Statistical Methods for Data Science: A Starter Kit

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Statistical Data Type

Categorical data: labels or tags

- Nominal: unordered labels, e.g. species of ducks
- Ordinal: ordered labels, e.g. {“duckling”, “teen duck”, “adult duck”}

Numerical data:

- Discrete (interval): countable, e.g. integers; numbers of ducks
- Continuous (ratio): uncountable, e.g. real values; weights of ducks

Data Container

Array (tensor):

- Scalar, vector, matrix, higher order array
- Same numerical data type
- Python library: numpy

Table:

- Described by columns and rows
- Mixed data types
- Python library: pandas

Descriptive Statistics: numerical data

Data set (a sample): numerical data $x_1, \cdots, x_N$

Centrality:

- sample mean: $\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$
- median: sort x_i and median is the value in the middle
- mode (discrete values): the most frequent value in a sample

Dispersion:

- min, max, range: $\min\{x_i\}$, $\max\{x_i\}$, $\max\{x_i\} - \min\{x_i\}$
- quantiles/percentiles: given $p \in (0,1)$, q is a p-quantile of the data if $p \times 100\%$ of the data are smaller than q
- sample variance: $s^2 = \frac{1}{N-1}\sum_{i=1}^{N}(x_i - \bar{x})^2$
- sample standard deviation: s

Dependence: given a data set with two paired values:

$$\{(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N)\}$$

- covariance:

$$cov(x,y) = \frac{1}{N-1}\sum_{i=1}^{N}(x_i - \bar{x})(y_i - \bar{y})$$

- correlation: measures how close data is to a linear relationship

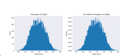
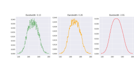
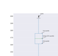
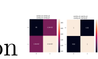
$$corr(x,y) = \frac{cov(x,y)}{\sigma_x \sigma_y}, \quad -1 \leq corr(x,y) \leq 1$$

Descriptive Statistics: categorical data

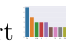
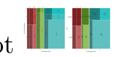
Data set (a sample): categorical data $x_1, \cdots, x_N$

- Count/frequency
- Transformed into numerical, discrete data

Visualization: numerical data

- Distribution:
  - Histogram/normalized histogram 
  - Kernel density estimator 
  - Box plot 
- Dependence (two variables):
  - Scatter plot 
  - Heat map for covariance/correlation 

Visualization: categorical data

- Distribution
  - Bar chart 
  - Pie chart 
- Dependence
  - Mosaic plot 

Probability distribution

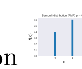
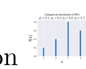
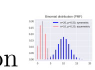
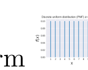
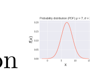
- Experiment, sample space, event, probability distribution (P(event)/PDF/PMF/CDF), random variable (discrete/continuous)
- Quantile function Q: the inverse CDF, i.e.

$$F_X(Q(p)) = p \text{ and } Q(F_X(q)) = q$$

- Conditional probability
- Independent and identically distributed (i.i.d.) random variables

Examples

Discrete/continuous, PMF/PDF, parameters, typical use cases (statistical data type, example scenarios)

- Bernoulli distribution 
- Categorical distribution 
- Binomial distribution 
- Discrete uniform 
- Gaussian distribution 

Generalize this learning routine to unknown distributions

Properties of Gaussian distributions

- Let $X \sim \mathcal{N}(\mu_X, \sigma_X^2)$ be a Gaussian random variable, then the following random variables are also Gaussian
  - Scaling: $tX \sim \mathcal{N}(t\mu_X, t^2\sigma_X^2)$, $t \neq 0$ is a constant
  - Translation: $X + c \sim \mathcal{N}(\mu_X + c, \sigma_X^2)$, c is a constant
  - $tX + c \sim \mathcal{N}(t\mu_X + c, t^2\sigma_X^2)$

- Let $X \sim \mathcal{N}(\mu_X, \sigma_X^2)$ and $Y \sim \mathcal{N}(\mu_Y, \sigma_Y^2)$ be two **independent** Gaussian random variables, then the following random variables are also Gaussian
  - $X + Y \sim \mathcal{N}(\mu_X + \mu_Y, \sigma_X^2 + \sigma_Y^2)$
  - $X - Y \sim \mathcal{N}(\mu_X - \mu_Y, \sigma_X^2 + \sigma_Y^2)$

Bayes' rule

- Parameter estimation:

$$f_{\Theta|data}(\theta \mid data) = \frac{\overbrace{f_{data|\Theta}(data \mid \theta)}^{\text{likelihood}}\overbrace{f_\Theta(\theta)}^{\text{prior}}}{f_{data}(data)}$$

  where $f(\cdot)$ is the PDF/PMF

- Multinomial naive Bayes classifier:

$$P(Y = y \mid X = x) = \frac{\overbrace{P(X = x \mid Y = y)}^{\text{likelihood}}\overbrace{P(Y = y)}^{\text{prior}}}{P(X = x)}$$

