

Prediction

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September 30, 2021

Outline



Simple linear regression

Multiple linear regression

Causal interpretation and extensions

Regression: General introduction



Regression analysis is the most widely used statistical tool for understanding relationships among variables

It provides a conceptually simple method for investigating functional relationships between one or more factors and an outcome of interest

The relationship is expressed in the form of an equation or a model connecting the response or dependent variable and one or more explanatory or predictor variable

Why?



Straight-up prediction:

- How much will I sell my house for?

Explanation and understanding:

- What is the impact of economic freedom on growth?

Example 1: Predicting house prices



Problem:

- Predict market price based on observed characteristics

Solution:

- Look at property sales data where we know the price and some observed characteristics.
- Build a decision rule that predicts price as a function of the observed characteristics.



Q: What characteristics do we use?

We have to define the variables of interest and develop a specific quantitative measure of these variables ...

Many factors or variables affect the price of a house:

- size
- number of baths
- garage, air conditioning, etc
- neighborhood



To keep things super simple, let's focus only on size. The value

that we seek to predict is called the dependent (or output) variable, and we denote this:

- Y =price of house (e.g. thousands of dollars)

The variable that we use to guide prediction is the explanatory (or input) variable, and this is labeled

-X =size of house (e.g. thousands of square feet)

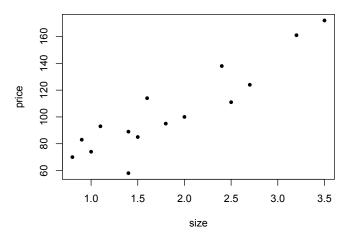


What does this data look like?

Size		Price	
	0.80		70
	0.90		83
	1.00		74
	1.10		93
	1.40		89
	1.40		58
	1.50		85
	1.60		114
	1.80		95
	2.00		100
	2.40		138
	2.50		111
	2.70		124
	3.20		161
	3.50		172



It is much more useful to look at a scatterplot



In other words, view the data as points in the $X \times Y$ plane.

Regression model



- Y =response or outcome variable
- X =explanatory or input variables

A linear relationship is written

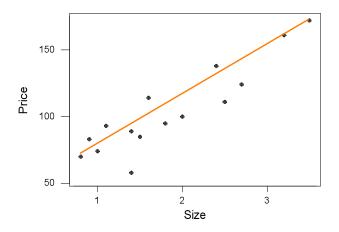
$$Y = b_0 + b_1 X + e$$

Linear prediction



There seems to be a linear relationship between price and size:

As size goes up, price goes up.



Linear prediction



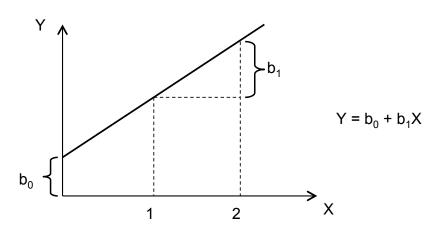
Recall that the equation of a line is:

$$Y = b_0 + b_1 X$$

Where b_0 is the intercept and b_1 is the slope.

- \rightarrow The intercept value is in units of Y (\$1,000)
- \rightarrow The slope is in units of *Y* per units of *X* (\$1,000/1,000 sq ft)







Q: How to find the "best line"?

We desire a strategy for estimating the slope and intercept parameters in the model $\hat{Y} = b_0 + b_1 X$

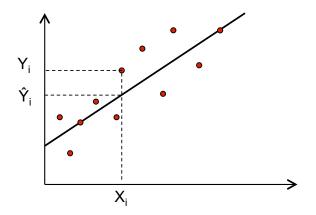
A reasonable way to fit a line is to minimize the amount by which the fitted value differs from the actual value.

This amount is called the residual.

Linear prediction



What is the "fitted value"?

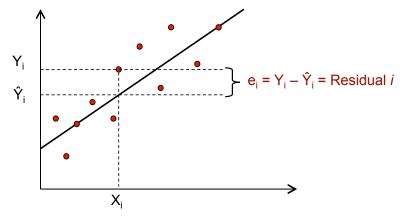


The dots are the observed values and the line represents our fitted values given by $\hat{Y}_i = b_0 + b_1 X_1$.

Linear prediction



What is the "residual" for the *i*th observation?



We can write $Y_i = \hat{Y}_i + (Y_i - \hat{Y}_i) = \hat{Y}_i + e_i$.

Least squares



Ideally, we want to minimize the size of all residuals:

- If they were all zero we would have a perfect line.
- Trade-off between moving closer to some points and at the same time moving away from other points.

Least squares



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The line fitting process:

- Give weights to all of the residuals.
- Minimize the "total" of residuals to get best fit.

Least squares



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The line fitting process:

- Give weights to all of the residuals.
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Least Squares chooses b_0 and b_1 to minimize $\sum_{i=1}^{N} e_i^2$

$$\sum_{i=1}^{N} e_i^2 = e_1^2 + e_2^2 + \dots + e_N^2 = (Y_1 - \hat{Y}_1)^2 + (Y_2 - \hat{Y}_2)^2 + \dots + (Y_N - \hat{Y}_N)^2$$

Least squares – R output



```
data = read.csv('housedata.csv')
fit = lm(Price~Size,data)
summary(fit)
##
## Call:
## lm(formula = Price ~ Size, data = data)
##
## Residuals:
##
      Min 10 Median 30
                                    Max
## -30.425 -8.618 0.575 10.766 18.498
##
## Coefficients:
             Estimate Std. Error t value Pr(>|t|)
##
## (Intercept) 38.885 9.094 4.276 0.000903 ***
## Size
           35.386 4.494 7.874 2.66e-06 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 14.14 on 13 degrees of freedom
## Multiple R-squared: 0.8267, Adjusted R-squared: 0.8133
## F-statistic: 62 on 1 and 13 DF, p-value: 2.66e-06
```

Example 2: Offensive performance in baseball



Problems:

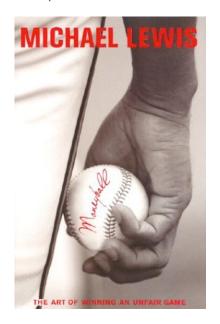
- Evaluate/compare traditional measures of offensive performance
- Help evaluate the worth of a player

Solutions:

 Compare prediction rules that forecast runs as a function of either AVG (batting average), SLG (slugging percentage – total bases divided by at bats) or OBP (on base percentage)

Example 2: Offensive performance in baseball

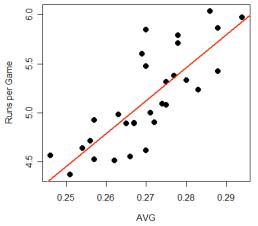




Baseball data - using AVG



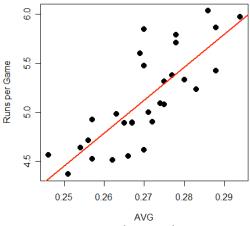
Each observation corresponds to a team in MLB. Each quantity is the average over a season.



Y = runs per game; X = AVG (average)LS fit: Runs/Game = -3.93 + 33.57 AVG

Baseball data - using AVG

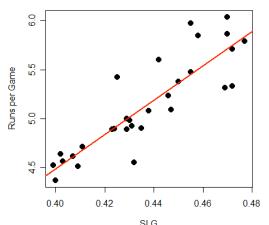




Y = runs per game; X = AVG (average)

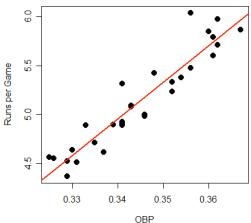
LS fit: Runs/Game = -3.93 + 33.57 AVG





Y = runs per game; X = SLG (slugging percentage)LS fit: Runs/Game = -2.52 + 17.54 SLG





Y = runs per game; X = OBP (on base percentage) LS fit: Runs/Game = -7.78 + 37.46 OBP



- What is the best prediction rule?
- Let's compare the predictive ability of each model using the average squared error

$$\sqrt{\frac{1}{N}\sum_{i=1}^{N}e_{i}^{2}} = \left(\frac{\sum_{i=1}^{N}\left(\widehat{\mathsf{Runs}_{i}} - \mathsf{Runs}_{i}\right)^{2}}{N}\right)^{\frac{1}{2}}$$





	Root Mean Squared Error
AVG	0.29
SLG	0.23
OBP	0.16



Remember how we get the slope (b_1) and intercept (b_0) . We minimize the sum of squared prediction errors.

The formulas for b_0 and b_1 that minimize the least squares criterion are:

$$b_1 = r_{xy} imes rac{s_y}{s_x} \qquad b_0 = \bar{Y} - b_1 \bar{X}$$

where,

- \bar{X} and \bar{Y} are the sample mean of X and Y
- $corr(x, y) = r_{xy}$ is the sample correlation
- $-s_x$ and s_y are the sample standard deviation of X and Y





- Sample Mean: measure of centrality

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

- Sample Variance: measure of spread

$$s_y^2 = \frac{1}{n-1} \sum_{i=1}^n (Y_i - \bar{Y})^2$$

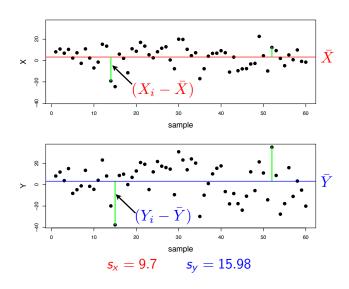
Sample Standard Deviation:

$$s_y = \sqrt{s_y^2}$$

Visual: standard deviation



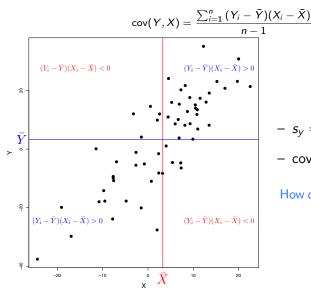
$$s_y^2 = \frac{1}{n-1} \sum_{i=1}^n (Y_i - \bar{Y})^2$$



Visual: Covariance



Measure the direction and strength of the linear relationship between Y and X



$$-s_y = 15.98, s_x = 9.7$$

$$- \operatorname{cov}(X, Y) = 125.9$$

How do we interpret that?



Correlation is the standardized covariance:

$$\operatorname{corr}(X,Y) = \frac{\operatorname{cov}(X,Y)}{\sqrt{s_x^2 s_y^2}} = \frac{\operatorname{cov}(X,Y)}{s_x s_y}$$

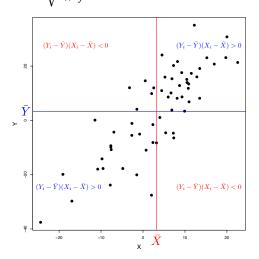
The correlation is scale invariant and the units of measurement don't matter: It is always true that $-1 \le corr(X, Y) \le 1$.

This gives the direction (negative or positive) and strength $(0 \to 1)$ of the linear relationship between X and Y.

Correlation

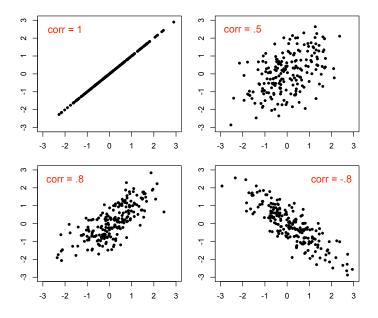


$$\operatorname{corr}(Y,X) = \frac{\operatorname{cov}(X,Y)}{\sqrt{s_x^2 s_y^2}} = \frac{\operatorname{cov}(X,Y)}{s_x s_y} = \frac{125.9}{15.98 \times 9.7} = 0.812$$



Correlation



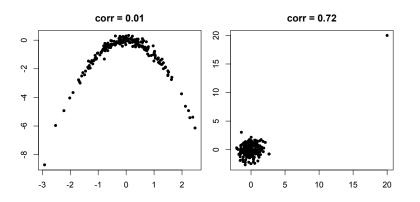


Correlation



Only measures linear relationships:

corr(X, Y) = 0 does not mean the variables are not related!



