SOME GEOMETRIC INTUITION IN REGRESSION AND PCA

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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

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

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

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

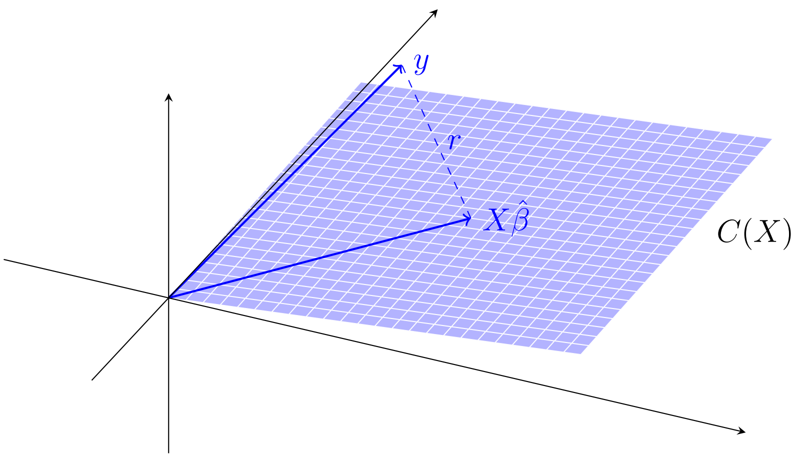
The output vector $y \sim \mathcal{N}(X\beta, \sigma^2 I)$ is normally distributed, so $\hat{\beta}$ is normally distributed as well with

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

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. $\square$

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 $e_1, \dots, e_{\dim(U)}$. Then by orthogonality

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

We additionally have the following equalities

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

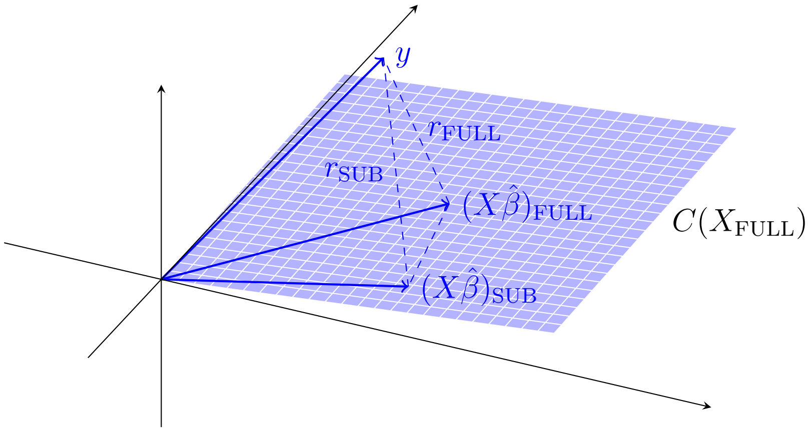
Since $\mathbb{E}(z_1) = 0$ and Qy has covariance matrix $\sigma^2 I$, we obtain

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

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

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 $\beta_{i_1} = \beta_{i_2} = \dots = \beta_{i_\ell} = 0$ 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 $X_{\mathrm{FULL}}\beta = X_{\mathrm{SUB}}\beta_{\mathrm{SUB}}$. Likewise, let $(X\hat{\beta})_{\mathrm{FULL}}$ and $(X\hat{\beta})_{\mathrm{SUB}}$ be the respective projections of y onto $C(X_{\mathrm{FULL}})$ and $C(X_{\mathrm{SUB}})$.



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 $X_{\text{FULL}}\beta = X_{\text{SUB}}\beta$, i.e. that $y = X_{\text{SUB}}\beta + \epsilon$, 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

$$\epsilon = \sigma^2(\sum_{i=1}^{m}\alpha_i q_i)$$

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 $N(\mu, \sigma)$ random variables. Letting X be the $m \times 1$ design matrix of ones $X = 1_{m\times 1}$ and also writing $\beta = \mu$ and $\epsilon \sim \mathcal{N}(0, \sigma^2 I)$, we see that the regression model holds $Y = X\beta + \epsilon$. 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.

2. A Note On PCA

Suppose we have an $m \times n$ design matrix X consisting of m mean-centered data points $x^{(1)}, \ldots, x^{(m)}$. PCA is a dimensionality-reduction technique which chooses a k-dimensional subspace $k < n$ and orthogonally projects the data onto that subspace. (Here k is a parameter chosen beforehand.)

PCA is usually formulated in two equivalent ways (e.g. in Bishop). The first is finding a subspace which maximizes the variance of the projected data. The second is finding a subspace which minimizes the reconstruction error of the original data. The straightforward equivalence between these two ideas seems not often made explicit, so we do that here.

For any subspace U, we can write the variance of the projected data as

$$\sum_{i=1}^m \|\mathrm{Proj}_U(x^{(i)})\|_2^2,$$

and we can write the reconstruction error as

$$\sum_{i=1}^{m} \|x^{(i)} - \mathrm{Proj}_U(x^{(i)})\|_2^2.$$

By orthogonality

$$\sum_{i=1}^{m} \|x^{(i)}\|_2^2 = \sum_{i=1}^{m} \|\mathrm{Proj}_U(x^{(i)})\|_2^2 + \sum_{i=1}^{m} \|x^{(i)} - \mathrm{Proj}_U(x^{(i)})\|_2^2,$$

so of course

$$\arg\max_U \sum_{i=1}^{m} \|\mathrm{Proj}_U(x^{(i)})\|_2^2 = \arg\min_U \sum_{i=1}^{m} \|x^{(i)} - \mathrm{Proj}_U(x^{(i)})\|_2^2.$$