- Gaussian naive Bayes classifier/Gaussian mixture models:

$$P(Y = y \mid X = x) = \frac{\overbrace{f_{X|Y=y}(x \mid Y = y)}^{\text{likelihood}}\overbrace{P(Y = y)}^{\text{prior}}}{f_X(x)}$$

Q-Q plot

- Use cases:
  - Compare a data distribution to a theoretical distribution (one sample test)
  - Compare two data distributions (two sample test)
- Steps:
  - Choose a set of m probabilities $p_1, \cdots, p_m \in [0, 1]$ (make sure they spread evenly between 0 and 1)
  - For $i = 1, 2, \cdots, m$:
    * Compute the quantile q_i^1 of the first distribution at p_i
    * Compute the quantile q_i^2 of the second distribution at p_i
    * Make a scatter plot of the pair (q_i^1, q_i^2)
- Interpretation
  - Case 1: if the two distributions are identical, the points in the Q-Q plot should follow a 45° straight line $y = x$
  - Case 2: if the two distributions are linearly related, the points in the Q-Q plot follow a straight line that is not necessarily $y = x$
  - Case 3: if the two distributions are from different families of distributions, the points in the Q-Q plot are not lying on a straight line.

Mathematical Modeling

$$y = g(x; \theta \mid h)$$

1. What do we want to predict, i.e. what is the target y?
2. What are the variables x?
3. What is the mathematical function g that relates variables x to the target y?
4. Are there any hyperparameters h in the function g? How do we choose them?
5. What are the unknown parameters θ in g? **How do we estimate them from data?**

Parameter estimation for probabilistic models

- Maximum likelihood estimation: frequentist approach - **θ is deterministic**
- Maximum A Posteriori estimation: Bayesian approach - **θ is probabilistic**

Maximum Likelihood Estimation

Given a model $y = g(x; \mathcal{O} \mid h)$, where $\mathcal{O}$ is a set of parameters

a) Describe the experiments

b) Describe the data generated from the experiments

c) Describe the random variables (typically with i.i.d. assumption)

d) Choose a parameter of interest $\theta \in \mathcal{O}$

e) Choose the maximum likelihood estimation as the estimation method:

   Given data $x_1, \cdots, x_N$ and assume i.i.d. random variables X_i with PDF/PMF $f(x_i)$,

$$L(\theta \mid x_1, \cdots, x_N) = \prod_{i=1}^{N} f(x_i; \theta)$$

f) Compute $\hat{\theta}_{MLE}$ by maximizing the likelihood function:

$$\begin{aligned}\hat{\theta}_{MLE} &= \arg\max_\theta L(\theta \mid x_1, \cdots, x_N) \\ &= \arg\max_\theta \prod_{i=1}^{N} f(x_i; \theta)\end{aligned}$$

   or equivalently, minimizing the **negative log likelihood function**:

$$\hat{\theta}_{MLE} = \arg\min_\theta \; -\sum_{i=1}^{N} \log\left(f(x_i; \theta)\right)$$

   - Simple case, e.g. i.i.d. Gaussian, find the closed-form solution by:
     * Taking the partial derivative with respect to the parameter
     * Setting the derivative to zero
     * Solving for the parameter
   - In general, the estimate needs to be found by iterative methods, e.g. gradient descent

Maximum A Posteriori Estimation

Given a model $y = g(x; \mathcal{O} \mid h)$, where $\mathcal{O}$ is a set of parameters

a) Describe the experiments

b) Describe the data generated from the experiments

c) Describe the random variables (typically with i.i.d. assumption)

d) Choose a parameter of interest $\theta \in \mathcal{O}$

e) Choose the maximum a posteriori estimation as the estimation method

   - **θ is assumed to be drawn from a random distribution**
   - Choose a prior distribution for θ along with the hyperparameters: $f_{\Theta}(\theta)$
     * Prior might be known by the problem setup
     * If prior unknown, conjugate priors are typically chosen for various reasons
   - Find the likelihood function: $f_{X|\Theta}(\boldsymbol{x} \mid \theta)$ (same as in MLE)
   - Express the posterior distribution in terms of the prior and the likelihood function

$$f_{\Theta|X}(\theta \mid \boldsymbol{x}) = \frac{f_{X|\Theta}(\boldsymbol{x} \mid \theta) f_{\Theta}(\theta)}{f_X(\boldsymbol{x})}$$

f) Compute $\hat{\theta}_{MAP}$ by maximizing the posterior function (or equivalently, minimizing the negative log posterior function without the normalization constant). The optimal solution can be found by a closed-form expression or using iterative techniques.