Also be careful with influential observations. Check out cor() in R.



Intercept:

$$b_0 = \bar{Y} - b_1 \bar{X} \Rightarrow \bar{Y} = b_0 + b_1 \bar{X}$$

The point (\bar{X}, \bar{Y}) is on the regression line!

Least squares finds the point of means and rotates the line through that point until getting the "right" slope

Slope:

$$b_{1} = \operatorname{corr}(X, Y) \times \frac{s_{Y}}{s_{X}} = \frac{\sum_{i=1}^{n} (X_{i} - \bar{X})(Y_{i} - \bar{Y})}{\sum_{i=1}^{n} (X_{i} - \bar{X})^{2}}$$
$$= \frac{\operatorname{cov}(X, Y)}{\operatorname{var}(X)}$$

So, the right slope is the correlation coefficient times a scaling factor that ensures the proper units for b_1

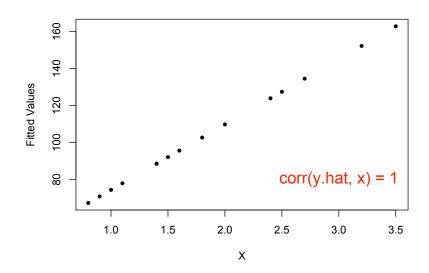
More on least squares



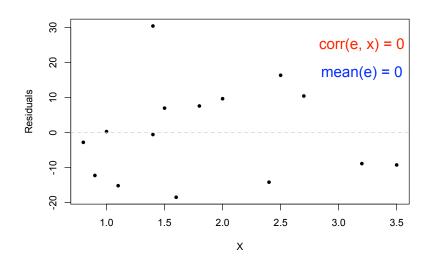
From now on, terms "fitted values" (\hat{Y}_i) and "residuals" (e_i) refer to those obtained from the least squares line.

The fitted values and residuals have some special properties. Let's look at the housing data analysis to figure out what these properties are...





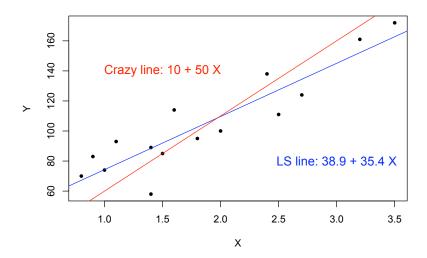




Why?

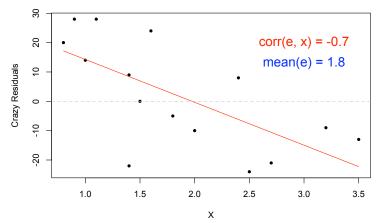


What is the intuition for the relationship between \hat{Y} and e and X? Lets consider some "crazy" alternative line:





This is a bad fit! We are underestimating the value of small houses and overestimating the value of big houses.



Clearly, we have left some predictive ability on the table!

Fitted values and residuals



As long as the correlation between e and X is non-zero, we could always adjust our prediction rule to do better.

We need to exploit all of the predictive power in the X values and put this into \hat{Y} , leaving no "Xness" in the residuals.

In summary: $Y = \hat{Y} + e$ where:

- \hat{Y} is "made from X"; $\operatorname{corr}(X, \hat{Y}) = 1$.
- e is unrelated to X; $\operatorname{corr}(X, e) = 0$.

Q: How well does the least squares line explain variation in Y?

