 = (y - X\beta)'(y - X\beta)$ .  $dL/d\beta = 0 \rightarrow \hat{\beta} = (X'X)^{-1}X'y$ 

Property: 
$$E(\hat{\beta}) = \beta$$
, Covariance Matrix:  $C = (X'X)^{-1}$ ;  $V(\hat{\beta}_j) = \sigma_e^2 C_{jj}$ ;  $cov(\hat{\beta}_i, \hat{\beta}_j) = \sigma_e^2 C_{ij}$ 

Estimate 
$$\sigma_e^2$$
,  $\hat{\sigma}_e^2 = SS_E/n - p$ , where  $p = k + 1$ 

$$R^2 = 1 - SS_E/SS_T$$
; adjusted R-square:  $R_{adj}^2 = 1 - SS_E/(n-p)$ 

$$\frac{SS_E/(n-p)}{SS_T/(n-1)}$$

## 26. Clustering algorithm

Hierarchical: agglomerative (eg, UPGMA), divisive

Non-hierarchical: PCA, K-means

- p x p symmetric matrix R of corr. coefficients  $r_{ij} = rac{\sigma_{ij}}{\sigma_i \sigma_j}$
- $R=n^{-1}Z'^*Z$  is a "square" of the matrix Z of standardized r.v.:  $z_{\alpha k}=\frac{x_{\alpha k}-\mu_k}{\sigma_k}$   $\Rightarrow$  all eigenvalues of R are non-negative
- Diagonal elements=1 → tr(R)=p
- Can be diagonalized:

R=V\*D\*V' where D is the diagonal matrix

- d(1,1) –largest eig. value, d(p,p) the smallest one
- The meaning of V(i,k) contribution of the data type i to the k-th eigenvector
- tr(D)=p, the largest eigenvalue d(1,1) absorbs a fraction =d(1,1)/p of all correlations can be ~100%
- Scores: Y=Z\*V: n x p matrix. Meaning of  $Y(\alpha,k)$  participation of the sample #  $\alpha$  in the k-th eigenvector

Distances: Euclidean: $\sqrt{\sum_i (x_i - y_i)^2}$ ; city block (Manhattan):

$$\sum_{i} |x_i - y_i|$$
; Canberra:  $\sum_{i} (\frac{x_i - y_i}{x_i + y_i})$ ; correlation coefficient:  $1 - \sum_{i} |x_i - y_i|$ 

$$\rho(x,y) = 1 - \frac{Cov(x,y)}{\sqrt{Var(x).Var(y)}}$$