DATA 3464: Fundamentals of Data Processing

Basic machine learning models

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Topic overview

- Some common machine learning tasks and models
- Evaluating model performance
- Limitations and assumptions

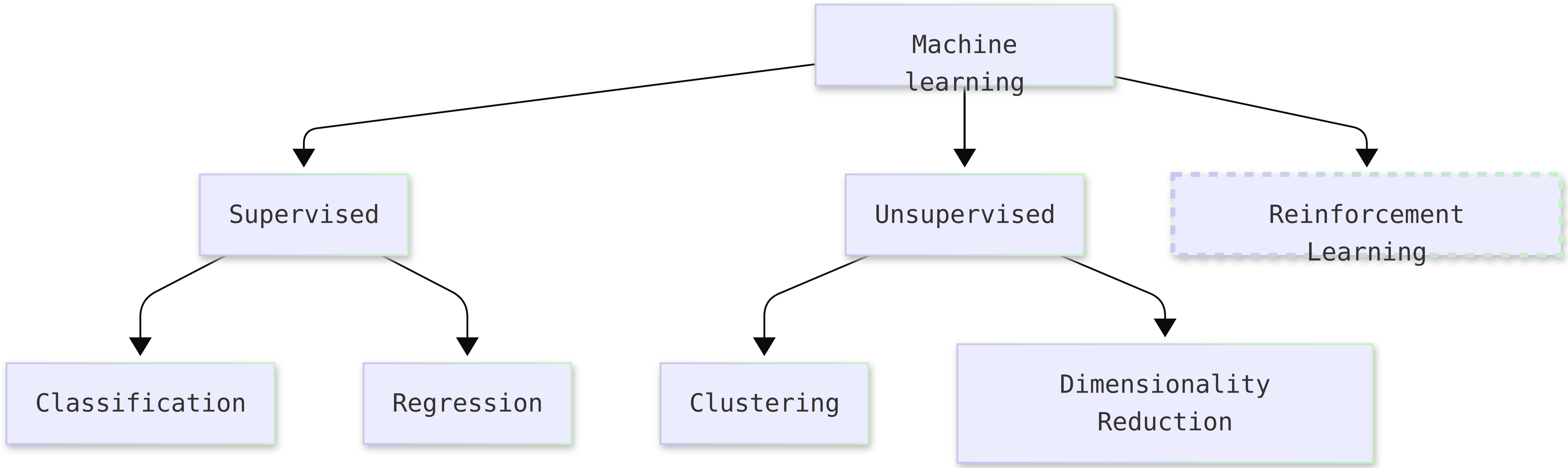
Resources used:

- Feature Engineering Chapter 1
- Introduction to Machine Learning with Python. Available at MRU Library
- Scikit-learn User Guide
- Hands on Machine Learning with Scikit-Learn and Tensorflow/PyTorch. Available at MRU Library

Machine learning

- To appropriately process the data, we need to know *why* we are doing it and what assumptions we're making
- Modern machine learning toolkits (such as scikit-learn) are so easy to use, they're easy to use inappropriately
- Goal: just enough understanding to use basic models **responsibly**

Why are we processing data?



- No reinforcement learning in this course, sorry

A selection of common models

Supervised

- Linear/logistic regression
- Decision trees
- Support vector machines

Unsupervised

- K-means clustering
- Principle component analysis

Source: Müller, A. C., & Guido, S. (2016). Introduction to Machine Learning with Python. O'Reilly Media, Incorporated. Available at MRU Library. 4

No free lunch

- A theory-heavy paper in 1996 showed that there is no one machine learning algorithm that excels in all situations
- Subsequent work has confirmed this, e.g. a 2018 analysis
- Tree-based methods, particularly **gradient boosted trees** *tend* to outperform other algorithms the most, but still have limitations
- What does it mean to "outperform"?

Further reading: http://www.feat.engineering/important-concepts#no-free-lunch

Model evaluation: Classification

- **True positive**: predicted positive, label was positive (TP) ✓
- **True negative**: predicted negative, label was negative (TN) ✓
- **False positive**: predicted positive, label was negative (FP) ✗ (type I)
- **False negative**: predicted negative, label was positive (FN) ✗ (type II)
- **Accuracy** is the fraction of correct predictions, given as:

$$\text{accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

Precision and recall

- **Precision**: Out of all the positive **predictions**, how many were correct?

$$\text{precision} = \frac{TP}{TP + FP}$$

- **Recall**: Out of all the positive **labels**, how many were correct?

$$\text{recall} = \frac{TP}{TP + FN}$$

- **Specificity**: Out of all the negative **labels**, how many were correct?

