REGRESSION

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1. Regression

1.1. **Overview.** Consider the linear regression model $y = X\beta + \epsilon$, where $X \in \mathbb{R}^{m\times n}$ $m \gg n$ is the design matrix of m data points, $\epsilon \sim \mathcal{N}(0, \sigma^2 I)$ is the noise vector, and y is the output vector. The goal is to estimate β.

The usual estimate $\hat{\beta}$ of β is obtained by minimizing the mean-squared error

$$\hat{\beta} = \arg\min_{\beta} \|y - X\beta\|_2^2$$

In statistics, it is usually assumed that X is full rank, and we get the estimate

$$\hat{\beta} = (X^T X)^{-1} X^T y.$$

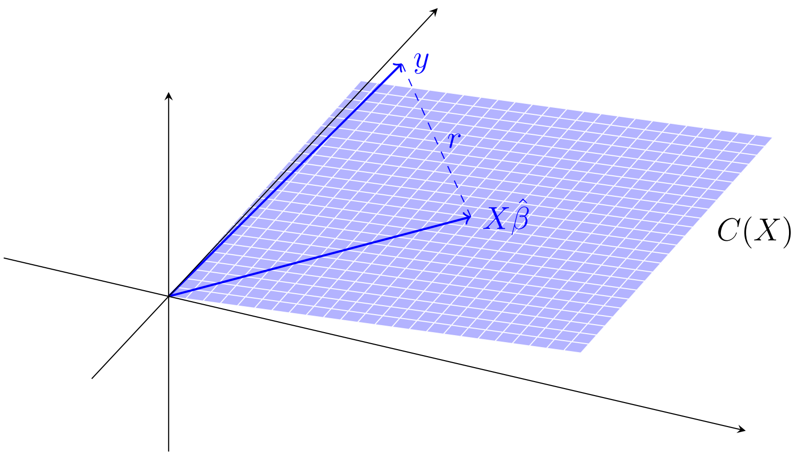
The output vector $y \sim \mathcal{N}(X\beta, \sigma^2 I)$ is normally distributed, so $\hat{\beta}$ is normally distributed as well with

$$\hat{\beta} \sim \mathcal{N}(\beta, \sigma^2 (X^T X)^{-1}).$$

Likewise the residual vector $r = y - X\hat{\beta}$ has a normal distribution

$$r \sim \mathcal{N}(0, \sigma^2(I - X(X^T X)X^T)).$$

Geometrically $X\hat{\beta}$ is the orthogonal projection of y onto the column space $C(X)$ of X.



1.2. **Distributional Results.**

1.2.1. *Estimating σ^2.* The dimension of the space $C(X)^\perp$ that contains the residual vector r is also called the degrees of freedom of r. This dimension is $m - n$.

Notice that r is normally distributed with $r \sim \mathcal{N}(0,\, \sigma^2(I - X(X^TX)X^T))$. Since $I - X(X^TX)X^T$ is the projection matrix onto $C(X)^\perp$, it can be diagonalized in the form $QI_{(m-n)}Q^T$ for some orthogonal matrix Q. Here $I_{(m-n)}$ is a diagonal matrix with $(m-n)$ ones and n zeros on the diagonal.

As a consequence, we see that $Q^Tr \sim \mathcal{N}(0,\, \sigma^2 I_{(m-n)})$. Since orthogonal matrices are norm-preserving, we can calculate the distribution of the sum of squared residuals:

$$\begin{aligned}\sum_{i=1}^m r_i^2 &= \|r\|_2^2 \\ &= \|Q^Tr\|_2^2 \\ &= \sigma^2 \sum_{i=1}^{m-n} z_i^2\end{aligned}$$

where $z_i \overset{iid}{\sim} \mathcal{N}(0,\, 1)$. So we get the distributional result

$$\sum_{i=1}^m r_i^2 \sim \sigma^2 \chi^2_{(m-n)}.$$

As a result, the estimator $\hat{\sigma}^2 = \frac{1}{m-n}\sum_{i=1}^m r_i^2$ has the distribution

$$\hat{\sigma}^2 \sim \sigma^2 \left(\frac{1}{m-n}\chi^2_{(m-n)}\right)$$

with expectation σ^2.