Remember that $Y = \hat{Y} + e$

Since \hat{Y} and e are uncorrelated, i.e. $\operatorname{corr}(\hat{Y},e)=0$,

$$var(Y) = var(\hat{Y} + e) = var(\hat{Y}) + var(e)$$

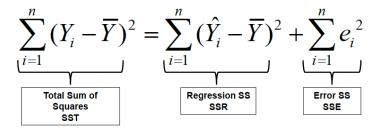
$$\frac{\sum_{i=1}^{n} (Y_i - \bar{Y})^2}{n-1} = \frac{\sum_{i=1}^{n} (\hat{Y}_i - \bar{\hat{Y}})^2}{n-1} + \frac{\sum_{i=1}^{n} (e_i - \bar{e})^2}{n-1}$$

Given that $\bar{e}=0$, and $\hat{\bar{Y}}=\bar{Y}$ (why?) we get to:

$$\sum_{i=1}^{n} (Y_i - \bar{Y})^2 = \sum_{i=1}^{n} (\hat{Y}_i - \bar{Y})^2 + \sum_{i=1}^{n} e_i^2$$

Decomposing the variance



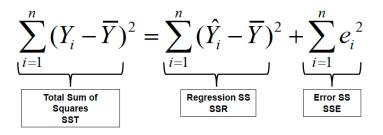


SSR: Variation in Y explained by the regression line.

SSE: Variation in Y that is left unexplained.

Decomposing the variance





SSR: Variation in Y explained by the regression line.

SSE: Variation in Y that is left unexplained.

$$SSR = SST \Rightarrow perfect fit.$$

Be careful of similar acronyms; e.g. SSR for "residual" SS.

The coefficient of determination, denoted by R^2 , measures goodness of fit:

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

- $-0 < R^2 < 1.$
- The closer R^2 is to 1, the better the fit.





Three very similar, related ways to look at a simple linear regression... with only one X variable, life is easy!

	R^2	corr	SSE
OBP	0.88	0.94	0.79
SLG	0.76	0.87	1.64
AVG	0.63	0.79	2.49



 $\label{eq:prediction} \textit{Prediction and Regression} + \textit{Probability}$



A prediction rule is any function where you input X and it outputs \hat{Y} as a predicted response at X.

The least squares line is a prediction rule:

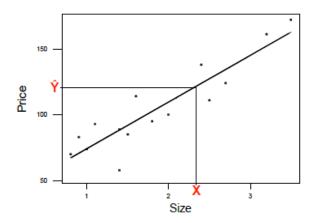
$$\hat{Y}=f(X)=b_0+b_1X$$





 \hat{Y} is not going to be a perfect prediction.

We need to devise a notion of forecast accuracy.



Prediction and the modeling goal



There are two things that we want to know:

- What value of Y can we expect for a given X?
- How <u>sure</u> are we about this forecast? Or how different could Y be from what we expect?

Our goal is to measure the accuracy of our forecasts or how much uncertainty there is in the forecast. One method is to specify a range of Y values that are likely, given an X value.

Prediction Interval: probable range for *Y*-values given *X*

Prediction and the modeling goal



Key Insight: To construct a prediction interval, we will have to assess the likely range of error values corresponding to a Y value that has not yet been observed!

We will build a probability model (e.g., normal distribution).

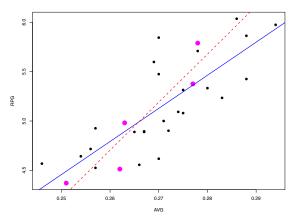
Then we can say something like "with 95% probability the error will be no less than -\$28,000 or larger than \$28,000".

We must also acknowledge that the "fitted" line may be fooled by particular realizations of the residuals.

Prediction and the modeling goal



We are always looking at samples! The dashed line fits the purple points. The solid line fits all the points. Which line is better? Why?



In summary, we need to work with the notion of a "true line" and a probability distribution that describes deviation around the line.





The power of statistical inference comes from the ability to make precise statements about the accuracy of the forecasts.

In order to do this we must invest in a probability model.

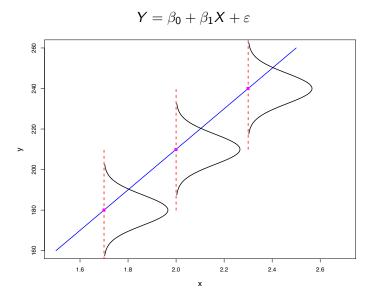
Simple Linear Regression Model:
$$Y = \beta_0 + \beta_1 X + \varepsilon$$

$$\varepsilon \sim \mathrm{N}(0, \sigma^2)$$

- $-\beta_0 + \beta_1 X$ represents the "true line"; The part of Y that depends on X.
- The error term ε is independent "idosyncratic noise"; The part of Y not associated with X.