$$\text{specificity} = \frac{TN}{TN + FP}$$

Confusion matrix

	Predicted Positive	Predicted Negative
True Positive	TP	FN
True Negative	FP	TN

- The axes might be reversed, but a good predictor will have strong diagonals
- There's also the **F1 score**, or harmonic mean of precision and recall:

$$F1 = 2 \cdot \frac{\mathrm{precision} \cdot \mathrm{recall}}{\mathrm{precision} + \mathrm{recall}}$$

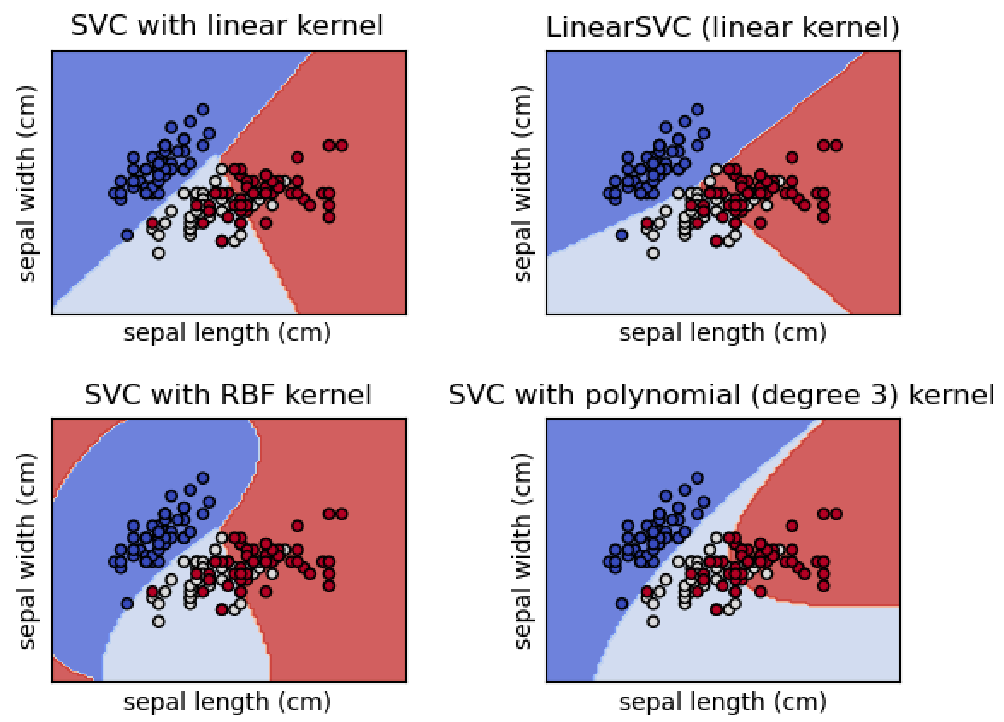
Check out the Wikipedia page for more ways of describing the same information

ROC Curves

- The receiver operating characteristic curve is a plot of the **true positive rate** (recall or sensitivity) vs. **false positive rate** (1 - specificity) as the detection threshold changes
- The diagonal is the same as random guessing
- A perfect classifier would hug the top left corner

> *Fun fact: the name comes from WWII radar operators, where true positives were airplanes and false positives were noise*

Classification model: Support Vector Classifier



- Linear model that finds vector(s) to best separate classes
- "Kernel trick" allows for nonlinear boundaries
- Check out the SVM Appendix of *Hands-on Machine Learning* by Aurélien Geron for more info

Image from Scikit-learn documentation

Classification Model: Decision Trees

- Family of models including:
  - decision trees
  - random forests
  - gradient boosted decision trees
- Finds thresholds for features that best separates classes
- Controllable through depth parameter

Model evaluation: regression

For a predicted $\hat{\mathbf{y}}$ and actual $\mathbf{y}$, metrics include:

- Mean squared error: $MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$
- Root mean squared error: $RMSE = \sqrt{MSE}$
- Mean absolute error: $MAE = \frac{1}{n}\sum_{i=1}^{n}\left|y_i - \hat{y}_i\right|$
- Mean absolute percentage error: $MAPE = \frac{100}{n}\sum_{i=1}^{n}\left|\frac{y_i - \hat{y}_i}{y_i}\right|$
- Coefficient of determination: $R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$

  (R^2 has some caveats)

Where we left off on January 13

Regression: ordinary least squares

- In 1D, estimate modeled as: $\hat{y_i} = wx_i + b$, where i denotes a sample
- Vector form: $\hat{\mathbf{y}} = w\mathbf{x} + b$
- Goal is to minimize the **Mean Square Error**:

$$MSE = \frac{1}{m}\sum_{i=1}^{m}(\hat{y} - y_i)^2 = \frac{1}{m}\sum_{i=1}^{m}(b + wx_i - y_i)^2$$

$$MSE = \frac{1}{m}(\hat{\mathbf{y}} - \mathbf{y})^T(\hat{\mathbf{y}} - \mathbf{y})$$

Regression: N-dimensional

- Most of the time we have $N > 1$ **features**
- N-D: $\hat{y}_i = w_1 x_{1i} + w_2 x_{2i} + \ldots + w_n x_{ni} + b$
- Common to use a **design matrix** $\mathbf{X}$ to represent the feature values:

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

where each row is an instance (sample) and each column is a feature.

