Ordinary Least Squares and Maximum Likelihood Estimation

David Carlson

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What are Regression Models Useful For

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- To make predictions
- To measure causal effects

Causal Inference

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- Natural experiments: Assignment into "treatment" and "control" is as if randomized by nature
- Observational studies: We do not know how assignment into "treatment" and "control" was achieved

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Smokers

Non-smokers

	Old	Young
GM	\hat{y}_1	\hat{y}_2
\sim GM	ŷ ₃	ŷ ₄

	Old	Young
GM	ŷ ₅	\hat{y}_6
\sim GM	ŷ ₇	ŷ ₈

We need not make too many assumptions about how \mathcal{T} affects \mathcal{Y} after controlling for \mathcal{X} . We could simply assume

$$p(Y|T,X) = g(T,X)$$

and use sample data to estimate p(Y|T,X) at different combinations of T and X.

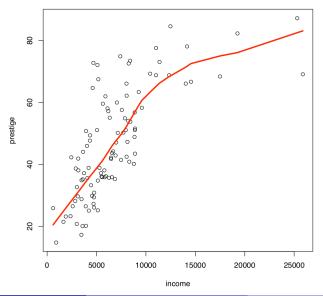
Smokers

Non-smokers

	Old	Young
GM	0.9	0.6
\sim GM	0.6	0.6

	Old	Young
GM	0.5	0.5
\sim GM	0.5	0.5

How can we learn anything about p(Y|X) when X is continuous?



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- NPR is computationally expensive
- NPR cannot be easily transmitted
- NPR collapes under "curse of dimensionality"
- We need to move from "natural" NPR to parametric approaches

Substantive Statements as Probability Models

Outcome (Y)	Predictor or Cause (X)
Votes for Party A	Platforms of parties A and B
Frequency of wars	Political regimes of neighboring countries
Campaign spending (\$)	Incumbent strength
Survival of democracy	Country's income level
Cancer rates	Number of phone lines

The **generalized linear model** notation makes it clear that we are building a model of the probability of Y conditional on X:

$$Y_i \sim f(\theta_i)$$

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- Stochastic component: $f(\cdot)$
- Systematic component: X
- Link function: $g(\cdot)$

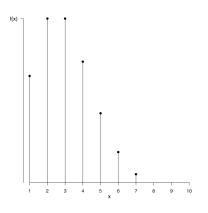
Distribution of Random Variables

• Random variable: A real-valued function that is defined on a sample space

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- Random variable: A real-valued function that is defined on a sample space
- Random variable X is characterized by a probability distribution over all possible values x that X can take

Discrete Random Variables



► The probability function of X is the function f such that for every x

$$f(x) = \Pr(X = x)$$

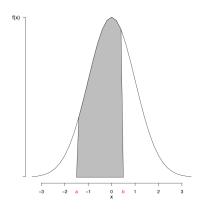
- 1. If x is outside the sample space, then f(x) = 0
- 2. If x_1, x_2, \ldots includes all values in the sample space, then

$$\sum_{i=1}^{\infty} f(x_i) = 1$$

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3.
$$Pr(X \in A) = \sum_{x_i \in A} f(x_i)$$

Continuous Random Variables



- The probability density function f(x) specifies the probability of X taking values on subsets of the sample space; e.g., for subset (a, b)
 - 1. $f(x) \geq 0, \forall x$
 - $2. \int_{-\infty}^{\infty} f(x) dx = 1$
 - 3. $Pr(a < x \le b) =$ $\int_a^b f(x) dx$

Joint Distribution of Discrete X, Y

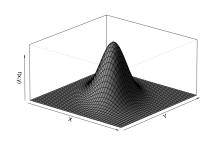
		X	
Y	1	2	3
1	0.1	0.3	0
2	0	0	0.2
3	0.1	0.1	0
4	0	0.2	0

- If X and Y are discrete random variables, their distribution is also discrete
- ► The joint p.f. of (X, Y) is the function f such that for every point (x, y)

$$f(x, y) = \Pr(X = x \text{ and } Y = y)$$

- 1. If x, y are outside the sample space, then f(x, y) = 0
- 2. $\sum_{(x,y)} f(x,y) = 1$

