14. Algebra of Least Squares

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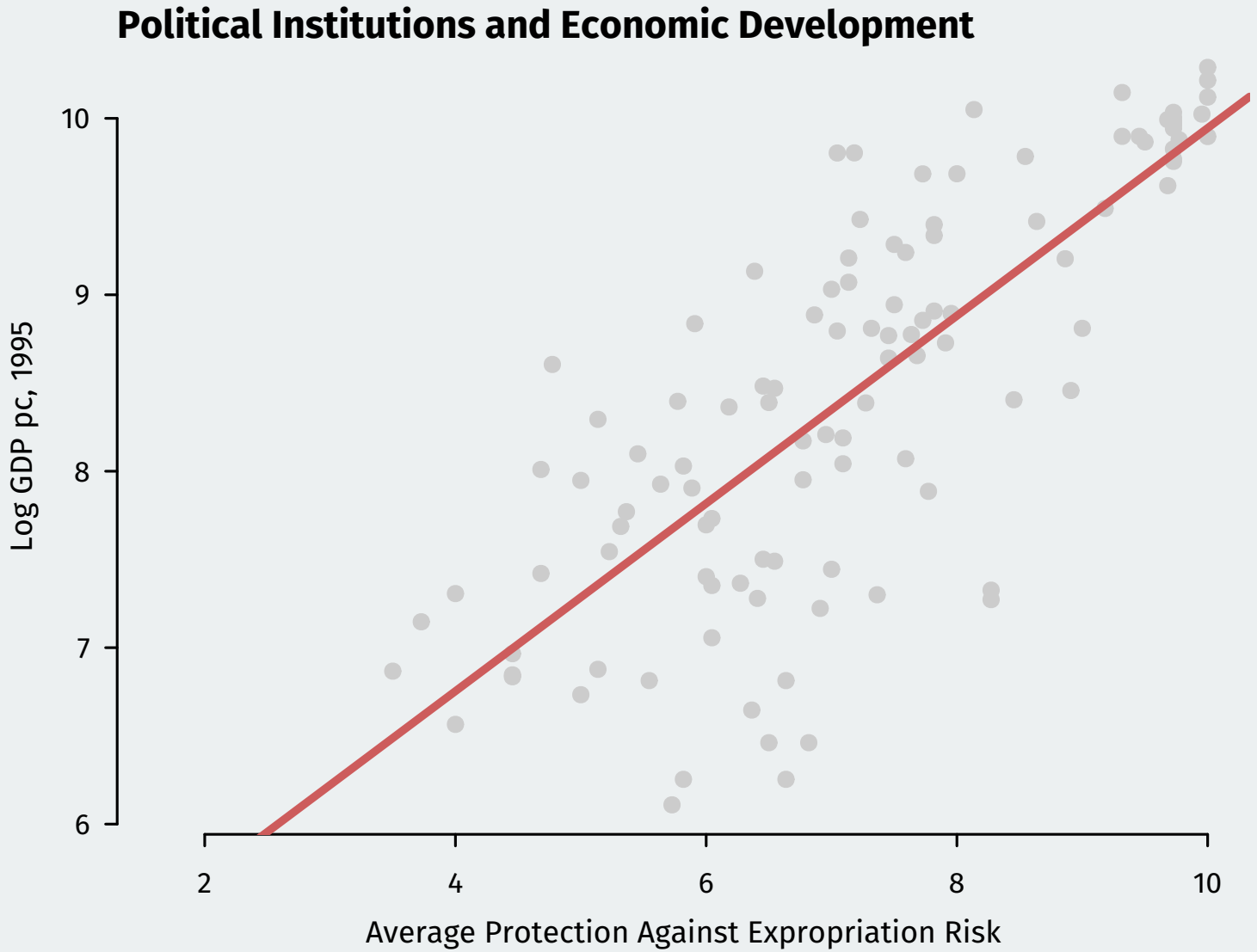
Gov 2002 (Harvard)

Where are we? Where are we going?

- We saw how the population linear projection works.
- How can we estimate the parameters of the linear projection or CEF?
- Now: least squares estimator and its algebraic properties.
- After that: the statistical properties of least squares.

Acemoglu, Johnson, and Robinson (2001)



Samples vs population

Assumption

The variables $\{(Y_1, \mathbf{X}_1), \ldots, (Y_i, \mathbf{X}_i), \ldots, (Y_n, \mathbf{X}_n)\}$ are i.i.d. draws from a common distribution F.

- F is the **population distribution** or **DGP**.
  - Without i subscripts, $(Y, \mathbf{X})$ are r.v.s and draws from F.
- $\{(Y_i, \mathbf{X}_i) : i = 1, \ldots, n\}$ is the **sample** and can be seen in two ways:
  - Numbers in your data matrix, fixed to the analyst.
  - From a statistical POV, they are realizations of a random process.
- Violations include time-series data and clustered sampling.
  - Weakening i.i.d. usually complicates notation but can be done.

Quantity of interest

- Population linear projection model:

$$Y = \mathbf{X}'\boldsymbol{\beta} + e$$

- Here $\boldsymbol{\beta}$ minimizes the **population** expected squared error:

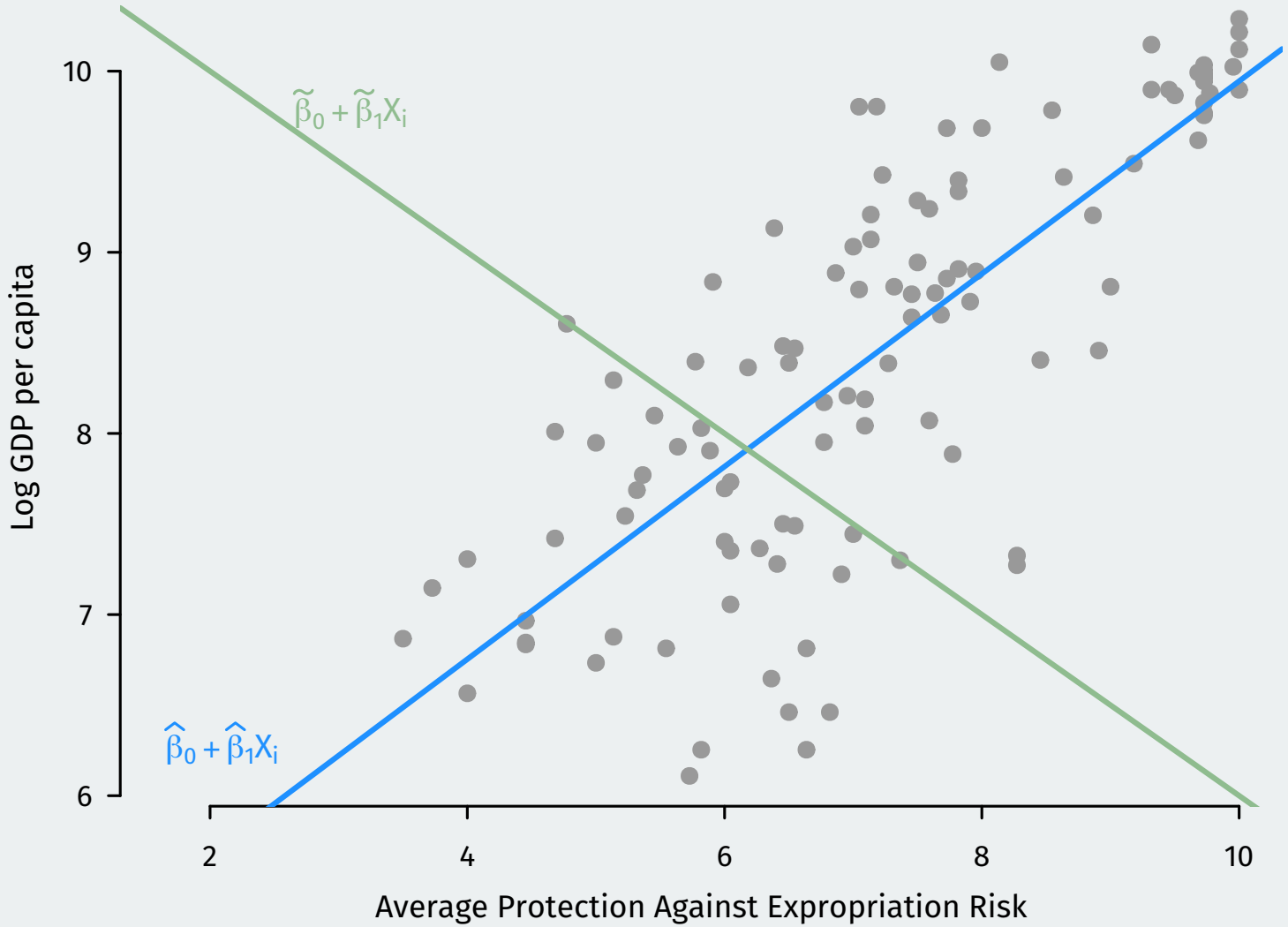
$$\boldsymbol{\beta} = \underset{\mathbf{b}\in\mathbb{R}^k}{\arg\min}\, S(\mathbf{b}), \qquad S(\mathbf{b}) = \mathbb{E}\left[(Y - \mathbf{X}'\mathbf{b})^2\right]$$

- Last time we saw that this can be written:

$$\boldsymbol{\beta} = \left(\mathbb{E}[\mathbf{X}\mathbf{X}']\right)^{-1}\mathbb{E}[\mathbf{X}Y]$$

- How do we estimate $\boldsymbol{\beta}$?

