ECE 20875
Python for Data Science
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regression
• **Inference** is one of the basic problems that we want to solve in data science

• Given a set of data that we know some facts about, what new conclusions can we draw, and with what certainty?

• We will investigate several approaches to drawing conclusions from given sets of data

• Over the next few lectures: Making **predictions** about new data points given existing data using **linear regression**
linear regression

• Basic modeling problem: I want to identify a relationship between …

  • **explanatory variables** (i.e., the “inputs”, often referred to as the **features** of a data point), and

  • a **target variable** (i.e., some “output” quantity that we want to estimate)

• Can we learn what this relationship is?

• If we have a **model** for this relationship, we can use it to predict the target variable for new data points
linear regression

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linear regression

- Can we learn the model from the data?

- Note that the model does not match the data exactly!
  - A model is (at best) a simplification of the real-world relationship

- What makes a good model?
  - Minimizes **observed error**: How far the model deviates from the observed data
  - Maximizes **generalizability**: How well the model is expected to hold up to unseen data
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We can view the error as the deviation between the model and the actual datapoints
simple linear regression model

• The **simple linear regression** model has a single explanatory variable:

\[ y_n = ax_n + b + \epsilon_n, \quad n = 1, \ldots, N \]

• \( y_n \) is the **measured value** of the target variable for the \( n \)th data point

• \( ax_n + b \) is the **estimated value** of the target, based on the explanatory \( x_n \)

• Each \( y_n \) is associated with a model prediction component \( ax_n + b \) plus some **error term** \( \epsilon_n \)

• How do we minimize this error?
minimizing error

- The **mean squared error** (MSE) for simple linear regression is

\[
E(a, b) = \frac{1}{N} \sum_{n=1}^{N} \left( y_n - (ax_n + b) \right)^2
\]

- Common error metric: We looked at already when we studied the choice of histogram bin widths

- We want to minimize \( E \), denoted: \( \min_{a,b} E(a, b) \)

- With two **model parameters** \( a \) and \( b \), this is reasonably easy to carry out by hand

- The square makes it easy to take the derivative
minimizing error: derivation

• Set the derivatives with respect to $a$ and $b$ to zero:

$$\frac{dE}{da} = \frac{1}{N} \sum_{n=1}^{N} - 2x_n \left( y_n - (ax_n + b) \right) = 0$$

$$\frac{dE}{db} = \frac{1}{N} \sum_{n=1}^{N} - 2 \left( y_n - (ax_n + b) \right) = 0$$
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• Focusing first on the second equation, we have:

$$- \frac{\sum_{n=1}^{N} y_n}{N} + a \frac{\sum_{n=1}^{N} x_n}{N} + b \frac{\sum_{n=1}^{N} 1}{N} = 0,$$

or

$$b = \frac{\sum_{n=1}^{N} y_n}{N} - a \frac{\sum_{n=1}^{N} x_n}{N} = \bar{y} - a\bar{x}$$
minimizing error: derivation

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\]

- Focusing first on the second equation, we have:

\[
-\frac{\sum_{n=1}^{N} x_n y_n}{N} + a \frac{\sum_{n=1}^{N} x_n^2}{N} + b \left( \sum_{n=1}^{N} \frac{1}{N} \right) = 0, \text{ so}
\]

\[
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\]

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\]

\[
b = \frac{\sum_{n=1}^{N} y_n}{N} - a\frac{\sum_{n=1}^{N} x_n}{N} = \bar{y} - a\bar{x}
\]

- As for the first equation,

\[
-\frac{\sum_{n=1}^{N} x_n y_n}{N} + a\frac{\sum_{n=1}^{N} x_n^2}{N} + b\frac{\sum_{n=1}^{N} x_n}{N} = 0, \text{ so}
\]

\[
a\frac{\sum_{n=1}^{N} x_n^2}{N} = \frac{\sum_{n=1}^{N} x_n y_n}{N} - b\bar{x}
\]

- Substituting our expression for \( b \), we have:

\[
a\left( \frac{\sum_{n=1}^{N} x_n^2}{N} - \bar{x}^2 \right) = \frac{\sum_{n=1}^{N} x_n y_n}{N} - \bar{y}\bar{x}
\]
minimizing error: formulas

