MS&E 226: "Small" Data

Lecture 2: Linear Regression (v2)

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Summarizing a sample

A sample

Suppose $\mathbf{Y} = (Y_1, \ldots, Y_n)$ is a sample of real-valued *observations*.

Simple statistics:

- *Sample mean*:

$$\overline{Y} = \frac{1}{n} \sum_{i=1}^{n} Y_i.$$

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Simple statistics:

- *Sample mean*:

$$\overline{Y} = \frac{1}{n} \sum_{i=1}^{n} Y_i.$$

- *Sample median*:
  - Order Y_i from lowest to highest.
  - Median is average of $n/2$'th and $(n/2 + 1)$'st elements of this list (if n is even)
    or $(n + 1)/2$'th element of this list (if n is odd)
  - More robust to "outliers"

A sample

Suppose $\mathbf{Y} = (Y_1, \ldots, Y_n)$ is a sample of real-valued *observations*.

Simple statistics:

- *Sample standard deviation*:

$$\hat{\sigma}_Y = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(Y_i - \overline{Y})^2}.$$

  Measures dispersion of the data.
  (Why $n-1$? See homework.)

Example in R

Children's IQ scores + mothers' characteristics
from National Longitudinal Survey of Youth (via [DAR])

Download from course site; lives in `child.iq/kidiq.dta`

```
> library(foreign)
> kidiq = read.dta("ARM_Data/child.iq/kidiq.dta")
> mean(kidiq$kid_score)
[1] 86.79724
> median(kidiq$kid_score)
[1] 90
> sd(kidiq$kid_score)
[1] 20.41069
```

Relationships

Modeling relationships

We focus on a particular type of summarization:

Modeling the relationship between observations.

Formally:

- Let Y_i, $i = 1, \ldots, n$, be the i'th observed (real-valued) *outcome*.
  Let $\mathbf{Y} = (Y_1, \ldots, Y_n)$
- Let X_{ij}, $i = 1, \ldots, n$, $j = 1, \ldots, p$ be the i'th observation of the j'th (real-valued) *covariate*.
  Let $\mathbf{X}_i = (X_{i1}, \ldots, X_{ip})$.
  Let $\mathbf{X}$ be the matrix whose *rows* are $\mathbf{X}_i$.

Pictures and names

How to visualize $\mathbf{Y}$ and $\mathbf{X}$?

Names for the Y_i's:
outcomes, *response variables*, *target variables*, *dependent variables*

Names for the X_{ij}'s:
covariates, *features*, *regressors*, *predictors*, *explanatory variables*, *independent variables*

$\mathbf{X}$ is also called the *design matrix*.

Example in R

The `kidiq` dataset loaded earlier contains the following columns:

`kid_score`	Child's score on IQ test
`mom_hs`	Did mom complete high school?
`mom_iq`	Mother's score on IQ test
`mom_work`	Working mother?
`mom_age`	Mother's age at birth of child

[*Note*: Always question how variables are defined!]

Reasonable question:

How is `kid_score` *related to the other variables?*

Example in R

```
> kidiq
  kid_score mom_hs    mom_iq mom_work mom_age
1        65      1 121.11753        4      27
2        98      1  89.36188        4      25
3        85      1 115.44316        4      27
4        83      1  99.44964        3      25
5       115      1  92.74571        4      27
6        98      0 107.90184        1      18
...
```

We will treat `kid_score` as our outcome variable.

Continuous variables

Variables such as `kid_score` and `mom_iq` are *continuous* variables: they are naturally real-valued.

For now we only consider outcome variables that are continuous (like `kid_score`).
Note: even continuous variables can be constrained:

- Both `kid_score` and `mom_iq` must be positive.
- `mom_age` must be a positive integer.

Categorical variables

Other variables take on only finitely many values, e.g.:

- `mom_hs` is 0 (resp., 1) if mom did (resp., did not) attend high school
- `mom_work` is a code that ranges from 1 to 4:
  - $1 =$ did not work in first three years of child's life
  - $2 =$ worked in 2nd or 3rd year of child's life
  - $3 =$ worked part-time in first year of child's life
  - $4 =$ worked full-time in first year of child's life

These are *categorical variables* (or *factors*).

Modeling relationships

Goal:

Find a functional relationship f such that:

$$Y_i \approx f(\mathbf{X}_i)$$

This is our first example of a "model."