Which line is better?



Plug-in principle returns!

- **Plug-in estimator**: solve the sample version of the population goal.
- Replace projection errors with observed errors, or **residuals**: $Y_i - \mathbf{X}_i'\mathbf{b}$
  - **Sum of squared residuals**, $SSR(\mathbf{b}) = \sum_{i=1}^{n}(Y_i - \mathbf{X}_i'\mathbf{b})^2$.
  - Total prediction error using $\mathbf{b}$ as our estimated coefficient.
- We can use these residuals to get a sample average prediction error:

$$\hat{S}(\mathbf{b}) = \frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \mathbf{X}_i'\mathbf{b}\right)^2 = \frac{1}{n}SSR(\mathbf{b})$$

- $\hat{S}(\mathbf{b})$ is an estimator of the expected squared error, $S(\mathbf{b})$.

Least squares estimator

- **Ordinary least squares estimator** minimizes $\hat{S}$ in place of S.

$$\boldsymbol{\beta} = \arg\min_{\mathbf{b} \in \mathbb{R}^k} \mathbb{E}\left[\left(Y - \mathbf{X}'\mathbf{b} \right)^2 \right]$$

$$\hat{\boldsymbol{\beta}} = \arg\min_{\mathbf{b} \in \mathbb{R}^k} \frac{1}{n} \sum_{i=1}^{n} \left(Y_i - \mathbf{X}_i'\mathbf{b} \right)^2$$

  - In words: find the coefficients that minimize the sum/average of the squared residuals.

- After some calculus, we can write this as a plug-in estimator:

$$\hat{\boldsymbol{\beta}} = \left(\frac{1}{n} \sum_{i=1}^{n} \mathbf{X}_i \mathbf{X}_i' \right)^{-1} \left(\frac{1}{n} \sum_{i=1}^{n} \mathbf{X}_i Y_i \right)$$

  - $n^{-1} \sum_{i=1}^{n} \mathbf{X}_i \mathbf{X}_i'$ is the sample version of $\mathbb{E}[\mathbf{X}\mathbf{X}']$
  - $n^{-1} \sum_{i=1}^{n} \mathbf{X}_i Y_i$ is the sample version of $\mathbb{E}[\mathbf{X}Y]$

Bivariate regressions

- **Bivariate regression** is the linear projection model with $\mathbf{X} = (1, X)$:

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

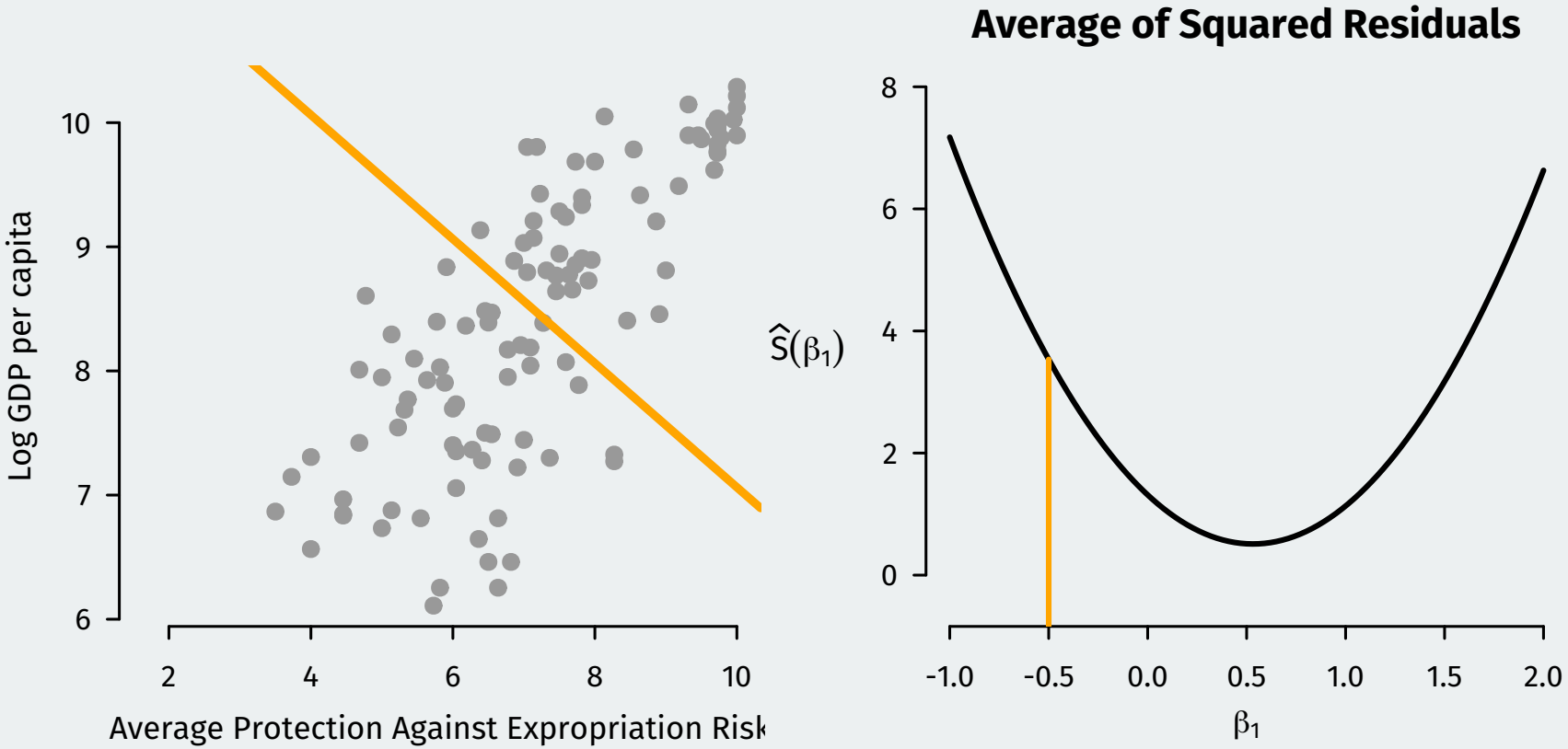
- Linear projection slope in the population from last times:

$$\beta_1 = \frac{\text{Cov}(X, Y)}{\mathbb{V}[X]}$$

- We can show the OLS estimator of the slope is:

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(Y_i - \overline{Y})(X_i - \overline{X})}{\sum_{i=1}^{n}(X_i - \overline{X})^2} = \frac{\widehat{\text{Cov}}(X, Y)}{\hat{\mathbb{V}}[X]}$$

Visualizing OLS



Residuals

- **Fitted value** $\widehat{Y}_i = \mathbf{X}_i'\hat{\boldsymbol{\beta}}$ is what the model predicts at $\mathbf{X}_i$
  - Not really a prediction for Y_i since that was used to generate $\hat{\boldsymbol{\beta}}$
- **Residuals** are the difference between observed and fitted values:

$$\hat{e}_i = Y_i - \widehat{Y}_i = Y_i - \mathbf{X}_i'\hat{\boldsymbol{\beta}}$$

  - We can write $Y_i = \mathbf{X}_i'\hat{\boldsymbol{\beta}} + \hat{e}_i$.
  - $\hat{e}_i$ are not the true errors e_i
- Key **mechanical properties** of OLS residuals:

$$\sum_{i=1}^{n} \mathbf{X}_i \hat{e}_i = 0$$

  - Sample covariance between $\mathbf{X}_i$ and $\hat{e}_i$ is 0.
  - If $\mathbf{X}_i$ has a constant, then $n^{-1}\sum_{i=1}^{n} \hat{e}_i = 0$

