# Assessing accuracy of linear regression

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#### Outline

Confidence intervals with linear regression

Measuring how well LSR line fits

**Example with Multiple variables** 

Polynomial fitting

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# Difference between parameters from "population" vs. from data

Modeling relationship between independent variables and y with a linear model (with noise in the y-coordinate direction). In other words, the modeled relationship is that

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for some parameters **w**, b.

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However, we find values for  $\mathbf{w}$  and b by using observed data, sampled from a "population." Among the entire population, there is a best fit linear model having some parameters. However, from the observed data  $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_P, y_P)$  if our procedure determines best fit parameters  $b^*$  and  $\mathbf{w}^*$ , these are not (necessarily) the parameters for the population linear model.

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```
1  x = np.random.uniform(0, 2, size=30)
2  def simulate_data(x, std):
4    return -1.6*x + 0.8 + np.random.normal(0, std, size=len(x))
5  y = simulate_data(x, 0.5)
```

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What is the mean of these slopes and intercepts that were found?

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  - ▶ Weak Law of Large Numbers: if s random samples of 2000 people taken, and each sample mean calculated then, as  $s \to \infty$ , the average of those s sample means limits (in probability) to the population mean.
- Analogous thing happens with data from linear relationship with noise think of parameters  $w^*$  and  $b^*$  as sample statistics (like the sample mean).

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Using  $\bar{x}$  for the average of  $x_1, \ldots, x_P$ ,

$$\begin{split} (SE(w^\star))^2 &= \frac{\sigma^2}{\sum_{i=1}^P (x_i - \bar{x})^2};\\ (SE(b^\star))^2 &= \sigma^2 \left(\frac{1}{P} + \frac{\bar{x}^2}{\sum_{i=1}^P (x_i - \bar{x})^2}\right). \end{split}$$

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Roughly, the Standard Error is the amount, on average, that  $w^*$  (resp.  $b^*$ ) differs from true slope w (resp. true intercept b).<sup>2</sup>

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 $\sigma$  is unknown, but can estimate it with **residual standard error**:

$$\hat{\sigma}^2 = RSE^2 = \frac{\sum_{i=1}^{P} (y_i - \hat{y}_i)^2}{P - 2}.$$

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Estimate:

$$\sigma^2 \approx RSE^2 = \frac{\sum_{i=1}^{P} (y_i - \hat{y}_i)^2}{P - 2}.$$

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Can get (roughly) 95% confidence interval<sup>3</sup> with  $\pm 2SE$ :

$$(\mathbf{w}^{\star} - 2SE(\mathbf{w}^{\star}), \mathbf{w}^{\star} + 2SE(\mathbf{w}^{\star}))$$

and

$$(b^* - 2SE(b^*), b^* + 2SE(b^*)).$$

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Closely related to RSE (residual standard error). Recall,

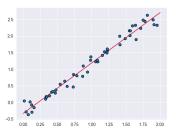
RSE = 
$$\sqrt{\frac{1}{P-2} \sum_{i=1}^{P} (y_i - \hat{y}_i)^2}$$
.

So MSE = 
$$\frac{P-2}{P}$$
RSE<sup>2</sup>.

## Mean Squared Error, example

Recall, 'Example1.csv' data. Its best fit line is

$$y = 1.520275x - 0.33458$$
.

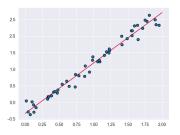


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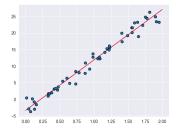
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The MSE for this data and its predictions is  $\approx$  0.0197. Does that mean that the linear model is a "good fit"?



# Mean Squared Error, scaling

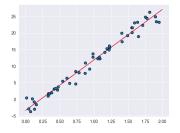
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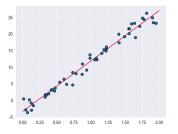
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MSE is still a good measure to think about, but its size depends on scale of y-coordinates (equivalently, depends on units y is measured in).

Get a measure that is unchanged by scaling: first, set **total sum of squares** (TSS) to

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  - Can you prove this?
- Checking that R<sup>2</sup> is "close" to 1 is often done to indicate that a linear model is a very good one.

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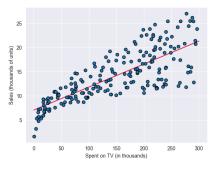
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- Model Sales (y) as a function of advertising budgets in TV  $(x_1)$ , Radio  $(x_2)$  and Newspaper  $(x_3)$ .
- Regression with just one of the variables ignores that all are contributing to Sales and doesn't predict y very well.



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As we discussed in Lecture 5, set A to be  $P \times (N+1)$  matrix with a column of ones, and a column for each independent variable (in this example, N=3). So,

$$A = \begin{bmatrix} \vec{1}, & \mathbf{x}_1, & \mathbf{x}_2, & \mathbf{x}_3 \end{bmatrix}$$
.

 $(b^*, w_1^*, w_2^*, w_3^*)$  is the solution to normal equations:  $(A^TA)^{-1}(A^T\mathbf{y})$ . General note: the matrix  $A^TA$  is invertible when A has rank N+1 (when  $\vec{1}, \mathbf{x}_1, \ldots, \mathbf{x}_N$  are linearly independent).<sup>4</sup>

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  - ► Larger  $N \rightarrow$  more likely there are numerical issues computing inverse of  $A^TA$ .

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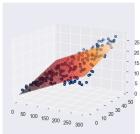
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Interpretation: given fixed budget for radio and newspaper ads, increasing TV ad budget by \$1000 will increase sales by around 46 units (in each market, on average).



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The value of  $R^2$  with all three predictor (independent) variables is: 0.89721. What conclusion can we draw?

<sup>&</sup>lt;sup>5</sup>Recall, on average, SE is how far  $w_i^*$  is from population coeff.  $w_i$ .

Hypothesis testing: choose a p-value threshold (often < 0.05 or < 0.01). The p-value corresponds to some t-statistic – use regression coefficient  $(w_i^* \text{ for } x_i)$  and Standard Error.

In example, if using simple linear regression on Newspaper, would get the variable is significant. However, using multiple regression with TV, Radio, and Newspaper, get very large p-value  $\rightarrow$  so, not significant.

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Alternative: if sample  $w_i^*$  varies a lot (relative to its size) compared to coeff's of the other var's, that variable is not significant.

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Hypothesis testing: choose a p-value threshold (often < 0.05 or < 0.01). The p-value corresponds to some t-statistic – use regression coefficient  $(w_i^* \text{ for } x_i)$  and Standard Error.

In example, if using simple linear regression on Newspaper, would get the variable is significant. However, using multiple regression with TV, Radio, and Newspaper, get very large p-value  $\rightarrow$  so, not significant.

The formula for  $SE(w_i)$  ...

Alternative: if sample  $w_i^*$  varies a lot (relative to its size) compared to coeff's of the other var's, that variable is not significant.

▶ p-value large when t-statistic is small, which is when  $SE(w_i^*)$  is large relative to size of  $w_i^*$ .

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### Intuitive estimate of significance (Bootstrapping)

Checking whether fluctuation of regression coefficient for an independent variable, relative to coeff.'s size, is large.

<sup>&</sup>lt;sup>6\*</sup>Some evidence in literature (Goodhue-Lewis, 2012) that not much precision is to be gained with more than 100 samples, for bootstrapping standard errors.

<sup>&</sup>lt;sup>7</sup>This is an example of a bootstrapping procedure: the whole sample is used as a proxy for the population and the subsamples, or resamplings, are simulating samples from the population.

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1. Take around 100 random subsamples<sup>6</sup> of data (or, resamplings with replacement); compute coefficient  $w_i^*$  for those. Standard deviation of those sample coefficients  $\approx SE(w_i^*)$ .

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- 2. Use regression coeff. from whole data set,  $\approx w_i$ . If standard dev. found in 1., divided by this coeff., is larger than about 0.5, variable is not significant.
  - Since we are estimating some things here, don't use as a hard cutoff. Getting 0.48, versus 0.59, would perhaps both be weakly significant. However, if larger than 1.5, say, definitely not significant.

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#### Outline

Confidence intervals with linear regression

Measuring how well LSR line fits

Example with Multiple variables

Polynomial fitting

If a linear model does not seem a good fit for our data, can try fitting to a polynomial. This is just like doing linear regression on transformed data, **except** with more than one function transformation: using x, and  $x^2$ , and  $x^3$ , etc.

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As a regression model, we use

$$y \approx w_d x^d + w_{d-1} x^{d-1} + \ldots + w_1 x + b$$

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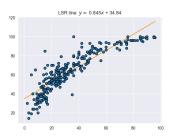
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$$A = \begin{bmatrix} x_1^d & \dots & x_1^2 & x_1 & 1 \\ x_2^d & \dots & x_2^2 & x_2 & 1 \\ \vdots & & \vdots & \vdots & \vdots \\ x_p^d & \dots & x_p^2 & x_p & 1 \end{bmatrix}$$

Taking the 'College.csv' data set from the DataSets folder. Two of the columns are 'Top10perc' and 'Top25perc'. For the schools in the data set, these columns give the percentage of the entering class that were in the top 10% (resp. 25%) of their graduating high school class.<sup>8</sup>

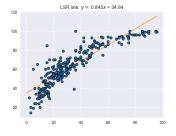
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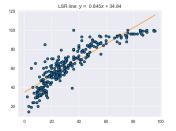


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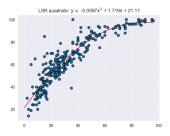
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Next, the data set with a least squares quadratic polynomial fit. The  $R^2$  value is 0.854.



What will happen to the value of  $R^2$  if we increase the degree of the polynomial that we fit to the data?

 $<sup>^{9}</sup>$ So,  $A_{1}$  has all the columns of  $A_{0}$ , and one additional column.

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set  $A_0$ : the Vandermonde matrix used to fit polynomial of degree d; set  $A_1$ : the one used for polynomial of degree d+1. <sup>9</sup> From Note, as long as enough of the  $x_i$  are distinct,  $\operatorname{rank}(A_1) = \operatorname{rank}(A_0) + 1$ .

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Meaning:  $Col(A_0)$  is proper subspace of  $Col(A_1)$ . So, using  $A_1$  makes  $|y - \hat{y}|^2$  smaller. Since  $\sum (y - \bar{y})^2$  is unchanged, makes  $R^2$  closer to 1.

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