CSC 461: Machine Learning

Fall 2024

Feature transformation

Prof. Marco Alvarez, Computer Science
University of Rhode Island

Data transformation

- Definition
  - converting or mapping data from its raw form into a format that better suits the learning algorithms
  - crucial step in the machine learning pipeline that can significantly improve model performance
- Why?
  - meet algorithm assumptions
  - handle non-linear relationships
  - scale features appropriately
  - handle different data types

Scaling

- Min-max scaling

$$\tilde{x} = \frac{x - x_{min}}{x_{max} - x_{min}}$$

- Standardization

$$\tilde{x} = \frac{x - \mu}{\sigma}$$

```
[[ -91   25  -85  -36]
 [  13   23   56   57]
 [  13  -92  -27 -100]
 [ -60   64   15  -84]
 [   0   39  -46  -12]]
```

```
MinMaxScaler()
[[0.         0.75       0.         0.40764331]
 [1.         0.73717949 1.         1.        ]
 [1.         0.         0.41134752 0.        ]
 [0.29807692 1.         0.70921986 0.10191083]
 [0.875      0.83974359 0.27659574 0.56050955]]
```

```
StandardScaler()
[[-1.54757414  0.24479055 -1.38466458 -0.01789141]
 [ 0.89102753  0.20770107  1.50346717  1.64600941]
 [ 0.89102753 -1.92494389 -0.19663876 -1.16294143]
 [-0.82068325  0.96803537  0.66365581 -0.87667893]
 [ 0.58620232  0.5044169  -0.58581963  0.41150235]]
```

Categorical transformations

- One-hot encoding
  - converts categorical variables into binary vectors
  - each category becomes a column, only one column contains 1, the rest are 0

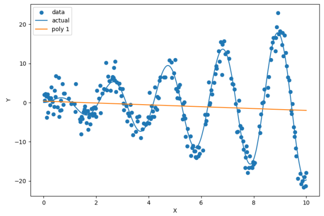
```
[['red']             [[0. 0. 1.]
 ['green']            [0. 1. 0.]
 ['blue']             [1. 0. 0.]
 ['red']              [0. 0. 1.]
 ['green']            [0. 1. 0.]
 ['blue']             [1. 0. 0.]
 ['red']              [0. 0. 1.]
 ['green']            [0. 1. 0.]
 ['blue']]            [1. 0. 0.]]
```

- Label encoding
  - converts categorical values into numerical by assigning a unique integer to each category

```
[['red']             [[2]
 ['green']            [1]
 ['blue']             [0]
 ['red']              [2]
 ['green']            [1]
 ['blue']             [0]
 ['red']              [2]
 ['green']            [1]
 ['blue']]            [0]]
```

Non-linear transformations

- Motivation
  - data is not always "linear"



$$\mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix} \quad \xrightarrow{\Phi} \quad \mathbf{z} = \begin{bmatrix} \Phi_1(\mathbf{x}) \\ \vdots \\ \Phi_{\tilde{d}}(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} z_1 \\ \vdots \\ z_{\tilde{d}} \end{bmatrix}$$