Prediction error

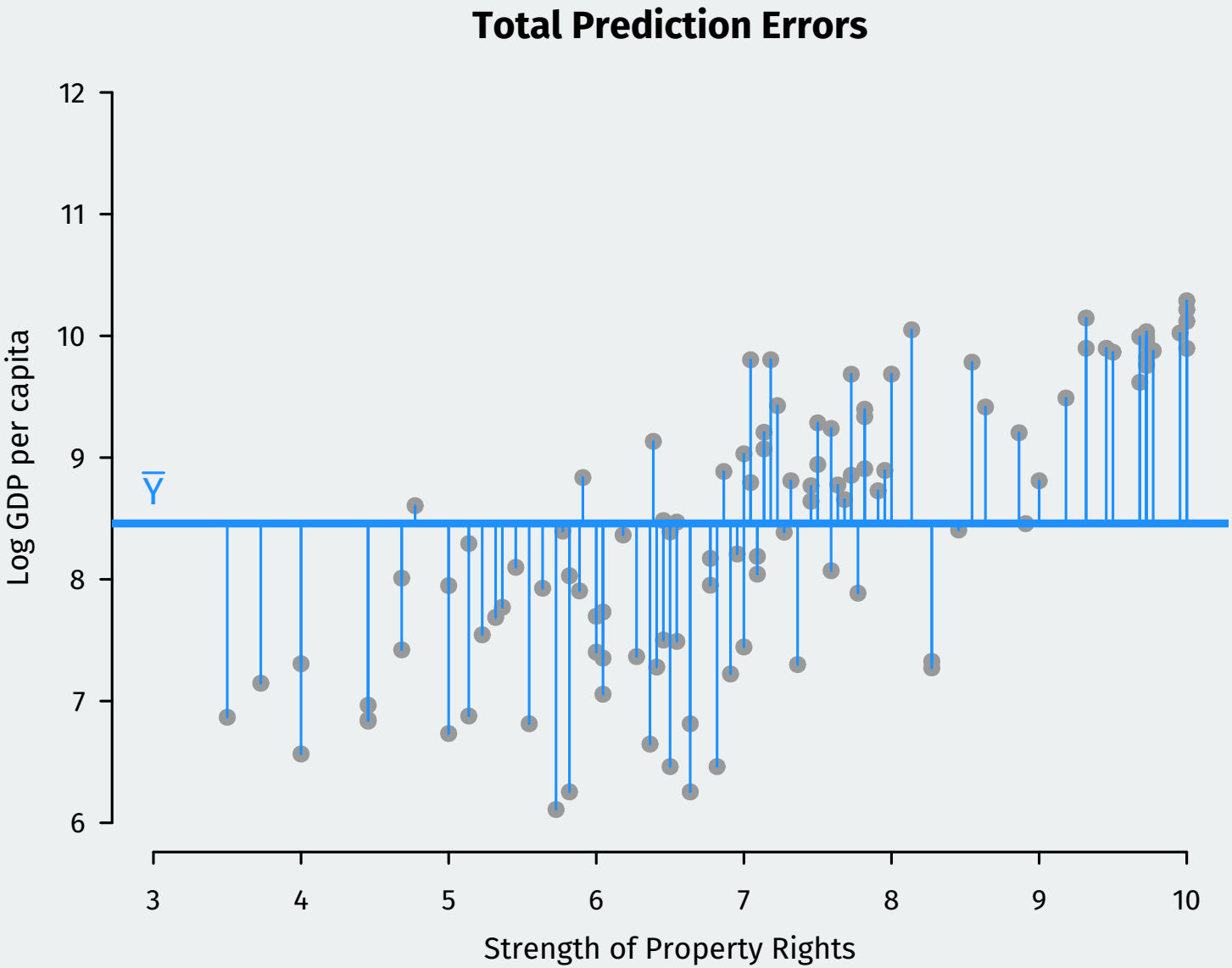
- How do we judge how well a regression fits the data?
- How much does $\mathbf{X}_i$ help us predict Y_i?
- **Prediction errors without $\mathbf{X}_i$**:
  - Best prediction is the mean, $\overline{Y}$
  - Prediction error is called the total sum of squares (SST) would be:

$$SST = \sum_{i=1}^{n} (Y_i - \overline{Y})^2$$

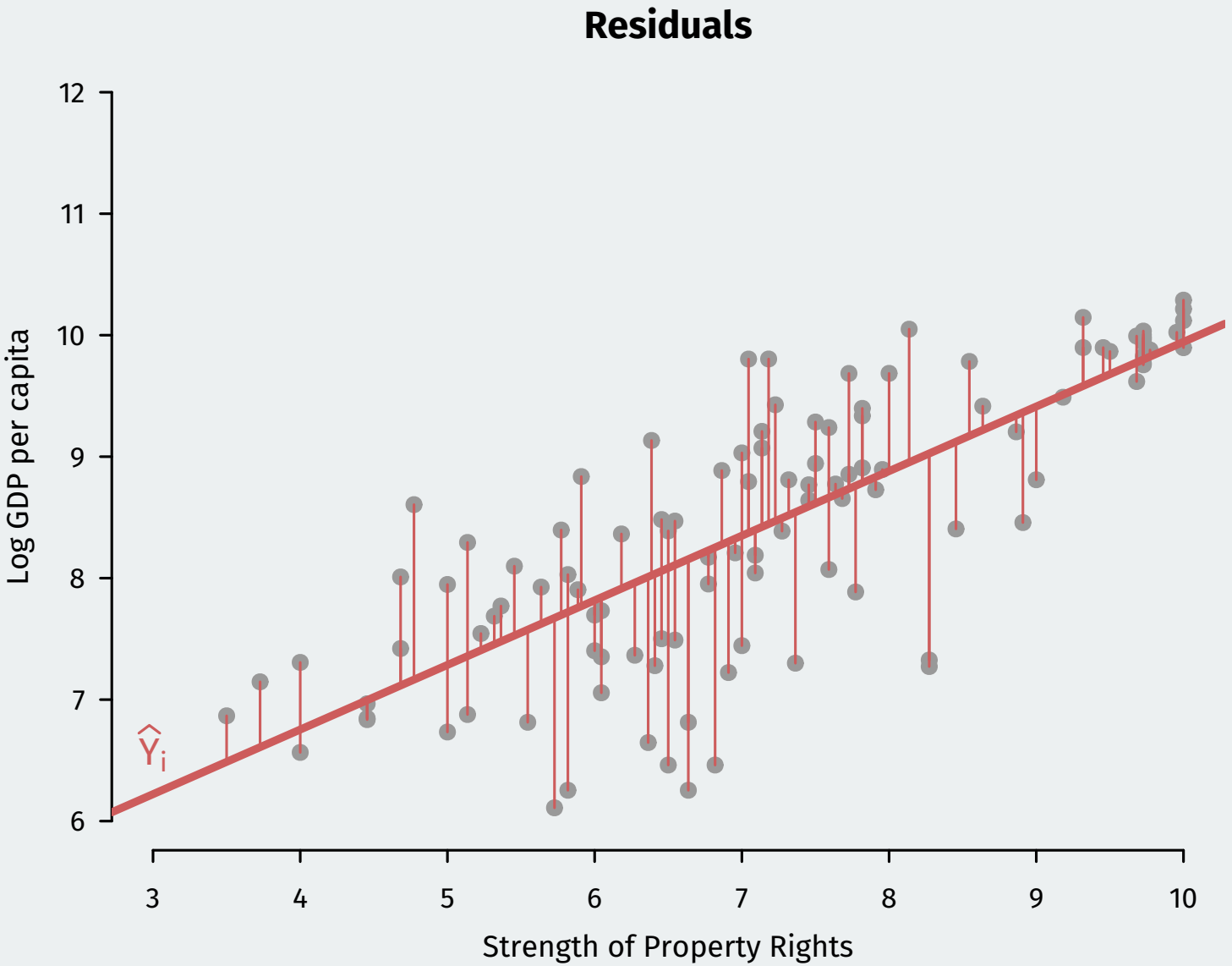
- **Prediction errors with $\mathbf{X}_i$**:
  - Best predictions are the fitted values, $\widehat{Y}_i$.
  - Prediction error is the the sum of the squared residuals or SSR:

$$SSR = \sum_{i=1}^{n} (Y_i - \widehat{Y}_i)^2$$

Total SS vs SSR



Total SS vs SSR



R-squared

- Regression will always improve in-sample fit: $SST > SSR$
- How much better does using $\mathbf{X}_i$ do? **Coefficient of determination** or R^2:

$$R^2 = \frac{SST - SSR}{SST} = 1 - \frac{SSR}{SST}$$

- $R^2 =$ fraction of the total prediction error eliminated by using $\mathbf{X}_i$.
- **Common interpretation:** R^2 is the fraction of the variation in Y_i is "explained by" $\mathbf{X}_i$.
    - $R^2 = 0$ means no relationship
    - $R^2 = 1$ implies perfect linear fit
- Mechanically increases with additional covariates (better fit measures exist)

Linear model in matrix form

- Linear model is a system of n linear equations:

$$\begin{aligned} Y_1 &= \mathbf{X}_1'\boldsymbol{\beta} + e_1 \\ Y_2 &= \mathbf{X}_2'\boldsymbol{\beta} + e_2 \\ &\vdots \\ Y_n &= \mathbf{X}_n'\boldsymbol{\beta} + e_n \end{aligned}$$

- We can write this more compactly using matrices and vectors:

$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}, \quad \mathbb{X} = \begin{pmatrix} \mathbf{X}_1' \\ \mathbf{X}_2' \\ \vdots \\ \mathbf{X}_n' \end{pmatrix} = \begin{pmatrix} 1 & X_{11} & X_{12} & \cdots & X_{1k} \\ 1 & X_{21} & X_{22} & \cdots & X_{2k} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & X_{n1} & X_{n2} & \cdots & X_{nk} \end{pmatrix}, \quad \mathbf{e} = \begin{pmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{pmatrix}$$

