Linear Regression

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Linear Regression

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Notations

Notations

A random variable or random vector:

- Y: response variable
- X: random variable or random vector
  - if a p-dim random vector, $X = (X_1, \ldots, X_p)^T$.

Suppose that we have a random sample, that is say n copies of (Y, X)'s from certain population.

- Subscript i sometimes used to emphasizes for the ith observation, say the pair (Y_i, X_i), where $X_i = (X_{i,1}, \cdots, X_{i,p})^T$.

Observed values:

- y_i: the value of response variable for ith observation
- $\boldsymbol{x}_i$: the ith observed value of X
  - $\boldsymbol{x}_i$ could be a scalar of a vector. If a scalar, just x_i.

- $\mathbf{y}$: the n-dim response vector consisting of y_i.

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

- $\mathbf{X}$: the $n \times p$ design matrix
  - ith row is $\boldsymbol{x}_i^T$
  - jth column is $\mathbf{x}_j$

$$\mathbf{X} = \begin{bmatrix} \boldsymbol{x}_1^T \\ \boldsymbol{x}_2^T \\ \vdots \\ \boldsymbol{x}_n^T \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1, \mathbf{x}_2 \cdots \mathbf{x}_p \end{bmatrix}$$

All vector are taken as column vectors by default. Generic capital letter or bold-face capital letter will often denote a matrix, e.g., A or $\mathbf{A}$.

Linear Regression Models

Linear Regression Models

Given a list of random variables $(Y, X) \in \mathbb{R} \times \mathbb{R}^p$. Here $X = (X_1, \ldots, X_p)^p$ is the covariate vector.

The covariates may come from different sources

- quantitative inputs; dummy coding qualitative inputs.
- transformed inputs: $\log(X_1), X_1^2, \sqrt{X_1}, \ldots$
- basis expansion: $X_1, X_1^2, X_1^3, \ldots$ (polynomial representation)
- interaction between variables: $X_1 X_2, \ldots$

Suppose we have a random sample $\{(Y_i, X_i)\}_{i=1}^n$. A standard linear regression model assumes

$$Y_i = X_i^T \boldsymbol{\beta} + \epsilon_i, \quad \epsilon_i \sim \text{ i.i.d }, \quad E(\epsilon_i) = 0, \text{Var}(\epsilon_i) = \sigma^2$$

- Y_i is the response for the ith observation, $X_i \in R^p$ is the covariates

classical model assumptions for simplicity:

- independence of errors ϵ_i
- constant error variance (homoscedasticity)
- ϵ_i independent of X_i.

note:

- normality of ϵ is not needed provided sample size is large.
- violation of homoscedasticity (heteroscedasticity) can be dealt with in general
- ϵ_i (mean) independent of X_i is the key for interpreting coefficients.

Review on matrix theory

Notations

- $\mathbf{x}$ is a nonzero $m \times 1$ vector
- $\boldsymbol{O}$ is a zero vector of $m \times 1$
- $\mathbf{e}_i, i = 1, \ldots, m$ is $m \times 1$ unit vector, with 1 in the ith position and zeros elsewhere.
- A an $m \times m$ matrix.
- The ith column of A can be expresed as $A\mathbf{e}_i$, for $i = 1, \ldots, m$
- col(A) : the subspace of R^m spanned by the columns of A.
- I_m is the identity matrix of size m.

Basic concepts

- The determinant of A is $\det(A) = |A|$.
- The trace of A is $\mathrm{tr}(A) =$ the sum of the diagonal elements.
- The roots of the m th degree of polynomial equation in λ.

$$|\lambda I_m - A| = 0$$

denoted by $\lambda_1, \cdots, \lambda_m$ are called the **eigenvalues** of A. The collection $\{\lambda_1, \cdots, \lambda_m\}$ is called the **spectrum** of A.

- Any nonzero $m \times 1$ vector $\mathbf{x}_i \neq \mathbf{0}$ such that

$$A\mathbf{x}_i = \lambda_i \mathbf{x}_i$$

is an **eigenvector** of A corresponding to the eigenvalue λ_i.

Orthogonal matrix

An $m \times n$ matrix U has orthonormal columns if $U^T U = I$.

An $m \times m$ matrix P is called an orthogonal matrix if

$$PP^T = P^T P = I_m, \quad \text{or } P^{-1} = P^T.$$

Any square matrix with orthonormal columns is an orthogonal matrix, and such a matrix must have orthonormal rows too.