- Isolating $a$ on the left hand side and simplifying, we get:

$$a = \frac{\sum_{n=1}^{N} x_n y_n - N\bar{y}\bar{x}}{\sum_{n=1}^{N} x_n^2 - N\bar{x}^2}$$

- Here, $\bar{x}$ and $\bar{y}$ are the averages of the $x_n$ and $y_n$, respectively

- We can then use $a$ to solve for $b$ according to:

$$b = \bar{y} - a\bar{x}$$

- And then our linear regression predictor for a new datapoint $i$ is

$$y_i = ax_i + b$$
minimizing error: formulas

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• What do we do if there is more than one explanatory variable?

• To generalize to this case, it is more convenient to work with matrix equations
matrix algebra review

- Let’s say \( \mathbf{x} = (x_1 \ x_2 \ \cdots \ x_n)^T \) and \( \mathbf{y} = (y_1 \ y_2 \ \cdots \ y_n)^T \) are both \( n \)-dimensional vectors. Then
  \[
  \mathbf{x}^T \mathbf{y} = x_1 y_1 + x_2 y_2 + \cdots + x_n y_n
  \]
  is the **inner product** or **dot product** of \( \mathbf{x} \) and \( \mathbf{y} \), which is the multiplication of a \( 1 \times n \) and \( n \times 1 \) vector and results in a scalar.

- For example, suppose \( \mathbf{x} = (3 \ 4 \ 5)^T, \mathbf{y} = (1 \ 0 \ 2)^T \). Then:
  \[
  \mathbf{x}^T \mathbf{y} = (3 \ 4 \ 5) \begin{pmatrix} 1 \\ 0 \\ 2 \end{pmatrix} = 3 \times 1 + 4 \times 0 + 5 \times 2 = 13
  \]

- The **L2-norm** of a vector \( \mathbf{x} = (x_1 \ x_2 \ \cdots \ x_n)^T \) is a generalization of the Pythagorean theorem for finding the “length”:
  \[
  \| \mathbf{x} \|_2 = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2}
  \]
• More generally, define two $m \times n$ matrices:

$$X = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & \cdots & x_{mn} \end{bmatrix}, \quad Y = \begin{bmatrix} y_{11} & y_{12} & \cdots & y_{1n} \\ y_{21} & y_{22} & \cdots & y_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ y_{m1} & y_{m2} & \cdots & y_{mn} \end{bmatrix}$$

Then the matrix multiplication of $X^T$ and $Y$, which results in an $n \times n$ matrix, is:

$$X^T Y = \begin{bmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_n^T \end{bmatrix} \begin{bmatrix} y_1 & y_2 & \cdots & y_n \\ y_2 & y_2 & \cdots & y_n \\ \vdots & \vdots & \ddots & \vdots \\ y_n & y_n & \cdots & y_n \end{bmatrix} = \begin{bmatrix} x_1^T y_1 & x_1^T y_2 & \cdots & x_1^T y_n \\ x_2^T y_1 & x_2^T y_2 & \cdots & x_2^T y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_n^T y_1 & x_n^T y_2 & \cdots & x_n^T y_n \end{bmatrix}$$

• For example, with $A$ and $B$ defined below, we get:

$$A = \begin{bmatrix} -1 & 0 & 1 \\ 0 & 2 & 3 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 2 & 3 \\ 3 & 0 & 1 \end{bmatrix} \quad \rightarrow \quad A^T B = \begin{bmatrix} -1 & 0 & 1 \\ 0 & 2 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 3 & 0 & 1 \end{bmatrix} = \begin{bmatrix} -1 & -2 & -3 \\ 6 & 0 & 2 \\ 10 & 2 & 6 \end{bmatrix}$$
matrix algebra review

- If $X$ has dimension $a \times b$, and $Y$ has dimension $c \times d$, then the matrix product $XY$ is only possible if $b = c$ (i.e., the inner dimensions match), which will have dimension $a \times d$ (outer dimensions).

- If $X$ is a square matrix (i.e., has dimension $n \times n$), then its inverse is $X^{-1}$ (if it exists), and:

$$X^{-1}X = XX^{-1} = I,$$

where $I = \begin{bmatrix} 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 1 \end{bmatrix}$

is the $n \times n$ identity matrix.