- Model is now just:

$$\mathbf{Y} = \mathbb{X}\boldsymbol{\beta} + \mathbf{e}$$

OLS estimator in matrix form

- Key relationship: sample sums can be written in matrix notation:

$$\sum_{i=1}^{n} \mathbf{X}_i \mathbf{X}_i' = \mathbb{X}'\mathbb{X}$$

$$\sum_{i=1}^{n} \mathbf{X}_i Y_i' = \mathbb{X}'\mathbf{Y}$$

- Implies we can write the OLS estimator as

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

- Residuals:

$$\hat{\mathbf{e}} = \mathbf{Y} - \mathbb{X}\hat{\boldsymbol{\beta}} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} - \begin{bmatrix} 1\hat{\beta}_0 + X_{11}\hat{\beta}_1 + X_{12}\hat{\beta}_2 + \cdots + X_{1k}\hat{\beta}_k \\ 1\hat{\beta}_0 + X_{21}\hat{\beta}_1 + X_{22}\hat{\beta}_2 + \cdots + X_{2k}\hat{\beta}_k \\ \vdots \\ 1\hat{\beta}_0 + X_{n1}\hat{\beta}_1 + X_{n2}\hat{\beta}_2 + \cdots + X_{nk}\hat{\beta}_k \end{bmatrix}$$

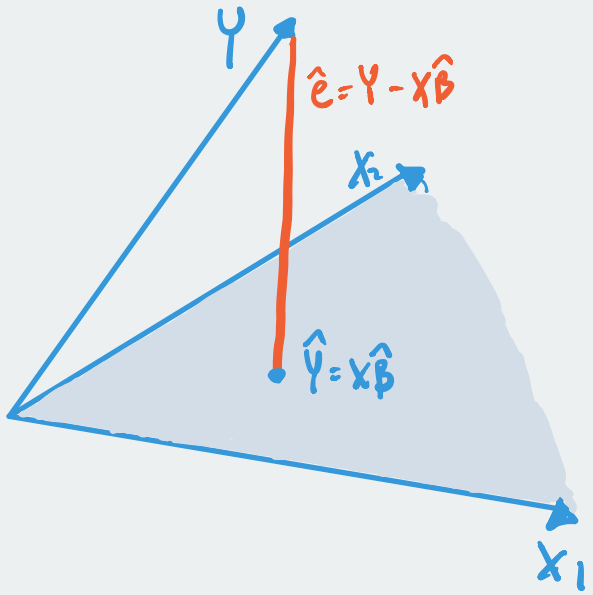
Least squares in matrix form

- OLS still minimizes sum of the squared residuals

$$\underset{\mathbf{b}\in\mathbb{R}^{k+1}}{\arg\min}\, \hat{\mathbf{e}}'\hat{\mathbf{e}} = \underset{\mathbf{b}\in\mathbb{R}^{k+1}}{\arg\min} (\mathbf{Y} - \mathbb{X}\mathbf{b})'(\mathbf{Y} - \mathbb{X}\mathbf{b})$$

- We can write the covariate-residual orthogonality as $\mathbb{X}'\hat{\mathbf{e}} = 0$.

Projection



- OLS can be seen as a projection of **Y** onto the column space of $\mathbb{X}$, $\mathcal{S}(\mathbb{X})$.
  - Picture with $n = 3$ and $k = 2$: points in 3D space,
  - Column space of $\mathbb{X}$ is a plane in this space.
- Intuition: $\hat{\boldsymbol{\beta}}$ defines the projection that gets is shortest distance between Y and prediction.

Projection/hat matrix

- There are a couple of very important matrices in OLS algebra.
- **Projection matrix** $\mathbf{P} = \mathbb{X}(\mathbb{X}'\mathbb{X})^{-1}\mathbb{X}'$
- Also called the **hat matrix** it puts the "hat" on $\mathbf{Y}$:

$$\mathbf{PY} = \mathbb{X}(\mathbb{X}'\mathbb{X})^{-1}\mathbb{X}'\mathbf{Y} = \mathbb{X}\hat{\boldsymbol{\beta}} = \widehat{\mathbf{Y}}$$

- Key properties:
  - $\mathbf{P}$ is an $n \times n$ symmetric matrix
  - $\mathbf{P}$ is **idempotent**: $\mathbf{PP} = \mathbf{P}$
  - Projecting $\mathbb{X}$ onto itself returns itself: $\mathbf{P}\mathbb{X} = \mathbb{X}$

Annihilator matrix

- **Annihilator matrix** projects onto the space spanned by the residual:

$$\mathbf{M} = \mathbf{I}_n - \mathbf{P} = \mathbf{I}_n - \mathbb{X}(\mathbb{X}'\mathbb{X})^{-1}\mathbb{X}'$$

- Also called the **residual maker**:

$$\mathbf{MY} = (\mathbf{I}_n - \mathbf{P})\mathbf{Y} = \mathbf{Y} - \mathbf{PY} = \mathbf{Y} - \widehat{\mathbf{Y}} = \mathbf{e}$$

- "Annihilates" any function in the column space of $\mathbb{X}$, $\mathcal{S}(\mathbb{X})$:

$$\mathbf{M}\mathbb{X} = (\mathbf{I}_n - \mathbf{P})\mathbb{X} = \mathbb{X} - \mathbf{P}\mathbb{X} = \mathbb{X} - \mathbb{X} = 0$$

- Properties:
  - $\mathbf{M}$ is a symmetric $n \times n$ matrix.
  - $\mathbf{M}$ is idempotent so that $\mathbf{MM} = \mathbf{M}$
  - Admits a nice expression for the residual vector: $\hat{\mathbf{e}} = \mathbf{Me}$

Partitioned regression

- Partition covariates and coefficients $\mathbb{X} = [\mathbb{X}_1 \ \mathbb{X}_2]$ and $\boldsymbol{\beta} = (\boldsymbol{\beta}_1, \boldsymbol{\beta}_2)'$:

$$\mathbf{Y} = \mathbb{X}_1\boldsymbol{\beta}_1 + \mathbb{X}_2\boldsymbol{\beta}_2 + \mathbf{e}$$

- Can we find expressions for $\hat{\boldsymbol{\beta}}_1$ and $\hat{\boldsymbol{\beta}}_2$?
- We can find $\hat{\boldsymbol{\beta}}_1$ by nested minimization:

$$\hat{\boldsymbol{\beta}}_1 = \arg\min_{\boldsymbol{\beta}_1} \left(\min_{\boldsymbol{\beta}_2} (\mathbf{Y} - \mathbb{X}_1\boldsymbol{\beta}_1 - \mathbb{X}_2\boldsymbol{\beta}_2)' (\mathbf{Y} - \mathbb{X}_1\boldsymbol{\beta}_1 - \mathbb{X}_2\boldsymbol{\beta}_2) \right)$$

  - First find the minimum of the sum of the squared residuals over $\boldsymbol{\beta}_2$ fixing $\boldsymbol{\beta}_1$
  - Then find $\boldsymbol{\beta}_1$ that minimizes the resulting SSR.

Partitioned regression results

- The projection and annihilator matrices are defined only by covariates.
  - $\mathbf{M}_1 = \mathbf{I}_n - \mathbb{X}_1(\mathbb{X}_1'\mathbb{X}_1)^{-1}\mathbb{X}_1'$
  - $\mathbf{M}_2 = \mathbf{I}_n - \mathbb{X}_2(\mathbb{X}_2'\mathbb{X}_2)^{-1}\mathbb{X}_2'$
  - Creates residuals from a regression on $\mathbb{X}_1$ or $\mathbb{X}_2$
- Solving the nested minimization gives:

$$\hat{\boldsymbol{\beta}}_1 = \left(\mathbb{X}_1'\mathbf{M}_2\mathbb{X}_1\right)^{-1}\left(\mathbb{X}_1'\mathbf{M}_2\mathbf{Y}\right)$$
$$\hat{\boldsymbol{\beta}}_2 = \left(\mathbb{X}_2'\mathbf{M}_1\mathbb{X}_2\right)^{-1}\left(\mathbb{X}_2'\mathbf{M}_1\mathbf{Y}\right)$$

- When will $\hat{\boldsymbol{\beta}}_1$ will be the same regardless of whether $\mathbb{X}_2$ is included?
  - If $\mathbb{X}_1$ and $\mathbb{X}_2$ are orthogonal so $\mathbb{X}_2'\mathbb{X}_1 = 0$ so $\mathbf{M}_2\mathbb{X}_1 = \mathbb{X}_1$

