Statistics for Data Science Concept Notes

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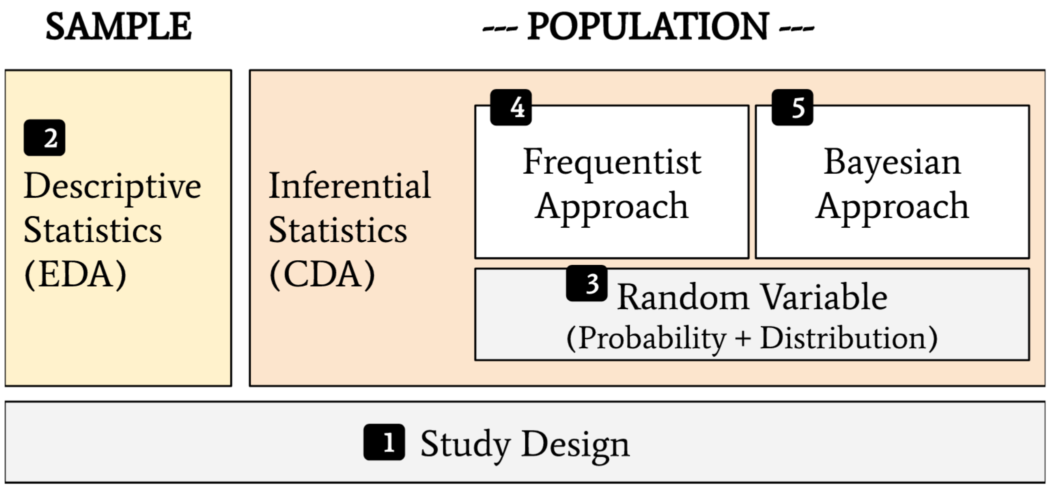

* EDA: Exploratory Data Analysis, CDA: Confirmatory Data Analysis

1. Study Design

a. Study Types & Sampling

b. Variable Types

2. Descriptive Statistics

a. Types of Descriptive Stats.

b. Charts & Graphs

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a. Estimation

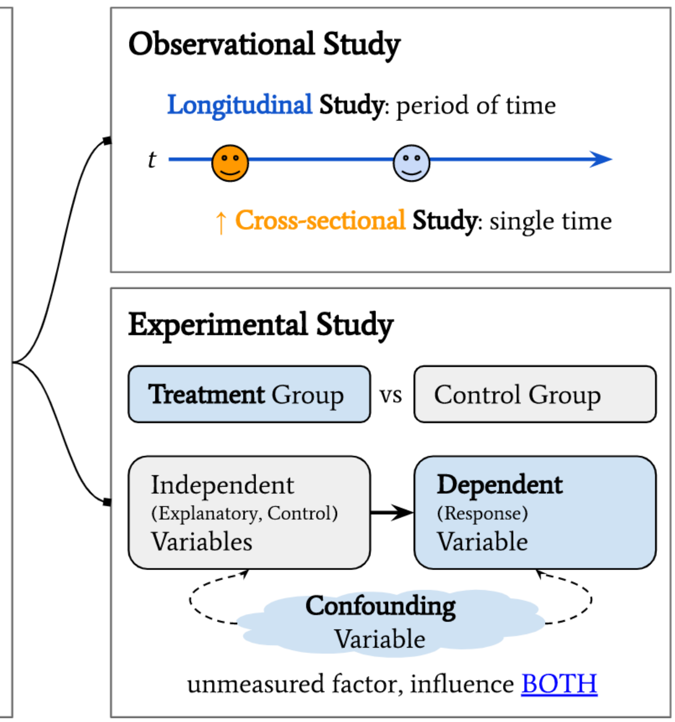
b. Bayesian Hypothesis Testing

1. Study Design

a. Study Types & Sampling Techniques

Sampling Techniques

1. **Simple Random Sampling**: equal chance for each individual
2. **Stratified Sampling**: grouping variable correlated with the measurement
3. **Cluster Sampling**: grouping variable NOT correlated with the measurement
4. **Systematic Sampling:** every nth member of the population
5. **Convenience Sampling**: unethical, biased



b. Variable Types

Types	Scale	Category	Order	Equal Intervals	True Zero	Example
Qualitative (Categorical)	Nominal	Y	N	N	N	Gender
	Ordinal	Y	Y	N	N	A, B, C
Quantitative (Numerical) Discrete/Continuous	Interval	Y	Y	Y	N	Year, IQ
	Ratio	Y	Y	Y	Y	Weight, Age

