BIOS 835: Linear Regression and Bayesian Decision Theory

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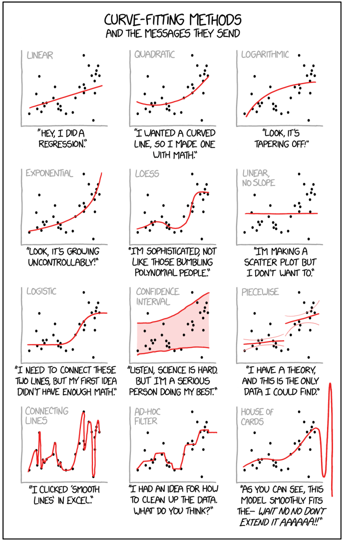
Outline


CURVE-FITTING METHODS
AND THE MESSAGES THEY SEND
LINEAR
"HEY, I DID A REGRESSION."
QUADRATIC
"I WANTED A CURVED LINE, SO I MADE ONE WITH MATH."
LOGARITHMIC
"LOOK, IT'S TAPERING OFF!"
EXPONENTIAL
"LOOK, IT'S GROWING UNCONTROLLABLY!"
LOESS
"I'M SOPHISTICATED, NOT LIKE THOSE BUMBLING POLYNOMIAL PEOPLE."
LINEAR, NO SLOPE
"I'M MAKING A SCATTER PLOT BUT I DON'T WANT TO."
LOGISTIC
"I NEED TO CONNECT THESE TWO LINES, BUT MY FIRST IDEA DIDN'T HAVE ENOUGH MATH."
CONFIDENCE INTERVAL
"LISTEN, SCIENCE IS HARD. BUT I'M A SERIOUS PERSON DOING MY BEST."
PIECEWISE
"I HAVE A THEORY, AND THIS IS THE ONLY DATA I COULD FIND."
CONNECTING LINES
"I CLICKED 'SMOOTH LINES' IN EXCEL."
AD-HOC FILTER
"I HAD AN IDEA FOR HOW TO CLEAN UP THE DATA. WHAT DO YOU THINK?"
HOUSE OF CARDS
"AS YOU CAN SEE, THIS MODEL SMOOTHLY FITS THE- WAIT NO NO DON'T EXTEND IT AAAAAA!!"

Linear Regression

- Linear regression models were developed before computers were around, but are still popular today.
- They are simple and (commonly) adequate and interpretable representations of the real world.
- They commonly work as well as difficult non-linear models for prediction, especially when there is limited data and low signal-to-noise ratio.
- Linear models do have assumptions, but many properties are robust to these assumptions (plus we can transform outcomes).

Linear Regression model

- A linear regression model is defined as

$$
\begin{aligned}
Y &= \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \epsilon \\
&= \beta_0 + \sum_{j=1}^{p} \beta_j X_j + \epsilon \\
&= f(\boldsymbol{X}) + \epsilon
\end{aligned}
$$

  - Y is our outcome of interest
  - $(X_1, X_2 \ldots, X_p)$ are our covariates of interest
  - β_0: intercept;
  - $\beta_j, j = 1, \cdots, p$: regression coefficients.
  - $E(\epsilon) = 0$ and $Var(\epsilon) = \sigma^2$.

Linear Regression model

- We can also define it in matrix form with the following

$$\boldsymbol{X} = \begin{pmatrix} 1 & X_{11} & \dots & X_{1p} \\ 1 & X_{21} & \dots & X_{2p} \\ \vdots & \vdots & & \\ 1 & X_{n1} & \dots & X_{np} \end{pmatrix} \quad \boldsymbol{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix} \quad \boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix} \quad \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}$$

  as the covariate data, observations, error term, and parameters in a linear regression model.
- The model can be expressed succinctly as