Joint Distribution of Continuous X, Y



- ▶ If X and Y are continuous random variables, their distribution is also continuous
- ► The joint pdf of (X, Y) is the function f such that for every region A

$$Pr(X, Y \in A) = \int_A \int f(x, y) dx dy$$

1.
$$f(x,y) \geq 0$$

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2. $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x,y) = 1$

Marginal Distribution of X

		X		
Y	1	2	3	$f_2(Y)$
1	0.1	0.3	0	0.4
2	0	0	0.2	0.2
3	0.1	0.1	0	0.2
4	0	0.2	0	0.2
$f_1(X)$	0.2	0.6	0.2	1

The distribution of X computed from the joint distribution of (X, Y) is the marginal distribution of X

Discrete distributions:

$$f_1(x) = \Sigma_y f(x, y)$$

Continuous distributions:

$$f_1(x) = \int_{-\infty}^{\infty} f(x, y) dy$$

Conditional Distributions

After observing Y = y, the probability that X = x is specified by the conditional probability

$$g_1(x|y) = p(X = x|Y = y) = \frac{p(X = x \text{ and } Y = y)}{p(Y = y)} = \frac{f(x,y)}{f(y)}$$

where $g_1(x|y) \geq 0$ and $\sum_{v} g_1(x|y) = 1$

Conditional Distributions (cont.)

			Χ		
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$$f_2(y=3)=0.2$$

•
$$f(x = 1 \text{ and } y = 3) = 0.1$$

•
$$f(x = 2 \text{ and } y = 3) = 0.1$$

•
$$f(x = 3 \text{ and } y = 3) = 0$$

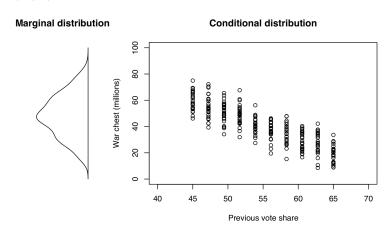
What's
$$g_1(X = 1 | Y = 3)$$
?

$$\frac{f(x=1 \text{ and } y=3)}{f_2(y=3)} = \frac{0.1}{0.2}$$

$$=\frac{1}{2}$$

Linear Regression as a Probability Model

War chest as a function of support in previous election The regression line joins E(Y|X) at different values of X



Alternative Notations for OLS Regression

GLM notation

$$Y_i \sim \mathcal{N}(\mu_i, \sigma^2)$$

 $\mu_i = \alpha + \beta X_i$

OLS notation

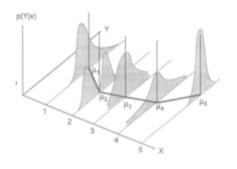
$$Y_i = \alpha + \beta X_i + \epsilon_i$$

$$\epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

In both cases, note the three main assumptions we impose:

- Normality
- Linearity
- Constant variance

Potential Pitfalls in Parametric Models



- 1. Failure of normality: p(Y|x=1), p(Y|x=2), and p(Y|x=3) are not normal
- 2. Failure of linearity: $E[p(Y|X)] \neq \alpha + \beta X$
- 3. Failure of constant variance: p(Y|x=4) and p(Y|x=5) do not have the same spread $(\sigma_{Y}|x=4 \neq \sigma_{Y}|x=5)$

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- This line could be constructed in many different ways, but we make three consequential decisions:
 - Vertical distances
 - Sum of errors
 - Sum of squared errors

Multiple Regression

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- In multiple regression, we fit a least squares "hyperplane" in k+1-dimensional space
- ullet \hat{eta}_0 is the expected value of Y when all variables X are jointly 0
- For any slope coefficient estimate $\hat{\beta}_k$: A unit increase in $X_{i,k}$ will yield on average a $\hat{\beta}_k$ increase in Y_i , all else constant

Multiple Regression (cont.)