Residual regression

- Define two sets of residuals:
  - $\widetilde{\mathbb{X}}_2 = \mathbf{M}_1\mathbb{X}_2$ = residuals from regression of $\mathbb{X}_2$ on $\mathbb{X}_1$
  - $\tilde{\mathbf{e}}_1 = \mathbf{M}_1\mathbf{Y}$ = residuals from regression of $\mathbf{Y}$ on $\mathbb{X}_1$.
- Then remembering that $\mathbf{M}_1$ is symmetric and idempotent:

$$\begin{aligned}\hat{\boldsymbol{\beta}}_2 &= \left(\mathbb{X}_2'\mathbf{M}_1\mathbb{X}_2\right)^{-1}\left(\mathbb{X}_2'\mathbf{M}_1\mathbf{Y}\right) \\ &= \left(\mathbb{X}_2'\mathbf{M}_1\mathbf{M}_1\mathbb{X}_2\right)^{-1}\left(\mathbb{X}_2'\mathbf{M}_1\mathbf{M}_1\mathbf{Y}\right) \\ &= \left(\widetilde{\mathbb{X}}_2'\widetilde{\mathbb{X}}_2\right)^{-1}\left(\widetilde{\mathbb{X}}_2'\tilde{\mathbf{e}}_1\right)\end{aligned}$$

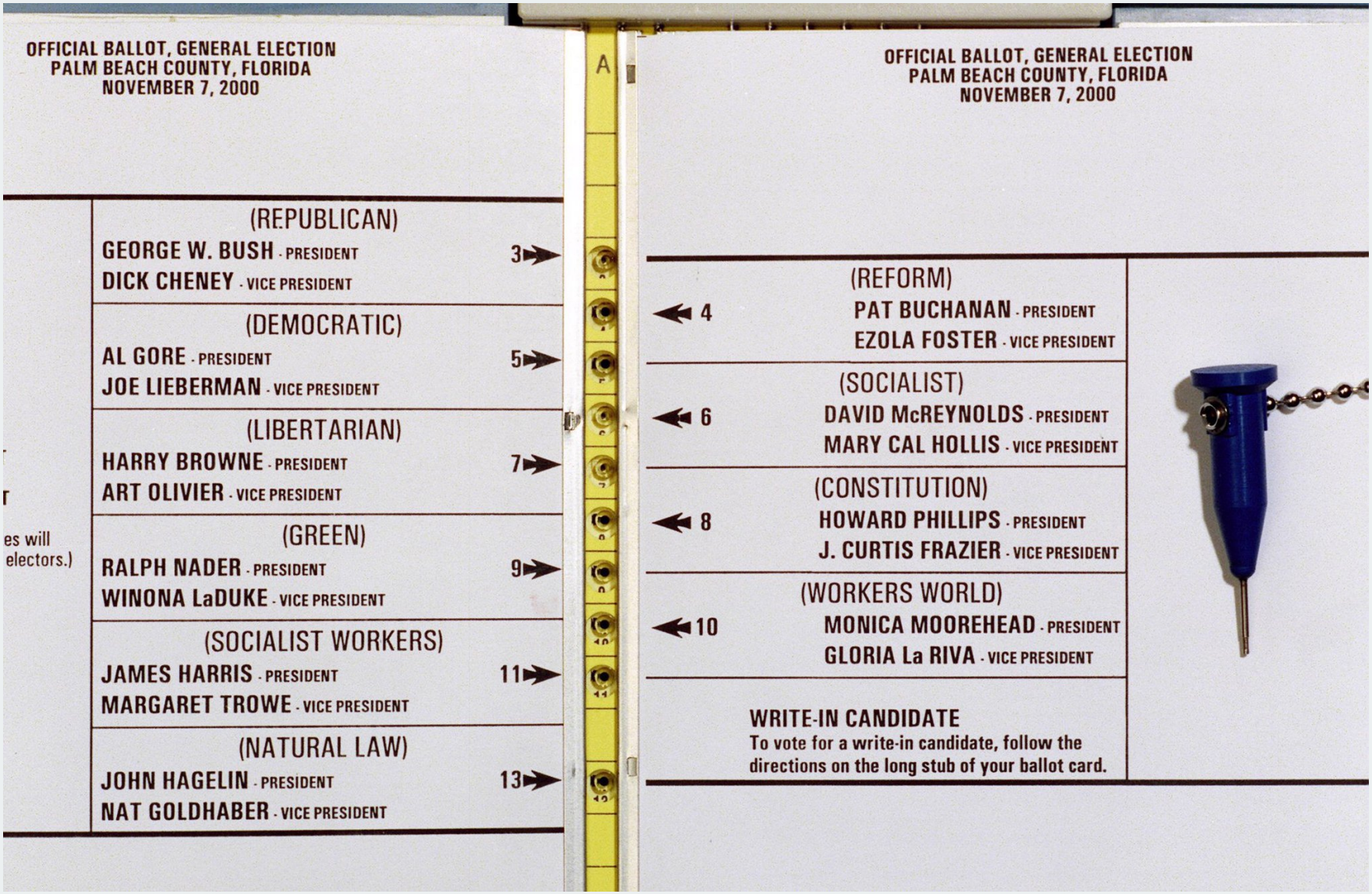
- $\hat{\boldsymbol{\beta}}_2$ can be obtained from a regression of $\tilde{\mathbf{e}}_1$ on $\widetilde{\mathbb{X}}_2$.
  - Same result applies when using $\mathbf{Y}$ in place of $\tilde{\mathbf{e}}_1$.
  - Intuition: residuals are orthogonal
  - Called the **Frisch-Waugh-Lovell Theorem**
  - Sample version of the results we saw for the linear projection.

Outliers, leverage points, and influential observations

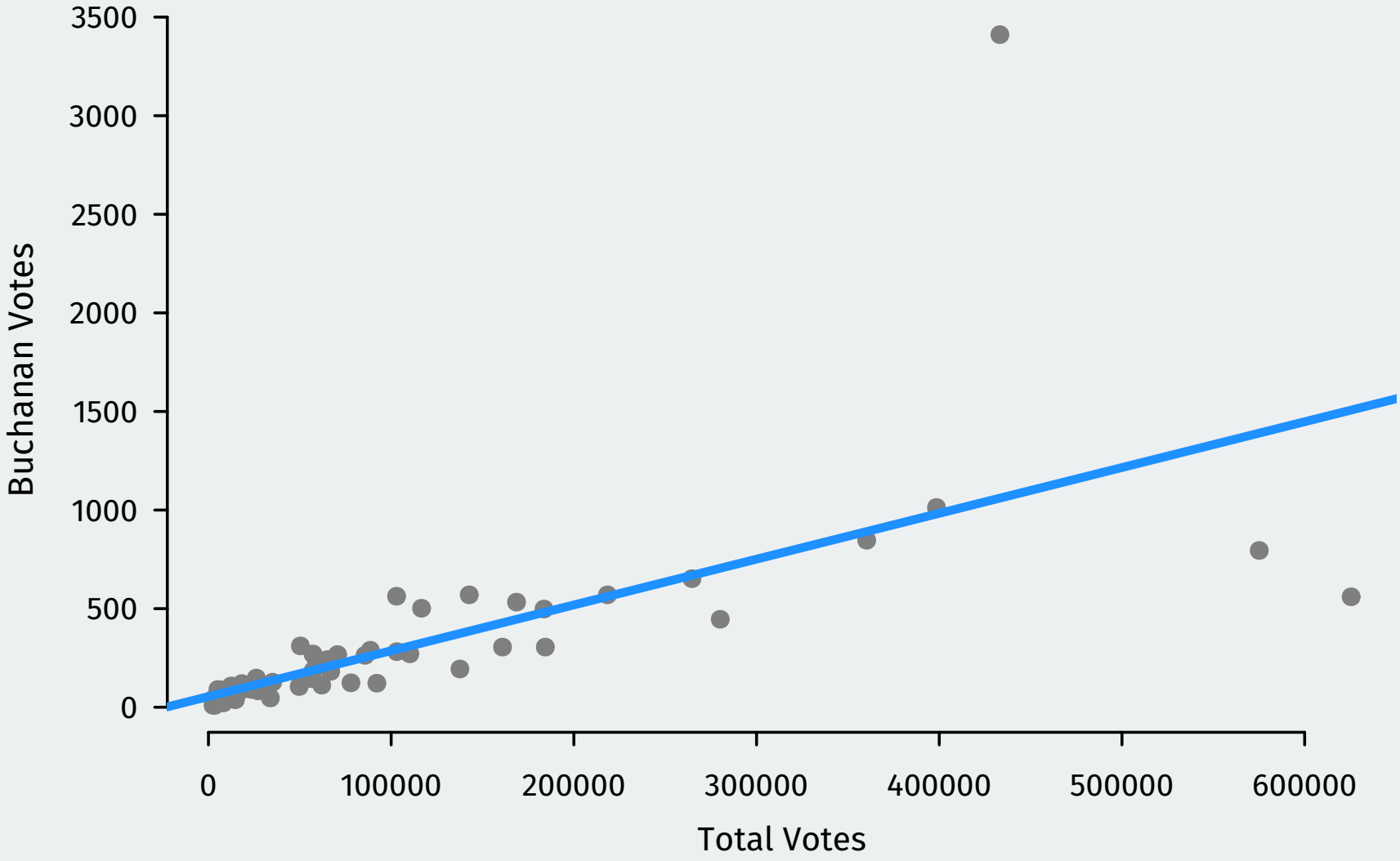
- Least square heavily penalizes large residuals.
- Implies a just a few unusual observations can be extremely influential.
    - Dropping them leads to large changes in the estimated $\hat{\boldsymbol{\beta}}$.
    - Not all "unusual" observations have the same effect, though.
- Useful to categorize:
    1. **Leverage point**: extreme in one X direction
    2. **Outlier**: extreme in the Y direction
    3. **Influence point**: extreme in both directions