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

Least squares and RSS

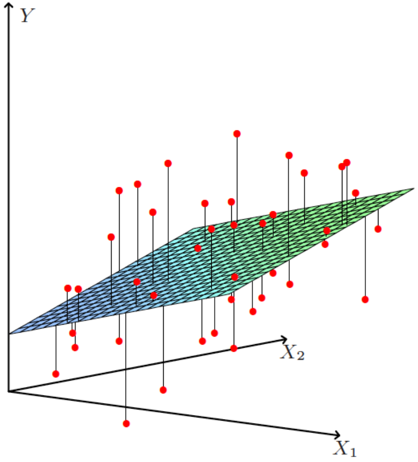
- The residual sum of squares for β is defined as

$$
\begin{aligned}
RSS(\beta) &= \sum_{i=1}^{n} (y_i - \boldsymbol{X}_i'\beta)^2 \\
&= \sum_{i=1}^{n} \{y_i - f(\boldsymbol{X}_i)\}^2 \\
&= (\boldsymbol{y} - \boldsymbol{X}\beta)'(\boldsymbol{y} - \boldsymbol{X}\beta) = ||\boldsymbol{y} - \boldsymbol{X}\beta||^2
\end{aligned}
$$

  where $\boldsymbol{X}_i = (X_{i1}, X_{i2}, \ldots, X_{ip})'$

- Using least squares criteria the estimate of β, denoted by $\hat{\beta}$, is the value that minimizes the RSS.

Least squares and RSS



The Least Squares Solution

- To minimize $RSS(\beta) = (\boldsymbol{y} - \boldsymbol{X}\beta)'(\boldsymbol{y} - \boldsymbol{X}\beta)$ we differentiate with respect to β to get

$$
\begin{aligned}
\frac{\partial RSS(\beta)}{\partial \beta} &= -2\boldsymbol{X}'(\boldsymbol{y} - \boldsymbol{X}\beta) \\
\frac{\partial^2 RSS(\beta)}{\partial \beta \partial \beta'} &= 2\boldsymbol{X}'\boldsymbol{X}.
\end{aligned}
$$

- If $\boldsymbol{X}$ has full column rank, setting the first derivative to zero yields,

$$
\begin{aligned}
0 &= \boldsymbol{X}'(\boldsymbol{y} - \boldsymbol{X}\beta) \quad \text{and} \\
\hat{\beta} &= (\boldsymbol{X}'\boldsymbol{X})^{-1}X'\boldsymbol{y}.
\end{aligned}
$$

Predicted values

- Predicted values at a point $\boldsymbol{x}_0$ are given by $\hat{f}(\boldsymbol{x}_0) = \boldsymbol{x}_0'\hat{\beta}$.
- The predicted values for the training data are given by

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

- $H = \boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'$ is referred to as the "Hat Matrix"
- Geometrically, $\hat{\beta}$ is chosen such that $\boldsymbol{y} - \hat{\boldsymbol{y}}$ is orthogonal to the subspace of $\boldsymbol{X}$.

Rank Deficiencies

- Recall, we said *"if $\boldsymbol{X}$ has full column rank"*
- When might this not be the case?

"Assumptions" standard regression models

Linear, Independent, Normality, and Equal variance (LINE)

- L: a linear relationship exists between Y and the X's.
- I: the data are independent.
- N: the residuals are normally distributed.
- E: the variance of the residuals is equal for all X's.

Properties of $\hat{\boldsymbol{y}}$, β and σ^2

- The variance of $\hat{\boldsymbol{\beta}}$ is

$$Var(\hat{\boldsymbol{\beta}}) = (\boldsymbol{X}'\boldsymbol{X})^{-1}\sigma^2$$

  which is estimated using

$$\hat{\sigma}^2 = \frac{1}{n-p-1}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

- Neither of these results requires any additional assumptions.

Properties of $\hat{\boldsymbol{y}}$, β and σ^2

Once we impose the LINE assumptions we get the following properties

- $\hat{\boldsymbol{\beta}} \sim MVN(\boldsymbol{\beta}, (X'X)^{-1}\sigma^2)$, hypothesis tests and confidence intervals for $\hat{\beta}_j$ can be based on
$$z_j = \frac{\hat{\beta}_j}{\hat{\sigma} v_j} \sim t_{n-p-1}$$
where v_j is the jth diagonal element of $(X'X)^{-1}$
- The predicted value at x_0 is $y \sim N\{f(\boldsymbol{x}_0), \sigma^2(1 + x_0(X'X)^{-1}x_0)\}$