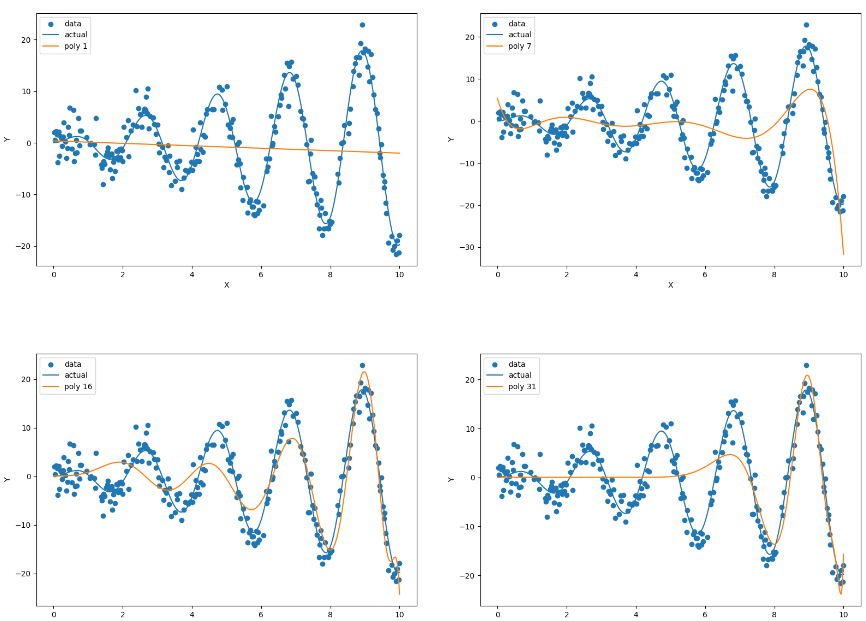
input space $\mathscr{X} = \mathbb{R}^d$ feature space $\mathscr{Z} = \mathbb{R}^{\tilde{d}}$

Non-linear transformations

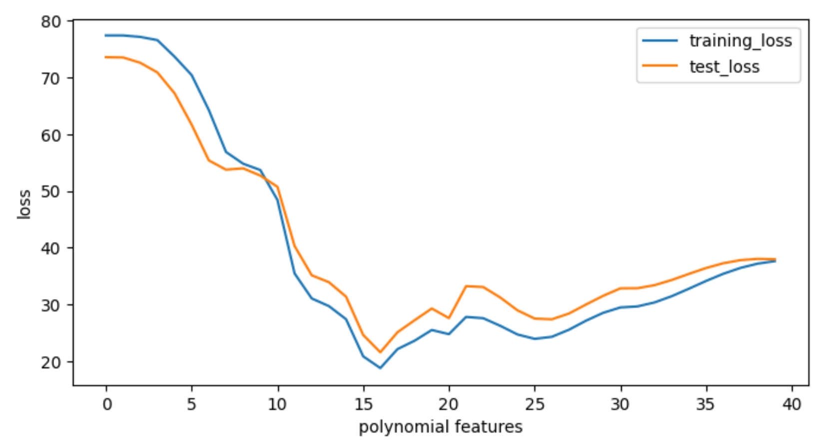
- k-th order polynomial features on one variable

$$\mathbf{x} = [x] \qquad \mathbf{z} = \begin{bmatrix} x^0 \\ x^1 \\ \vdots \\ x^k \end{bmatrix}$$

```
                  PolynomialFeatures(degree=4)
[[  7]        [[       1.        7.       49.       343.      2401.]
 [ 22]         [       1.       22.      484.     10648.    234256.]
 [-38]         [       1.      -38.     1444.    -54872.   2085136.]
 [-67]         [       1.      -67.     4489.   -300763.  20151121.]
 [  0]]        [       1.        0.        0.         0.         0.]]
```



Evaluating different degrees



Non-linear transformations

- k-th order polynomial features on two variables

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \qquad \mathbf{z} = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ x_1 x_2 \\ x_2^2 \end{bmatrix} \quad \text{degree k=2}$$

```
                          PolynomialFeatures(degree=2)
[[ 77  79]               [[    1.    77.    79.  5929.  6083.  6241.]
 [-46 -23]                [    1.   -46.   -23.  2116.  1058.   529.]
 [ 97 -87]                [    1.    97.   -87.  9409. -8439.  7569.]
 [ 53  26]                [    1.    53.    26.  2809.  1378.   676.]
 [ 41  -8]]               [    1.    41.    -8.  1681.  -328.    64.]]
```