We define the multiple regression model as follows:

$$Y_{i} = \beta_{0} + \beta_{1}X_{i1} + \ldots + \beta_{k}X_{ik} + \epsilon_{i}$$

$$\epsilon_{i} \sim \mathcal{N}(0, \sigma^{2})$$

In this model, we have:

- i = 1, ..., n observations
- k independent variables
- ullet k+1 slope and intercept parameters eta_j
- ullet one variance parameter σ^2

Statistical Theory for Linear Models

The scalar notation is cumbersome, but the model can be simplified by defining the following vectors and matrices:

- $\mathbf{y} = [y_1, y_2, \dots, y_n]'$ is a vector of observations on the dependent variable
- $X = [1, x_1, x_2, ..., x_k]$ is a matrix with a column of 1's and k columns of independent variables
- $\bullet \ \boldsymbol{\beta} = [\beta_0, \beta_1, \beta_2, \dots, \beta_k]'$
- $\epsilon = [\epsilon_1, \epsilon_2, \dots, \epsilon_n]'$ is a vector of random errors

Statistical Theory for Linear Models (cont.)

The linear model can then be represented succinctly as:

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

$$E(\boldsymbol{\epsilon}) = [0, 0, \dots, 0]' = \mathbf{0}$$

$$\operatorname{var}(\boldsymbol{\epsilon}) = E(\boldsymbol{\epsilon}\boldsymbol{\epsilon}') = \begin{bmatrix} \sigma^2 & 0 & 0 & \cdots & 0 \\ 0 & \sigma^2 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \sigma^2 \end{bmatrix} = \sigma^2 \boldsymbol{I}_n$$

Statistical Theory for Linear Models (cont.)

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

$$\underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}}_{n \times 1} = \underbrace{\begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix}}_{n \times (k+1)} \underbrace{\begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{bmatrix}}_{(k+1) \times 1} + \underbrace{\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}}_{n \times 1}$$

For observation 2:

$$y_2 = \beta_0 \cdot 1 + \beta_1 X_{2,1} + \beta_2 X_{2,2} + \ldots + \beta_k X_{2,k} + \epsilon_2$$

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Derivation of OLS Estimators

• Define the vector of residuals as

$$e = Y - Xb$$

• The sum of squared errors is defined as

$$\mathbf{e'e} = (\mathbf{Y} - \mathbf{X}\mathbf{\beta})'(\mathbf{Y} - \mathbf{X}\mathbf{\beta})$$

• Compute $\frac{\partial}{\partial \boldsymbol{b}}(\boldsymbol{e'e})$

$$\frac{\partial}{\partial \mathbf{b}}(\mathbf{e}'\mathbf{e}) = \frac{\partial}{\partial \mathbf{b}}(\mathbf{Y} - \mathbf{X}\mathbf{b})'(\mathbf{Y} - \mathbf{X}\mathbf{b})
= \frac{\partial}{\partial \mathbf{b}}(\mathbf{Y}' - \mathbf{b}'\mathbf{X}')(\mathbf{Y} - \mathbf{X}\mathbf{b})
= \frac{\partial}{\partial \mathbf{b}}(\mathbf{Y}'\mathbf{Y} - \mathbf{Y}'\mathbf{X}\mathbf{b} - \mathbf{b}'\mathbf{X}'\mathbf{Y}' + \mathbf{b}'\mathbf{X}'\mathbf{X}\mathbf{b})
= \frac{\partial}{\partial \mathbf{b}}(\mathbf{Y}'\mathbf{Y} - 2\mathbf{b}'\mathbf{X}'\mathbf{Y} + \mathbf{b}'\mathbf{X}'\mathbf{X}\mathbf{b})
= -2\mathbf{X}'\mathbf{Y} + 2\mathbf{X}'\mathbf{X}\mathbf{b}$$

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Derivation of OLS Estimators (cont.)

• Set the first derivative of e'e with respect to b equal to 0

$$-2X'Y + 2X'Xb = 0$$
$$2X'Xb = 2X'Y$$
$$X'Xb = X'Y$$

• Compute the inverse $(\mathbf{X}'\mathbf{X})^{-1}$ of $\mathbf{X}'\mathbf{X}$ and use it to pre-multiply both sides of the previous equation:

$$(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$$

 $\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$

• **b** is uniquely defined as long as **X'X** is a full-rank matrix

Derivation of OLS Estimators (cont.)