2. Descriptive Statistics

a. Types of Descriptive Statistics

Measures of Central Tendency

- **Mean / median / mode**
  * uni-/bi-/multi-modal or no mode
- **Hildebrand Rule**: is it symmetric?
  : H=(mean-median) / std
  → sufficiently symmetric if |H| < 0.2

Measures of Frequency

- **Frequency** (Counts)
- **Relative frequency** (in %)
- **Cumulative frequency**
  (only when ordered)

Measures of Position

- **Percentile**
- **Quartile**
- **IQR (Q3-Q1)**
- **z-score**

$$Z = \frac{x - \mu}{\sigma}$$

Measures of Dispersion

$$s^2 = \frac{\Sigma(x_i - \bar{x})^2}{n-1}$$

- **Range / variance / standard deviation**
  * std: same unit → easier to interpret
- To compare between variables,
  Coefficient of variation = std / mean
  ("risk/reward ratio")
- **Empirical Rule:** 68-95-99.7%
  * can apply only to bell-shaped curves
- **Chebyshev's Theorem**:
  P(within K stds) > 1-(1/K2)
  * can apply to any type of distribution

Measures of Dependence

- **Covariance**: measure of joint variability
- **Correlation coefficient**: cov / std(x)std(y)
- **Covariance matrix**:
  covariance between every pair of features

$$cov_{x,y} = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{N-1}$$

b. Charts & Graphs

Qualitative	Pie chart, Bar chart, Pareto chart (bars in descending order)
Quantitative	Histogram(1D), Boxplot (five-number summary) (1D) Scatter plot (2D), Line Graph (2D)

Appendix. Sample Covariance Matrix

$$C = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})(X_i - \bar{X})^T$$

- Using the sample covariance matrix, we can express the variation in every direction
  $$var(\vec{v}^T\vec{x}_1, \cdots, \vec{v}^T\vec{x}_n) = \vec{v}^T\ \Sigma(\vec{x}_1, \cdots, \vec{x}_n)\ \vec{v}$$
- Using eigendecomposition of the covariance matrix,
  $CV = VL \Rightarrow C = V\,L\,V^{-1}$: particular case of Singular Value Decomposition
  1) **PCA**: eigenvectors & eigenvalues characterize the variation of the data in every direction
  2) **Whitening**: decorrelate (eliminate the linear skew) to reveal underlying nonlinear structure
  $\vec{y}_i = \sqrt{L}^{-1}\,V^T\vec{x}_i$ (the covariance of y becomes an identity matrix)

3. Random Variables

a. Probability

Interpretation	• **Frequentists**: relative frequency in the long run : n(E) / n(S) • **Propensity**: experimental probability : freq / #OfSamples • **Bayesian** (Subjectivists): degree of belief
Rules	---------- **Probability Axioms** ---------- 1. For any event A, 0 ≤ P(A) ≤ 1 2. ΣP(A) = 1 3. Complement Rule: P(not A) = 1 – P(A) ---------- **Probability Rules** ---------- 4. Addition Rule: P(A or B) = P(A) + P(B) – P(A and B) for Disjoint: P(A or B) = P(A) + P(B) 5. Conditional Probability: P(A|B) = P(A and B) / P(B) C. Independence: P(A.B|C) = P(A|C)P(B|C) 6. Multiplication Rule: P(A and B) = P(A)P(B|A) for Independence: P(A and B) = P(A)P(B) Chain Rule: P(A and B and C) = P(A)P(B|A)P(C|A,B) (cf) Pairwise independence does not imply joint independence. Independence does not imply conditional independence or vice versa. ---------- **Applications** ---------- 7. Bayes' Rule: P(A|B) = P(A)P(B|A) / P(B) - by Rule #5 and #6 - 8. Law of Total Probability: P(S) = ΣP(S and Ai) = ΣP(Ai)P(S|Ai) - by Rule #4 and #6 -

Appendix. Basic Counting Rules

- **Combination**: order DOES NOT matter (→ divide more!)
- **Permutation**: order matters
- **Special Permutation**: number of distinguishable permutations

$${}_nC_r = \frac{n!}{r!(n-r)!} \qquad {}_nP_r = \frac{n!}{(n-r)!} \qquad \frac{n!}{n_1!n_2!\ldots n_k!}$$

b. Random Variable

Random Variables (cf) RV (uncertainty) vs Realization (revealed outcome/value)

Discrete Random Variables (Probability Mass Function)

- **Bernoulli**: $P(X=x) = p^x(1-p)^{1-x}$ $E[X] = p$ $V[X] = p(1-p)$
  only two possible outcomes

Σ

- **Binomial** B(n,p): $P(X=x) = {}_nC_x\, p^x (1-p)^{n-x}$ $E[Y] = np$ $V[Y] = np(1-p)$
  sum of n i.i.d Bernoulli (count of success)

$\fallingdotseq$

- **Poisson** Pois(λ): $P(X=x) = \frac{\lambda^k e^{-\lambda}}{k!}$ $E[X] = \lambda$ $V[X] = \lambda$
  count of successes over area/time (no upper limit)
  can be modeled as a B(n, λ/n): (success or failure within 1/n interval) * repeat n times

- **Geometric** Geo(p): $P(K=k) = (1-p)^{k-1}p$ $E[X] = 1/p$ $V[X] = (1-p)/p^2$
  success on kth Bernoulli trial
  memorylessness: the distribution of waiting time until a certain event DOES NOT depend on how much time has elapsed already ⇒ P(X>m+n | X≥m) = P(X>n)

- **Hypergeometric**: $P(X=x) = \frac{\binom{K}{k}\binom{N-K}{n-k}}{\binom{N}{n}}$ $E[X] = n\frac{K}{N}$ $V[X] = n\frac{K}{N}\frac{(N-K)}{N}\frac{N-n}{N-1}$

  k success in n draws w/o replacement from N population (K is total possible success)

Continuous Random Variables (Probability Density Function)

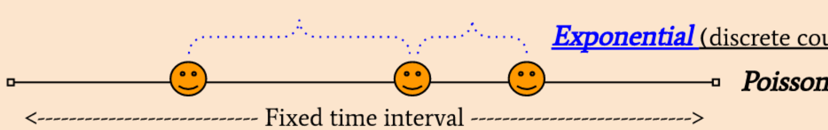
- **Uniform** unif(a,b): $P(X=x) = \begin{cases} \frac{1}{b-a} & \text{for } x \in [a,b] \\ 0 & \text{otherwise} \end{cases}$ $E[X] = \frac{1}{2}(a+b)$ $V[X] = \frac{1}{12}(b-a)^2$
  constant likelihood across interval
  Equivalent to a beta distribution with a=b=1

- **Exponential** exp(λ): $P(X=x) = \lambda e^{-\lambda x}$ $E[Y] = \frac{1}{\lambda}$ $V[Y] = \frac{1}{\lambda^2}$
  time between the events in a Poisson process
  memorylessness: the distribution of waiting time until a certain event DOES NOT depend on how much time has elapsed already ⇒ P(X>m+n | X≥m) = P(X>n)

- **Normal** N(μ, σ2): $P(X=x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$

- **Beta** Beta(α, β): $P(X=x) = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{\int_0^1 u^{\alpha-1}(1-u)^{\beta-1}\,du}$

TIPs



Exponential (discrete counterpart: ***Geometric***)

memoryless

Appendix 1. Gaussian Mixture Model

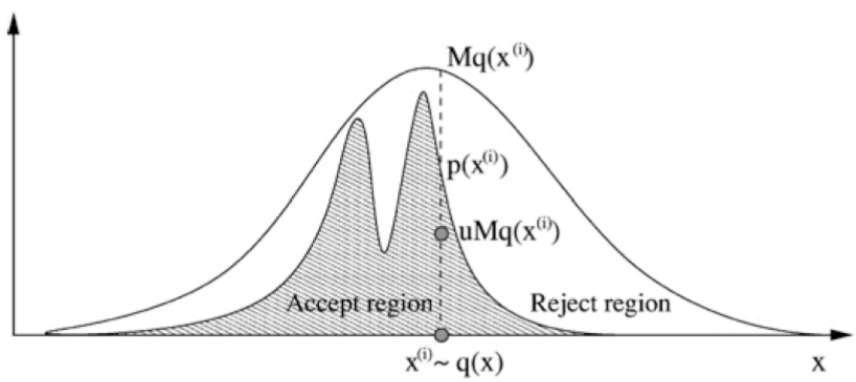
- **Gaussian random vectors**: multidimensional generalization of Gaussian random variables
  - Property 1) linear transformation of Gaussian random vectors are also Gaussian
  - Property 2) marginals of Gaussian random vectors are also Gaussian
- **Gaussian Mixture Model**: discrete marginal + continuous conditional