Example: Buchanan votes in Florida, 2000

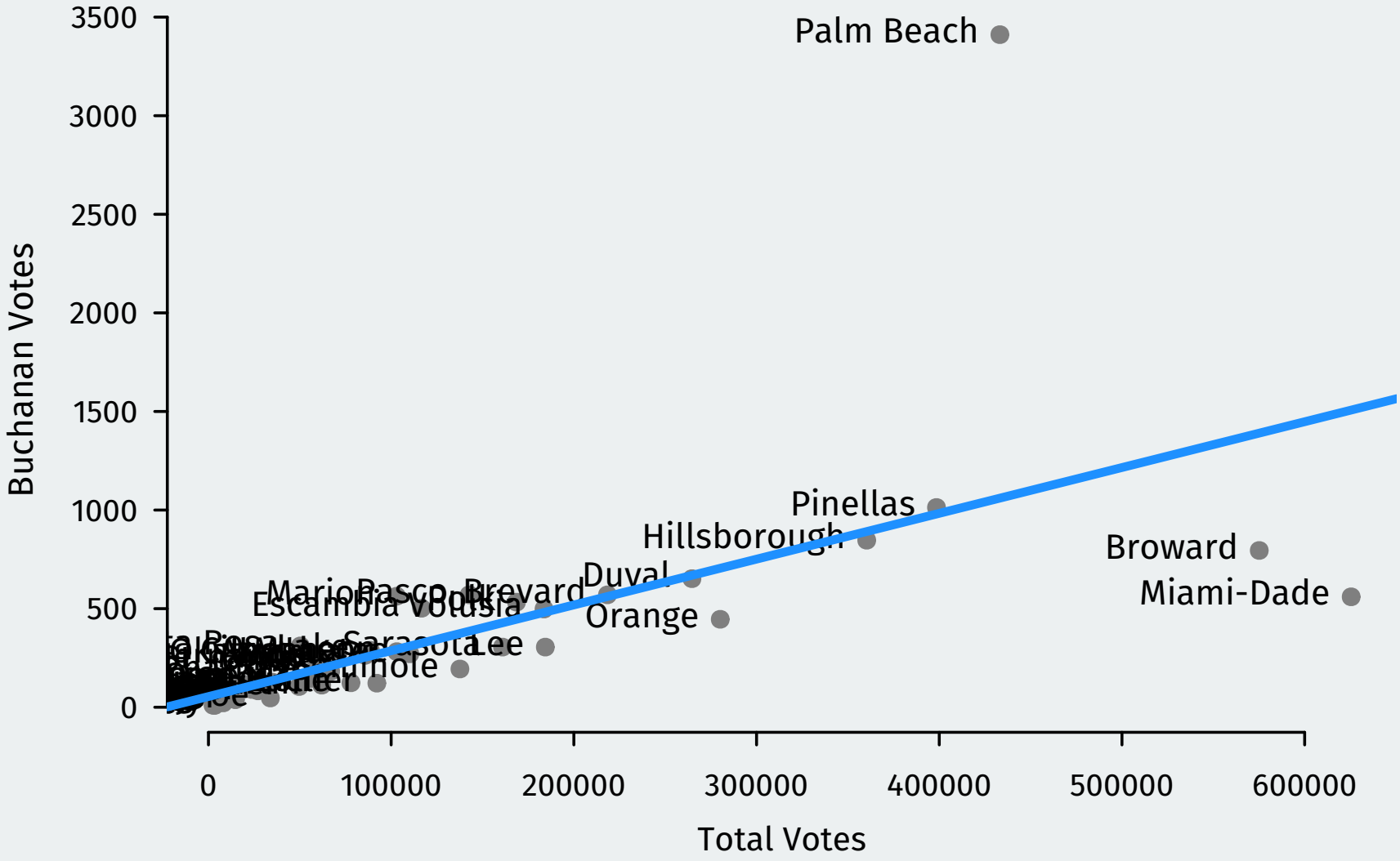
- 2000 Presidential election in FL (Wand et al., 2001, APSR)



Example: Buchanan votes in Florida, 2000



Example: Buchanan votes in Florida, 2000

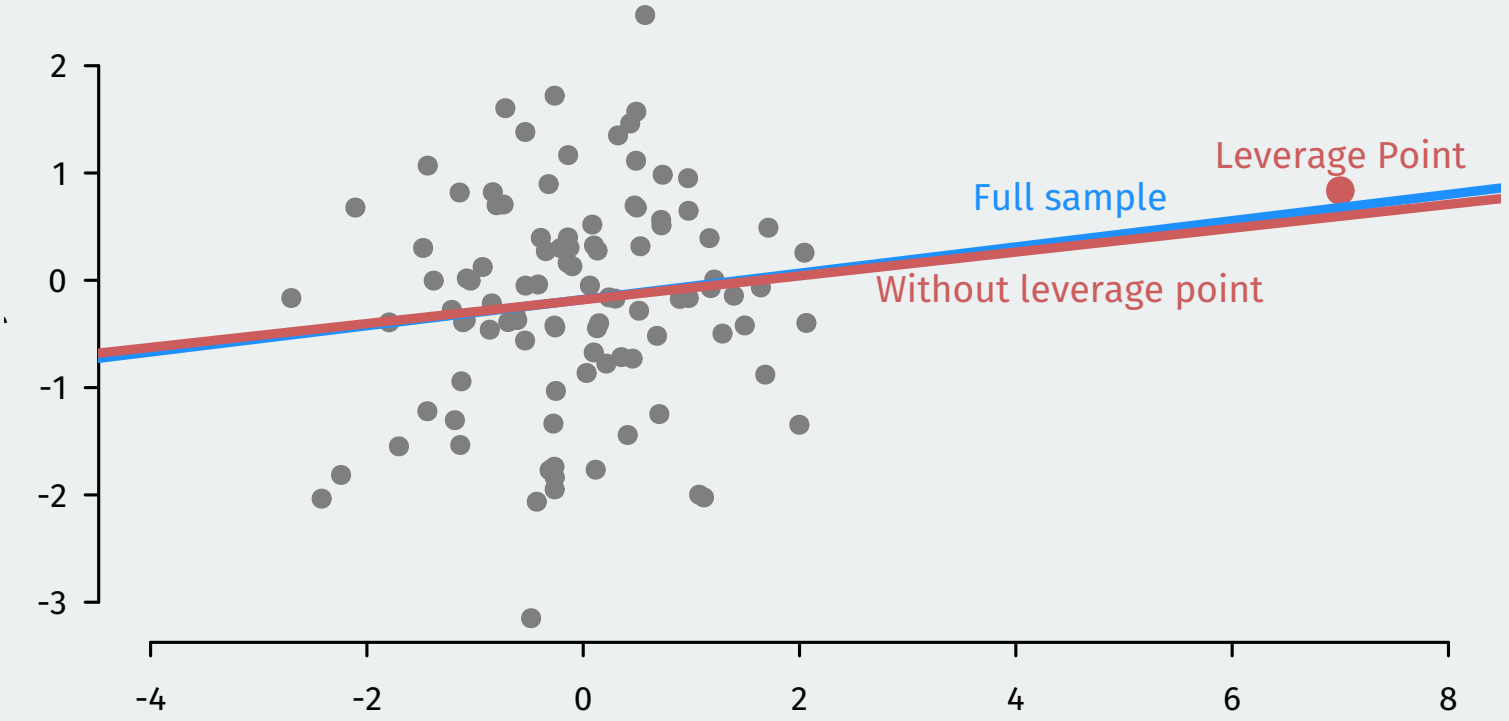


Example: Buchanan votes

```
mod <- lm(edaybuchanan ~ edaytotal, data = flvote)
summary(mod)
```

```
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 54.22945   49.14146    1.10     0.27
## edaytotal    0.00232    0.00031    7.48  2.4e-10 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 333 on 65 degrees of freedom
## Multiple R-squared:  0.463,  Adjusted R-squared:  0.455
## F-statistic:   56 on 1 and 65 DF,  p-value: 2.42e-10
```

Leverage point definition



- Values that are extreme in the X dimension
- That is, values far from the center of the covariate distribution