We use models for lots of things:

- *Associations* and *correlations*
- *Predictions*
- *Causal relationships*

Linear regression models

Linear relationships

We first focus on modeling the relationship between outcomes and covariates as *linear*.

In other words: find coefficients $\hat{\beta}_0, \dots, \hat{\beta}_p$ such that: [1]

$$Y_i \approx \hat{\beta}_0 + \hat{\beta}_1 X_{i1} + \cdots + \hat{\beta}_p X_{ip}.$$

This is a *linear regression model*.

[1] We use "hats" on variables to denote quantities computed from data. In this case, whatever the coefficients are, they will have to be computed from the data we were given.

Matrix notation

We can compactly represent a linear model using matrix notation:

- Let $\hat{\boldsymbol{\beta}} = [\hat{\beta}_0, \hat{\beta}_1, \cdots \hat{\beta}_p]^\top$ be the $(p+1) \times 1$ column vector of coefficients
- Expand $\mathbf{X}$ to have $p+1$ columns, where the first column (indexed $j = 0$) is $X_{i0} = 1$ for all i.
- Then the linear regression model is that for each i:

$$Y_i \approx \mathbf{X}_i \hat{\boldsymbol{\beta}},$$

or even more compactly

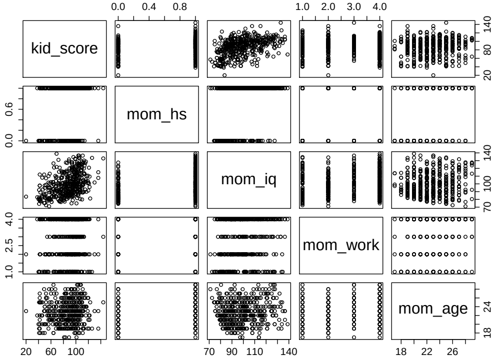
$$\mathbf{Y} \approx \mathbf{X}\hat{\boldsymbol{\beta}}.$$

Matrix notation

A picture of $\mathbf{Y}$, $\mathbf{X}$, and $\hat{\boldsymbol{\beta}}$:

Example in R

Running `pairs(kidiq)` gives us this plot:



Looks like `kid_score` is positively correlated with `mom_iq`.

Example in R

Let's build a simple regression model of `kid_score` against `mom_iq`.

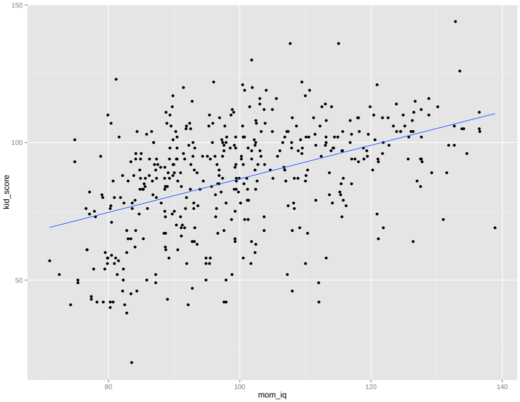
```
> fm = lm(formula = kid_score ~ 1 + mom_iq, data = kidiq)
> display(fm)
lm(formula = kid_score ~ 1 + mom_iq, data = kidiq)
            coef.est coef.se
(Intercept) 25.80     5.92
mom_iq       0.61     0.06
...
```

In other words: `kid_score` $\approx 25.80 + 0.61 \times$ `mom_iq`.

Note: You can get the `display` function and other helpers by installing the `arm` package in R (using `install.packages('arm')`).

Example in R

Here is the model plotted against the data:




```
> library(ggplot2)
> ggplot(data = kidiq, aes(x = mom_iq, y = kid_score)) +
  geom_point() +
  geom_smooth(method="lm", se=FALSE)
```

Note: Install the ggplot2 package using install.packages('ggplot2').

Example in R: Multiple regression

We can include multiple covariates in our linear model.

```
> fm = lm(data = kidiq,
          formula = kid_score ~ 1 + mom_iq + mom_hs)
> display(fm)
lm(formula = kid_score ~ 1 + mom_iq + mom_hs, data = kidiq)
            coef.est coef.se
(Intercept) 25.73    5.88
mom_iq       0.56    0.06
mom_hs       5.95    2.21
```

(Note that the coefficient on `mom_iq` is different now...we will discuss why later.)