If P is an orthogonal matrix, then $\left|PP^T\right| = |P|\left|P^T\right| = |P|^2 = |I| = 1$, so $|P| = \pm 1$

- For any A, we have $\operatorname{tr}\left(PAP^T\right) = \operatorname{tr}\left(AP^T P\right) = \operatorname{tr}(A)$.
- PAP^T and A have the same eigenvalues, since

$$\left|\lambda I_m - PAP^T\right| = \left|\lambda PP^T - PAP^T\right| = |P|^2 \left|\lambda I_m - A\right| = \left|\lambda I_m - A\right|$$

Spectral decomposition of a symmetric matrix

If A is symmetric, there exists an orthogonal matrix P such that

$$P^T AP = \Lambda = \text{diag}\{\lambda_1, \cdots, \lambda_m\}$$

- λ_i 's are the eigenvalues of A.
- The eigenvectors of A are the column vectors of P.
- Denote the ith column of P by $\mathbf{p}_i$, then

$$PP^T = \sum_{i=1}^{m} \mathbf{p}_i \mathbf{p}_i^T = I_m$$

- The **spectral decomposition** of A is

$$A = P\Lambda P^T = \sum_{i=1}^{m} \lambda_i \mathbf{p}_i \mathbf{p}_i^T$$

- $\text{tr}(A) = \text{tr}(\Lambda) = \sum_{i=1}^{n} \lambda_i$ and $|A| = |\Lambda| = \prod_{i=1}^{m} \lambda_i$

Idempotent Matrices

An $m \times m$ matrix A is idempotent if

$$A^2 = AA = A$$

- The eigenvalues of an idempotent matrix are either zero or one

$$\begin{aligned} \lambda \mathbf{x} = A\mathbf{x} = A(A\mathbf{x}) = A(\lambda \mathbf{x}) = \lambda^2 \mathbf{x} \\ \Longrightarrow \lambda = \lambda^2 \end{aligned}$$

- If A is idempotent, so is $I_m - A$.

Projection Matrices

A symmetric, idempotent matrix A is called a **projection matrix**.

If A is a $m \times m$ symmetric idempotent , then

- If $\text{rank}(A) = r$, then A has r eigenvalues equal to 1 and $m - r$ zero eigenvalues.
- $\text{tr}(A) = \text{rank}(A)$
- $I_m - A$ is also symmetric idempotent, of rank $m - r$.

Given $\mathbf{x} \in R^m$, define $\mathbf{y} = A\mathbf{x}, \mathbf{z} = (I - A)\mathbf{x} = \mathbf{x} - \mathbf{y}$. Then

- $\mathbf{y} \perp \mathbf{z}$
- $\mathbf{y}$ is the orthogonal projection of x onto the subspace $\text{col}(A)$.
- $\mathbf{z} = (I - A)\mathbf{x}$ is the orthogonal projection of x onto the complementary subspace such that

$$\mathbf{x} = \mathbf{y} + \mathbf{z} = A\mathbf{x} + (I - A)\mathbf{x}$$

Linear regression (details)

Linear regression (details)

- The response vector $\mathbf{y} = (y_1, \cdots, y_n)^T$
  - The design matrix $\mathbf{X}$.
  - Assume the first column of $\mathbf{X}$ is $\mathbf{1}$
  - The dimension of $\mathbf{X}$ is $n \times (1 + p)$.
  - The regression coefficients $\boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \boldsymbol{\beta}_1 \end{pmatrix}$.
  - The error vector $\boldsymbol{\epsilon} = (\epsilon_1, \cdots, \epsilon_n)^T$

The linear model is written as:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