Regression: N-dimensional

- We can rewrite the estimate in matrix notation:

$$\hat{\mathbf{y}} = \mathbf{X}\theta$$

- The MSE can be written as:

$$MSE = \frac{1}{m}\sum_{i=1}^{m}(\hat{y}_i - y_i)^2 = \frac{1}{m}(\mathbf{X}\theta - \mathbf{y})^T(\mathbf{X}\theta - \mathbf{y})$$

- This has a closed form solution, but it is computationally expensive

Regression: Decision trees

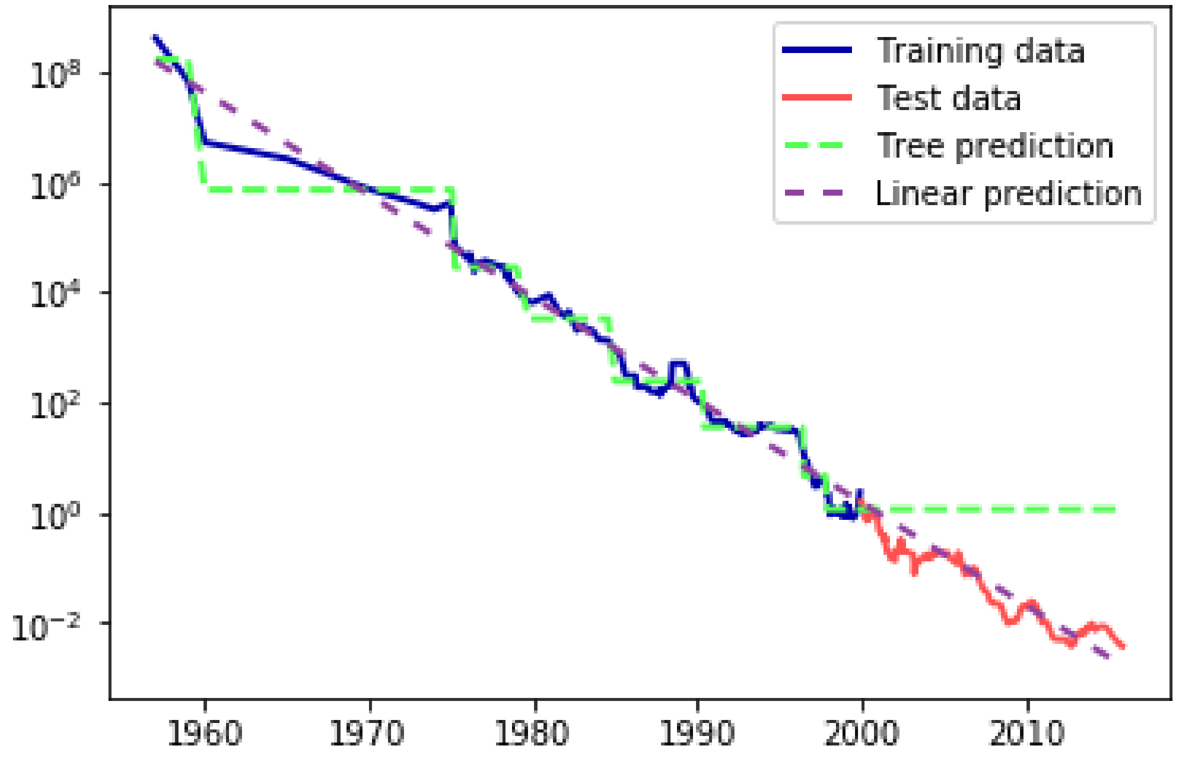


Figure 2-32. Comparison of predictions made by a linear model and predictions made by a regression tree on the RAM price data. Source: Introduction to Machine Learning with Python

Comparison of model families

Linear models

+ Very fast, particularly inference
+ Scalable to large number of features
+ Can model nonlinearity with kernel trick
+ Easy to regularize

- Difficult to interpret
- Sensitive to parameters and preprocessing
- Data needs to be on same scale
- Slow to train on large datasets

Decision Trees

+ Highly explainable
+ Fast to train
+ Few parameters to tune
+ Little preprocessing needed
+ Provides feature importance

- Prone to overfitting
- High variance
- Poor extrapolation

Coming up next

- Exploring and understanding your data
- Splitting your data
  - Repeatability considerations
  - Stratified sampling
- Assignment 1: Exploring Calgary traffic data