

Lecture 1: Logistics and Preliminaries

Instructor: Yifan Chen

Scribes: Yujia Yin

Proof reader: Yifan Chen, Xiong Peng

Note: *LaTeX template courtesy of UC Berkeley EECS dept.***Disclaimer:** *These notes have not been subjected to the usual scrutiny reserved for formal publications. They may be distributed outside this class only with the permission of the Instructor.*

1.1 Gaussian Distribution

The Gaussian distribution, also known as the normal distribution, is a continuous probability distribution that is symmetric around its mean. It is characterized by its mean ($\boldsymbol{\mu}$) and covariance matrix ($\boldsymbol{\Sigma}$). In this section, we study the matrix form of the distribution for the random variable $\mathbf{X} \in \mathbb{R}^n$ as follows:

$$p(\mathbf{X}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(\sqrt{2\pi})^n} \cdot \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \cdot \exp\left(-\frac{1}{2}(\mathbf{X} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{X} - \boldsymbol{\mu})\right),$$

here, $\boldsymbol{\mu}$ is the mean vector of size $n \times 1$, and $\boldsymbol{\Sigma}$ is the covariance matrix, which describes the shape and orientation of the distribution. The term $|\boldsymbol{\Sigma}|$ represents the determinant of the covariance matrix.

1.1.1 T-test

In a t-test, we consider two independent groups of observations. Suppose each group consists of n observations, and let \mathbf{X}_n^y and \mathbf{X}_n^b be two independent random vectors, following a multivariate normal distribution:

$$\mathbf{X}_n^y \sim N(\boldsymbol{\mu}_y, \sigma_y^2 \mathbf{I}), \quad \mathbf{X}_n^b \sim N(\boldsymbol{\mu}_b, \sigma_b^2 \mathbf{I}),$$

where $\boldsymbol{\mu}_y$ and $\boldsymbol{\mu}_b$ are both mean vectors, \mathbf{I} is the identity matrix.

Under the null hypothesis $H_0 : \boldsymbol{\mu}_y = \boldsymbol{\mu}_b$ and alternative hypothesis $H_1 : \boldsymbol{\mu}_y > \boldsymbol{\mu}_b$, we define a new random variable $\mathbf{X}_n^y - \mathbf{X}_n^b$. Since under H_0 both \mathbf{X}_n^y and \mathbf{X}_n^b are normally distributed and independent, their difference also follows a normal distribution:

$$\mathbf{X}_n^y - \mathbf{X}_n^b \sim N(\mathbf{0}, (\sigma_y^2 + \sigma_b^2) \mathbf{I}).$$

1.1.2 t distribution

The basic form of the t distribution is:

$$T = \frac{z}{\sqrt{s/d}},$$

where the random variables z and s satisfy the following conditions:

1. $z \sim N(0, 1)$,
2. $s \sim \chi^2(d)$, where d is the degrees of freedom,
3. z and s are independent.

In the case of estimating a population mean, the t distribution arises in the following way:

$$T = \frac{\bar{X} - \mu}{\hat{\sigma}/\sqrt{n}} \sim T(n-1), \quad \text{where } \hat{\sigma}^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{X})^2. \quad (1.1)$$

Proof. We can rewrite eq. (1.1) to match the basic form of the t distribution:

$$T = \frac{(\bar{X} - \mu)/\sqrt{\sigma^2/n}}{\hat{\sigma}/\sqrt{n}/\sqrt{\sigma^2/n}} \triangleq \frac{z}{\sqrt{s/(n-1)}}. \quad (1.2)$$

1. We can easily verify that condition item 1 holds because the numerator in eq. (1.2) follows a standard normal distribution.
2. Next, we prove condition item 2 holds in our case. we need to show that: $s = \frac{n-1}{\sigma^2} \hat{\sigma}^2 = \frac{1}{\sigma^2} \sum_{i=1}^n (x_i - \bar{X})^2$ follows a chi-square distribution with $n-1$ degrees of freedom.
Let $\mathbf{X} = \{x_1, x_2, \dots, x_n\}^\top$ be the vector of observed data points. Using vector notation, we have:

$$\begin{aligned} s &= \frac{n-1}{\sigma^2} \hat{\sigma}^2 = \frac{1}{\sigma^2} \sum_{i=1}^n (x_i - \bar{X})^2 \\ &= \frac{1}{\sigma^2} (\mathbf{X} - \frac{1}{n} \cdot \mathbf{1} \cdot \mathbf{1}^\top \mathbf{X})^\top (\mathbf{X} - \frac{1}{n} \cdot \mathbf{1} \cdot \mathbf{1}^\top \mathbf{X}) \\ &= \frac{1}{\sigma^2} \left[(\mathbf{I} - \frac{1}{n} \cdot \mathbf{1} \cdot \mathbf{1}^\top) \mathbf{X} \right]^\top \left[(\mathbf{I} - \frac{1}{n} \cdot \mathbf{1} \cdot \mathbf{1}^\top) \mathbf{X} \right]. \end{aligned} \quad (1.3)$$