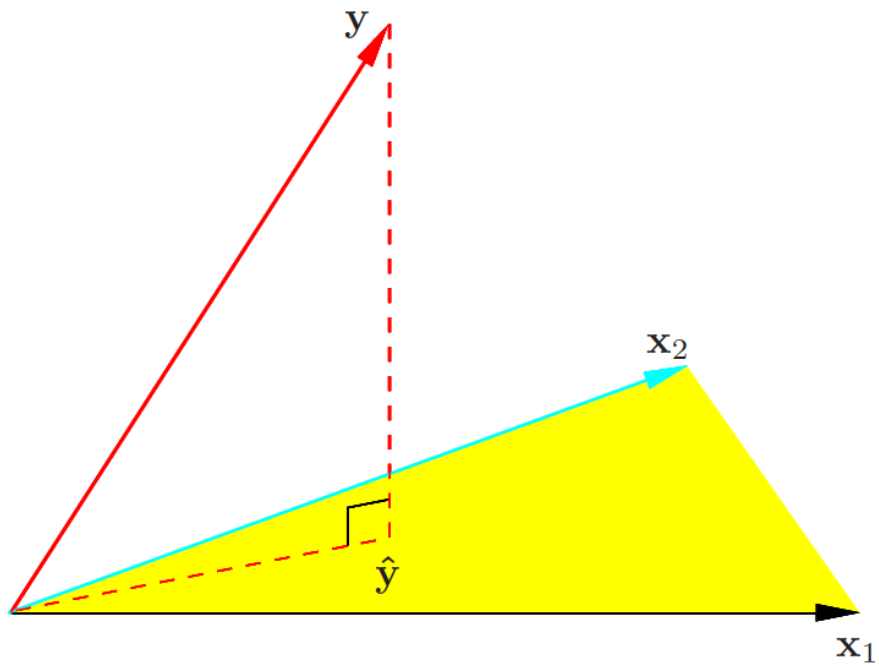
- the estimated coefficients $\hat{\boldsymbol{\beta}}$
- the predicted response $\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}}$.

$$\min_{\boldsymbol{\beta}} \mathrm{RSS}(\boldsymbol{\beta}) = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

- Normal equations: $\mathbf{X}^T(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) = 0$
- $\hat{\boldsymbol{\beta}} = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^T \mathbf{y}$ and $\hat{\mathbf{y}} = \mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y} = P_{\mathbf{X}}\mathbf{y}$
- Residual vector is $\mathbf{r} = \mathbf{y} - \hat{\mathbf{y}} = (I - P_{\mathbf{X}})\,\mathbf{y}$.
- Residual sum squares $RSS = \mathbf{r}^T\mathbf{r}$.

Call the following square matrix the projection or hat matrix:

$$P_{\mathbf{X}} = \mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T$$



ESL: Fig 3.2

Properties:

- symmetric and non-negative definite
- idempotent: $P_{\mathbf{X}}^2 = P_{\mathbf{X}}$. The eigenvalues are 0 's and 1 's.
- $P_{\mathbf{X}}\mathbf{X} = \mathbf{X}, \quad (I - P_{\mathbf{X}})\,\mathbf{X} = 0$

We have

$$\mathbf{r} = (I - P_{\mathbf{X}})\,\mathbf{y}, \quad RSS = \mathbf{y}^T\,(I - P_{\mathbf{X}})\,\mathbf{y}$$

Note

$$\mathbf{X}^T\mathbf{r} = \mathbf{X}^T\,(I - P_{\mathbf{X}})\,\mathbf{y} = 0$$

The residual vector is orthogonal to the column space spanned by $\mathbf{X}$, col($\mathbf{X}$).

sampling properties of $\hat{\boldsymbol{\beta}}$

- $\text{Var}(\hat{\boldsymbol{\beta}}) = \sigma^2 \left(\mathbf{X}^T\mathbf{X}\right)^{-1}$
- The variance σ^2 can be estimated as

$$\hat{\sigma}^2 = RSS/(n-p-1)$$

This is an unbiased estimator, i.e.,$\text{E}\left(\hat{\sigma}^2\right) = \sigma^2$

Inferences under Gaussian Errors:

Under the Normal assumption on the error ϵ, we have

- $\hat{\boldsymbol{\beta}} \sim N\left(\boldsymbol{\beta}, \sigma^2 \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\right)$
- $(n-p-1)\hat{\sigma}^2 \sim \sigma^2\chi^2_{n-p-1}$
- $\hat{\boldsymbol{\beta}}$ is independent of $\hat{\sigma}^2$

To test $H_0 : \beta_j = 0$, we use

- if σ^2 is known, $z_j = \frac{\hat{\beta}_j}{\sigma\sqrt{v_j}}$ has a standard normal distribution under H_0 where v_j is the j th diagonal element of $\left(\mathbf{X}^T\mathbf{X}\right)^{-1}$;
- if σ^2 is unknown, $t_j = \frac{\hat{\beta}_j}{\hat{\sigma}\sqrt{v_j}}$ has a t_{n-p-1} distribution under H_0.