Leverage values

- Let h_{ij} be the (i, j) entry of $\mathbf{P}$. Then:

$$\widehat{\mathbf{Y}} = \mathbf{PY} \qquad \Longrightarrow \qquad \widehat{Y}_i = \sum_{j=1}^{n} h_{ij} Y_j$$

  - $h_{ij} =$ importance of observation j is for the fitted value $\widehat{Y}_i$

- **Leverage/hat values:** h_{ii} diagonal entries of the hat matrix

- With a simple linear regression, we have

$$h_{ii} = \frac{1}{n} + \frac{(X_i - \overline{X})^2}{\sum_{j=1}^{n} (X_j - \overline{X})^2}$$

  - $\rightsquigarrow$ how far i is from the center of the X distribution

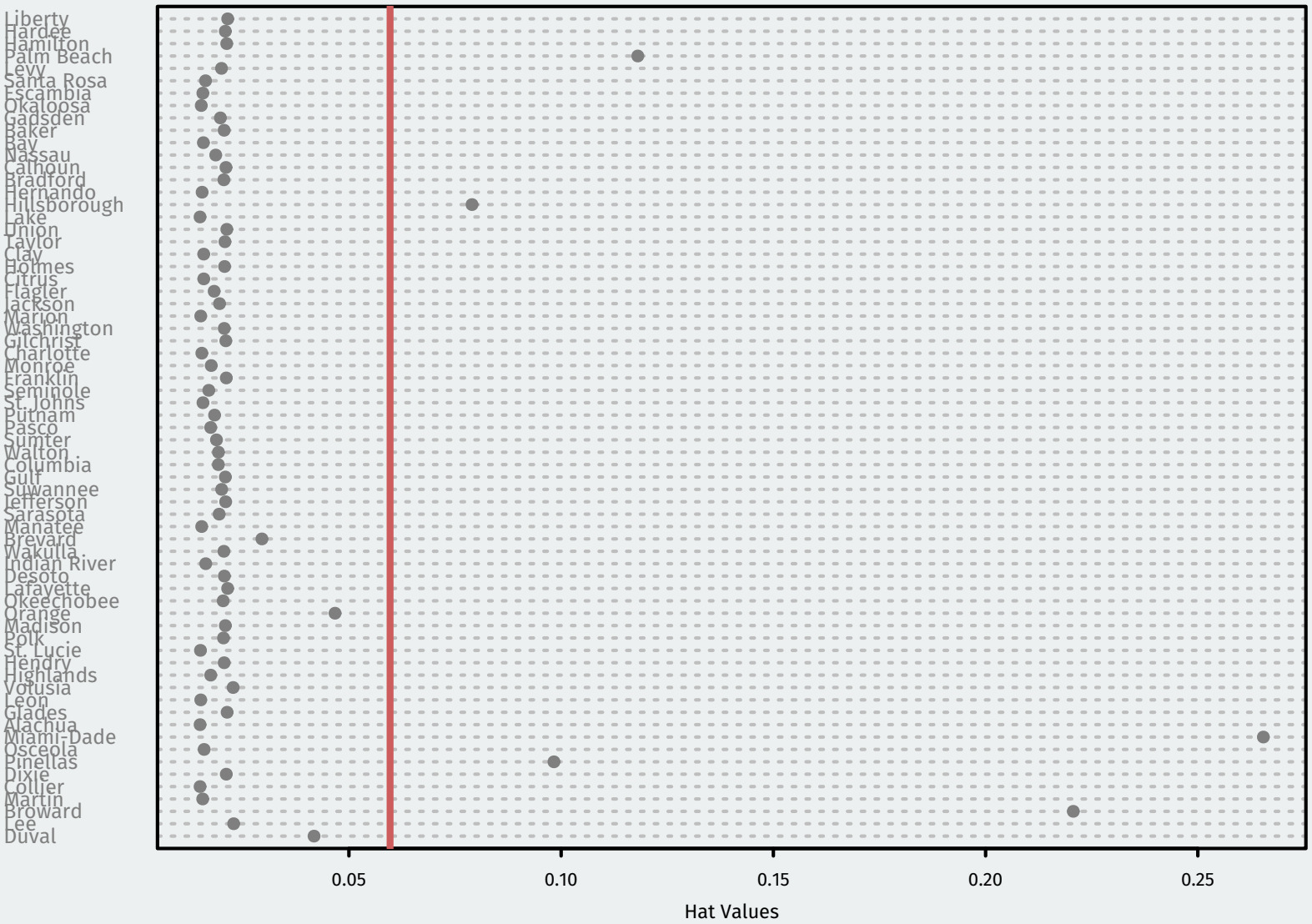
- **Rule of thumb:** examine hat values greater than $2(k + 1)/n$

Buchanan hats

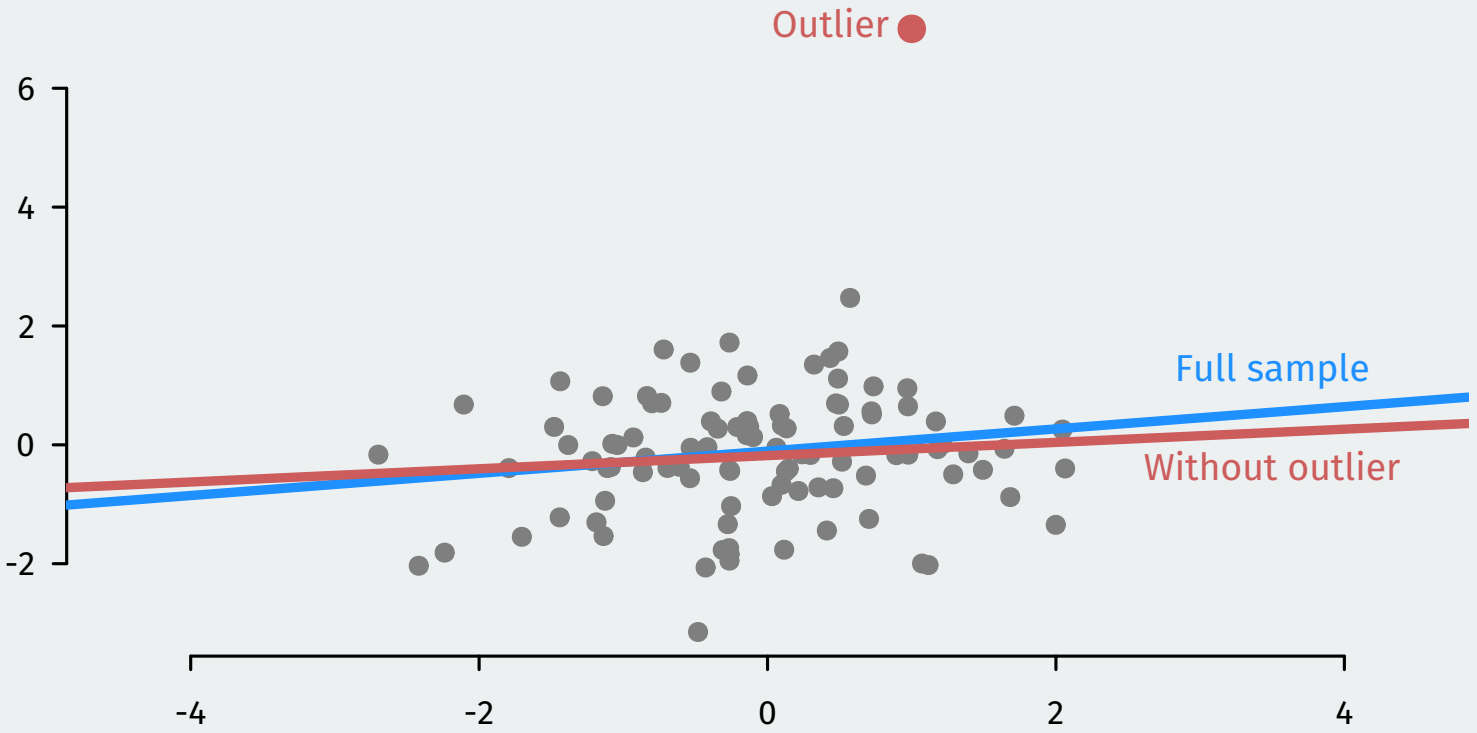
```
head(hatvalues(mod), 5)
```

```
##      1      2      3      4      5
## 0.0418 0.0228 0.2207 0.0156 0.0149
```

Buchanan hats



Outlier definition



- An **outlier** is far away from the center of the Y distribution.
- Intuitively: a point that would be poorly predicted by the regression.