Let $\mathbf{P} := \mathbf{I} - \frac{1}{n} \cdot \mathbf{1} \cdot \mathbf{1}^\top$, which is a projection matrix satisfying $\mathbf{P}^2 = \mathbf{P}$ and $\mathbf{P} \cdot \mathbf{1} = 0$:

$$\mathbf{P} = \bar{\mathbf{U}} \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & 0 \end{pmatrix} \bar{\mathbf{U}}^\top = \mathbf{U} \mathbf{U}^\top, \quad (1.4)$$

where $\mathbf{U} \in \mathbb{R}^{n \times (n-1)}$ is orthogonal. From eqs. (1.3) and (1.4), we obtain:

$$s = \frac{1}{\sigma^2} \mathbf{X}^\top \mathbf{P}^\top \mathbf{P} \mathbf{X} = \frac{1}{\sigma^2} \mathbf{X}^\top \mathbf{U} (\mathbf{U}^\top \mathbf{X}).$$

Let $\mathbf{Y}_{n-1} := \mathbf{U}^\top \mathbf{X} \sim N(\mu \cdot \mathbf{U}^\top \cdot \mathbf{1}, \sigma^2 \cdot \mathbf{U}^\top \mathbf{U})$, where $\mathbf{U}^\top \mathbf{U} = \mathbf{I}_{n-1}$. We can also infer that $\mathbf{P} \cdot \mathbf{1} = 0$ based on the properties of the projection matrix, which implies that $\mathbf{U}^\top \cdot \mathbf{1} = 0$. Finally, we have:

$$s = \frac{1}{\sigma^2} \mathbf{X}^\top \mathbf{U} (\mathbf{U}^\top \mathbf{X}) = \frac{1}{\sigma^2} \mathbf{Y}_{n-1}^\top \mathbf{Y}_{n-1} = \frac{1}{\sigma^2} \sum_{i=1}^{n-1} Y_i^2 \sim \chi^2(n-1).$$

Thus, condition item 2 holds.

3. To prove the independence between z and s , we calculate the covariance between \bar{X} and \mathbf{Y} .

$$\begin{aligned} \text{Cov}(\mathbf{Y}, \bar{X}) &= E[\mathbf{Y} \cdot \bar{X}] - E[\mathbf{Y}] \cdot E[\bar{X}] \\ &= E[\mathbf{U}^\top \mathbf{X} \cdot \frac{1}{n} \cdot \mathbf{X}^\top \cdot \mathbf{1}] && (E[\mathbf{Y}] = 0) \\ &= \frac{1}{n} \mathbf{U}^\top (E[\mathbf{X} \mathbf{X}^\top]) \cdot \mathbf{1} && (\text{linearity of expectation}) \\ &= \frac{1}{n} \mathbf{U}^\top \left[(\mu \cdot \mathbf{1})(\mu \cdot \mathbf{1})^\top + \sigma^2 \mathbf{I} \right] \cdot \mathbf{1} && (\text{covariance structure of } \mathbf{X}) \\ &= \frac{1}{n} \mathbf{U}^\top \mu^2 \cdot \mathbf{1} \cdot \mathbf{1}^\top \cdot \mathbf{1} + \frac{1}{n} \mathbf{U}^\top \sigma^2 \cdot \mathbf{I} \cdot \mathbf{1} = \mathbf{0}_{n-1}. && (\mathbf{U}^\top \mathbf{1} = 0) \end{aligned} \quad (1.5)$$

The eq. (1.5) shows that condition item 3 holds.

□

The t distribution is commonly used in hypothesis testing and in the construction of t-tests. It allows for inference about population means when the population standard deviation is unknown.