Partial F-test for multiple variables

- Suppose we'd like to test $H_0 : \beta_j = \beta_{j+1} = \ldots = \beta_{j+k-1} = 0$ v.s $H_1 : \beta_l \neq 0$ for some $l = j, \ldots, j+k-1$ given the other $(p-k)$ variables.
- This can be tested via

$$F_0 = \frac{(RSS_0 - RSS_1)/(p1 - p0)}{RSS_1/(N - p_1 - 1)}$$

where RSS_1 and $p_1 + 1$ are the RSS and number of parameters for the bigger model (similarly for RSS_0 and p_0).
- Under the Gaussian assumption and the null hypotheses $F_0 \sim F_{p_1 - p_0, N - p_1 - 1}$
- Reject if

$$F_0 > F_{p_1 - p_0, N - p_1 - 1}(1 - \alpha)$$

Gauss-Markov Theorem

- The Gauss-Markov Theorem is one of the most famous results in statistics.
- It states that the least squares estimate $\hat{\boldsymbol{\beta}}$ has the smallest variance among all linear unbiased estimates.
- Specifically, suppose we wish to estimate $\theta = a'\boldsymbol{\beta}$. The least squares estimate is

$$\hat{\theta} = a'\hat{\boldsymbol{\beta}} = a'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}$$

  which is unbiased when the linear model is correct.
- The Gauss-Markov Theorem shows that another estimator $\tilde{\theta} = \boldsymbol{c}'\boldsymbol{y}$, which is unbiased for $a'\boldsymbol{\beta}$, will have

$$Var(a'\hat{\boldsymbol{\beta}}) \leq Var(\boldsymbol{c}'\boldsymbol{y})$$

Gauss-Markov Theorem

- What does the Gauss-Markov Theorem not say?
- Consider
$$MSE(\hat{\theta}) = E\{(\hat{\theta} - \theta)^2\}$$

Simple (simple) LR and notation

- Consider the following (very) simple LR model with 1 covariate and no intercept

$$Y = X\beta + \epsilon$$

- The LS estimate and residual are

$$\hat{\beta} = \frac{\sum_1^n x_i y_i}{\sum_1^n x_i^2}$$
$$r_i = y_i - x_i\hat{\beta}$$

- It is convenient (and more general) to use the following notation

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \sum_{i=1}^{n} x_i y_i = \boldsymbol{x}'\boldsymbol{y}, \quad \text{so} \quad \hat{\beta} = \frac{\langle \boldsymbol{x}, \boldsymbol{y} \rangle}{\langle \boldsymbol{x}, \boldsymbol{x} \rangle} = \frac{\boldsymbol{x}'\boldsymbol{y}}{\boldsymbol{x}'\boldsymbol{x}}$$

MLR for orthgonal vectors

- Suppose we have $1 = x_0, x_1, \ldots, x_p$ inputs are all orthogonal
  - $\langle \boldsymbol{x}_j, \boldsymbol{x}_k \rangle = 0$ for all $j \neq k$
- Then
$$\hat{\beta}_j = \frac{\langle \boldsymbol{x}_j, \boldsymbol{y} \rangle}{\langle \boldsymbol{x}_j, \boldsymbol{x}_j \rangle}$$
- What are the impacts of this?
- Will this ever happen?

Simple Gram-Schmidt process

- Now, suppose we have the SLR model

$$Y = \beta_0 + X\beta_1 + \epsilon$$

How can we make 1 *and* X *orthogonal?*

- By orthogonalizing we get the coefficient as

$$\hat{\beta}_1 = \frac{\langle \boldsymbol{x} - \bar{x}\mathbf{1}, \boldsymbol{y} \rangle}{\langle \boldsymbol{x} - \bar{x}\mathbf{1}, \boldsymbol{x} - \bar{x}\mathbf{1} \rangle}$$

which is the coefficient for the model $Y = (x - \bar{x})\beta_1 + \epsilon$

Simple Gram-Schmidt process

- So a way to calculate β_1 is to do the following:
  1. regress $\boldsymbol{x}$ on $\mathbf{1}$, and get the residual $\boldsymbol{z} = \boldsymbol{x} - \bar{x}\mathbf{1}$
  2. regress $\boldsymbol{y}$ on the residual $\boldsymbol{z}$ to give the coefficient $\hat{\beta}_1$

  where regress $\boldsymbol{y}$ on $\boldsymbol{z}$ means to estimate the "no intercept model" we initially started with.