- For example, with $A$ and $B$ defined as below, we can verify $B = A^{-1}$, since $AB = I$:

$$A = \begin{bmatrix} 3 & 0 & 2 \\ 2 & 0 & -2 \\ 0 & 1 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 0.2 & 0.2 & 0 \\ -0.2 & 0.3 & 1 \\ 0.2 & -0.3 & 0 \end{bmatrix}, \quad AB = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
But how do we perform matrix manipulations, like taking inverses, on large matrices in general?

In Python, we can use the numpy library to do matrix operations

```python
import numpy as np

np.array(A)  //Convert list to numpy array
np.matmul(A,B)  //Matrix multiplication (or A@B)
np.linalg.inv(A)  //Matrix inverse
A.sum(axis=0)  //Sum over rows of matrix
```

See https://scipy-lectures.org/intro/numpy/operations.html for more examples, as well as the notebook.
• Now, back to regression

• For **simple linear regression**, if we define

\[
X = \begin{bmatrix}
    x_1 & 1 \\
    x_2 & 1 \\
    \vdots & \vdots \\
    x_N & 1
\end{bmatrix}
\]

\[
\beta = \begin{bmatrix} a \\ b \end{bmatrix}
\]

\[
y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}
\]

then we can write the equations for all data points compactly using the following matrix equation:

\[
y = X\beta + \epsilon
\]

• The **multivariable linear regression model** with \( M \) explanatory variables is

\[
y_n = a_1 x_{n,1} + a_2 x_{n,2} + \cdots + a_M x_{n,M} + b + \epsilon_n, \quad n = 1, \ldots, N
\]

• In this case, we define

\[
X = \begin{bmatrix}
    x_{1,1} & x_{1,2} & \cdots & x_{1,M} & 1 \\
    x_{2,1} & x_{2,2} & \cdots & x_{2,M} & 1 \\
    \vdots & \vdots & \ddots & \vdots & \vdots \\
    x_{N,1} & x_{N,2} & \cdots & x_{N,M} & 1
\end{bmatrix}
\]

\[
\beta = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_M \\ b \end{bmatrix}
\]

\[
y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}
\]

where \( X \) is the **feature matrix**. Then, as before, we can write

\[
y = X\beta + \epsilon
\]
least squares equations

- With this matrix notation, we can write our original optimization for minimizing MSE as:

$$\min_{\beta} \frac{1}{N} \sum_{n=1}^{N} (y_n - x_n^T \beta)^2$$

- Or, equivalently, this can be written using the vector norm:

$$\min_{\beta} \frac{1}{N} \|y - X\beta\|_2^2$$

- Similar to 1D case, we can take the gradient (multidimensional derivative) and set to 0 (i.e., the vector of zeros) to find minimum:

$$\nabla \left( \frac{1}{N} \|y - X\beta\|_2^2 \right) = \frac{2}{N} X^T X\beta - \frac{2}{N} X^T y = 0$$

- This yields the least squares equations for solving for $\beta$:

$$X^T X\beta = X^T y$$
solving for $\beta$

- If $X^TX$ is invertible, we can take a matrix inverse to solve for the model parameters $\beta$:
  \[ \beta = (X^TX)^{-1}X^Ty \]

- But $X^TX$ is not always invertible
  - The inverse exists if and only if the columns of $X$ are linearly independent of one another
  - This means that we cannot have the case where one column can be written as a linear combination of the others

- What does it mean when $X^TX$ is not invertible?
  - Infinitely many possible solutions
  - We typically choose the one where $\|\beta\|$ is smallest. Why?
Suppose we collect five data points consisting of two features $x_1, x_2$ and a target variable $y$ in the form $(x_1, x_2, y): (1, 2, 10), (-3, 6, 0), (0, 0, 3), (1, -1, 4), (5, -2, 20)$. We want to fit a linear regression model to this dataset.

What are the least squares equations?

What is the resulting model?

What would be the prediction for a new datapoint with $x_1 = -1, x_2 = 1$?
The model we want to fit is $\hat{y} = a_1 x_1 + a_2 x_2 + b$, where $\beta = (a_1 \ a_2 \ b)^T$ is the parameter vector.

