The OLS Estimator (1)

STA 211: The Mathematics of Regression

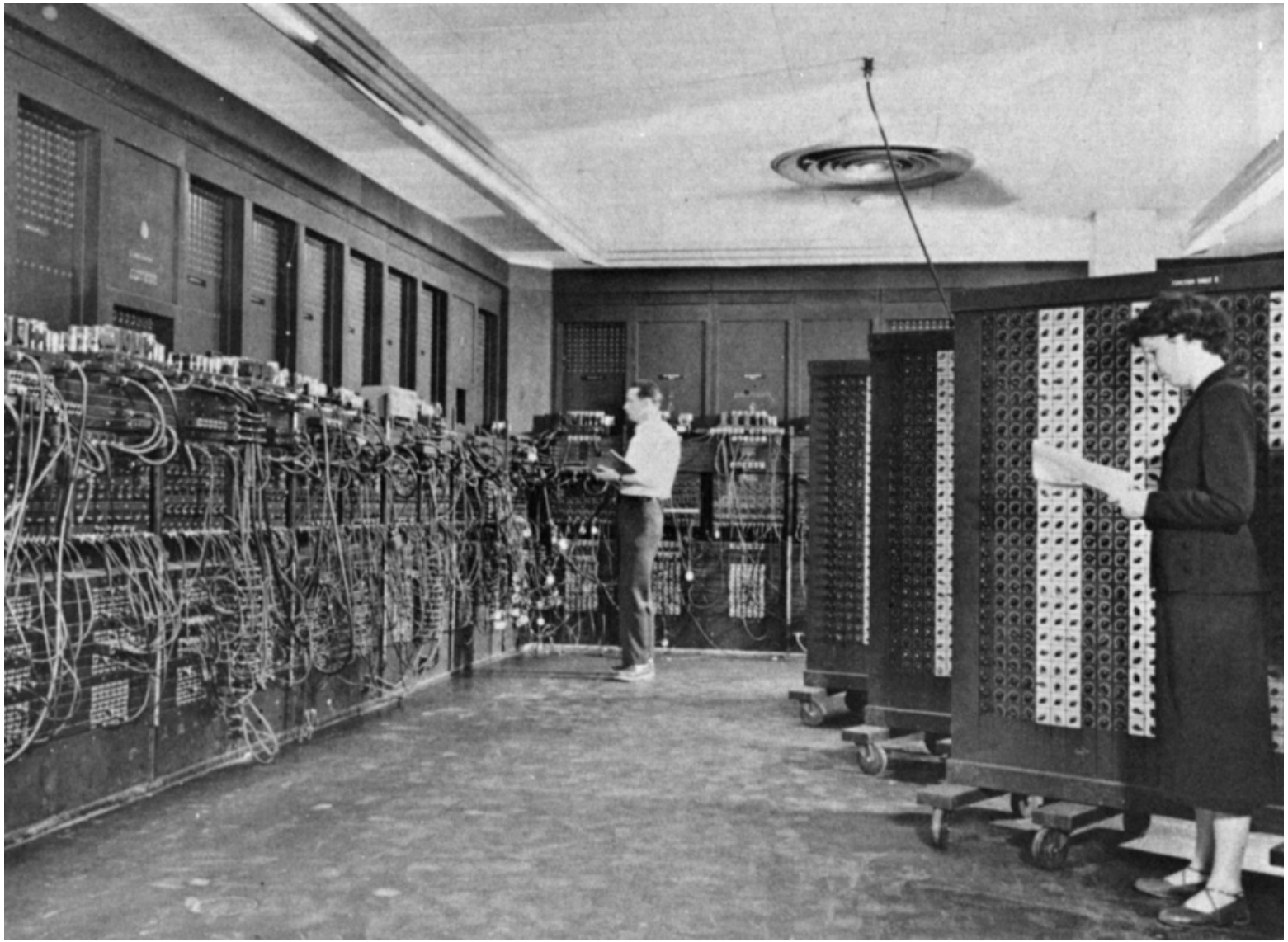
Yue Jiang

January 17, 2023

The following material was used by Yue Jiang during a live lecture.

Without the accompanying oral comments, the text is incomplete as a record of the presentation.

Why care about linear models?



Review: vector operations

Let $\mathbf{x}$ be a k-vector (this is to say, with dimensions $k \times 1$):

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix}$$

Review: vector operations

Suppose we have some function of $\mathbf{x}$, $f(\mathbf{x})$. Then the gradient ∇f (with respect to $\mathbf{x}$) is the k-vector of partial derivatives:

$$\nabla_x f = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_k} \end{bmatrix}$$

Review: vector operations

Similarly, the Hessian $\nabla^2 f$ is the $k \times k$ matrix of second partial derivatives:

$$\nabla_x^2 f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_k} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_k} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_k \partial x_1} & \frac{\partial^2 f}{\partial x_k \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Review: vector operations

The gradient has some convenient properties. For instance, suppose we wish to differentiate the linear form $\mathbf{x}^T\mathbf{z}$, where $\mathbf{z}$ is also a k-vector (and not a function of $\mathbf{x}$):

$$\mathbf{x}^T\mathbf{z} = \begin{bmatrix} x_1 & \cdots & x_k \end{bmatrix} \begin{bmatrix} z_1 \\ \vdots \\ z_k \end{bmatrix} = x_1 z_1 + \cdots + x_k z_k$$

Review: vector operations

The gradient has some convenient properties. For instance, suppose we wish to differentiate the linear form $\mathbf{x}^T\mathbf{z}$, where $\mathbf{z}$ is also a k-vector (and not a function of $\mathbf{x}$):

$$\mathbf{x}^T\mathbf{z} = \begin{bmatrix} x_1 & \cdots & x_k \end{bmatrix} \begin{bmatrix} z_1 \\ \vdots \\ z_k \end{bmatrix} = x_1 z_1 + \cdots + x_k z_k$$

Then the gradient with respect to $\mathbf{x}$ is

$$\nabla \mathbf{x}^T\mathbf{z} = \begin{bmatrix} \frac{\partial \mathbf{x}^T\mathbf{z}}{\partial x_1} \\ \vdots \\ \frac{\partial \mathbf{x}^T\mathbf{z}}{\partial x_k} \end{bmatrix} = \begin{bmatrix} \frac{\partial}{\partial x_1}(x_1 z_1 + \cdots + x_k z_k) \\ \vdots \\ \frac{\partial}{\partial x_k}(x_1 z_1 + \cdots + x_k z_k) \end{bmatrix} = \begin{bmatrix} z_1 \\ \vdots \\ z_k \end{bmatrix} = \mathbf{z}$$

Review: vector operations

Similarly, if $\mathbf{A}$ is a $k \times k$ matrix that is not a function of $\mathbf{x}$, then the gradient of the quadratic form $\mathbf{x}^T\mathbf{A}\mathbf{x}$ (again, with respect to $\mathbf{x}$) is

$$\nabla\left(\mathbf{x}^T\mathbf{A}\mathbf{x}\right) = \left(\mathbf{A} + \mathbf{A}^T\right)\mathbf{X},$$

which is $2\mathbf{A}\mathbf{x}$ if $\mathbf{A}$ is symmetric.

The linear model in matrix form

We have n observations of a response variable Y and each predictor X_1, X_2, $\cdots$, X_p. As well, each observation has some unobserved error ϵ (which may have certain properties, which we'll talk about later this semester).

The linear model in matrix form

We have n observations of a response variable Y and each predictor X_1, X_2, $\cdots$, X_p. As well, each observation has some unobserved error ϵ (which may have certain properties, which we'll talk about later this semester).

We wish to fit the model

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \epsilon$$

The linear model in matrix form

$$\underbrace{\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}}_{\mathbf{y}} = \underbrace{\begin{bmatrix} 1 & x_{11} & \cdots & x_{1p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \cdots & x_{np} \end{bmatrix}}_{\mathbf{X}} \underbrace{\begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}}_{\boldsymbol{\beta}} + \underbrace{\begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}}_{\boldsymbol{\epsilon}}$$

- What are the dimensions of each of the pieces above?

The mean squared error

Note the error term, ϵ; suppose we are interested in the mean squared error (MSE), given by

$$\frac{1}{n}\epsilon^T\epsilon$$

- What is the dimension of the MSE?
- How would you express the MSE in terms of $\mathbf{y}$, $\mathbf{X}$, and β?