Confidence intervals for coefficients:

- Under Normal assumption, the $100(1-\alpha)\%$ C.I. of β_j is

$$\hat{\beta}_j \pm t_{n-p-1,\frac{\alpha}{2}} \hat{\sigma} \sqrt{v_j}$$

  where $t_{k,\nu}$ is ν upper-percentile of t_k distribution.

- In practice, we use the approximate $100(1-\alpha)\%$ C.I. of β_j

$$\hat{\beta}_j \pm z_{\frac{\alpha}{2}} \hat{\sigma} \sqrt{v_j}$$

  where $Z_{\frac{\alpha}{2}}$ is $\frac{\alpha}{2}$ upper percentile of the standard Normal distribution.

- Even if the Gaussian assumption does not hold, this interval is approximately right, with the coverage probability $1-\alpha$ as $n \to \infty$.

Confidence intervals and prediction intervals for means:

Let for some fixed values $\mathbf{x}_0$ for $\mathbf{x}$.

- The $100(1-\alpha)\%$ confidence interval for $E(Y|X=\mathbf{x}_0)$ is given by

$$\hat{y}_0 \pm z_{\alpha/2}\hat{\sigma}\sqrt{\mathbf{x}_0^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_0}$$

  where $\hat{y}_0 = \mathbf{x}_0^T\hat{\boldsymbol{\beta}}$.
- The $100(1-\alpha)\%$ prediction interval for the value of Y when $X=\mathbf{x}_0$ is given by

$$\hat{y}_0 \pm z_{\alpha/2}\hat{\sigma}\sqrt{1+\mathbf{x}_0^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_0}$$

F distribution:

Distributions of Quadratic Form:

- If $X \sim N_p(\boldsymbol{\mu}, I_p)$, then

$$W = X^T X = \sum_{i=1}^{p} X_i^2 \sim \chi_p^2(\lambda), \quad \lambda = \boldsymbol{\mu}^T \boldsymbol{\mu}$$

- Special case: If $X \sim N_p(\mathbf{0}, I_p)$, then $W = X^T X \sim \chi_p^2$
- If $U_1 \sim \chi_p^2, U_2 \sim \chi_q^2$ and $U_1 \perp U_2$, then

$$F = \frac{U_1/p}{U_2/q} \sim F_{p,q}$$

- If $U_1 \sim \chi_p^2(\lambda), U_2 \sim \chi_q^2$ and $U_1 \perp U_2$, then

$$F = \frac{U_1/p}{U_2/q} \sim F_{p,q}(\lambda), \quad (\text{ noncentral } F)$$

Example: Assume $\mathbf{y} \sim N_n\left(\mathbf{X}\boldsymbol{\beta}, \sigma^2 I_n\right)$.

$$RSS = \mathbf{y}^T(I - P_{\mathbf{X}})\mathbf{y} = \|\mathbf{r}\|^2, \quad SSR = \mathbf{y}^T P_{\mathbf{X}}\mathbf{y} = \|\hat{\mathbf{y}}\|^2$$

Then

$$F = \frac{SSR/(p+1)}{RSS/(n-p-1)} \sim F_{p+1,n-p-1}(\lambda), \quad \lambda = \|X\beta\|^2/\sigma^2$$

Nested Model Selection:

To test for significance of groups of coefficients simultaneously, we use F-statistic

$$F = \frac{(RSS_0 - RSS_1)/(p_1 - p_0)}{RSS_1/(n - p_1 - 1)}$$

where

- RSS_1 is the RSS for the bigger model with $p_1 + 1$ parameters
- RSS_0 is the RSS for the **nested** smaller model with $p_0 + 1$ parameter, have $p_1 - p_0$ parameters constrained to zero.

F-statistic measure the change in RSS per additional parameter in the bigger model, and it is normalized by $\hat{\sigma}^2$.