The feature matrix $X$, target vector $y$, and least squares equations are:

$$X = \begin{bmatrix}
1 & 2 & 1 \\
-3 & 6 & 1 \\
0 & 0 & 1 \\
1 & -1 & 1 \\
5 & -2 & 1
\end{bmatrix}, \quad y = \begin{bmatrix}
10 \\
0 \\
3 \\
4 \\
20
\end{bmatrix}.$$  

$$X^T X \beta = X^T y$$
solution: model and test prediction

Using the numpy commands for inverse, transpose, and multiplication, we compute the solution: $\beta = (X^T X)^{-1} X^T y$

$$\beta = (4.2308, 1.7538, 2.2615)^T$$

Which means that our model is

$$\hat{y} = 4.2308x_1 + 1.7538x_2 + 2.2615$$

And the prediction for $x_1 = -1$, $x_2 = 1$ is

$$\hat{y} = 4.2308 \cdot -1 + 1.7538 \cdot 1 + 2.2615 = -0.2154$$
interpreting results

• How should we interpret the results of linear regression?

• Recall multi-feature model, e.g.,
  \[ y_n = a_1 x_{n,1} + a_2 x_{n,2} + b \]

• If one feature weight (e.g., \( a_1 \)) is higher than another (e.g., \( a_2 \)), this can indicate that this feature is more important than the other (contributes more to the value of \( y \))

• Need to be careful, though! If different features have different scales, then weights will naturally be different!

• Normalization is useful as it standardizes the feature ranges

Here, \( x_1 \) has a range of 8, while \( x_2 \) only has a range of 2
normalization for interpretation

• **Problem:** Suppose I fit a linear regression model and get

\[ \hat{y} = 10x_1 + 100x_2 + 5 \]

• Does this mean that \( x_2 \) has a bigger impact on \( y \) than \( x_1 \)?

• Not necessarily, because we have said nothing about the ranges of \( x_1 \) and \( x_2 \) that resulted in \( a_1 = 10 \) and \( a_2 = 100 \).

• **One solution:** Normalize the data before doing linear regression so that coefficients are comparable over a consistent range.
standard normalization

- For every feature column, do the following to make them all have a mean of 0 and standard deviation of 1:

  1. **Center values**: Subtract the column average from each feature sample
     - Useful to eliminate any bias contained in the features
  2. **Scale values**: Divide each feature sample by the column standard deviation
     - Re-scales features so that each is expressed in new units: standard deviations from the mean (similar to how we calculate z-scores)

- Mathematically, we are defining the following operation for each feature column $\mathbf{x}_m$:

  $$\tilde{x}_m = \frac{x_m - \bar{x}_m}{s_m},$$
  where $\bar{x}_m$ and $s_m$ are the sample mean and standard deviation of feature $m$
How good is the fit of the regression to the dataset?

To answer this, one possibility is using the MSE

Another commonly used quantity is the coefficient of determination, called $r^2$

$$r^2 = 1 - \frac{\sum_{n=1}^{N} (y_n - \hat{y}_n)^2}{\sum_{n=1}^{N} (y_n - \bar{y})^2} = 1 - \frac{MSE}{\sigma_Y^2}$$

- $y_n$: Measured value, $\hat{y}_n$: Predicted value
- $\bar{y}$: Mean measured value, $\sigma_Y^2$: Variance of measured value

$r^2$ gives the fraction of variance in the data that is explained by the model

Typically between 0 (bad, no better than horizontal line) and 1 (perfect fit)

Sometimes preferred to MSE in regression problems for this reason
After fitting a linear regression model, you can **estimate** (or predict) the target $y$ of new data points using your model.