Second order condition: The matrix of second derivatives of e'e (Hessian matrix) should be positive definite, hence a global minimum:

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Derivation of the Moments of **b**

We can also find the variance of **b**:

$$var(\mathbf{b}) = var(\mathbf{AY})$$

$$= \mathbf{A}var(\mathbf{Y})\mathbf{A}'$$

$$= [(\mathbf{X'X})^{-1}\mathbf{X'}]var(\mathbf{Y})[(\mathbf{X'X})^{-1}\mathbf{X'}]'$$

$$= [(\mathbf{X'X})^{-1}\mathbf{X'}]\sigma^{2}\mathbf{I}[(\mathbf{X'X})^{-1}\mathbf{X'}]'$$

$$= \sigma^{2}[(\mathbf{X'X})^{-1}\mathbf{X'}][(\mathbf{X'X})^{-1}\mathbf{X'}]'$$

$$= \sigma^{2}[(\mathbf{X'X})^{-1}\mathbf{X'}][\mathbf{X}(\mathbf{X'X})^{-1}]$$

$$= \sigma^{2}(\mathbf{X'X})^{-1}$$

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- Non-stochastic X: X is fixed in repeated sampling

Basic Assumptions of OLS ("conditional" approach)

- No perfect multicollinearity
- Variability in X: var(X) > 0 but finite
- Linearity: $Y_i = \alpha + \beta X_i + \epsilon_i$
- Conditional zero mean: $E(\epsilon_i|\mathbf{X}) = 0$
- Conditional homoskedasticity: $var(\epsilon_i|\mathbf{X}) = \sigma^2$
- Conditional non-autocorrelation: $cov(\epsilon_i, \epsilon_i | \mathbf{X}) = 0, \forall i \neq j$

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Maximum-Likelihood Estimation

- We use data to make inferences about a set θ of parameters (ex., $\theta = (\beta_0, \beta_1, \dots, \beta_k)$)
- We observe

$$Y = (y_1, y_2, ..., y_n)'$$

 $X = (x_1, x_2, ..., x_k)$

and assume

- lacktriangleright that each draw y_i is drawn from the same distribution with parameter heta and
- ▶ that the draws i = (1, ..., n) are independent
- In short: $y_i \stackrel{iid}{\sim} f(\theta, \mathbf{X}_i)$

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- Which parameters $\theta = (\mu, \sigma^2)$ are most likely to have generated the values $\mathbf{y} = (3, 5, 7)$ if $Y \sim \mathcal{N}(\mu, \sigma^2)$?

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- Which parameters $\theta = (\mu, \sigma^2)$ are most likely to have generated the values $\mathbf{y} = (3, 5, 7, 6, 1, 2, 4, 5, 5, 9, 8)$ if $Y \sim \mathcal{N}(\mu, \sigma^2)$?

• We can rewrite the linear regression model as a probability model:

$$\mathbf{Y} \sim \mathcal{N}_n(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{I})$$

• Which means that, for any observation:

$$\begin{aligned} y_i &\sim \mathcal{N}(\boldsymbol{x_i'\beta}, \sigma^2) \\ p(y_i|\boldsymbol{x_i}, \boldsymbol{\beta}, \sigma^2) &= \frac{1}{(2\pi\sigma^2)^{1/2}} exp\left[-\frac{1}{2\sigma^2}(y_i - \boldsymbol{x_i'\beta})^2\right] \end{aligned}$$

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MLE for the Linear Regression Model

Because of our assumption of independence, we can write the joint pdf of \boldsymbol{Y} as

$$p(\mathbf{Y}|\mathbf{X},\boldsymbol{\beta},\sigma^{2}) = p(y_{1}) \times p(y_{2}) \times \cdots \times p(y_{n}) = \prod_{i=1}^{n} p(y_{i})$$

$$= \prod_{i=1}^{n} \frac{1}{(2\pi\sigma^{2})^{1/2}} exp \left[-\frac{1}{2\sigma^{2}} (y_{i} - \mathbf{x}'_{i}\boldsymbol{\beta})^{2} \right]$$

$$= \frac{1}{(2\pi\sigma^{2})^{n/2}} exp \left[-\frac{1}{2\sigma^{2}} \sum_{i=1}^{n} (y_{i} - \mathbf{x}'_{i}\boldsymbol{\beta})^{2} \right]$$

$$= \frac{1}{(2\pi\sigma^{2})^{n/2}} exp \left[-\frac{1}{2\sigma^{2}} (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})' (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) \right]$$

MLE for the Linear Regression Model (cont.)