1.1.3 Maximum Likelihood Estimator

The Maximum Likelihood Estimator (MLE) of μ is the value that maximizes the likelihood function, i.e.,

$$\hat{\mu} = \arg \max_{\mu} \prod_{i=1}^n p(\mathbf{x}_i; \mu, \Sigma).$$

Next, we simplify the likelihood function by applying a logarithm, which converts the product into a sum. This transformation facilitates computation and differentiation. For example, taking the logarithm of an exponential function often leads to a more tractable additive form. In the case of MLE, this allows us to rewrite the optimization problem as follows:

$$\sum \ln p(\mathbf{x}; \mu, \Sigma) \propto \sum_{i=1}^n (\mathbf{x}_i - \mu)^\top \Sigma^{-1} (\mathbf{x}_i - \mu).$$

Next, we use matrix trace to simplify the problem:

$$\begin{aligned} & \min_{\mu} \sum_{i=1}^n (\mathbf{x}_i - \mu)^\top \Sigma^{-1} (\mathbf{x}_i - \mu) \\ \iff & \min \text{Tr} \left[(\mathbf{X} - \mathbf{1} \cdot \mu^\top)^\top \Sigma^{-1} (\mathbf{X} - \mathbf{1} \cdot \mu^\top) \right] \\ & := f(\mu). \end{aligned}$$

After defining $f(\mu)$, we calculate its derivative:

$$df = \text{Tr} \left[\left(\frac{\partial f}{\partial \mu} \right)^\top d\mu \right].$$

To compute the derivative of $f(\mu)$, let's recall how to differentiate the trace of a matrix. For matrices \mathbf{ABC} , the trace of the product is denoted as $\text{Tr}(\mathbf{ABC})$, and its derivative is:

$$df = \text{Tr} [d\mathbf{A} \cdot \mathbf{BC} + \mathbf{A} \cdot d\mathbf{B} \cdot \mathbf{C} + \mathbf{AB} \cdot d\mathbf{C}]. \quad (1.6)$$

Additionally, based on properties of matrix traces, we know that:

$$\text{Tr}(\mathbf{AB}) = \text{Tr}(\mathbf{BA}). \quad (1.7)$$

Using eqs. (1.6) and (1.7), the derivative of the MLE is:

$$df = \text{Tr} \left[d(\mathbf{X} - \mathbf{1} \cdot \mu^\top)^\top \Sigma^{-1} (\mathbf{X} - \mathbf{1} \cdot \mu^\top) + \mathbf{0} + (\mathbf{X} - \mathbf{1} \cdot \mu^\top)^\top \Sigma^{-1} d(\mathbf{X} - \mathbf{1} \cdot \mu^\top) \right],$$

let $\mathbf{A}^\top = \Sigma^{-1}(\mathbf{X} - \mathbf{1} \cdot \mu^\top)$, so we have:

$$\begin{aligned} df &= \text{Tr} \left[d(\mathbf{X} - \mathbf{1} \cdot \mu^\top)^\top \cdot \mathbf{A}^\top + \mathbf{0} + \mathbf{A} \cdot d(\mathbf{X} - \mathbf{1} \cdot \mu^\top) \right] \\ &= \text{Tr} \left[-\mathbf{1} \cdot d\mu^\top \cdot \mathbf{A}^\top + \mathbf{A} \cdot (-d\mu) \cdot \mathbf{1}^\top \right] \\ &= \text{Tr} \left[-2 \cdot -\mathbf{1}^\top \cdot \mathbf{A} \cdot d\mu \right]. \end{aligned}$$

Thus, we derive the first derivative of $f(\mu)$. Since $f(\mu)$ is a convex function, the point at which the first derivative is zero corresponds to the global minimum. Therefore, we deduce:

$$\begin{aligned}
\frac{\partial f}{\partial \mu} &= -2 \cdot \mathbf{A} \cdot \mathbf{1} = 0 \\
&\Rightarrow \Sigma^{-1}(\mathbf{X} - \mathbf{1} \cdot \mu^\top) \cdot \mathbf{1} = 0 \\
&\Rightarrow \mu = \frac{1}{n} \cdot \mathbf{X}^\top \cdot \mathbf{1}.
\end{aligned}$$

Thus, we obtain the value of μ .

1.2 Linear Regression

1.2.1 Linear Model

Assume we have a linear model described by the equation:

$$\mathbf{Y} = (\mathbf{1}_n \quad \mathbf{X}) \cdot \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} + \mathbf{e}, \quad \mathbf{X} \in \mathbb{R}^{n \times d}, \quad \beta_1 \in \mathbb{R}^{d \times 1}. \quad (1.8)$$

In the eq. (1.8), \mathbf{X} is the design matrix of independent variables, and β_0, β_1 are the regression coefficients. The error term \mathbf{e} typically assumed to satisfy the Gaussian-Markov conditions:

1. Zero mean: $E[\mathbf{e}] = \mathbf{0}$,
2. Homoscedasticity and no autocorrelation: $\text{Var}[\mathbf{e}] = \sigma^2 \mathbf{I}_{n \times n}$.