- New data point: $(x_1, x_2, \ldots)$
- Prediction: $\hat{y} = a_1x_1 + a_2x_2 + \cdots + b$
- How good is the prediction?
  - Squared error between $\hat{y}$ and $y$ (once it is known)
  - MSE or $r^2$ over a set of new data points
- When using the model, make sure to take into account any normalization that was used (i.e., normalize new data points before inputting them, “un-normalize” the $\hat{y}$ you get back)
linear regression in python

- You can solve the least squares equations directly using numpy
- Given how common linear regression is, several variants are built in to the sklearn (scikit learn) library directly:

```python
from sklearn import linear_model, from sklearn.metrics import mean_squared_error, r2_score

regr = linear_model.LinearRegression(fit_intercept=True)  # Define linear regression object
regr.fit(X_train,y_train)  # Fit model to training set
regr.coef_  # View coefficients (a_1,…,a_M) of trained model
regr.intercept_  # View intercept (b) of trained model
y_pred = regr.predict(X_test)  # Apply model to test set
r2_score(y_true,y_pred)  # r2 score between true and predicted
```
more interpretation

• Is a feature significant?
  • Just because a feature is used in a model doesn’t mean it is important in predicting the value of the output
  • But the model will try to account for the feature anyway!
• Can perform a hypothesis test (see previous lectures):
  • **Null hypothesis** \( H_0 \): Coefficient \( a_m \) is 0 (feature has no predictivity, \( y \) does not depend on \( x_m \))
  • **Alternative hypothesis** \( H_1 \): Coefficient \( a_m \) is not 0 (feature has predictivity, \( y \) does depend on \( x_m \))
hypothesis test for regression

- Test statistic is always: \( \frac{\hat{a}_m - a_m}{SE_{a_m}} \)

- What is the standard error for a regression coefficient \( a_m \)?

\[
SE_{a_m} = \sqrt{\frac{\sum_{n=1}^{N} (y_n - \hat{y}_n)^2}{N - 2}}
\]

- For a \( z \)-test, find \( p \)-value of \( SE_{a_m} \) against the \( z \)-distribution

- For a \( t \)-test, find \( p \)-value against a \( t \)-distribution with \( N - k - 1 \) degrees of freedom, where \( k \) is the number of features
a linear model may be wrong

• In these graphs, all 4 datasets have the same …
  • linear regression line
  • coefficient of determination
  • mean and variance of both x and y
• Yet clearly, the relationship between x and y is different in each case
• It is important to visualize the results, and possibly try non-linear models!
what about non-linear?

- A common (and understandable) misconception is that linear regression can only find linear relationships.
  - The “linear” part refers to the parameter vector $\beta$, not the input features in $X$.
- We can readily take nonlinear functions of our features.
- For example, suppose we want to fit a quadratic model:
  $$y_n = a_1(x_n)^2 + a_2x_n + b$$
- We create a “synthesized” feature matrix that has the quadratic form:

\[
X = \begin{bmatrix}
(x_1)^2 & x_1 & 1 \\
(x_2)^2 & x_2 & 1 \\
\vdots & \vdots & \vdots \\
(x_N)^2 & x_N & 1 \\
\end{bmatrix} \quad \beta = \begin{bmatrix}
a_1 \\
a_2 \\
b \\
\end{bmatrix} \quad y = \begin{bmatrix}
y_1 \\
y_2 \\
\vdots \\
y_N \\
\end{bmatrix}
\]
more and more complexity

• If we use a higher degree $d$ of polynomials, we can reduce MSE:

\[
\begin{align*}
\text{MSE} &= 0.90 \\
\quad d &= 0 \\
\text{MSE} &= 0.64 \\
\quad d &= 1 \\
\text{MSE} &= 0.04 \\
\quad d &= 2 \\
\text{MSE} &= 0.04 \\
\quad d &= 4 \\
\text{MSE} &= 0.01 \\
\quad d &= 8 \\
\text{MSE} &= 0.00 \\
\quad d &= 16
\end{align*}
\]

• But, is this a good thing to do?
overfitting

• If our goal was just to minimize error on the existing dataset, we’d keep adding features (e.g., increasing the degree $d$ of a polynomial)

• But this sacrifices the generalizability of the model

• An **overfitted** model is one which contains too many parameters than can be justified by the data
  
  • High $r^2$ and low MSE on training data, but low $r^2$ and high MSE on testing data

• We can contrast this with **underfitting**, where we don’t have enough parameters to drive down MSE on either training or testing data
When we have a lot of features, we can use **regularization**, a class of techniques for mitigating overfitting by penalizing non-zero model coefficients.