Gram-Schmidt algorithm

We can generalize this for p non-orthogonal inputs $1 = x_0, x_1, \ldots, x_p$

1. Set $\boldsymbol{z}_0 = \boldsymbol{x}_0 = \mathbf{1}$
2. For $j = 1, 2, \ldots, p$:

   regress $\boldsymbol{x}_j$ on $\boldsymbol{z}_0, \ldots, \boldsymbol{z}_{j-1}$, and get the residual $\boldsymbol{z}_j = \boldsymbol{x}_j - \sum_{k=0}^{j-1} \hat{\gamma}_{kj} \boldsymbol{z}_k$ where $\hat{\gamma}_{kj} = \langle \boldsymbol{z}_k, \boldsymbol{x}_j \rangle / \langle \boldsymbol{z}_k, \boldsymbol{z}_k \rangle$.
3. regress $\boldsymbol{y}$ on the residual $\boldsymbol{z}_p$ to give the coefficient

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

Implications

- Another way to express the variability in $\hat{\beta}_p$ is

$$Var(\hat{\beta}_p) = \frac{\sigma^2}{\langle \boldsymbol{z}_p, \boldsymbol{z}_p \rangle} = \frac{\sigma^2}{||\boldsymbol{z}_p||^2}$$

- What will $\boldsymbol{z}_p$ look like if $\boldsymbol{x}_p$ is accurately predicted from $x_0, x_1, \ldots, x_{(p-1)}$?
- What about $||\boldsymbol{z}_p||^2$?
- How do we get back to the original $\boldsymbol{x}$ coefficients?
    - Let $\boldsymbol{x}_{0,1,\ldots,(j-1),(j+1),\ldots,p}$ denote the residual after regression $\boldsymbol{x}_j$ on $\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{(j-1)}, \boldsymbol{x}_{(j+1)}, \ldots, \boldsymbol{x}_p$
    - The jth multiple regression coefficient is the univariate regression coefficient of $\boldsymbol{y}$ on $\boldsymbol{x}_{0,1,\ldots,(j-1),(j+1),\ldots,p}$.

Matrix GS with QR decomp

- In matrix form, we can represent the second step of the GS algorithm with

$$\boldsymbol{X} = \boldsymbol{Z}\Gamma$$

where $\boldsymbol{Z}$ has columns $\boldsymbol{z}_j$, and Γ is the upper triangular matrix with entries $\hat{\gamma}_{kj}$.

- Let's add in $\boldsymbol{D}$ a diagonal matrix with entries $D_{jj} = ||\boldsymbol{z}_j||$ to get

$$\begin{aligned} \boldsymbol{X} &= \boldsymbol{Z}\boldsymbol{D}^{-1}\boldsymbol{D}\Gamma \\ &= \boldsymbol{Q}\boldsymbol{R} \end{aligned}$$

The $\boldsymbol{QR}$ decomposition of $\boldsymbol{X}$

Matrix GS with QR decomp

- Using the $\boldsymbol{QR}$ decomposition of $\boldsymbol{X}$ we get the following form for $\hat{\beta}$ and $\hat{\boldsymbol{y}}$

$$
\begin{aligned}
\hat{\beta} &= (\boldsymbol{X}'\boldsymbol{X})^{-1}X'\boldsymbol{y} = \{(\boldsymbol{QR})'\boldsymbol{QR}\}^{-1}(\boldsymbol{QR})'\boldsymbol{y} = \boldsymbol{R}^{-1}\boldsymbol{Q}'\boldsymbol{y}, \\
\hat{\boldsymbol{y}} &= \boldsymbol{QQ}'\boldsymbol{y}
\end{aligned}
$$

This form of $\hat{\beta}$ is a lot easier to solve because $\boldsymbol{R}$ is upper triangular.