- Under the assumption that the smaller model is correct,

$$F \sim F_{p_1 - p_0, n - p_1 - 1}$$

Confidence set

- The approximate confidence set of $\boldsymbol{\beta}$ is

$$C_{\boldsymbol{\beta}} = \left\{ \boldsymbol{\beta} \mid (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})^T \left(\mathbf{X}^T \mathbf{X} \right) (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) \leq \hat{\sigma}^2 \chi^2_{p+1,\alpha} \right\}$$

  where $\chi^2_{k,\alpha}$ is α upper percentile of χ^2_k distribution.
- The confidence interval for the true function $f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{\beta}$ is

$$\left\{ \boldsymbol{x}^T \boldsymbol{\beta} \mid \boldsymbol{\beta} \in C_{\boldsymbol{\beta}} \right\}$$

Linear regression with orthogonal design

Linear regression with orthogonal design

- If X is univariate, the least square estimate is

$$\hat{\beta} = \frac{\sum_i x_i y_i}{\sum_i x_i^2} = \frac{< \mathbf{x}, \mathbf{y} >}{< \mathbf{x}, \mathbf{x} >}$$

- if $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_d]$ has orthogonal columns, i.e.,

$$< \mathbf{x}_j, \mathbf{x}_k >= 0, \quad \forall j \neq k$$

or equivalently, $\mathbf{X}^T\mathbf{X} = \text{diag}\left(\|\mathbf{x}_1\|^2, \ldots, \|\mathbf{x}_d\|^2\right)$. The OLS estimates are given as

$$\hat{\beta}_j = \frac{\langle \mathbf{x}_j, \mathbf{y} \rangle}{\langle \mathbf{x}_j, \mathbf{x}_j \rangle} \quad \text{for} \quad j = 1, \ldots, d$$

  - Each input has no effect on the estimation of other parameters.
  - Multiple linear regression reduces to univariate regression.

Regression by Successive Orthogonalization

To orthogonalize $\mathbf{X}$

Consider $\mathbf{y} = \beta_0\mathbf{x}_0 + \beta_1\mathbf{x}_1 + \beta_2\mathbf{x}_2 + \boldsymbol{\epsilon}$. $(\mathbf{x}_0 = \mathbf{1})$ Orthogonization process:

(1) We regress $\mathbf{x}_1$ onto $\mathbf{x}_0$, compute the residual

$$\mathbf{z}_1 = \mathbf{x}_1 - \gamma_{01}\mathbf{x}_0. \quad (\text{ note } \mathbf{z}_1 \perp \mathbf{x}_0)$$

(2) We regress $\mathbf{x}_2$ onto $(\mathbf{x}_0, \mathbf{z}_1)$, compute the residual

$$\mathbf{z}_2 = \mathbf{x}_2 - \gamma_{02}\mathbf{x}_0 - \gamma_{12}\mathbf{z}_1. \quad (\text{ note } \mathbf{z}_2 \perp \{\mathbf{x}_0, \mathbf{z}_1\})$$

Note: $\text{span}\{\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2\} = \text{span}\{\mathbf{x}_0, \mathbf{z}_1, \mathbf{z}_2\}$.

More generally, we may use Gram-Schmidt procedure, to transform $\mathbf{X} = (\mathbf{x}_0, \ldots, \mathbf{x}_p)$ to $\mathbf{Z} = (\mathbf{z}_0, \ldots, \mathbf{z}_p)$ where $\mathbf{z}_j$ is the residual of regress $\mathbf{x}_j$ on $\mathbf{x}_0, \ldots, \mathbf{x}_{j-1}$ In fact, such a $\mathbf{Z}$ has orthogonal columns. $\{\mathbf{z}_0, \mathbf{z}_1, \ldots, \mathbf{z}_p\}$ forms orthogonal basis for $\mathrm{Col}(\mathbf{X})$.

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \epsilon.$$

1. Initialize $\mathbf{z}_0 = \mathbf{x}_0 = \mathbf{1}$
2. For $j = 1, \ldots, p$, successively perform the following: regress $\mathbf{x}_j$ on $\mathbf{z}_0, \mathbf{z}_1, \ldots, \mathbf{z}_{j-1}$ to produce coefficients

$$\hat{\gamma}_{kj} = \frac{\langle \mathbf{z}_k, \mathbf{x}_j \rangle}{\langle \mathbf{z}_k, \mathbf{z}_k \rangle}$$

   for $k = 0, \ldots, j-1$, and residual vector $\mathbf{z}_j = \mathbf{x}_j - \sum_{k=0}^{j-1} \hat{\gamma}_{kj} \mathbf{z}_k$.
3. Regress $\mathbf{y}$ on $\mathbf{z}_p$ to get

$$\hat{\beta}_p = \hat{\eta}_p = \frac{\langle \mathbf{y}, \mathbf{z}_p \rangle}{\langle \mathbf{z}_p, \mathbf{z}_p \rangle}.$$