How to choose $\hat{\beta}$?

There are many ways to choose $\hat{\boldsymbol{\beta}}$.

We focus primarily on *ordinary least squares* (OLS):

Choose $\hat{\beta}$ so that

$$\text{SSE} = \text{sum of squared errors} = \sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2$$

is minimized, where

$$\hat{Y}_i = \mathbf{X}_i\hat{\boldsymbol{\beta}} = \hat{\beta}_0 + \sum_{i=1}^{p}\hat{\beta}_j X_{ij}$$

is the *fitted* value of the i'th observation.

This is what R (typically) does when you call `lm`.
(Later in the course we develop one justification for this choice.)

Questions to ask

Here are some important questions to be asking:

- Is the resulting model a good fit?
- Does it make sense to use a linear model?
- Is minimizing SSE the right objective?

We start down this road by working through *the algebra of linear regression*.

Ordinary least squares: Solution

OLS solution

From here on out we assume that $p < n$ and $\mathbf{X}$ has *full rank* $= p + 1$.

(What does $p < n$ mean, and why do we need it?)

Theorem
The vector $\hat{\boldsymbol{\beta}}$ *that minimizes* SSE *is given by:*

$$\hat{\boldsymbol{\beta}} = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \mathbf{Y}.$$

(Check that dimensions make sense here: $\hat{\boldsymbol{\beta}}$ is $(p + 1) \times 1$.)

OLS solution: Intuition

The SSE is the squared Euclidean norm of $\mathbf{Y} - \hat{\mathbf{Y}}$:

$$\mathsf{SSE} = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 = \|\mathbf{Y} - \hat{\mathbf{Y}}\|^2 = \|\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}\|^2.$$

Note that as we vary $\hat{\boldsymbol{\beta}}$ we range over *linear combinations of the columns of* $\mathbf{X}$.

The collection of all such linear combinations is the *subspace* spanned by the columns of $\mathbf{X}$.

So the linear regression question is

What is the "closest" such linear combination to $\mathbf{Y}$*?*

OLS solution: Geometry

OLS solution: Algebraic proof [$*$]

Based on [SM], Exercise 3B14:

- Observe that $\mathbf{X}^\top\mathbf{X}$ is symmetric and invertible. (Why?)
- Note that: $\mathbf{X}^\top\hat{\mathbf{r}} = 0$, where $\hat{\mathbf{r}} = \mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}$ is the vector of *residuals*.
  In other words: *the residual vector is orthogonal to every column of $\mathbf{X}$.*
- Now consider any vector $\boldsymbol{\gamma}$ that is $(p+1)\times 1$. Note that: $\mathbf{Y} - \mathbf{X}\boldsymbol{\gamma} = \hat{\mathbf{r}} + \mathbf{X}(\hat{\boldsymbol{\beta}} - \boldsymbol{\gamma})$.
- Since $\hat{\mathbf{r}}$ is orthogonal to $\mathbf{X}$, we get:

$$\|\mathbf{Y} - \mathbf{X}\boldsymbol{\gamma}\|^2 = \|\hat{\mathbf{r}}\|^2 + \|\mathbf{X}(\hat{\boldsymbol{\beta}} - \boldsymbol{\gamma})\|^2.$$

- The preceding value is minimized when $\mathbf{X}(\hat{\boldsymbol{\beta}} - \boldsymbol{\gamma}) = 0$.
- Since $\mathbf{X}$ has rank $p+1$, the preceding equation has the unique solution $\boldsymbol{\gamma} = \hat{\boldsymbol{\beta}}$.

Hat matrix (useful for later) [$*$]

Since: $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{Y}$, we have:

$$\hat{\mathbf{Y}} = \mathbf{H}\mathbf{Y},$$

where:

$$\mathbf{H} = \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top.$$

$\mathbf{H}$ is called the *hat* matrix.
It *projects* $\mathbf{Y}$ into the subspace spanned by the columns of $\mathbf{X}$.
It is symmetric and *idempotent* ($\mathbf{H}^2 = \mathbf{H}$).

Residuals and R^2

Residuals

Let $\hat{\mathbf{r}} = \mathbf{Y} - \hat{\mathbf{Y}} = \mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}$ be the vector of *residuals*.

Our analysis shows us that: $\hat{\mathbf{r}}$ *is orthogonal to every column of* $\mathbf{X}$.