Minimizing the mean squared error

$$\frac{1}{n}\boldsymbol{\epsilon}^T\boldsymbol{\epsilon} = \frac{1}{n}\left(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\right)^T\left(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\right)$$

Minimizing the mean squared error

$$\begin{aligned}\frac{1}{n}\boldsymbol{\epsilon}^T\boldsymbol{\epsilon} &= \frac{1}{n}\left(\mathbf{y}-\mathbf{X}\boldsymbol{\beta}\right)^T\left(\mathbf{y}-\mathbf{X}\boldsymbol{\beta}\right) \\ &= \frac{1}{n}\left(\mathbf{y}^T-\boldsymbol{\beta}^T\mathbf{X}^T\right)\left(\mathbf{y}-\mathbf{X}\boldsymbol{\beta}\right)\end{aligned}$$

Minimizing the mean squared error

$$\begin{aligned}
\frac{1}{n}\boldsymbol{\epsilon}^T\boldsymbol{\epsilon} &= \frac{1}{n}\left(\mathbf{y}-\mathbf{X}\beta\right)^T\left(\mathbf{y}-\mathbf{X}\beta\right) \\
&= \frac{1}{n}\left(\mathbf{y}^T-\beta^T\mathbf{X}^T\right)\left(\mathbf{y}-\mathbf{X}\beta\right) \\
&= \frac{1}{n}\left(\mathbf{y}^T\mathbf{y}-2\beta^T\mathbf{X}^T\mathbf{y}+\beta^T\mathbf{X}^T\mathbf{X}\beta\right)
\end{aligned}$$

Minimizing the mean squared error

$$\begin{aligned}\frac{1}{n}\boldsymbol{\epsilon}^T\boldsymbol{\epsilon} &= \frac{1}{n}\left(\mathbf{y}-\mathbf{X}\boldsymbol{\beta}\right)^T\left(\mathbf{y}-\mathbf{X}\boldsymbol{\beta}\right)\\ &= \frac{1}{n}\left(\mathbf{y}^T-\boldsymbol{\beta}^T\mathbf{X}^T\right)\left(\mathbf{y}-\mathbf{X}\boldsymbol{\beta}\right)\\ &= \frac{1}{n}\left(\mathbf{y}^T\mathbf{y}-2\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{y}+\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{X}\boldsymbol{\beta}\right)\end{aligned}$$

Suppose we wanted to minimize the MSE with respect to $\boldsymbol{\beta}$.

- What is the gradient of the MSE with respect to $\boldsymbol{\beta}$?

The mean squared error

$$\nabla_\beta \frac{1}{n}\boldsymbol{\epsilon}^T\boldsymbol{\epsilon} = \frac{1}{n}\left(\nabla \mathbf{y}^T\mathbf{y} - 2\nabla\beta^T\mathbf{X}^T\mathbf{y} + \nabla\beta^T\mathbf{X}^T\mathbf{X}\beta\right)$$

The mean squared error

$$\begin{aligned}\nabla_\beta \frac{1}{n}\boldsymbol{\epsilon}^T\boldsymbol{\epsilon} &= \frac{1}{n}\left(\nabla \mathbf{y}^T\mathbf{y} - 2\nabla\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{y} + \nabla\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{X}\boldsymbol{\beta}\right) \\ &= \frac{1}{n}\left(0 - 2\mathbf{X}^T\mathbf{y} + 2\mathbf{X}^T\mathbf{X}\boldsymbol{\beta}\right)\end{aligned}$$

The mean squared error

$$\begin{aligned}
\nabla_\beta \frac{1}{n}\boldsymbol{\epsilon}^T\boldsymbol{\epsilon} &= \frac{1}{n}\left(\nabla \mathbf{y}^T\mathbf{y} - 2\nabla\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{y} + \nabla\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{X}\boldsymbol{\beta}\right) \\
&= \frac{1}{n}\left(0 - 2\mathbf{X}^T\mathbf{y} + 2\mathbf{X}^T\mathbf{X}\boldsymbol{\beta}\right) \\
&\propto \mathbf{X}^T\mathbf{X}\boldsymbol{\beta} - \mathbf{X}^T\mathbf{y}
\end{aligned}$$

The mean squared error

$$\begin{aligned}\nabla_\beta \frac{1}{n}\boldsymbol{\epsilon}^T\boldsymbol{\epsilon} &= \frac{1}{n}\left(\nabla \mathbf{y}^T\mathbf{y} - 2\nabla\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{y} + \nabla\boldsymbol{\beta}^T\mathbf{X}^T\mathbf{X}\boldsymbol{\beta}\right) \\ &= \frac{1}{n}\left(0 - 2\mathbf{X}^T\mathbf{y} + 2\mathbf{X}^T\mathbf{X}\boldsymbol{\beta}\right) \\ &\propto \mathbf{X}^T\mathbf{X}\boldsymbol{\beta} - \mathbf{X}^T\mathbf{y}\end{aligned}$$

