Summarizing a sample
A sample

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

- **Sample mean:**

\[
\bar{Y} = \frac{1}{n} \sum_{i=1}^{n} Y_i.
\]
A sample

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

- **Sample mean:**
  
  $$\overline{Y} = \frac{1}{n} \sum_{i=1}^{n} Y_i.$$

- **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:**

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

Measures dispersion of the data.
(Why \( n - 1 \)? See first problem set.)
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 $Y$ and $X$?

\[
\begin{bmatrix}
Y_1 \\
\vdots \\
Y_i \\
\vdots \\
Y_n
\end{bmatrix} = 
\begin{bmatrix}
X_{i1} & \cdots & X_{ip} \\
X_{i1} & \cdots & X_{ip} \\
\vdots & \cdots & \vdots \\
X_{i1} & \cdots & X_{ip}
\end{bmatrix} \rightarrow X
\]

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*

$X$ 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

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*).
Goal:

Find a functional relationship \( f \) such that:

\[
Y_i \approx f(X_i)
\]

This is our first example of a “model.”

We use models for lots of things:

- Associations and correlations
- Predictions
- Causal relationships
Linear regression models
We first focus on modeling the relationship between outcomes and covariates as *linear*.

In other words: find coefficients $\hat{\beta}_0, \ldots, \hat{\beta}_p$ such that: 

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

This is a *linear regression model*.

---

1We 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 \( \hat{\beta} = [\hat{\beta}_0, \hat{\beta}_1, \cdots, \hat{\beta}_p]^\top \) be the \((p + 1) \times 1\) column vector of coefficients.

- Expand \( X \) 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 \( i \):

\[
Y_i \approx X_i \hat{\beta},
\]

or even more compactly

\[
Y \approx X \hat{\beta}.
\]
Matrix notation

\[ Y_i = \hat{\beta}_0 + \hat{\beta}_1 X_{i1} + \cdots + \hat{\beta}_p X_{ip} \]

A picture of \( Y, X, \) and \( \hat{\beta} \):
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`.

```r
> 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:

```r
> 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.

```r
> 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 $\hat{\beta}$.

We focus primarily on ordinary least squares (OLS):

Choose $\hat{\beta}$ so that

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

is minimized, where

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

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
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 $\hat{\beta}$ that minimizes SSE is given by:*

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

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

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

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

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

\[ y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} \]

\[
\begin{bmatrix}
  y_1 \\
  \vdots \\
  y_n
\end{bmatrix} = 
\begin{bmatrix}
  1 & x_{11} & \cdots & x_{1p} \\
  \vdots & \vdots & \ddots & \vdots \\
  1 & x_{n1} & \cdots & x_{np}
\end{bmatrix}
\begin{bmatrix}
  \beta_0 \\
  \beta_1 \\
  \vdots \\
  \beta_p
\end{bmatrix}
\]

all linear comb of cols of X

(residuals) \[ \bar{y} \]
OLS solution: Algebraic proof

Based on [SM], Exercise 3B14:

- Observe that $\mathbf{X}^\top \mathbf{X}$ is symmetric and invertible.
- Note that: $\mathbf{X}^\top \hat{\mathbf{r}} = 0$, where $\hat{\mathbf{r}} = \mathbf{Y} - \mathbf{X} \hat{\mathbf{\beta}}$ is the vector of residuals.

In other words: the residual vector is orthogonal to every column of $\mathbf{X}$.

- Now consider any vector $\mathbf{\gamma}$ that is $(p + 1) \times 1$. Note that:
  $\mathbf{Y} - \mathbf{X} \mathbf{\gamma} = \hat{\mathbf{r}} + \mathbf{X}(\hat{\mathbf{\beta}} - \mathbf{\gamma})$.

- Since $\hat{\mathbf{r}}$ is orthogonal to $\mathbf{X}$, we get:
  $$\| \mathbf{Y} - \mathbf{X} \mathbf{\gamma} \|^2 = \| \hat{\mathbf{r}} \|^2 + \| \mathbf{X}(\hat{\mathbf{\beta}} - \mathbf{\gamma}) \|^2.$$  

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

Hat matrix (useful for later)

Since: $\hat{Y} = X\hat{\beta} = X(X^TX)^{-1}X^TY$, we have:

$$\hat{Y} = HY,$$

where:

$$H = X(X^TX)^{-1}X^T.$$

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

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

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

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

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

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

$$\sum_i (1 \ldots 1) = 0 \Rightarrow \sum_i Y_i - \hat{Y}_i = 0$$
Residuals

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

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

Using equality of sample means we get:

$$||Y||^2 - \bar{Y}^2 = ||\hat{r}||^2 + ||\hat{Y}||^2 - \bar{Y}_\hat{r}^2.$$
Residuals

How do we interpret:

\[ \| \mathbf{Y} \|^2 - \bar{\mathbf{Y}}^2 = \| \mathbf{r} \|^2 + \| \hat{\mathbf{Y}} \|^2 - \bar{\hat{\mathbf{Y}}}^2 \]

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

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

So this relation suggests how much of the variation in \( \mathbf{Y} \) is “explained” by \( \hat{\mathbf{Y}} \).
Formally:

\[ R^2 = \frac{\sum_{i=1}^{n} (\hat{Y}_i - \bar{Y})^2}{\sum_{i=1}^{n} (Y_i - \bar{Y})^2} \]

is a measure of the fit of the model.

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.*
Example in R

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

```r
> 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:

```r
> 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?