1.2.2. *The F-test.* The vector $y \sim \mathcal{N}(X\beta,\, \sigma^2 I)$ is multivariate normal. We can make use of the following property of multivariate normal variables.

Property 1. *Suppose $y \in \mathbb{R}^m$ is a multivariate normal random variable with covariance matrix $\sigma^2 I$ and $U, V \subset \mathbb{R}^m$ are orthogonal subspaces. Then $z_1 = Proj_U(y)$ and $z_2 = Proj_V(y)$ are each (possibly degenerate) multivariate normal random variables. Moreover, z_1 and z_2 are independent.*

Proof. First consider the case where U, V are subspaces spanned by standard basis vectors. Then the result holds since $y_1, \ldots, y_m$ are independent random normal variables (because the covariance matrix of y is $\sigma^2 I$). The general case reduces to the previous case by multiplying by an orthogonal matrix so that U and V are spanned by standard basis vectors, and noting that the covariance matrix of y is unchanged by this transformation. □

We get the following distributional results.

Property 2. *Consider the setting of Property 1, and suppose additionally that* $\mathbb{E}(z_1) = \mathbb{E}(z_2) = 0$. *Then the following distributional results hold:*

$$\|z_1\|_2^2 \sim \sigma^2 \chi^2_{\dim(U)}$$

$$\|z_2\|_2^2 \sim \sigma^2 \chi^2_{\dim(V)}$$

In particular,

$$\frac{\|z_1\|_2^2/\dim(U)}{\|z_2\|^2/\dim(V)} \sim F_{\dim(U),\dim(V)}.$$

Proof. As in the proof of Property 1, let Q be an orthogonal matrix so that QU is spanned by the first $\dim(U)$ standard basis vectors $e_1, \ldots, e_{\dim(U)}$. Then by orthogonality

$$\|z_1\|_2^2 = \|Qz_1\|_2^2.$$

We additionally have the following equalities

$$\begin{aligned} Qz_1 &= Q\mathrm{Proj}_U(y) \\ &= \mathrm{Proj}_{QU}(Qy) \\ &= ((Qy)_1, \ldots, (Qy)_{\dim(U)}, 0, \ldots, 0) \end{aligned}$$

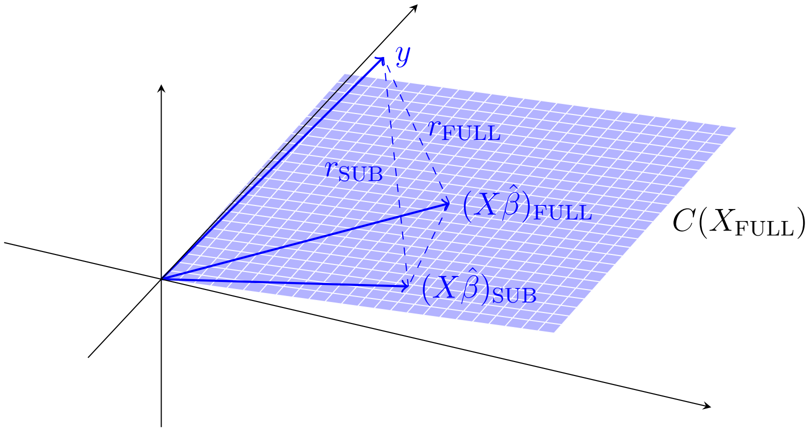
Since $\mathbb{E}(z_1) = 0$ and Qy has covariance matrix $\sigma^2 I$, we obtain

$$\|z_1\|_2^2 = \|((Qy)_1, \ldots, (Qy)_{\dim(U)})\|_2^2 \sim \sigma^2 \chi^2_{\dim(U)}.$$

The rest of the result follows by applying the definition of the F distribution and noting that z_1 and z_2 are independent. □

The F distribution in the F-test and ANOVA arises exactly from Property 2.

For the F test, we consider a model obtained by linear regression but with some of the columns of X removed. We are testing the null hypothesis that $\beta_{i_1} = \beta_{i_2} = \ldots = \beta_{i_\ell} = 0$ for the coefficients corresponding to these columns. Denote the full design matrix by X_{FULL} and the design matrix with columns removed by X_{SUB}, so that under the null hypothesis $X_{\text{FULL}}\beta = X_{\text{SUB}}\beta_{\text{SUB}}$. Likewise, let $(X\hat{\beta})_{\text{FULL}}$ and $(X\hat{\beta})_{\text{SUB}}$ be the respective projections of y onto $C(X_{\text{FULL}})$ and $C(X_{\text{SUB}})$.