If a solution $\widehat{\boldsymbol{\beta}}$ exists, it occurs when this quantity is zero:

$$\mathbf{0} \overset{set}{=} \mathbf{X}^T\mathbf{X}\widehat{\boldsymbol{\beta}} - \mathbf{X}^T\mathbf{y}$$

- What is the (candidate) solution?

Minimizing the mean squared error

$$\mathbf{0} \stackrel{set}{=} \mathbf{X}^T\mathbf{X}\widehat{\beta} - \mathbf{X}^T\mathbf{y}$$

Minimizing the mean squared error

$$\mathbf{0} \stackrel{set}{=} \mathbf{X}^T\mathbf{X}\widehat{\beta} - \mathbf{X}^T\mathbf{y}$$

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

Minimizing the mean squared error

$$\begin{aligned} \mathbf{0} &\stackrel{set}{=} \mathbf{X}^T\mathbf{X}\widehat{\beta} - \mathbf{X}^T\mathbf{y} \\ \mathbf{X}^T\mathbf{y} &= \mathbf{X}^T\mathbf{X}\widehat{\beta} \\ \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y} &= \widehat{\beta} \end{aligned}$$

- Is this proposed solution a minimum?

The ordinary least squares estimate

$$\nabla_\beta \left(\mathbf{X}^T \mathbf{X} \beta - \mathbf{X}^T \mathbf{y} \right) = \mathbf{X}^T \mathbf{X}$$

If $\mathbf{X}$ has full column rank, then we have indeed found a *minimizing* solution, since for any non-zero $\mathbf{z}$ $\mathbf{z}^T \left(\mathbf{X}^T \mathbf{X} \right) \mathbf{z} > 0$ (that is, the Hessian is positive definite). In fact, this is the unique global solution.

Fitted values

Suppose we use our OLS estimates $\widehat{\beta}$ to try and predict $\mathbf{y}$ from $\mathbf{X}$: $\widehat{\mathbf{y}} = \mathbf{X}\widehat{\beta}$. This gives us a vector of fitted values:

$$\begin{aligned}\widehat{\mathbf{y}} &= \mathbf{X}\widehat{\beta} \\ &= \underbrace{\mathbf{X}\left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T}_{\mathbf{H}}\mathbf{y}\end{aligned}$$

where $\mathbf{H}$ is known as the "hat matrix" (it puts the hat on the $\mathbf{y}$). Note that this is only a function of $\mathbf{X}$, NOT of $\mathbf{y}$. From this matrix, we can see how our predictions change as $\mathbf{X}$ varies.

Residuals

The *difference* between the observed outcome $\mathbf{y}$ and the predicted outcome $\widehat{\mathbf{y}}$ is known as the residual:

$$\begin{aligned}\mathbf{e} &= \mathbf{y} - \widehat{\mathbf{y}} \\ &= \mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}\end{aligned}$$

We can equivalently use the hat matrix here:

$$\mathbf{e} = (\mathbf{I} - \mathbf{H})\mathbf{y}$$

Homework 1: Due Jan. 24

1. Show that $\nabla \left(\mathbf{x}^T \mathbf{A} \mathbf{x} \right) = 2\mathbf{A}\mathbf{x}$ for a k-vector $\mathbf{x}$ and symmetric $k \times k$ matrix $\mathbf{A}$.
2. Show that $\mathbf{H}$ and $\mathbf{I} - \mathbf{H}$ are symmetric (i.e., $\mathbf{H}^T = \mathbf{H}$, etc.) and idempotent (i.e., $\mathbf{H}^2 = \mathbf{H}$, etc.).
3. Instead of the MSE, suppose we wanted to minimize the following function with respect to $\boldsymbol{\beta}$, for some scalar $\lambda > 0$ (assuming full rank $\mathbf{X}$):

$$(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) + \lambda \boldsymbol{\beta}^T \boldsymbol{\beta}.$$

   Is there an analytical solution to this objective function? If so, provide the solution and demonstrate that it indeed minimizes the objective function. Otherwise, explain why not.

Some housekeeping