The general expression we work with in regularization is:

\[
\text{minimize} \ (\text{model error}) + \lambda (\text{coefficient weights})
\]

\(\lambda \geq 0\) is the **regularization parameter**

- Higher \(\lambda\): Minimizing model parameters becomes more important
- Lower \(\lambda\): Minimizing model error becomes more important

Several different regularization techniques: Lasso, **Ridge**, Elastic-Net, …
In **ridge regression**, the regularization term is the sum of squares of the coefficients:

\[
\minimize_{\beta} \| X\beta - y \|_2^2 + \lambda \| \beta \|_2^2
\]

- This makes it easy to solve in matrix form as:

\[
\beta^* = (X^T X + \lambda I)^{-1} X^T y
\]

- In Python (where \( \alpha \) is the regularization parameter):

```python
from sklearn import linear_model
reg = linear_model.Ridge(alpha=0.1, fit_intercept=True)
```
regularization can alleviate overfitting

- Polynomial of degree $d = 10$, with different amounts of regularization:

- A higher value of $\lambda$ has a “smoothing” effect on the model
evaluating predictive performance

• Descriptive and diagnostic analysis (classical statistics, data mining)
  • Focus: Understand and interpret statistical relationships in observed dataset
  • Evaluation: e.g., MSE or $r^2$ on training data (data used to fit the model)

• Predictive and prescriptive analysis (machine learning)
  • Focus: Predict target value for new or future unseen data
  • Evaluation: e.g., MSE or $r^2$ on test data (data not used to fit the model)
why evaluate on test data?

• Analogy to class
  • Training data is like homeworks, sample problems and sample exams
  • Testing data is like the real exam
• If we train and evaluate on the same data, the model may not generalize well
• Reasons for computing performance on test data (the standard ML approach):
  • Model evaluation: Quantify the model’s predictive performance if deployed
    • e.g., describing the model and its business implications to the CEO
  • Model selection: Select which model should be deployed
    • e.g., which polynomial degree or regularization value should be used?
choosing model based on test MSE

- We can use MSE on a held-out test set to determine the best model:

- Blue points: Training set
- Orange points: Held-out test set
We can use MSE on a held-out test set to determine the best model:

- The best model has the lowest test MSE
- This is often achieved when there is a small difference between training and test MSE
simulating testing data

• Ultimately, we’d like to actually test the model in the real world (e.g., predict tomorrow’s temperature)

• However, this is usually quite costly, time consuming, or downright impossible, so we have to simulate it

• To do this, we can split our dataset into:
  • **Training data:** A subset we use to train/fit the model
  • **Testing data:** A subset we used to report the generalized performance
    • Common splits: 90/10 (i.e., 90% training and 10% test) and 80/20

• **Note:** It is important that the algorithm never sees the testing data (just like it is important that students don’t see the real midterm)
**cross validation**

- **k-fold cross validation** (often abbreviated **CV**) repeats the train/test split idea *k* times, across different **folds** of the data.
  - The data is divided into *k* parts.
  - In each fold, one part is used as the testing set, and the other *k* − 1 are used as the training set.
  - Thus, there are *k* models fit throughout this process, and we can average testing performance (and sometimes the coefficients).
  - How many folds should be used?
    - 3-fold, 5-fold and 10-fold are common.
  - **Leave-one-out CV**: *k* is the number of datapoints, i.e., one is held out in each fold (computationally expensive).
cross validation for model selection

- How do we determine the right value of $\lambda$?

- Test a wide range of $\lambda$ typically log scale, e.g., $0.01, \ldots, 0.1, \ldots, 1, \ldots, 10, \ldots, 100$

- Use multiple CV iterations, one for each value of $\lambda$:

  - Train all folds with $\lambda = 0.01$
  - Train all folds with $\lambda = 0.1$
  - Train all folds with $\lambda = 1$
  - Train all folds with $\lambda = 10$

- Choose $\lambda^*$ whose CV performance is the best

- For final model, train model with all data using $\lambda^*$
Suppose we collect three data points with a single feature $x$ and target variable $y$. In the form $(x, y)$, they are, approximately: $(2.18, 2.26)$, $(0.13, -14.57)$, $(2.75, 16.74)$.

Find the linear regression model $\hat{y} = ax + b$ and corresponding regularization parameter $\lambda$ which has minimum cross validation error.