$$\sum_{d \in R_D} p_D(d) F_{C|D}(c|d)$$

  - data from continuous distribution whose parameters are chosen from a discrete set
  - a popular technique for clustering

Appendix 2. Sampling from Distribution

- **Inverse-transform sampling**: a sample of Uniform → set $x := F_X^{-1}(u)$
- **Rejection sampling**:
  - Why do we need it? When we cannot easily sample from f(x), there exists another density g(x) from which it is easy for us to sample (ex. Normarl, t-distribution as built-in functions)
  - How does it work? sample from a proposal function q(x) → sample from u(0,1) → y = u * M * q(x) → accept if u * M * q(x) ≤ p(x)



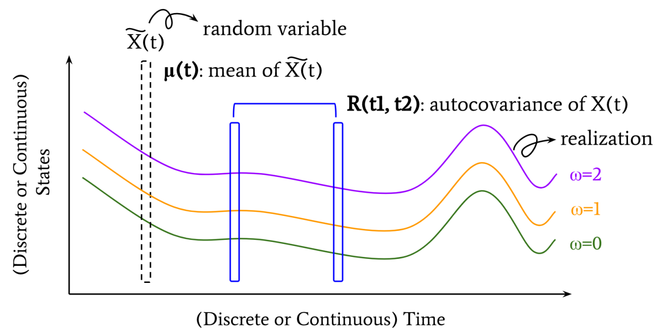
c. Expectation of Random Variables

Mean	• E[X] = $\sum$ x P(X=x) "first moment"
Median	• {x | P(X ≤ x) ≥ 0.5, P(X ≥ x) ≥ 0.5} → May not be unique for discrete R.V.
Variance	• V[X] = $\sum(x-\mu)^2$ P(X=x) "second centered moment"
Covariance	• Cov(X,Y) = E((X-E(X))(Y-E(Y)))= E(XY)-E(X)E(Y) • Var(X+Y) = Var(X) + Var(Y) + 2Cov(X,Y)
Correlation Coefficient	• = Cov(X,Y) / $\sigma_X\sigma_Y$ "normalized covariance" • To what extent X and Y are "linearly" related • Between -1 and 1 (can be proven with Cauchy-Schwarz inequality) • Independence implies un-correlation, but un-correlation does not imply independence (ex. U=X+Y, V=X-Y) (however, *under Gaussian*, un-correlation implies independence)
Conditional Expectation	• E(g(X,Y)|X):= h(X) where h(x):=E(g(X,Y)|X=x) • Conditional expectation is a random variable! ("function of X") • Iterated expectation: E(g(X,Y)) = E(E(g(X,Y)|X))

Appendix. Bounding Probabilities using Mean and Variance

- **Markov's inequality**: $X - a\,1_{X\geq a} \geq 0 \Rightarrow P(X \geq a) \leq \frac{E(X)}{a}$ (X is a nonnegative random variable)
- **Chebyshev's inequality**: $P(|X - E(X)| > a) \leq \frac{Var(X)}{a^2}$
  If Var(X)=Std(X)=1, equivalent to "Chebyshev's Theorem" from Part 2