The Simple Linear Regression Model









You are told (without looking at the data) that

$$\beta_0 = 40$$
; $\beta_1 = 45$; $\sigma = 10$

and you are asked to predict price of a 1500 square foot house.

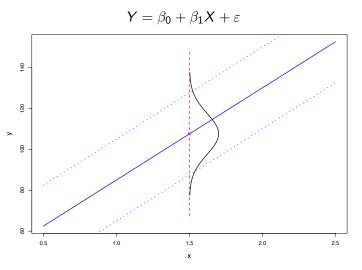
What do you know about Y from the model?

$$Y = 40 + 45(1.5) + \varepsilon$$
$$= 107.5 + \varepsilon$$

Thus our prediction for price is $Y|(X=1.5) \sim N(107.5, 10^2)$ and a 95% *Prediction Interval* for Y is 87.5 < Y < 127.5

Conditional distributions





The conditional distribution for Y given X is Normal:

$$Y|X = x \sim N(\beta_0 + \beta_1 x, \sigma^2).$$

Conditional distributions



The model says that the mean value of a 1500 sq. ft. house is \$107,500 and that deviation from mean is within \approx \$20,000.

We are 95% sure that

- $-20 < \varepsilon < 20$
- -87.5 < Y < 127.5

In general, the 95 % Prediction Interval is $PI = \beta_0 + \beta_1 X \pm 2\sigma$.



Put differently, why do we have $\varepsilon \sim N(0, \sigma^2)$?

- $E[\varepsilon] = 0 \Leftrightarrow E[Y \mid X] = \beta_0 + \beta_1 X$ ($E[Y \mid X]$ is "conditional expectation of Y given X").
- Many things are close to Normal (central limit theorem).
- It works! This is a very robust model for the world.

We can think of $\beta_0 + \beta_1 X$ as the "true" regression line.

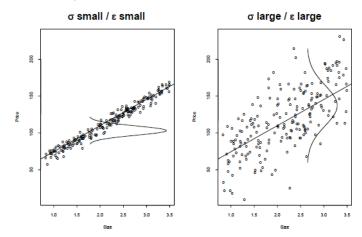
Conditional distributions



The conditional distribution for Y given X is Normal:

$$Y|X \sim N(\beta_0 + \beta_1 X, \sigma^2).$$

 σ controls dispersion:





More on the conditional distribution:

$$Y|X \sim N(E[Y|X], var(Y|X)).$$

- The conditional mean is $E[Y|X] = E[\beta_0 + \beta_1 X + \varepsilon] = \beta_0 + \beta_1 X$.
- The conditional variance is $var(Y|X) = var(\beta_0 + \beta_1 X + \varepsilon) = var(\varepsilon) = \sigma^2$.
- $-\sigma^2 < \text{var}(Y)$ if X and Y are related.



Assume that all observations are drawn from our regression model and that errors on those observations are independent.

The model is

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$

where ε is independent and identically distributed $N(0, \sigma^2)$.

- independence means that knowing ε_i doesn't affect your views about ε_j
- identically distributed means that we are using the same Normal for every ε_i



The model is

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$

$$\varepsilon_i \sim \mathrm{N}(0, \sigma^2).$$

The SLR has 3 basic parameters:

- $-\beta_0$, β_1 (linear pattern)
- σ (variation around the line).

Key characteristics of linear regression model



Mean of Y is linear in X.

- Error terms (deviations from line) are Normally distributed (very few deviations are more than 2 standard devations away from the regression mean).
- Error terms have constant variance.



SLR assumes every observation in the dataset was generated by the model:

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$

This is a model for the conditional distribution of Y given X.