Introduction to Multivariate Regression

- Now let's consider the more classical multivariate case where we have $Y_1, Y_2, \ldots, Y_K$ and $X_0, \boldsymbol{X}_1, \ldots, \boldsymbol{X}_p$ and the linear model

$$Y_k = \beta_{0k} + \sum_{j=1}^{p} X_j \beta_{jk} + \epsilon_k = f_k(\boldsymbol{X}) + \epsilon_k \quad \text{for } k = 1, 2, \ldots, K$$

or in matrix form

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{B} + \boldsymbol{E}$$

where $\boldsymbol{Y}$ is $n \times K$ are the outcomes, $\boldsymbol{X}$ is $n \times (p+1)$ are the inputs, $\boldsymbol{B}$ is an $(p+1) \times K$ matrix of β coefficients and $\boldsymbol{E}$ is an $n \times K$ matrix of residuals.

RSS and solution

- The RSS for the multivariate case is given by

$$\begin{aligned} RSS(\boldsymbol{B}) &= \sum_{k=1}^{K} \sum_{i=1}^{n} \{y_{ik} - f_k(x_i)\}^2 \\ &= tr\{(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{B})'(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{B})\} \end{aligned}$$

- It's rather straightforward to show that $RSS(\boldsymbol{B})$ is minimized with

$$\hat{\boldsymbol{B}} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{Y}$$

Implications

- More specifically, for the kth outcome the coefficient is

$$\hat{\beta}_k = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}_k$$

- If we were to use the general linear model where $Cov(\epsilon) = \Sigma$ and

$$RSS(\boldsymbol{B}, \Sigma) = tr\{(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{B})'\Sigma^{-1}(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{B})\},$$

  .... the solution is still the same.

- What does this imply about doing regression with multiple outcomes?

Introduction

- **Bayesian Decision Theory** is a decision-making framework that combines probability theory and decision theory.
- It is based on the Bayesian approach to probability, where prior beliefs are updated with new evidence in the form of data to produce posterior beliefs.
- Bayesian Decision Theory provides a formal mechanism for making decisions under uncertainty, weighing the risks of different actions against the posterior beliefs about the state of the world.

Probabilistic Setup

- Let θ be a parameter or state of nature we want to learn about (it could represent various things: the true state of a system, a model parameter, etc.)
- $p(\theta)$ is the prior probability distribution over θ which reflects our beliefs about θ before observing data.
- $p(x|\theta)$ is the likelihood function which provides the probability of observing data x given θ.
- $p(\theta|x)$ is the posterior probability distribution over θ given data x, which is computed using Bayes' theorem:

$$p(\theta|x) = \frac{p(x|\theta)p(\theta)}{p(x)}$$

where $p(x)$ is the evidence or marginal likelihood.

Decision Making

- Suppose we have a set of possible actions A we can take.
- A loss function $L(\theta, a)$ represents the cost or loss of taking action a when the true state is θ.
- The loss function quantifies the "penalty" for making decisions; related to the norms we discussed but more general (e.g., for binary data).
- The goal in Bayesian decision theory is to minimize the expected loss. The decision rule is given by:

$$a^* = \arg\min_a \mathbb{E}[L(\theta, a)|x]$$

where the expectation is over the posterior distribution of θ given data x.

Example: Binary Hypothesis Testing

Let's consider a simple case where θ can be either H_0 or H_1.

- Prior Probabilities: $p(H_0)$ and $p(H_1)$.
- Likelihoods: $p(x|H_0)$ and $p(x|H_1)$.
- Actions: here we'll consider $A \in \{a_0, a_1\}$, i.e., a "hard" decision.
- Loss function might be defined such that $L(H_0, a_0) = 0$ (no loss for correctly deciding H_0), $L(H_0, a_1) = 1$ (loss for wrongly deciding H_1 when truth is H_0), and similar definitions for decisions regarding H_1.
  - if $A \in (0, 1)$ the other loss functions would be used.

Example: Binary Hypothesis Testing

- The Bayesian decision rule will decide a_1, i.e., H_1, if:

$$\frac{p(x|H_1)p(H_1)}{p(x)} > \frac{p(x|H_0)p(H_0)}{p(x)}$$

This simplifies to:

$$\frac{p(x|H_1)}{p(x|H_0)} > \frac{p(H_0)}{p(H_1)}$$

Here, $\frac{p(x|H_1)}{p(x|H_0)}$ is the likelihood ratio and $\frac{p(H_0)}{p(H_1)}$ is the prior odds ratio.