We want to apply Property 2 to obtain the F distribution. To do so, we need to choose suitable orthogonal subspaces U and V. Let $U = C(X_{\text{SUB}})^{\perp} \cap C(X_{\text{FULL}})$ and let $V = C(X_{\text{FULL}})^{\perp}$. Then we have

$$\begin{aligned}(X\hat{\beta})_{\text{FULL}} - (X\hat{\beta})_{\text{SUB}} &= \text{Proj}_U(y)\\ r_{\text{FULL}} &= \text{Proj}_V(y)\end{aligned}$$

Next, observe that under the null hypothesis, we can write

$$y = X_{\text{FULL}}\beta + \epsilon = X_{\text{SUB}}\beta_{\text{SUB}} + \epsilon,$$

and it follows that the projected means $\mathbb{E}(\text{Proj}_U(y))$ and $\mathbb{E}(\text{Proj}_V(y))$ are 0. As a result, we can apply Property 2 to get the F-distribution

$$\frac{\|(X\hat{\beta})_{\text{FULL}} - (X\hat{\beta})_{\text{SUB}}\|_2^2/\dim(U)}{\|r_{\text{FULL}}\|_2^2/\dim(V)} \sim F_{\dim(U),\dim(V)}.$$

Finally, by orthogonality $\|r_{\text{SUB}}\|_2^2 - \|r_{\text{FULL}}\|_2^2 = \|(X\hat{\beta})_{\text{FULL}} - (X\hat{\beta})_{\text{SUB}}\|_2^2$, so we get the F-test

$$\frac{(\|r_{\text{SUB}}\|_2^2 - \|r_{\text{FULL}}\|_2^2)/\dim(U)}{\|r_{\text{FULL}}\|_2^2/\dim(V)} \sim F_{\dim(U),\dim(V)}.$$

In particular, if X_{FULL} is a full rank $m \times n$ matrix and X_{SUB} is $m \times p$, we get $\dim(U) = n - p$ and $\dim(V) = m - n$ so

$$\frac{(\|r_{\text{SUB}}\|_2^2 - \|r_{\text{FULL}}\|_2^2)/(n-p)}{\|r_{\text{FULL}}\|_2^2/(m-n)} \sim F_{n-p,m-n},$$

which is the familiar formula for the F-test.

1.2.3. *One-way ANOVA.* The F-distribution for one-way ANOVA arises in the same manner as the F test. Suppose we have a one-way ANOVA model with k groups and let X_{FULL} be the $m \times k$ matrix such that

$$(X_{\text{FULL}})_{i,j} = \begin{cases} 1 & \text{if measurement } i \text{ belongs to the } j\text{th group} \\ 0 & \text{otherwise} \end{cases}$$

Likewise, index y by letting $y_{i,j}$ correspond to the ith measurement of the jth group. The null hypothesis is that $\beta_j = \mathbb{E}(y_{\cdot,\cdot})$ for $j = 1, \ldots, k$, i.e. that the expected measurement for each group is the same.

Next, let $X_{\text{SUB}} = \mathbf{1}_{m\times 1}$ and observe that under the null hypothesis $X_{\text{FULL}}\beta = X_{\text{SUB}}\beta_1 \subseteq C(X_{\text{SUB}})$. As a result, one can show that the arguments from Section 2 apply here as well. Writing $\bar{y}^{(j)}$ as the mean for the j-th group and noting that $(X\hat{\beta})_{\text{SUB}} = \mathbf{1}_{m\times 1}\bar{y}$, we find

$$\|(X\hat{\beta})_{\text{FULL}} - (X\hat{\beta})_{\text{SUB}}\|_2^2 = \sum_{j=1}^{k}\sum_{i=1}^{m_j}(\bar{y}^{(j)} - \bar{y})^2$$

$$\|r_{\text{FULL}}\|_2^2 = \sum_{j=1}^{k}\sum_{i=1}^{m_j}(y_{i,j} - \bar{y}^{(j)})^2.$$

From the previous section,

$$\frac{\|(X\hat{\beta})_{\text{FULL}} - (X\hat{\beta})_{\text{SUB}}\|_2^2/\dim(U)}{\|r_{\text{FULL}}\|_2^2/\dim(V)} \sim F_{\dim(U),\dim(V)},$$

so we obtain the familiar one-way ANOVA test

$$\frac{\left(\sum_{j=1}^{k}\sum_{i=1}^{m_j}(\bar{y}^{(j)} - \bar{y})^2\right)/(k-1)}{\left(\sum_{j=1}^{k}\sum_{i=1}^{m_j}(y_{i,j} - \bar{y}^{(j)})^2\right)/(m-k)} \sim F_{k-1,m-k}.$$

1.2.4. *Intuition.* Intuitively, what's going on in the previous two sections is as follows. The null hypothesis is that $X_{\text{FULL}}\beta = X_{\text{SUB}}\beta_{\text{SUB}}$, i.e. that $y = X_{\text{SUB}}\beta_{SUB} + \epsilon$, where $\epsilon \sim \mathcal{N}(0, \sigma^2 I)$. In this scenario, Property 1 says that the component z_1 of the noise ϵ in the subspace $U = C(X_{\text{FULL}}) \cap C(X_{\text{SUB}})^{\perp}$ and the component z_2 in the subspace $V = C(X_{\text{FULL}})^{\perp}$ are independent Gaussians whose covariance matrices are essentially $\sigma^2 I_{\dim(U)}$ and $\sigma^2 I_{\dim(V)}$. As a result,

$$\frac{\|z_1\|_2^2/\dim(U)}{\|z_2\|_2^2/\dim(V)} \sim F_{\dim(U),\dim(V)}.$$

A helpful way to think of the distribution of $\epsilon \sim \mathcal{N}(0, \sigma^2 I)$ is that ϵ is a random variable that can be written as

$$\epsilon = \sigma(\sum_{i=1}^{m}\alpha_i q_i)$$

where $\alpha_1 \ldots \alpha_m$ are independent $\mathcal{N}(0, 1)$ random variables and $q_1 \ldots q_m$ is any arbitrary orthonormal basis. After selecting $q_1, \ldots, q_m$ by extending orthonormal bases for U and V (note U, V are orthogonal), one can see that $\|z_1\|_2^2/\dim(U) \sim \sigma^2\chi^2_{\dim(U)}$ and $\|z_2\|_2^2/\dim(V) \sim \sigma^2\chi^2_{\dim(V)}$ are independent so their ratio has distribution $F_{\dim(U),\dim(V)}$.

1.2.5. *Sample Variance.* Suppose $Y_1, \ldots, Y_m$ are *i.i.d.* random variables. The naive estimator $\frac{1}{m}\sum_{i=1}^{m}(Y_i - \hat{\mu})^2$ for the variance is biased, and instead the sample variance $\hat{\sigma}^2$ is defined as

$$\hat{\sigma}^2 = \frac{1}{m-1}\sum_{i=1}^{m}(Y_i - \hat{\mu})^2,$$

which is unbiased. The usual intuition is that the sample mean $\hat{\mu}$ is correlated with each Y_i. Consequently, each term in the sum is slightly smaller than if one were to replace $\hat{\mu}$ instead of μ, and then some algebra is done to compute that $m - 1$ is the correct normalizing factor.

Our previous work provides another way to obtain this $(m-1)$ factor. Consider the case where $Y_1 \ldots Y_m$ are independent $N(\mu, \sigma^2)$ random variables. Letting X be the $m \times 1$ design matrix of ones $X = \mathbf{1}_{m\times 1}$ and also writing $\beta = \mu$ and $\epsilon \sim \mathcal{N}(0, \sigma^2 I)$, we obtain the regression model $Y = X\beta + \epsilon$. So our unbiased estimate for the variance from section 1.2.1 yields

$$\begin{aligned}\hat{\sigma}^2 &= \frac{1}{m-1}\sum_{i=1}^{m} r_i^2 \\ &= \frac{1}{m-1}\sum_{i=1}^{m}(Y_i - \hat{\mu})^2\end{aligned}$$

To make things clear here, $n = 1$ because X has one column. This means $C(X)$ is one dimensional so $r \in C(X)^{\perp}$ lives in an $m-1$ dimensional subspace.