Assessing accuracy of linear regression

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Oct 9, 2025

Outline

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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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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 $b^\star$ and $\mathbf{w}^\star$, these are not (necessarily) the parameters for the population linear model.

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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 $w^\star$ and $b^\star$ as sample statistics (like the sample mean).

Confidence intervals

How close do we suspect $w^\star$ and $b^\star$ to be to the *true* (population) slope and intercept?

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$$(SE(w^\star))^2 = \frac{\sigma^2}{\sum_{i=1}^{P}(x_i - \bar{x})^2};$$

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

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Roughly, the Standard Error is the amount, on average, that $w^\star$ (resp. $b^\star$) differs from true slope w (resp. true intercept b).[2]

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σ 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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Confidence intervals, cont'd

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Formulae:

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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[3] with $\pm 2SE$:

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

and

$$(b^\star - 2SE(b^\star), b^\star + 2SE(b^\star)).$$

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Mean Squared Error

How to measure how well the data fits to regression line?

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In linear regression, we found "predicted" $\hat{y}_i = b^\star + \mathbf{x}_i^T \mathbf{w}^\star, 1 \leq i \leq P$ so that the points $\left(\mathbf{x}_1, \hat{y}_1\right), \ldots, \left(\mathbf{x}_P, \hat{y}_P\right)$ fit a line. Could use the Mean Squared Error as our measure.

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

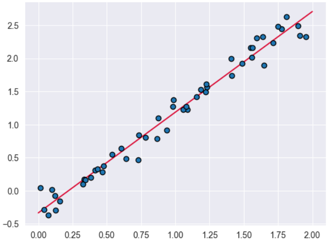
$$\text{RSE} = \sqrt{\frac{1}{P-2} \sum_{i=1}^{P} (y_i - \hat{y}_i)^2}.$$

So MSE $= \frac{P-2}{P}\text{RSE}^2$.

Mean Squared Error, example

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

$$y = 1.520275x - 0.33458.$$



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

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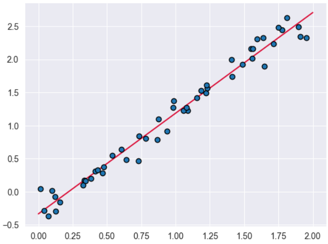
The MSE for this data and its predictions is ≈ 0.0197.
Does that mean that the linear model is a "good fit"?



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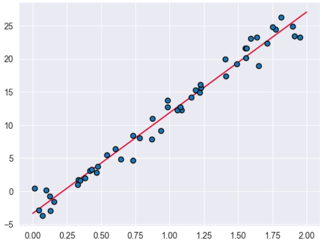

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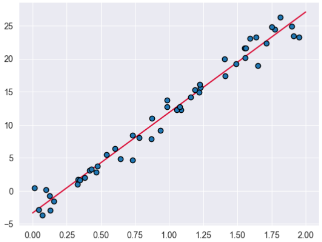

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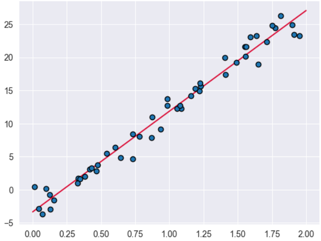

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MSE is still a good measure to think about, but its size depends on scale of y-coordinates (equivalently, depends on units y is measured in).

R^2: Proportion of "variance explained"

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^2 is "close" to 1 is often done to indicate that a linear model is a very good one.

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- Fitting `Sales` to each one with single-variable regression (one for `TV`, one for `Radio`, one for `Newspaper`) is inadequate.
  - Ignores that all are contributing together to `Sales`.
  - Doesn't give predictive ability that matches data.

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As we discussed, set A to be $P \times (N+1)$ matrix with a column of ones, and a column for each independent variable. That is,

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

$(b^\star, w_1^\star, \ldots, w_N^\star)$ is the solution to normal equations: $(A^TA)^{-1}(A^T\mathbf{y})$.

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).[4]

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

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Contrast with result of three separate linear regressions, below.

Variable	TV	Radio	Newspaper
LSR line	$0.0475x_0 + 7.0326$	$0.2025x_1 + 9.3116$	$0.0547x_2 + 12.3514$
R^2	0.612	0.332	0.052

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

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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 ($\hat{p}_i$ 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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- 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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- p-value large when t-statistic is small, which is when SE is large *relative to size of* $\hat{p}_i$. [5]

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

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2. Use regression coeff. from whole data set, $\approx p_i$. 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.

[7]

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Outline

Powers of x in place of multiple variables

Often, a linear model does not seem like a good fit for our data. What about trying to fit the data to a polynomial?

[8] Could do mix, multivariate regression and powers.

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i.e., consider the model

$$y = p_0 x^d + p_1 x^{d-1} + \ldots + p_{d-1} x + p_d + \varepsilon$$

for some degree d, and find the coefficients which give best fit polynomial.

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For the procedure, use essentially the same idea for the matrix A, but using powers of single variable x instead of using different independent variables[8]. Given data with x-coordinates $x_1, x_2, \ldots, x_n$, the matrix A is known as a **Vandermonde matrix**.

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

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Example

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.[9]

[9] Removed rows that contained schools receiving fewer than 2500 applications.

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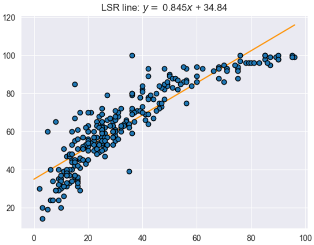

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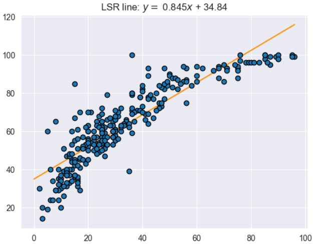

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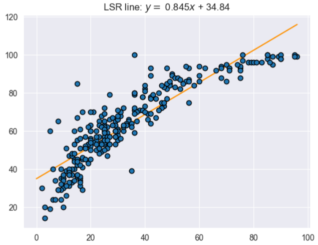
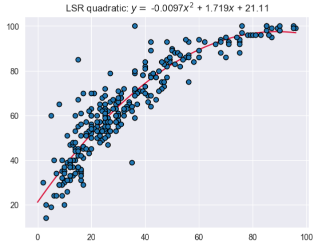


Next, the data set with a least squares quadratic polynomial fit. The R^2 value is 0.854.



Value of R^2 as polynomial degree increases

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

[10] So, A_1 has all the columns of A_0, and one additional column.

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- Note: Suppose that $n > d$. A Vandermonde matrix for x-values $x_1, x_2, \ldots, x_n$, which has $d + 1$ columns (so, highest power is x_i^d), will have rank $d + 1$ if and only if there are $d + 1$ of the x_i that are distinct.

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$\mathrm{rank}(A_1) = \mathrm{rank}(A_0) + 1$.
Meaning: $\mathrm{Col}(A_0)$ is proper subspace of $\mathrm{Col}(A_1)$. 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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