When the parameters β , σ^2 are expressed as a function of the data Y, X, the joint pdf is called the likelihood function:

$$\mathcal{L}(oldsymbol{eta}, \sigma^2 | oldsymbol{Y}, oldsymbol{X}) = rac{1}{(2\pi\sigma^2)^{n/2}} exp\left[-rac{1}{2\sigma^2} (oldsymbol{Y} - oldsymbol{X}oldsymbol{eta})' (oldsymbol{Y} - oldsymbol{X}oldsymbol{eta})
ight]$$

- Note that $\mathcal{L}(\cdot)$ returns a real number for every combination of $\mathbf{Y}, \mathbf{X}, \boldsymbol{\beta}, \sigma^2$
- Maximum likelihood estimates of $\boldsymbol{\beta}$ are simply the values of \boldsymbol{b} , $\hat{\sigma}^2$ that maximize $\mathcal{L}(\cdot)$ given $\boldsymbol{Y}, \boldsymbol{X}$

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MLE for the Linear Regression Model (cont.)

- In the linear model, $\mathcal{L}(\cdot)$ is a concave function (thus **b** and $\hat{\sigma}^2$ exist and are unique) but has a very difficult form
- Fortunately, we can appeal to the invariance property of maximum likelihood estimators to transform $\mathcal{L}(\cdot)$ into something manageable, like the log (ℓ) :

$$\begin{split} \ell(\pmb{\beta}, \sigma^2 | \pmb{Y}, \pmb{X}) &= \textit{In} \mathcal{L}(\cdot) \\ &= \textit{In} \left(\frac{1}{(2\pi\sigma^2)^{n/2}} exp \left[-\frac{1}{2\sigma^2} (\pmb{Y} - \pmb{X} \pmb{\beta})' (\pmb{Y} - \pmb{X} \pmb{\beta}) \right] \right) \\ &= -\frac{n}{2} \textit{In} (2\pi\sigma^2) - \frac{1}{2\sigma^2} (\pmb{Y} - \pmb{X} \pmb{\beta})' (\pmb{Y} - \pmb{X} \pmb{\beta}) \end{split}$$

MLE for the Linear Regression Model (cont.)

• We can now solve the (relatively) simpler problem of choosing β and σ^2 to maximize ℓ :

$$\frac{\partial \ell}{\partial \boldsymbol{\beta}} = \frac{1}{2\sigma^2} (2\boldsymbol{X}'\boldsymbol{Y} - 2\boldsymbol{X}'\boldsymbol{X}\boldsymbol{\beta} = 0$$

$$\frac{\partial \ell}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4} (\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})'(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}) = 0$$

The ML estimates are:

$$\begin{aligned} & \boldsymbol{b}_{ML} = (\boldsymbol{X'X})^{-1}\boldsymbol{X'Y} \\ & \hat{\sigma}_{ML}^2 = \frac{(\boldsymbol{Y} - \boldsymbol{Xb})'(\boldsymbol{Y} - \boldsymbol{Xb})}{n} = \frac{\boldsymbol{e'e}}{n} \end{aligned}$$

Dichotomous Dependent Variables: LPM

The linear probability model is based on the assumption of linearity to model dichotomous dependent variables

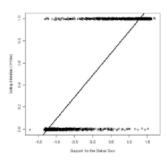
$$Y_{i} = \underbrace{\alpha + \beta x_{i}}_{\mathsf{E}(Y|x_{i}) = \pi_{i}} + \varepsilon_{i}$$
$$\varepsilon_{i} \sim \mathcal{N}(0, \sigma^{2})$$

LPM is BLAT, but:

- 1. Errors are not normally distributed
- 2. Heteroskedasticity

$$\operatorname{var}(\varepsilon_i) = \pi_i (1 - \pi_i)$$

3. Linearity assumption



Generalized Linear Models

So far, we have discussed the identity link, but many possible options for $\mathbf{g}(\cdot)$

- Binary (dichotomous)
 - ► Logit, Probit, or c-log-log
- Unordered categorical (polytomous)
 - ► Multinomial logit
- Ordered categorical
 - Ordered logit or Probit
- Counts
 - Poisson
- Rare counts
 - Negative binomial
- Zero-inflated models for rare non-zero outcomes (e.g. war)