Non-linear transformations

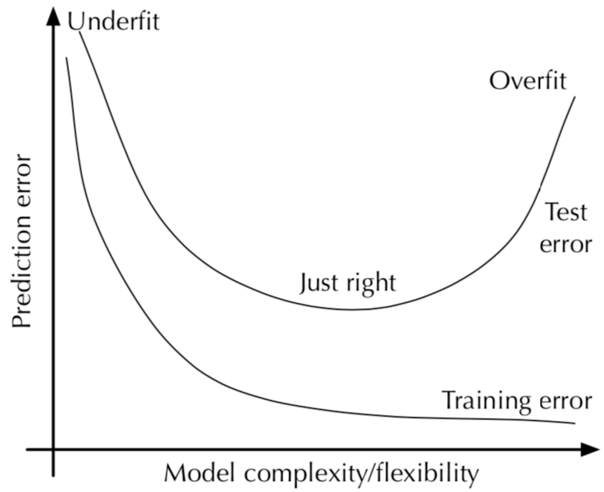
- k-th order polynomial features on d variables
  - "all polynomial combinations of the features with degree less than or equal to the specified degree"
- Issues:
  - be aware of computational cost
  - be aware of overfitting
- Alternatives?
  - use other non-linear functions: logarithmic, power, etc.

Data transformation

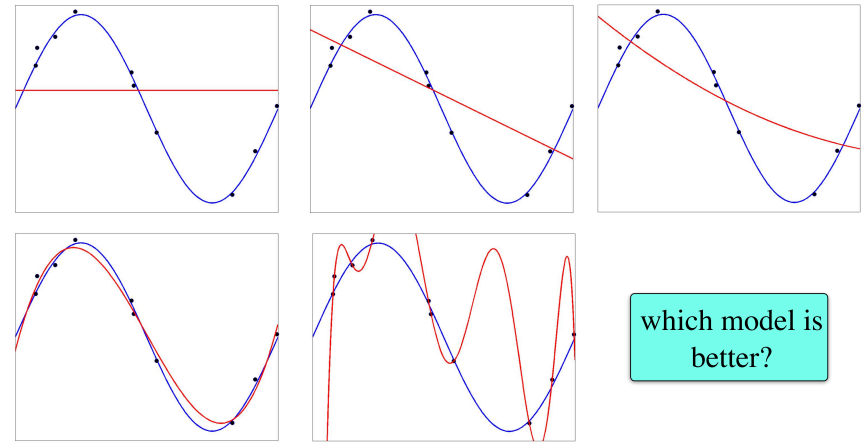
- Best Practices
  - transform after splitting data
  - fit transformers on **training data only**
  - handle missing values before transformation and use appropriate imputation
  - use pipelines to ensure reproducibility and to prevent data leakage

Overfitting

Model complexity



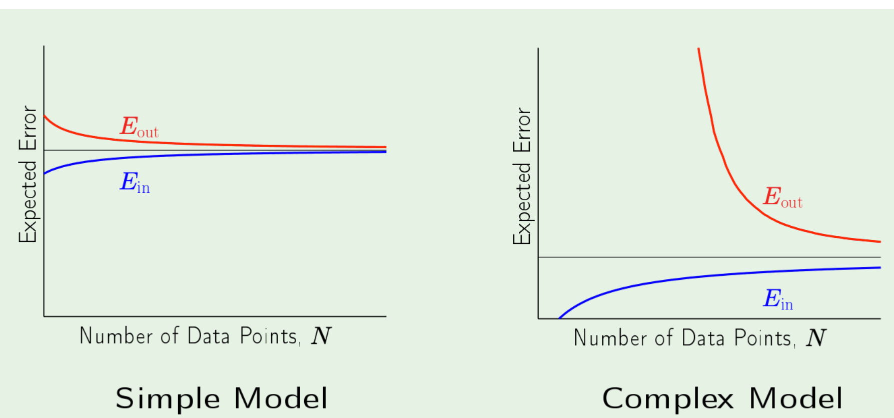
Overfitting and model complexity



which model is better?

Underfitting: model is too simple
Overfitting: model is too complex

Overfitting and data size



https://work.caltech.edu/lectures.html

Overfitting

- Reasons
  - model is too complex
  - model is fitting noise present in the training data
  - training data is not a representative sample of the distribution
- How to prevent?
  - use more training data
  - use fewer features
  - **regularize** your model