CS-UY 4563: Lecture 4
Finish Linear Regression, Model Selection

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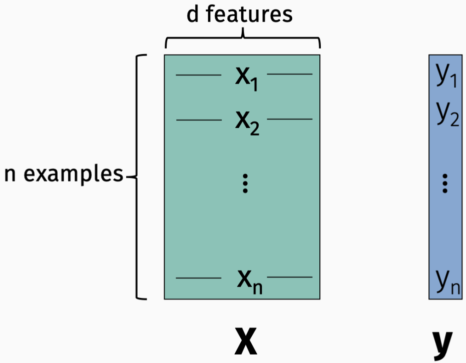
- First written assignment due **Thursday, by midnight.**
- Second lab posted `lab_robot_partial.ipynb` due **next Tuesday 2/11, by midnight.**

Target variable:

- Scalars $y_1, \ldots, y_n$ for n data examples (a.k.a. samples).

Predictor variables:

- d dimensional vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n$ for n data examples and d features

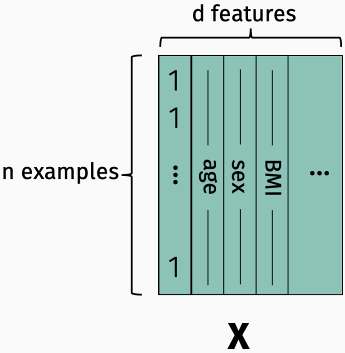


Motivating example: Predict diabetes progression in patients after 1 year based on health metrics. (Measured via numerical score.)

Features: Age, sex, body mass index, average blood pressure, six blood serum measurements (e.g. cholesterol, lipid levels, iron, etc.)

Demo in `demo1_diabetes.ipynb`.

Predictor variables:



Linear Least-Squares Regression.

- Model:

$$f_{\boldsymbol{\beta}}(\mathbf{x}) = \langle \mathbf{x}, \boldsymbol{\beta} \rangle$$

- Model Parameters:

$$\boldsymbol{\beta} = [\beta_1, \beta_2, \ldots, \beta_d]$$

- Loss Function:

$$L(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2$$

Machine learning goal: minimize the loss function $L(\boldsymbol{\beta}) : \mathbb{R}^d \rightarrow \mathbb{R}$.

Find optimum by determining for which $\boldsymbol{\beta} = [\beta_1, \ldots, \beta_d]$ the gradient is 0. I.e. when do we have:

$$\nabla L(\beta) = \begin{bmatrix} \frac{\partial L}{\partial \beta_1} \\ \frac{\partial L}{\partial \beta_2} \\ \vdots \\ \frac{\partial L}{\partial \beta_d} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Function:

$$f(\mathbf{z}) = \mathbf{a}^T\mathbf{z} \text{ for some fixed column vector } \mathbf{a} \in \mathbb{R}^d$$

Gradient:

Function:

$$f(\mathbf{z}) = \|\mathbf{z}\|_2^2$$

Gradient:

Function:

$$f(\mathbf{z}) = g(\mathbf{A}\mathbf{z}) = \text{ for fixed } \mathbf{A} \in \mathbb{R}^{n \times d} \text{ and function } g$$

Gradient:

Loss function:

$$L(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2$$

Loss function: $\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2$.

Goal: minimize the loss function $L(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2$.

$$\nabla L(\boldsymbol{\beta}) = 2\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} - 2\mathbf{X}^T\mathbf{y} = \mathbf{0}$$

Solve for optimal $\boldsymbol{\beta}^*$:

$$\mathbf{X}^T\mathbf{X}\boldsymbol{\beta}^* = \mathbf{X}^T\mathbf{y}$$

$$\boldsymbol{\beta}^* = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y}$$

What is the sign of β_1 when we run a simple linear regression using the following predictors for diabetes progression in isolation:

- Body mass index (BMI): **Positive**
- Sex (values of 1 indicates male, value of 2 indicates female): **Positive**

What is the sign of the corresponding β's when we run a multiple linear regression using the following predictors together:

- Body mass index (BMI): **Positive**
- Sex (values of 1 indicates male, value of 2 indicates female): **Negative**

Can you explain this? Try to think of your own example of a regression problem where this phenomenon might show up.

The sex variable in the diabetes problem was binary.

Suppose we go back to the MPG prediction problem. What if we had a categorical predictor variable for car make with more than 2 options: e.g. Ford, BMW, Honda. **How would you encode as a numerical column?**

$$\begin{bmatrix} \texttt{ford} \\ \texttt{ford} \\ \texttt{honda} \\ \texttt{bmw} \\ \texttt{honda} \\ \texttt{ford} \end{bmatrix} \rightarrow \begin{bmatrix} \\ \\ \\ \\ \\ \end{bmatrix}$$

Better approach: One Hot Encoding.