1.2.2 Square Loss

To estimate $\bar{\beta}$, we minimize the squared loss function, which is given by:

$$L(\bar{\beta}) = \frac{1}{2n} (\mathbf{Y} - \bar{\mathbf{X}} \bar{\beta})^\top (\mathbf{Y} - \bar{\mathbf{X}} \bar{\beta}), \quad \text{where } \bar{\mathbf{X}} = (\mathbf{1}_n, \mathbf{X}), \quad \bar{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}.$$

Since the squared loss function is convex, we find its global minimum by setting its gradient to zero. Taking the derivative with respect to $\bar{\beta}$ and setting it to zero, we obtain:

$$\nabla_{\bar{\beta}} L(\bar{\beta}) = -\frac{1}{n} \bar{\mathbf{X}}^\top (\mathbf{Y} - \bar{\mathbf{X}} \bar{\beta}) = \mathbf{0}.$$

Solving for $\bar{\beta}$, we derive the closed-form solution:

$$\bar{\mathbf{X}}^\top \bar{\mathbf{X}} \bar{\beta} = \bar{\mathbf{X}}^\top \mathbf{Y}. \quad (1.9)$$

Since eq. (1.9) uniquely determines the optimal estimate of $\bar{\beta}$, we denote the solution as $\hat{\beta}$:

$$\hat{\beta} = (\bar{\mathbf{X}}^\top \bar{\mathbf{X}})^{-1} \bar{\mathbf{X}}^\top \mathbf{Y}.$$

Next, we analyze the properties of $\hat{\beta}$, focusing on its unbiasedness and variance.

Lemma 1.1. *The estimator $\hat{\beta}$ is unbiased.*

Proof. For $\mathbf{Y} = \bar{\mathbf{X}} \bar{\beta} + \mathbf{e}$, we can deduce:

$$\begin{aligned}
E[\hat{\beta}] &= E \left[(\bar{\mathbf{X}}^\top \bar{\mathbf{X}})^{-1} \bar{\mathbf{X}}^\top (\bar{\mathbf{X}} \bar{\beta} + \mathbf{e}) \right] \\
&= (\bar{\mathbf{X}}^\top \bar{\mathbf{X}})^{-1} (\bar{\mathbf{X}}^\top \bar{\mathbf{X}}) \bar{\beta} + (\bar{\mathbf{X}}^\top \bar{\mathbf{X}})^{-1} (\bar{\mathbf{X}}^\top \bar{\mathbf{X}}) E[\mathbf{e}].
\end{aligned}$$

Since $E[\mathbf{e}] = \mathbf{0}$, we have:

$$E[\hat{\beta}] = \bar{\beta}.$$

□

Lemma 1.2. *The variance of $\hat{\beta}$ is given by $\text{Var}(\hat{\beta}) = \sigma^2(\bar{\mathbf{X}}^\top \bar{\mathbf{X}})^{-1}$.*

Proof. Using the formula for the variance of a linear transformation, we deduce:

$$\begin{aligned}\text{Var}(\hat{\beta}) &= (\bar{\mathbf{X}}^\top \bar{\mathbf{X}})^{-1} \bar{\mathbf{X}}^\top \cdot \text{Var}(\mathbf{Y}) \cdot \bar{\mathbf{X}} (\bar{\mathbf{X}}^\top \bar{\mathbf{X}})^{-1} \\ &= \sigma^2 (\bar{\mathbf{X}}^\top \bar{\mathbf{X}})^{-1} \bar{\mathbf{X}}^\top \bar{\mathbf{X}} (\bar{\mathbf{X}}^\top \bar{\mathbf{X}})^{-1} \\ &= \sigma^2 (\bar{\mathbf{X}}^\top \bar{\mathbf{X}})^{-1}.\end{aligned}$$

□

While we obtained $\hat{\beta}$ by minimizing the squared loss, we now show that this solution also corresponds to the Maximum Likelihood Estimator (MLE) under the assumption of Gaussian errors.