Detecting outliers

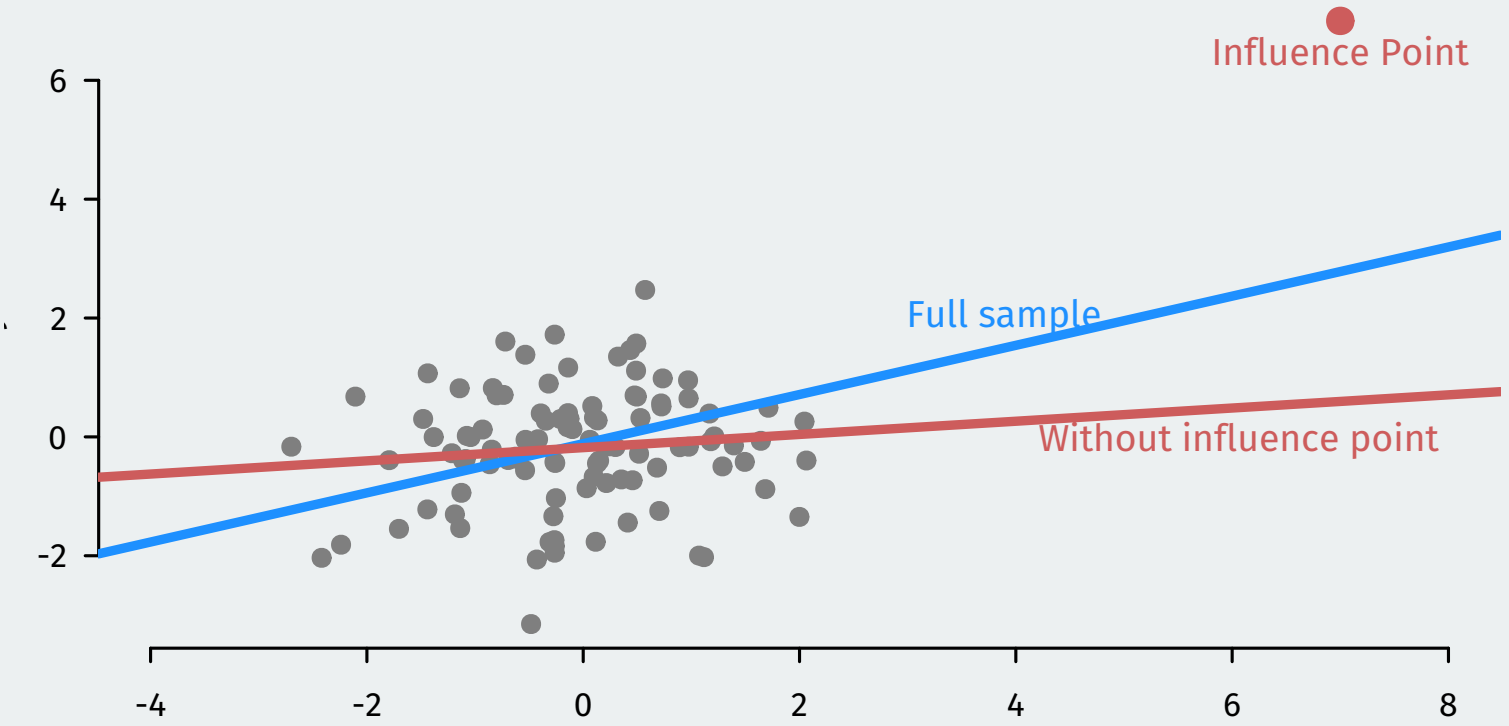
- Want values poorly predicted? Look for big residuals, right?
  - Problem: we use i to estimate $\hat{\boldsymbol{\beta}}$ so $\widehat{\mathbf{Y}}$ aren't valid predctions.
  - unit might pull the regression line toward itself $\rightsquigarrow$ small residual
- Better: **leave-one-out prediction errors**,
  1. Regress $\mathbb{X}_{(-i)}$ on $\mathbf{Y}_{(-i)}$, where these omit unit i:

$$\hat{\boldsymbol{\beta}}_{(-i)} = \left(\mathbb{X}'_{(-i)}\mathbb{X}_{(-i)}\right)^{-1}\mathbb{X}_{(-i)}\mathbf{Y}_{(-i)}$$

  2. Calculate predicted value of Y_i using that regression: $\widetilde{Y}_i = \mathbf{X}'_i\hat{\boldsymbol{\beta}}_{(-i)}$
  3. Calculate prediction error: $\tilde{e}_i = Y_i - \widetilde{Y}_i$
- Simple closed-form expressions:

$$\hat{\boldsymbol{\beta}}_{(-i)} = \hat{\boldsymbol{\beta}} - \left(\mathbb{X}'\mathbb{X}\right)^{-1}\mathbf{X}_i\tilde{e}_i \qquad \tilde{e}_i = \frac{\hat{e}_i}{1 - h_{ii}}$$

Influence points



- An **influence point** is one that is both an outlier and a leverage point.
- Extreme in both the X and Y dimensions

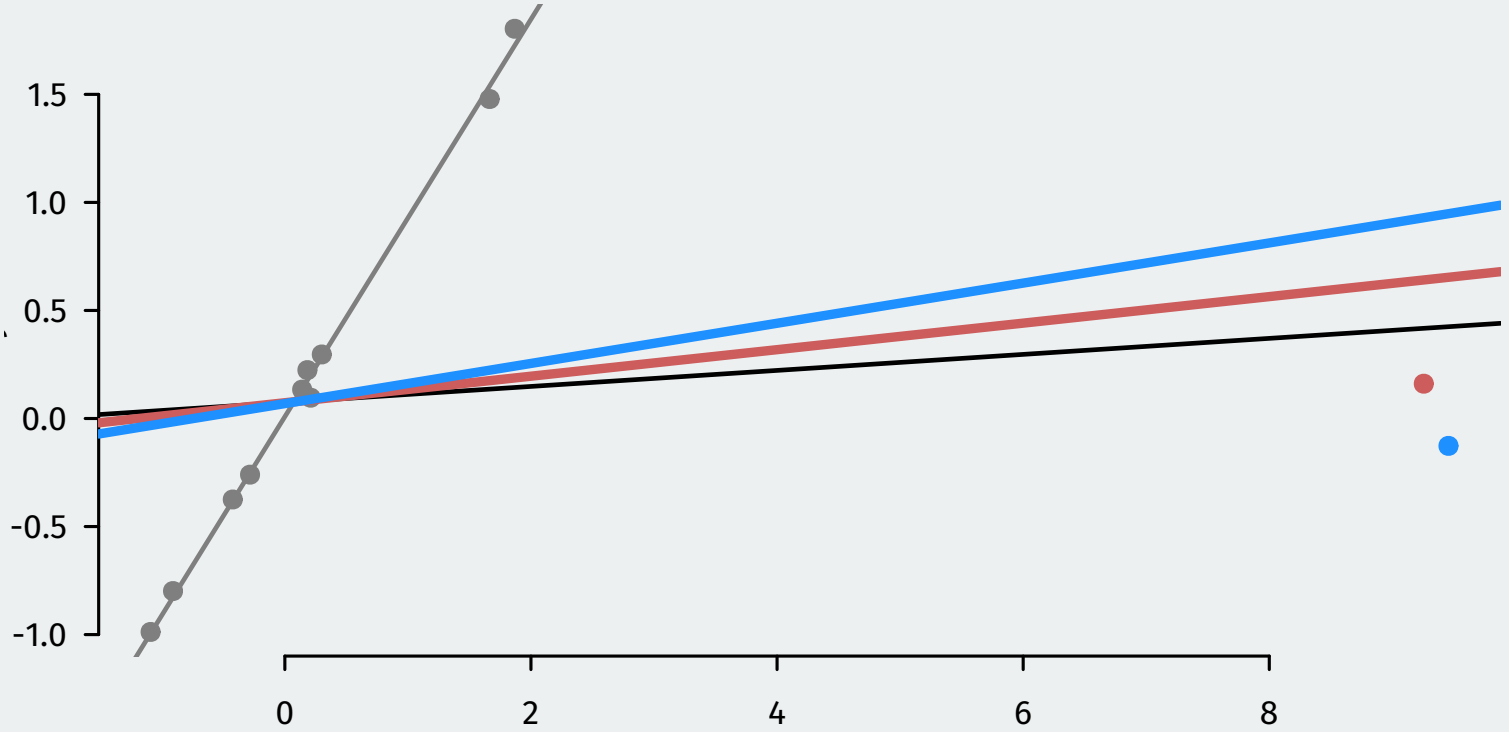
Overall measures of influence

- Influence of i can be measured by change in predictions:

$$\widehat{Y}_i - \widetilde{Y}_i = h_{ii}\tilde{e}_i$$

  - How much does excluding i from the regression change its predicted value?
  - Equal to "leverage $\times$ outlier-ness"
- Lots of diagnostics exist, but are mostly heuristic.
  - Does removing the point change a coefficient by a lot?

Limitations of the standard tools



- What happens when there are two influence points?
- Red line drops the red influence point
- Blue line drops the blue influence point

What to do about outliers and influential units?

- Is the data corrupted?
    - Fix the observation (obvious data entry errors)
    - Remove the observation
    - Be transparent either way
- Is the outlier part of the data generating process?
    - Transform the dependent variable ($\log(y)$)
    - Use a method that is robust to outliers (robust regression, least absolute deviations)