4. To compute $\hat{\beta}_j$, for $j = p-1, \ldots, j = 0$: regress Regress $\mathbf{y}$ on $\mathbf{z}_j$ to get $\hat{\eta}_j$ for all $j = 0, \ldots, p-1$,

$$\hat{\eta}_j = \frac{\langle \mathbf{z}_j, \mathbf{y} \rangle}{\langle \mathbf{z}_j, \mathbf{z}_j \rangle}.$$

Let Γ be the $(p+1) \times (p+1)$ upper triangular matrix with all diagonal elements equal to 1 and $\Gamma_{ij} = \hat{\gamma}_{i-1,j-1}$ for $j > i \geq 1$. Solve for $\hat{\beta}_j$, for $j = p-1, \ldots, j = 0$ recursively from $\Gamma \hat{\boldsymbol{\beta}} = \hat{\boldsymbol{\eta}}$.

In general, for arbitrary index j, we can put the j-th regression in the **last** column, then do the orthogonalizaiotn process to obtain $\hat{\beta}_j$.

Multicollinearity

For the term $j = p$ (the step 3 in above procedure), the p-th coefficient (the last coefficient)

$$\hat{\beta}_p = \frac{\langle \mathbf{z}_p, \mathbf{y} \rangle}{\langle \mathbf{z}_p, \mathbf{z}_p \rangle}$$

If $\mathbf{x}_p$ is highly correlated with some of the other $\mathbf{x}_j's$, then

- The residual vector $\mathbf{z}_p$ is close to zero
- The coefficient $\hat{\beta}_p$ will be very unstable
- The variance estimate

$$\text{Var}\left(\hat{\beta}_p\right) = \frac{\sigma^2}{\|\mathbf{z}_p\|^2}$$

The precision for estimating $\hat{\beta}_p$ depends on the length of $\mathbf{z}_p$, or, how much $\mathbf{x}_p$ is unexplained by the other (or previous) $\mathbf{x}_k$'s

Computational algorithms

Consider the Normal Equation

$$\mathbf{X}^T\mathbf{X}\beta = \mathbf{X}^T\mathbf{y}$$

We like to avoid computing $\left(\mathbf{X}^T\mathbf{X}\right)^{-1}$ directly.

(1) QR decomposition of $\mathbf{X}$:

- $\mathbf{X} = QR$ where Q is orthonormal and R is upper triangular

(2) Cholesky decomposition of $\mathbf{X}^T\mathbf{X}$:

- $\mathbf{X}^T\mathbf{X} = \tilde{R}\tilde{R}^T$ where $\tilde{R}$ is lower triangular

QR algorithm

We can represent step 2 of the above Algorithm in matrix form:

$$\mathbf{X} = \mathbf{Z}\Gamma$$
$$\mathbf{X} = [\mathbf{x}_0, \ldots, \mathbf{x}_p] \text{ and } \mathbf{Z} = [\mathbf{z}_0, \ldots, \mathbf{z}_p]$$

Standardizing $\mathbf{Z}$ using $D = \text{diag}\{\|\mathbf{z}_0\|, \ldots, \|\mathbf{z}_p\|\}$,

$$\mathbf{X} = \mathbf{Z}\Gamma = \mathbf{Z}D^{-1}D\Gamma \equiv QR, \quad \text{with } Q = ZD^{-1}, \quad R = D\Gamma$$

- The columns of Q consists of an orthonormal basis for the column space of X.
- Q is orthonormal matrix of $n \times (p+1)$, satisfying $Q^TQ = I$.
- R is upper triangular matrix of $(p+1) \times (p+1)$, full-rank.

We then can show

$$R\boldsymbol{\beta} = Q^T\mathbf{y}$$

Based on this, we solve for $\hat{\boldsymbol{\beta}}$ as follows:

(1) Conduct QR decomposition of $\mathbf{X} = QR$. (Gram-Schmidt Orthogonalization)
(2) Compute $Q^T\mathbf{y}$
(3) Solve the triangular system $R\boldsymbol{\beta} = Q^T\mathbf{y}$.