d. Random Process

Random Variable Model uncertain quantities that "evolve in time"	 ● Wide/Weakly stationary: $\mu_{\tilde{X}}(t) = \mu$ **(constant)**, $R_{\tilde{X}}(t_1, t_2) = R_{\tilde{X}}(t_1 + \tau, t_2 + \tau)$ **(shift invariant)**
Examples	**IID Sequences** ● *Identical* and mutually *independent* distribution for any i (discrete-time) ● Fully characterised by the associated pdf/pmf (strictly stationary) ● $\mu_{\tilde{X}}(i) := E(\tilde{X}(i)) = \mu$ $\quad$ $R_{\tilde{X}}(i, j) = \sigma^2$ *if* $i = j$, 0 *otherwise* **Gaussian Process** ● Fully characterised by its mean function and autocovariance function ● Strict- and wide-sense stationary **Poisson Process** ● (1) $\tilde{N}(t_2) - \tilde{N}(t_1)$ is a Poisson RV with parameter $\lambda(t_2 - t_1)$ (2) $\tilde{N}(t_2) - \tilde{N}(t_1)$ & $\tilde{N}(t_4) - \tilde{N}(t_3)$ independent (if no time overlaps) ● $\mu_{\tilde{X}}(t) := E(\tilde{X}(t)) = \lambda t$ $\quad$ $R_{\tilde{X}}(t_1, t_2) := \lambda\, min(t_1, t_2)$ ● not stationary (mean not constant) **Random Walk** ● Models a sequence of steps in random directions ● $\mu_{\tilde{X}}(t) := 0$ $\quad$ $R_{\tilde{X}}(i, j) := min(i, j)$ ● not stationary (not shift invariant)
Convergence	**Convergence in Distribution** ● Cdf of $\tilde{X}(i)$ converges pointwise to the cdf of another random variable X ● Weaker than convergence with P=1 / in mean square / in probability ● ex) Binomial approximation of Poisson **Law of Large Numbers** ● Assume: (1) well-defined mean, (2) finite variance ● Weak LLN: moving average converges in mean square to μ ● Strong LLN: average converges to μ in probability

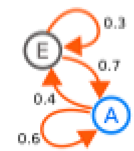
	Central Limit Theorem ● Assume: (1) finite variance, (2) independent sample w/ replacement ● The distribution of sample means tend towards Normal $\sum_{i=1}^{n} X_i \rightarrow N(n\mu,\ n\sigma^2) \Rightarrow \frac{\sum_{i=1}^{n} X_i}{n} \rightarrow N(\mu,\ \frac{\sigma^2}{n})$ ⇒ Justifies the use of Gaussian distributions to model data ● ex) Normal approximation to Binomial $X \sim Bin(n, p) \simeq N(np,\ npq) \Rightarrow\ p = X/n\ \sim\ N(p,\ pq/n)$

e. Markov Chains

Markov Chains

- **Markov property**: the future is conditionally independent from the past given the present (ex) IID sequences, Random Walk
- **Time-homogeneous Markov Chains**: the same transition probabilities for all t
  - Initial state vector and Transition matrix completely specify THMC

$$\vec{p}_{\tilde{X}(i)} = T^{i}_{\tilde{X}}\, \vec{p}_{\tilde{X}(0)}.$$



State vector for E $\begin{bmatrix} 0.3 \\ 0.7 \end{bmatrix}$

Property

Irreducible

- for any state x, the probability of reaching every other state in a finite number of steps is non-zero (can reach every state)
- All states are recurrent
  (cf) recurrent: P(coming back)=1 *vs* transient state: P(coming back) < 1
- Have a single stationary distribution by P-F Theorem (Appendix)
  - Stationary distribution = eigenvector of T with eigenvalue = 1
  - Reversibility ($(T_{\tilde{X}})_{kj}\, \vec{p}_j = (T_{\tilde{X}})_{jk}\, \vec{p}_k.$) implies stationarity

Aperiodic

Period = 1

* **period**: the largest integer m such that it is only possible to return to x in a number of steps that is a multiple of m

Ergodic Markov Chains

its state vector converges to the stationary distribution for any initial state vector

Application: Markov Chain Monte Carlo (MCMC) Sampling

- Design an irreducible aperiodic Markov chain and sample from the stationary distribution
- Mixing(burn-in) time: takes time until convergence → discard the samples from this period
- **Metropolis-Hastings algorithm**:
  1) Generate a candidate by using the transition matrix $P(C=k|X(i-1)=j) = T_{kj}$
  2) Set X(i) = C with the acceptance probability $P_{acc}(j,k)=\min(T_{jk}P_k/T_{kj}P_j, 1)$
  → Produce a reversible, therefore stationary, Markov Chain
- Advantages:
  1) Works well when sampling from high-dimensional distributions
  2) Depends on the distribution only through the ratio (full pmf/pdf not needed)
  → Useful for sampling from posterior distributions in the Bayseian framework