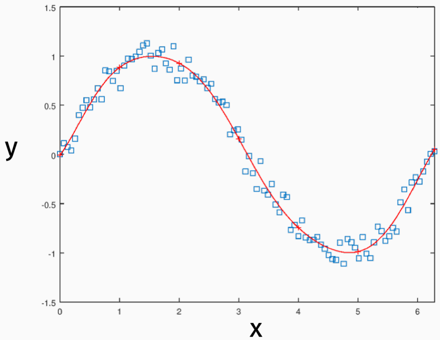
$$\begin{bmatrix} \texttt{ford} \\ \texttt{ford} \\ \texttt{honda} \\ \texttt{bmw} \\ \texttt{honda} \\ \texttt{ford} \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

- Create a separate feature for every category, which is 1 when the variable is in that category, zero otherwise.
- Not too hard to do by hand, but you can also use library functions like `sklearn.preprocessing.OneHotEncoder`.

Avoids adding inadvertent linear relationships.

Suppose we have singular variate data examples (x, y). How could we fit the non-linear model:

$$y \approx \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3.$$



Transform into a multiple linear regression problem:

$$\mathbf{X} = \begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^1 & x_2^3 \\ 1 & x_3 & x_3^2 & x_3^3 \\ \vdots & \vdots & & \vdots \\ 1 & x_n & x_n^2 & x_n^3 \end{bmatrix}$$

Each column j is generated by a different basis function $\phi_j(x)$.

Could have:

- $\phi_j(x) = x^q$
- $\phi_j(x) = sin(x)$
- $\phi_j(x) = cos(10x)$
- $\phi_j(x) = 1/x$

Transformations can also be for multivariate data.

Example: Multinomial model.

- Given a dataset with <u>target y</u> and <u>predictors x, z</u>.
- For inputs $(x_1, z_1), \ldots, (x_n, z_n)$ construct the data matrix:

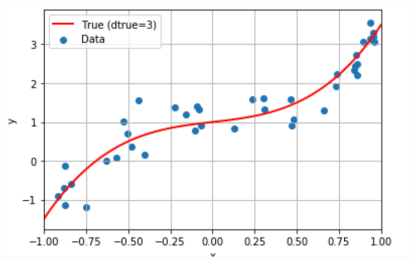
$$\begin{bmatrix} 1 & x_1 & x_1^2 & z_1 & z_1^2 & x_1 z_1 \\ 1 & x_2 & x_2^2 & z_2 & z_2^2 & x_2 z_2 \\ \vdots & \vdots & & \vdots & & \\ 1 & x_n & x_n^2 & z_n & z_n^2 & x_n z_n \end{bmatrix}$$

- Captures non-linear interaction between x and y.

Remainder of lecture: Learn about model selection, test/train paradigm, and cross-validation through a simple example.

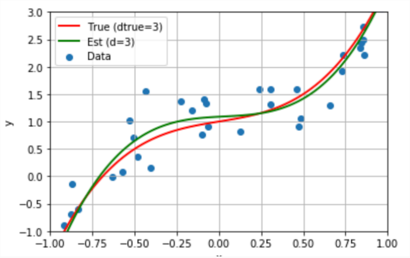
Simple experiment:

- Randomly select data points $x_1, \ldots, x_n \in [-1, 1]$.
- Choose a degree 3 polynomial $p(x)$.
- Create some fake data: $y_i = p(x_i) + \eta$ where η is a random number (e.g random Gaussian).



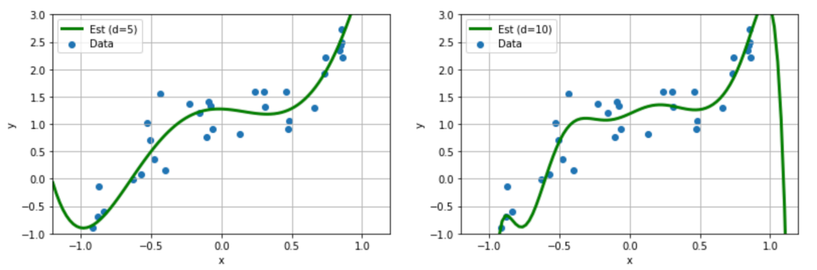
Simple experiment:

- Use multiple linear regression to fit a degree 3 polynomial.



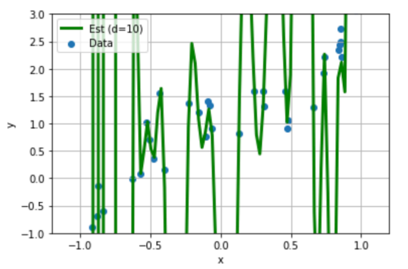
What if we fit a higher degree polynomial?