We use Least Squares to estimate β_0 and β_1 :

$$\hat{\beta}_1 = b_1 = r_{xy} \times \frac{s_y}{s_x}$$

$$\hat{\beta}_0 = b_0 = \bar{Y} - b_1 \bar{X}$$

We estimate s^2 with:

$$s^2 = \frac{1}{n-2} \sum_{i=1}^{n} e_i^2 = \frac{SSE}{n-2}$$

(2 is the number of regression coefficients; i.e. 2 for β_0 and β_1).

We have n-2 degrees of freedom because 2 have been "used up" in the estimation of b_0 and b_1 .

We usually use $s = \sqrt{SSE/(n-2)}$, in the same units as Y. It's also called the regression standard error.

Uncertainty in estimates



We now know how to make statements about uncertainty in forecasts aka predictions. But what about our parameter estimates?

Q: How much do our estimates depend on the particular random sample that we happen to observe?

Uncertainty in estimates



Imagine:

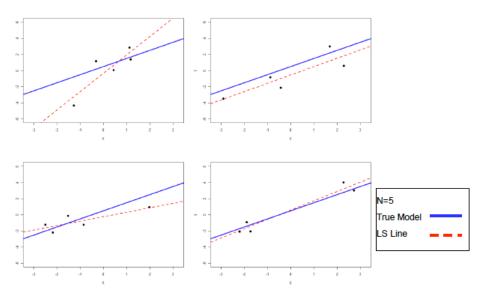
- Randomly draw different samples of the same size.
- For each sample, compute the estimates b_0 , b_1 , and s.

If the estimates don't vary much from sample to sample, then it doesn't matter which sample you happen to observe.

If the estimates do vary a lot, then it matters which sample you happen to observe.

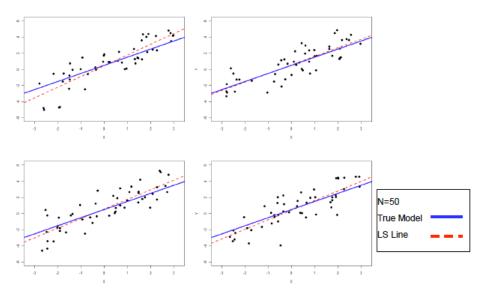
Sampling distribution of least squares estimates





Sampling distribution of least squares estimates





Sampling distribution of least squares estimates



Least squares lines are much closer to the true line when N = 50.

For N = 5, some lines are close, others aren't:

We need to get "lucky!"

So, to sum up ...



Parameter estimates are uncertain because we only have sample from the population

We can characterize a sampling distribution of each parameter based on the assumptions of the SLR model

The standard deviation of the sampling distribution is called the standard error

 $\to R$ directly reports standard errors. They can also be calculated with other methods, like bootstrapping.

Least squares – R output



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data = read.csv('housedata.csv')
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summary(fit)
##
## Call:
## lm(formula = Price ~ Size, data = data)
##
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## Multiple R-squared: 0.8267, Adjusted R-squared: 0.8133
## F-statistic: 62 on 1 and 13 DF, p-value: 2.66e-06
```



The bootstrap

Quantifying uncertainty



In data science, we equate trustworthiness with stability:

Key question: If our data had been different merely due to chance, would our answer have been different, too? Or would the answer have been stable, even with different data?

Confidence in your estimates \iff Stability of those estimates under the influence of chance

Example: Quantifying uncertainty



For example:

- If doctors had taken a different sample of 503 cancer patients and gotten a drastically different estimate of the new treatment's effect, then the original estimate isn't very trustworthy.
- If, on the other hand, pretty much any sample of 503 patients would have led to the same estimates, then their answer for this particular subset of 503 is probably accurate.

Some notation



Suppose we are trying to estimate some population-level feature of interest, θ . This might be something very complicated!

So we take a sample from the population: X_1, X_2, \ldots, X_N . We use the data to form an estimate $\hat{\theta}_N$ of the parameter.

Key insight: $\hat{\theta}_N$ is a random variable.

 $(\hat{\theta}_N$ can be the slope of a least squares regression)

Some notation



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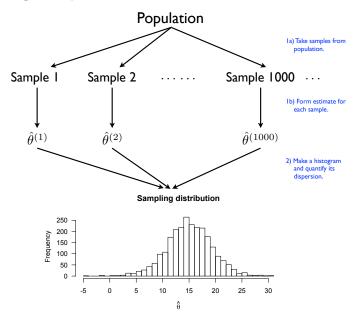
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 \rightarrow Now imagine repeating this process thousands of times! Since $\hat{\theta}_N$ is a random variable, it has a probability distribution: the sampling distribution.

Visualizing this procedure







Standard error: the standard deviation of an estimator's sampling distribution:

$$\begin{split} \operatorname{se}(\hat{\theta}_N) &= \sqrt{\operatorname{var}(\hat{\theta}_N)} \\ &= \sqrt{E[(\hat{\theta}_N - \bar{\theta}_N)^2]} \\ &= \operatorname{Typical\ deviation\ of\ } \hat{\theta}_N \text{ from its\ average} \end{split}$$

"If I were to take repeated samples from the population and use this estimator for every sample, how much does the answer vary, on average?"

Standard error



But there's a problem here...

Knowing the standard error requires knowing what happens across many separate samples. But we've only got our one sample!

So how can we ever calculate the standard error?

Standard error



Two roads diverged in a yellow wood And sorry I could not travel both And be one traveler, long I stood And looked down one as far as I could To where it bent in the undergrowth...

- Robert Frost, The Road Not Taken, 1916

Quantifying our uncertainty would seem to require knowing all the roads not taken—an impossible task.

The bootstrap

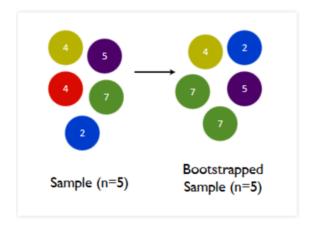


Problem: we can't take repeated samples of size N from the population, to see how our estimate changes across samples.

Seemingly hacky solution: Take repeated samples of size N, with replacement, from the sample itself, and see how our estimate changes across samples. This is something we can easily simulate on a computer (with R).

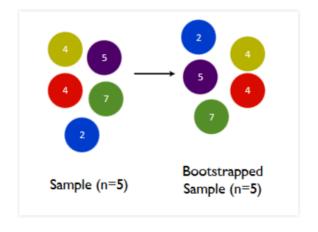
Basically, we pretend that our sample is the whole population and we charge ahead! This is called bootstrap resampling, or just bootstrapping.

boostrapped sample 1



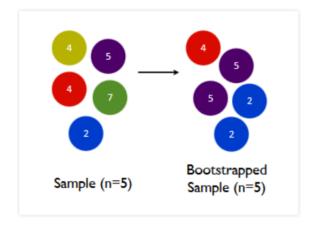


boostrapped sample 2



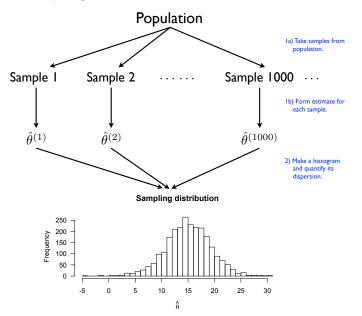


boostrapped sample 3



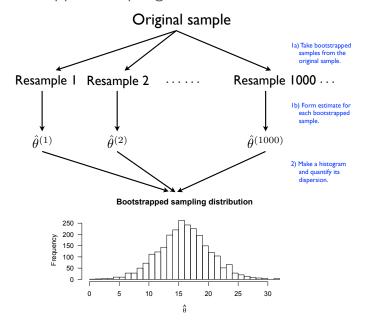
The true sampling distribution





The bootstrapped sampling distribution





The bootstrapped sampling distribution



 Each bootstrapped sample has its own pattern of duplicates and omissions from the original sample.

• These duplicates and omissions create variability in $\hat{\theta}$ from one bootstrapped sample to the next.

 This variability mimics the true sampling variability you'd expect to see across real repeated samples from the population.