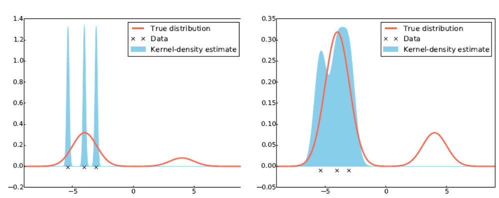
Appendix. Perron-Frobenius Theorem

If P is a stochastic matrix such that all the entries are strictly positive,

1) 1 is an eigenvalue of P and there exists an eigenvector $\mu \in \triangle n$ associated with 1
2) The eigenvector associated with 1 are unique up to scalar multiple
3) For all $x \in \triangle n$, $P^t x \rightarrow \mu$ in limit

4. Frequentist Statistics

a. Estimation

Assumption	• Parameters are unknown but fixed → cannot make probabilistic statements about the parameters
Point Estimate	**Method of Moments** • Adjust the parameters of a distribution so that the moments of the distribution coincide with the sample moments of the data • (ex) sample mean & variance: unbiased and consistent **Maximum Likelihood Estimate (MLE)** • Consistent but not always unbiased • (ex) least-square estimator, lasso estimator $\hat{\theta} = \underset{\theta \in \Theta}{\arg\max}\, \widehat{L}_n(\theta\,; \mathbf{y})$
Interval Estimate	**Confidence Interval** • Quantify the estimator's accuracy ("soft estimate") ** if we had <u>infinite</u> data, we do not need a CI • Approximated using Central Limit Theorem because the sample mean follows Normal(μ, σ^2/n) • If σ is unknown, use t-score * StandardError $\left(\bar{x} - z^* \frac{\sigma}{\sqrt{n}}, \bar{x} + z^* \frac{\sigma}{\sqrt{n}}\right)$ $\left(\bar{x} - t^* \frac{s}{\sqrt{n}}, \bar{x} + t^* \frac{s}{\sqrt{n}}\right)$
Non-parametric Distribution Estimate	• **[CDF] Empirical cdf**: unbiased and consistent estimator of the true cdf • **[PDF] Kernel Density Estimation** (KDE): many samples close to x → the estimate at x should be large  $\widehat{f}_{h,n}(x) := \frac{1}{n\,h} \sum_{i=1}^{n} k\left(\frac{x - x_i}{h}\right)$

Appendix. Analyzing Estimators

- **Mean Square Error** MSE[Y] = E[(Y-E(Y))2] + (E(Y)-γ)2 = variance + bias
- **Unbiased** E(Y) = γ
- **Consistent** converges to the true value as n → ∞

  * the sample median is always a consistent estimator unlike the sample mean

b. Hypothesis Testing: Reject or Fail to Reject

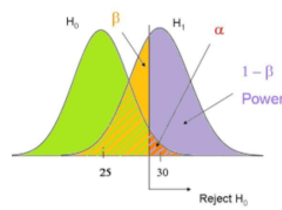
Hypothesis Testing: Did the patterns in the data came from random fluctuations?

** Frequentist perspective: either reject or fail to reject (can't compute probability)

- **Null Hypothesis** (=,≤,≥) vs. Alternative Hypothesis
- **P-value**: the probability of observing a result more extreme than the observations under H0
- **Type I Error** (α; false positive; significance level)

  Type II Error (β; false negative)

  Power (1-β): probability of rejecting H0 when it is indeed false



Parametric Testing

One sample *for mean and proportion*

z-test $$z = \frac{\bar{x} - \mu_0}{\sigma/\sqrt{n}}$$

t-test $$t = \frac{\bar{x} - \mu_0}{s/\sqrt{n}}$$ with df = n-1

Two sample

z-test $$z = \frac{\overline{x_1} - \overline{x_2}}{\sqrt{\sigma_1^2/n_1 + \sigma_2^2/n_2}}$$

Unpaired t-test $$t = \frac{\bar{x}_1 - \bar{x}_2}{\sqrt{s^2\left(\frac{1}{n_1} + \frac{1}{n_2}\right)}}$$ with df = n_1+n_2-2

$$s^2 = \frac{\sum_{i=1}^{n_1}(x_i - \bar{x}_1)^2 + \sum_{j=1}^{n_2}(x_j - \bar{x}_2)^2}{n_1 + n_2 - 2}$$