Lemma 1.3. *$\hat{\beta}$ is the MLE of $\bar{\beta}$ under the Gaussian error term \mathbf{e} .*

Proof. From the linear model in eq. (1.8), we can easily get that \mathbf{Y} is following a normal distribution. The likelihood function of \mathbf{Y} given $\bar{\mathbf{X}}$ is:

$$L(\bar{\beta}, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left(-\frac{1}{2\sigma^2}(\mathbf{Y} - \bar{\mathbf{X}}\bar{\beta})^\top (\mathbf{Y} - \bar{\mathbf{X}}\bar{\beta})\right).$$

Taking the logarithm, we have:

$$\log L(\bar{\beta}, \sigma^2) = -\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2}(\mathbf{Y} - \bar{\mathbf{X}}\bar{\beta})^\top (\mathbf{Y} - \bar{\mathbf{X}}\bar{\beta}).$$

To find MLE of $\bar{\beta}$, we maximize $\log L(\bar{\beta}, \sigma^2)$. Since the first term is independent of $\bar{\beta}$, we only need to minimize $(\mathbf{Y} - \bar{\mathbf{X}}\bar{\beta})^\top (\mathbf{Y} - \bar{\mathbf{X}}\bar{\beta})$. We take its derivative with respect to $\bar{\beta}$ and set it to $\mathbf{0}$:

$$\begin{aligned}\nabla_{\bar{\beta}}(\mathbf{Y} - \bar{\mathbf{X}}\bar{\beta})^\top (\mathbf{Y} - \bar{\mathbf{X}}\bar{\beta}) &= \mathbf{0} \\ \Rightarrow -2\bar{\mathbf{X}}^\top (\mathbf{Y} - \bar{\mathbf{X}}\hat{\beta}) &= \mathbf{0}\end{aligned}$$

Thus, we obtain the solution:

$$\hat{\beta} = (\bar{\mathbf{X}}^\top \bar{\mathbf{X}})^{-1} \bar{\mathbf{X}}^\top \mathbf{Y}.$$

□

1.2.3 Population Risk

In this section, we investigate the population risk of our linear model. We remark that during the training process, we are minimizing the *empirical risk* on the fixed design matrix $\bar{\mathbf{X}}$.

Specifically, we assume a new random sample \mathbf{x} and the corresponding label $y = \mathbf{x}^\top \beta + \epsilon$; the risk is expressed as below:

$$E_{\mathbf{x}, y, \hat{\beta}}(y - \mathbf{x}^\top \hat{\beta})^2 = E_{\hat{\beta}} \left[E_{\mathbf{x}, y} (y - \mathbf{x}^\top \hat{\beta})^2 \mid \hat{\beta} \right].$$

Considering that the noise term ϵ is a random variable independent of the feature vector \mathbf{x} , and that its expectation is zero, the population risk depends on: $E_{\mathbf{x}, \hat{\beta}} [\mathbf{x}^\top (\beta - \hat{\beta})(\beta - \hat{\beta})^\top \mathbf{x}]$. For simplicity, we refer to this as the prediction error in the well-specified case, where the model is correctly specified. We are equivalently minimizing:

$$\begin{aligned}\min E_{\mathbf{x}, \hat{\beta}} [\mathbf{x}^\top (\beta - \hat{\beta})(\beta - \hat{\beta})^\top \mathbf{x}] \\ &= E_{\hat{\beta}} \left[E_{\mathbf{x}} \text{Tr}(\mathbf{x}\mathbf{x}^\top (\beta - \hat{\beta})(\beta - \hat{\beta})^\top \mid \hat{\beta}) \right] \\ &= E_{\hat{\beta}} \left[\text{Tr}(E[\mathbf{x}\mathbf{x}^\top] (\beta - \hat{\beta})(\beta - \hat{\beta})^\top \mid \hat{\beta}) \right] \\ &= \text{Tr}(E[\mathbf{x}\mathbf{x}^\top] \cdot E[(\beta - \hat{\beta})(\beta - \hat{\beta})^\top]) \\ &= \sigma^2 \text{Tr}(E[\mathbf{x}\mathbf{x}^\top] (\bar{\mathbf{X}}^\top \bar{\mathbf{X}})^{-1}).\end{aligned}\tag{1.10}$$

In eq. (1.10), we recall that $\bar{\mathbf{X}}$ is the fixed design matrix in the training process. In other words, during the training, we can manipulate $\bar{\mathbf{X}}$ to minimize the population risk, while other quantities remain fixed. The expectation $E[\mathbf{x}\mathbf{x}^\top]$ represents the second-moment matrix of the feature distribution and remains constant across realizations of \mathbf{x} , whereas individual samples \mathbf{x} are random. Assuming $E[\mathbf{x}\mathbf{x}^\top] = \mathbf{I}$, the preceding expression simplifies to: $\sigma^2 \text{Tr}[(\bar{\mathbf{X}}^\top \bar{\mathbf{X}})^{-1}] = \text{Tr}[\text{Var}(\hat{\boldsymbol{\beta}})]$, indicating the connection between population risk and parameter variance in the case of linear regression.