Cholesky Decomposition algorithm

For any positive definite square matrix A, we have

$$A = RR^T$$

where R is a lower triangular matrix of full rank.

(1) Compute $\mathbf{X}^T\mathbf{X}$ and $\mathbf{X}^T\mathbf{y}$
(2) Factoring $\mathbf{X}^T\mathbf{X} = RR^T$, then $\hat{\beta} = \left(R^T\right)^{-1} R^{-1}\mathbf{X}^T\mathbf{y}$
(3) Solve the triangular system $R\mathbf{w} = \mathbf{X}^T\mathbf{y}$ for $\mathbf{w}$.
(4) Solve the triangular system $R^T\boldsymbol{\beta} = \mathbf{w}$ for $\boldsymbol{\beta}$.

Choleksy decompostion algorithm can be faster than QR for small d, but can be less stable.

Some further remarks

The role of $E(Y|X)$ in our interpretation

It is common to interpret the coefficient, say β_1 as the "'effect" on the average value of Y from increasing X_1 by one unit while holding the other predictors or covariates unchanged. This interpretation however hings upon the assumption that ϵ_i is independent of all X's, or more precisely,

$$E(\epsilon|X) = 0.$$

It is important to emphasize that linear regression models seldom satisfy this assumption in practice.

It is always possible to write

$$Y = \mu(X) + \epsilon$$

where $\mu(X) = E(Y|X)$ and ϵ satisfies $E(\epsilon|X) = 0$.

Here $\mu(X)$ is called the **regression function**, with which we like to predict Y.

For a linear regression coefficients to have meaningful interpretation, one essentially believe that the linear model $X^T\beta$ is correctly specified for $E(Y|X)$.

The statistical meaning of $\mu(X)$

$$\begin{aligned}\text{MSE}(f) &= E\left[(Y - f(X))^2\right] \\ &= E\left[V[Y \mid X] + (E[Y - f(X) \mid X])^2\right]\end{aligned}$$

The optimal function $\hat{f}$ is given by

$$\mu(x) = E[Y \mid X = x]$$

In other words, given X, the best predictor for Y is the conditional expectation $E[Y \mid X]$ (in mean-squared sense).

Causal relationship?

In most classical courses in linear regression, X is viewed as "independent variable", while Y viewed as "dependent" variable, which may seems to suggest some **causal relationship** between them. However this is not necessarily so.

The conditional expectation $E(Y|X)$ or $E(X|Y)$ may be defined regardless of the actual causal relationship between X and Y.

In the so-called structural equations framework, $\mu(X)$ may have structural meaning (often suggested by theory), which means X is viewed as a **direct cause** of Y. In that case, it might only make sense to consider $E(Y|X)$. But a causal relationship can be studied in a different framework that subsumes the structural equations framework.

Linear Smoothers

To predict at some arbitrary point x using a simple linear regression,

$$\hat{\mu}(x) = \hat{\alpha} + \hat{\beta}x = \sum_{i=1}^{n} \frac{1}{n} \left(1 + \frac{(x - \bar{x})(x_i - \bar{x})}{\hat{\sigma}_X^2} \right) y_i$$

where $\hat{\sigma}_X^2 = \sum_i (x_i - \bar{x})^2 / n$. Note that it takes the form

$$\hat{\mu}(x) = \sum_{i=1}^{n} w(x, x_i) \cdot y_i = \mathbf{w}(x)\mathbf{y}$$

Using a multiple linear regression,

$$\hat{\mu}(x) = x^T \left(\mathbf{X}^T \mathbf{X} \right)^{-1} \mathbf{X}^T \mathbf{y} = \mathbf{w}(x)\mathbf{y}$$

We call a regression function of this form a **linear smoother** (note this is so-named because it is linear in y, but need not behave linearly as a function of x!).

Another example: k-nearest-neighbors regression

$$w\left(x, x_i\right) = \begin{cases} 1/k & \text{if } x_i \text{ is one of the } k \text{ nearest points to } x \\ 0 & \text{otherwise} \end{cases}$$

that is,

$$\hat{\mu}(x) = \frac{1}{k} \sum_{i \in N_k(x)} y_i$$

where $N_k(x)$ gives the k nearest neighbors of x.

Linear smoothers include many important classes of estimators: kernel regression, locally weighted regression, Gaussian process regression, smoothing splines, series or sieve regression.