Paired t-test $$t = \frac{\bar{d}}{s_d/\sqrt{n}}$$ with df = n-1

Non-parametric Testing

One sample *Target variance*

Chi-square for variance $$\chi^2 = \frac{(n-1)\cdot s^2}{\sigma^2}$$

Chi-square Goodness-of-fit (right-tail)
H_0: from the hypothesized distribution

$$\chi_c^2 = \sum \frac{(O_i - E_i)^2}{E_i}$$ with df = class-1

Two sample

Chi-square for Independence (right-tail)
H_0: two categorical variables are ind.

$$\chi^2 = \sum_{i=1}^{r}\sum_{j=1}^{c} \frac{(O_{i,j} - E_{i,j})^2}{E_{i,j}}$$ with df = (r-1)(c-1)

Permutation Test
H_0: two datasets are from the same dist.
(invariant to permutations)

Statistics of interest

$t_{\text{diff}}(\vec{x}) := t(\vec{x}_A) - t(\vec{x}_B)$ for each permutation

$$p = \mathrm{P}\left(t_{\text{diff}}(\vec{X}) \geq t_{\text{diff}}(\vec{x})\right) = \frac{1}{m}\sum_{i=1}^{m} 1_{t_{\text{diff},i} \geq t_{\text{diff}}(\vec{x})}$$

Multiple Testing

Generalization to >= 2

Analysis of Variance (ANOVA)

H_0: no difference in the means between groups (right-tail)

Source	SS	df	MS	F	Sig.
Between	SS_b	k-1	MS_b	MS_b/MS_w	p value
Within	SS_w	N-k	MS_w		
Total	$SS_b + SS_w$	N-1			

Bonferroni's Method

Guarantees that the desired significance level α holds simultaneously for all the tests.

Reject the null hypothesis if $$p_i \leq \frac{\alpha}{n}$$ *Can be proven by the union bound*

5. Bayesian Statistics

a. Estimation

Assumption	● Parameters are unknown and random → can be described probabilistically Bayes' Theorem: P(Θ|X) ∝ P(X|Θ)P(Θ) ● **Prior distribution** P(Θ): encodes uncertainty about the model ● **Likelihood** P(X|Θ): how the data(evidence) depend on the parameters ● **Posterior distribution** P(Θ|X): update uncertainty about the model ★ Conjugate priors: the prior and the posterior belong to the same family (ex) Beta distributions are conjugate priors when likelihood is binomial $\frac{x^{\alpha-1}(1-x)^{\beta-1}}{\mathrm{B}(\alpha,\beta)}$ $\beta\left(a,b\right) := \int_u u^{a-1}\left(1-u\right)^{b-1}\,\mathrm{d}u$
Point Estimate	**Minimum mean-square-error estimation (MMSE)** ● Posterior mean E(Θ|X=x) minimizes the mean square error **Maximum-a-posteriori estimation (MAP)** ● Posterior mode (maximum of the pdf/pmf of the posterior) minimizes the probability of error $\mathrm{P}\left(\theta_{\text{other}}(\vec{X}) \neq \vec{\Theta}\right) \geq \mathrm{P}\left(\theta_{\text{MAP}}(\vec{X}) \neq \vec{\Theta}\right)$ ● Under a uniform prior, MAP equals to MLE → frequentist view can be understood as having a uniform prior
Interval Estimate	**Credible Interval** ● Interval in the posterior distribution within which an unobserved parameter value falls with a particular probability

b. Bayesian Hypothesis Testing

- Quantitative measure of much evidence there is for H_a relative to H_b given the data

$$K = \frac{P(H_b|\mathbf{y})}{P(H_a|\mathbf{y})} = \frac{P(H_b)}{P(H_a)}\boxed{\frac{P(\mathbf{y}|H_b)}{P(\mathbf{y}|H_a)}}$$

Bayes Factor
Can be calculated using MCMC method

- Model selection based on Bayes factors:
  1) calculate the expected loss for choosing H_a := $P(H_b|y)L(H_a|H_b)$ and similarly for H_b
  2) take the model which minimizes the expected loss (Bayesian decision)