Use the Ridge model, $k = 3$ folds, and test $\lambda = 0, 0.1, 1$. Note that the coefficient $b$ should NOT be regularized.
solution

- We need to solve the least squares equations for three values of lambda, and three folds each (i.e., 9 cases total). Here is the math for \( \lambda = 0, 0.1 \) and the second fold:

```
fold=2, lambda=0.0

x ~ [2.18, 0.13, 2.75]
y ~ [2.26, -14.57, 16.74]

fold=2, lambda=0.1

x:
[[2.17997451 1.]
 [2.74831239 1.]]

X.T @ X:
[[12.30550986  4.9282869]
 [ 4.9282869  2.]]

X.T @ X + lambda*I:
[[12.30550986  4.9282869]
 [ 4.9282869  2.]]

(X.T @ X + lambda*I)^(-1):
[[ 6.19179817 -9.42296757]
 [-9.42296757 23.71954383]]

(X.T @ X + lambda*I)^(-1)@ X^T:
[[-1.0866716  1.0866716]
 [ 3.1777147 -2.1777147]]

(X.T @ X + lambda*I)^(-1)@ X^T @ y:
[25.47215001 -53.26685674]

Only coefficient is changed by \( \lambda \), intercept is not regularized

Notice how different the inverse is just from a small \( \lambda \)
```

• We need to solve the least squares equations for three values of lambda, and three folds each (i.e., 9 cases total). Here is the math for \( \lambda = 0, 0.1 \) and the second fold:
fold=2, lambda=0.0

\[
\begin{align*}
x &= [2.18, 0.13, 2.75] \\
y &= [2.26, -14.57, 16.74]
\end{align*}
\]

\[
X = \begin{bmatrix}
  2.17997451 & 1.00 \\
  2.74831239 & 1.00
\end{bmatrix}
\]

\[
X^T \times X =
\begin{bmatrix}
  12.3050986 & 4.9282869 \\
  4.9282869 & 2.00
\end{bmatrix}
\]

\[
X^T \times X + \lambda I =
\begin{bmatrix}
  12.3050986 & 4.9282869 \\
  4.9282869 & 2.00
\end{bmatrix}
\]

\[
(X^T \times X + \lambda I)^{-1} =
\begin{bmatrix}
  3.8240337 & -9.422968 \\
  -9.422968 & 23.719544
\end{bmatrix}
\]

\[
(X^T \times X + \lambda I)^{-1} \times X^T \times y =
\begin{bmatrix}
  -1.086672 & 3.1777147 \\
  3.1777147 & -2.1777147
\end{bmatrix}
\]

\[
(X^T \times X + \lambda I)^{-1} \times X^T \times y =
\begin{bmatrix}
  15.73151403 & -29.2645324
\end{bmatrix}
\]

\[
\lambda^* = 0.10 \text{ has best average test MSE}
\]

fold=2, lambda=0.1

\[
\begin{align*}
x &= [2.18, 0.13, 2.75] \\
y &= [2.26, -14.57, 16.74]
\end{align*}
\]

\[
X = \begin{bmatrix}
  2.17997451 & 1.00 \\
  2.74831239 & 1.00
\end{bmatrix}
\]

\[
X^T \times X =
\begin{bmatrix}
  12.3050986 & 4.9282869 \\
  4.9282869 & 2.00
\end{bmatrix}
\]

\[
X^T \times X + \lambda I =
\begin{bmatrix}
  12.4050986 & 4.9282869 \\
  4.9282869 & 2.00
\end{bmatrix}
\]

\[
(X^T \times X + \lambda I)^{-1} =
\begin{bmatrix}
  3.8240337 & -9.422968 \\
  -9.422968 & 23.719544
\end{bmatrix}
\]

\[
(X^T \times X + \lambda I)^{-1} \times X^T \times y =
\begin{bmatrix}
  -0.866672 & 1.0866716 \\
  1.0866716 & 3.1777147
\end{bmatrix}
\]

\[
(X^T \times X + \lambda I)^{-1} \times X^T \times y =
\begin{bmatrix}
  15.73151403 & -29.2645324
\end{bmatrix}
\]

\[
\lambda^* = 0.10 \text{ has best average test MSE}
\]