In particular, $\hat{\mathbf{r}}$ is orthogonal to the all 1's vector
(first column of $\mathbf{X}$), so:

$$\overline{Y} = \frac{1}{n}\sum_{i=1}^{n} Y_i = \frac{1}{n}\sum_{i=1}^{n} \hat{Y}_i = \overline{\hat{Y}}.$$

In other words, *the residuals sum to zero*, and
the original and fitted values have the same sample mean.

Residuals

Since $\hat{\mathbf{r}}$ is orthogonal to every column of $\mathbf{X}$,
we use the Pythagorean theorem to get:

$$\|\mathbf{Y}\|^2 = \|\hat{\mathbf{r}}\|^2 + \|\hat{\mathbf{Y}}\|^2.$$

Using equality of sample means we get:

$$\|\mathbf{Y}\|^2 - n\overline{Y}^2 = \|\hat{\mathbf{r}}\|^2 + \|\hat{\mathbf{Y}}\|^2 - n\overline{\hat{Y}}^2.$$

Residuals

How do we interpret:

$$\|\mathbf{Y}\|^2 - n\overline{Y}^2 = \|\hat{\mathbf{r}}\|^2 + \|\hat{\mathbf{Y}}\|^2 - n\overline{\hat{Y}}^2 \ ?$$

Note $\frac{1}{n-1}(\|\mathbf{Y}\|^2 - n\overline{Y}^2)$ is the *sample variance of* $\mathbf{Y}$. [2]

Note $\frac{1}{n-1}(\|\hat{\mathbf{Y}}\|^2 - n\overline{\hat{Y}}^2)$ is the *sample variance of* $\hat{\mathbf{Y}}$.

So this relation suggests how much of the variation in $\mathbf{Y}$ is "explained" by $\hat{\mathbf{Y}}$.

[2] Note that the (adjusted) sample variance is usually defined as $\frac{1}{n-1}\sum_{i=1}^{n}(Y_i - \overline{Y})^2$. You should check this is equal to the expression on the slide!

R^2

Formally:

$$R^2 = \frac{\sum_{i=1}^n (\hat{Y}_i - \overline{\hat{Y}})^2}{\sum_{i=1}^n (Y_i - \overline{Y})^2}$$

is a measure of the *fit* of the model, with $0 \leq R^2 \leq 1$.[3]

When R^2 is large, much of the outcome sample variance is "explained" by the fitted values.

Note that R^2 is an *in-sample* measurement of fit:

We used the data itself to construct a fit to the data.

[3]Note that this result depends on $\overline{Y} = \overline{\hat{Y}}$, which in turn depends on the fact that the all 1's vector is part of $\mathbf{X}$, i.e., that our linear model has an intercept term.

Example in R

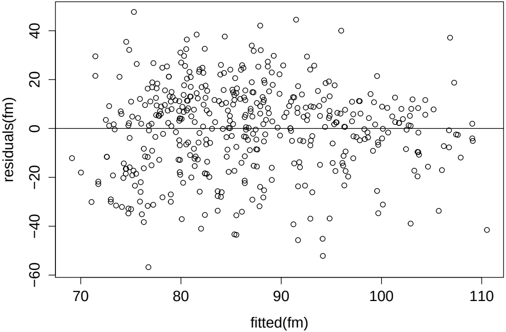
The full output of our model earlier includes R^2:

```
> fm = lm(data = kidiq, formula = kid_score ~ 1 + mom_iq)
> display(fm)
lm(formula = kid_score ~ 1 + mom_iq, data = kidiq)
            coef.est coef.se
(Intercept) 25.80     5.92
mom_iq       0.61     0.06
---
n = 434, k = 2
residual sd = 18.27, R-Squared = 0.20
```

Note: `residual sd` is the sample standard deviation of the residuals.

Example in R

We can plot the residuals for our earlier model:




```
> fm = lm(data = kidiq, formula = kid_score ~ 1 + mom_iq)
> plot(fitted(fm), residuals(fm))
> abline(0,0)
```

Note: We generally plot residuals against *fitted* values, not the original outcomes. You will investigate why on your next problem set.

Questions

- What do you hope to see when you plot the residuals?
- Why might R^2 be high, yet the model fit poorly?
- Why might R^2 be low, and yet the model be useful?
- What happens to R^2 if we add additional covariates to the model?