- Fit degree 5 polynomial under squared loss.
- Fit degree 10 polynomial under squared loss.

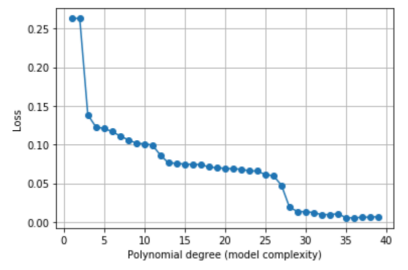


Even higher?

- Fit degree 40 polynomial under squared loss.



The more **complex** our model class (i.e. the higher degree we allow) the better our loss:

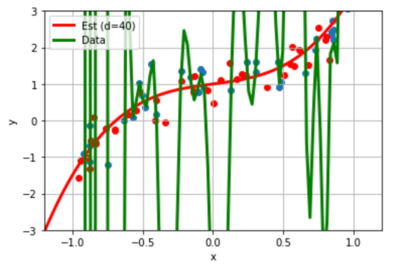


Is our model getting better and better?

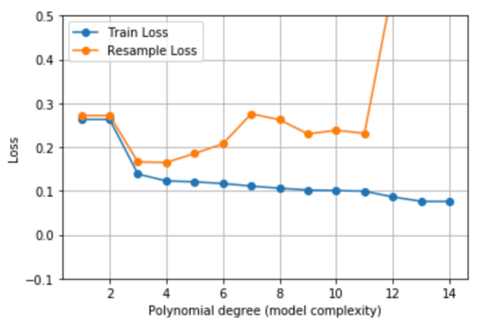
Given the raw data, how do we know which model to choose?
Degree 3? Degree 5? Degree 40?

Problem: Loss alone is not informative for choosing model.

For more complex models, we get smaller loss on the training data, but don't expect to perform well on "new" data:



Solution: Directly test model on "new data".



- Loss continues to decrease as model complexity grows.
- Performance on new data "turns around" once our model gets too complex. Minimized around degree 4.

In most situations, we cannot simply collect or generate "new data". Here's an alternative:

Test/train split:

- Given data set $(\mathbf{X}, \mathbf{y})$, split into two sets $(\mathbf{X}_{tr}, \mathbf{y}_{tr})$ and $(\mathbf{X}_{ts}, \mathbf{y}_{ts})$.
- Train q models $f_1, \ldots, f_q$ by finding parameters which minimize the loss on $(\mathbf{X}_{tr}, \mathbf{y}_{tr})$.
- Evaluate loss of each trained model on $(\mathbf{X}_{ts}, \mathbf{y}_{ts})$.

Justification:

- Assume each data example is randomly drawn from some distribution $(\mathbf{x}, y) \sim \mathcal{D}$: we don't care about any particulars of this distribution.
- **Goal:** Find model $f \in \{f_1, \ldots, f_q\}$ and parameter vector $\boldsymbol{\theta}$ to minimize the Risk:

$$R(f, \boldsymbol{\theta}) = \mathbb{E}_{(\mathbf{x}, y) \sim \mathcal{D}} \left[L\left(f(\mathbf{x}, \boldsymbol{\theta}) - y \right) \right]$$

where L is some loss function (e.g. $L(z) = |z|$ or $L(z) = z^2$).

Justification:

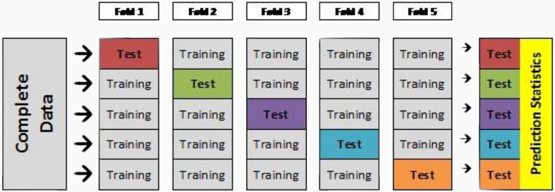
- Suppose the testing dataset $(\mathbf{X}_{ts}, \mathbf{y}_{ts})$ has m examples.
- Given any model f and parameters $\boldsymbol{\theta}$, let

$$L_{ts}(f, \boldsymbol{\theta}) = \frac{1}{m} \sum_{\mathbf{x}, y \in (\mathbf{X}_{ts}, \mathbf{y}_{ts})} L\left(f(\mathbf{x}, \boldsymbol{\theta}) - y\right)$$

- **Claim:**

$$\mathbb{E}\left[L_{ts}(f, \boldsymbol{\theta})\right] = R(f, \boldsymbol{\theta}).$$

- So our testing error is an unbiased estimate for the true risk which measures how well a function performs on average for any "new" data point.



- Randomly divide data in K parts.
    - Typical choice: $K = 5$ or $K = 10$.
- Use $K - 1$ parts for training, 1 for test.
- For each model, compute test loss L_{ts} for each "fold".
- Choose model with best average loss.
- Retrain best model on entire dataset.

Leave-one-out cross validation: take $K = n$, where n is our total number of samples.

Is there any disadvantage to choosing K larger?