MATH 567: Mathematical Techniques in Data Science
Linear Regression: old and new

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- In the example, we want:
  $\text{price} = \beta_1 \cdot \text{mileage} + \beta_2 \cdot \text{cylinder} + \ldots$

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Modern setting:

- In modern problems, it is often the case that $n \ll p$.
- Requires supplementary assumptions (e.g. sparsity).
- Can still build good models with very few observations.

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where $\mathbf{x_1}, \dots, \mathbf{x_p} \in \mathbb{R}^{n\times 1}$ are the observations of $X_1, \dots X_p$.

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- We want $Y = \beta_1 X_1 + \dots + \beta_p X_p$.
- Equivalent to solving

$$Y = X\beta \qquad \beta = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{pmatrix}.$$

Classical setting (cont.)

We need to solve $Y = X\beta$.

- In general, the system has **no solution** ($n \gg p$) or **infinitely many solutions** ($n \ll p$).

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$$\hat{\beta} = \operatorname*{argmin}_{\beta \in \mathbb{R}^p} \|Y - X\beta\|^2.$$

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$$0 = \frac{\partial}{\partial \beta_i} \|Y - X\beta\|^2 = \frac{\partial}{\partial \beta_i} \sum_{k=1}^{n} (y_k - X_{k1}\beta_1 - X_{k2}\beta_2 - \cdots - X_{kp}\beta_p)^2$$

$$= 2 \sum_{k=1}^{n} (y_k - X_{k1}\beta_1 - X_{k2}\beta_2 - \cdots - X_{kp}\beta_p) \times (-X_{ki})$$

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Therefore,

$$\sum_{k=1}^{n} X_{ki}(X_{k1}\beta_1 + X_{k2}\beta_2 + \cdots + X_{kp}\beta_p) = \sum_{k=1}^{n} X_{ki} y_k$$

Calculus approach (cont.)

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- Proved by computing the Hessian matrix:

$$\frac{\partial^2}{\partial\beta_i\beta_j}\|Y - X\beta\|^2 = 2X^T X.$$

Linear algebra approach

Want to solve $Y = X\beta$.

Linear algebra approach: Recall: If $V \subset \mathbb{R}^n$ is a subspace and $w \notin V$, then the best approximation of w be a vector in V is

$$\text{proj}_V(w).$$

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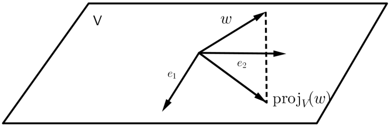

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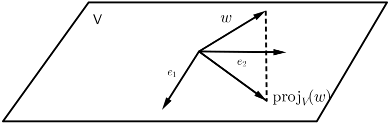

$$X\beta \in \text{col}(X) = \text{span}(\mathbf{x_1}, \ldots, \mathbf{x_p}).$$

- If $Y \notin \text{col}(X)$, then the best approximation of Y by a vector in $\text{col}(X)$ is

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Linear algebra approach (cont.)

So
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With a little more work, we can find an explicit solution:
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Equivalently,
$$X^T X\hat{\beta} = X^T Y \qquad \text{(Normal equations)}.$$

The least squares theorem

Theorem (Least squares theorem)

Let $A \in \mathbb{R}^{n \times m}$ *and* $b \in \mathbb{R}^n$. *Then*

1. $Ax = b$ *always has a least squares solution* $\hat{x}$.
2. *A vector* $\hat{x}$ *is a least squares solution iff it satisfies the normal equations*
$$A^T A\hat{x} = A^T b.$$
3. $\hat{x}$ *is unique* $\Leftrightarrow$ *the columns of* A *are linearly independent* $\Leftrightarrow$ $A^T A$ *is invertible. In that case, the unique least squares solution is given by*
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In R:

`model <- lm(`$Y \sim X_1 + X_2 + \cdots + X_p$`).`

How good is our linear model?

- We examine the *mean squared error*:

$$\mathrm{MSE}(\hat{\beta}) = \frac{1}{n}\|y - X\hat{\beta}\|^2 = \frac{1}{n}\sum_{k=1}^{n}(y_i - \hat{y}_i)^2.$$

Measuring the fit of a linear model

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- Example:

```
model <- lm(Auto$mpg ~ Auto$horsepower + Auto$weight)
sm <- summary(model)
mean(sm$residuals^2)   # The MSE
```

The coefficient of determination

- The *coefficient of determination*, called “R squared” and denoted R^2:

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- In some sense, the R^2 measures "how much better" is the prediction, compared to a constant prediction equal to the average of the $y_i s$.

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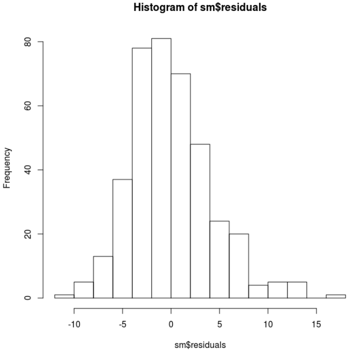
- A model with a R^2 close to 1 fits the data well.

Measuring the fit of a linear model (cont.)

We can examine the distribution of the residuals:

```
hist(sm$residuals)
```



Desirable properties:

- Symmetry
- Light tail.

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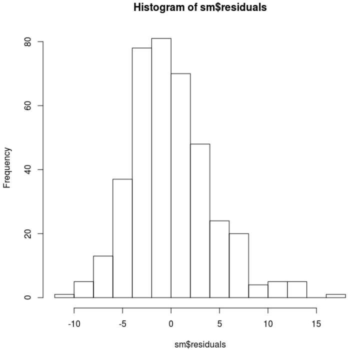


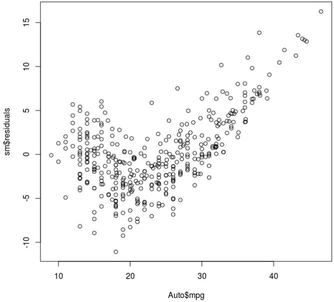
Desirable properties:

- Symmetry
- Light tail.

- A heavy tail suggests there may be outliers.
- Can use transformations such as $\log$, $\sqrt{\cdot}$, or $1/x$ to improve the fit.

Measuring the fit of a linear model (cont.)

Plotting the residuals as a function of the mpg (or fitted values), we immediately observe some patterns.



Outliers? Separate categories of cars?

Improving the model

- Add more variables to the model.
- Select the best variables to include.
- Use transformations.
- Separate cars into categories.
- etc.

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For example, let us fit a model only for cars with a `mpg` less than 25: