Decision Trees, Linear Algebra and Bias-Variance Decomposition

CSC311 Summer 2025

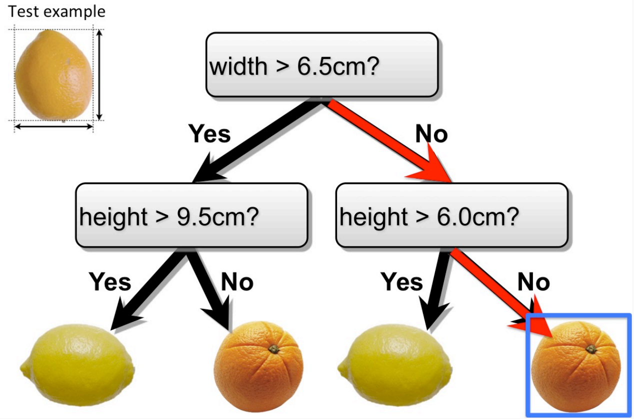
University of Toronto

Decision Trees Review

Decision Trees Review

- A non-linear algorithm for classification and regression.
- Represents features of data in a tree-structure.
- Each node corresponds to one feature and thresholds that cover its possible values.
- Each branch from a node divides the data into bins based on its feature and thresholds.
- Leaves of the tree correspond to targets or outputs.

Decision Trees Review



Features

Features may be discrete or continuous.

- Discrete: Takes values in some discrete finite set. “Thresholds” just assign each branch to a different value. For example, a feature may be boolean and take values in

$$\{\text{True}, \text{False}\}$$

.

- Continuous: Takes a range of continuous values. “Thresholds” divide the range based on some value. For example, a feature like height may have thresholds $6, 9.5$, dividing the data into the bins:

$$\{\text{Height} \leq 6, 6 \leq \text{Height} \leq 9.5, \text{Height} \geq 9.5\}$$

Outputs

Outputs may be discrete or continuous.

- Discrete: Classification Tree
- Continuous: Regression Tree

Splits

We need some heuristic to determine good splits that guide decision making.

- Choose feature that will maximize *information gain* greedily.
- Repeat at every node.
- Stop when leaves are empty or contain examples of the same class.

Linear Algebra

We will use linear algebra tools to concisely depict data, parameters and measure different quantities like norms, similarity, projections, etc.
Some basic elements:

- Scalar: A number. Denoted by lowercase letters like a.
- Vector: A 1-D array of numbers. Denoted by bold lowercase $\mathbf{a}$.
- Matrix: A 2-D array of numbers. Denoted by bold uppercase $\mathbf{A}$.

Norms

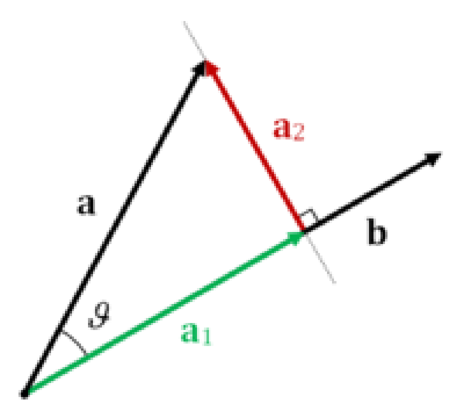
Norm is a measure of how "large" a vector is.

$$l_p\text{-norm } ||x||_p = \left[\sum_i |x_i|^p \right]^{1/p}$$

- l_2-norm is called the Euclidean norm: $\sqrt{\sum_i x_i^2}$.
- l_1-norm is called the Manhattan norm: $\sum_i |x_i|$.
- l_∞-norm is called the max norm: $\max_i |x_i|$.

Projections

When studying linear models, we will encounter vector projections[1].



[1] Image from Wikipedia

Projections

- Each vector is determined by its magnitude and direction.
- Projection of one vector on another can be thought of as dropping a perpendicular from one to the other.
- The magnitude of the projection is determined by the magnitude of the first vector and the angle between the two vectors.
- The direction of the projection is the same as that of the second vector.
- Mathematically, the projection of $\mathbf{a}$ on $\mathbf{b}$ is given by $\frac{\mathbf{a}^T\mathbf{b}}{||\mathbf{b}||_2}$.

Exercise: Linear Algebra Notation

Suppose we are trying to predict commute times based on the distance traveled and day of the week. We have the following data:

dist	day	commute time
2.7	1	25
3.4	1	31
5.2	2	45
1.0	3	16
2.8	5	22

We estimate that commute times have the following relationship:

$$\text{commute time} = 10 \times \text{dist} - \text{day}$$

What are our predicted commute times? How can we use matrices to compute this quickly?

Exercise: Linear Algebra Notation

(Solution: Let X denote our matrix of features i.e.

$$\begin{bmatrix} 2.7 & 1 \\ 3.4 & 1 \\ \ldots & \\ 2.8 & 5 \end{bmatrix}$$

Denoting

$$w = \begin{bmatrix} 10 \\ -1 \end{bmatrix},$$

we compute Xw to get our predictions. Note that we often append an additional column of 1s (a bias term) so that our linear model is not constrained to passing through the origin.
In numpy, we use np.dot(X, w).
)

Exercise: Linear Algebra Notation

Suppose we want to calculate the average mean squared error between the predictions and the ground truth. How do we do this?

(Solution: Letting y denote the vector of ground truth commute times, we compute

$$\frac{1}{n}|Xw - y|_2^2 = \frac{1}{5}(Xw - y)^T(Xw - y)$$

We can do this in code with np.mean((np.dot$(X, w) - y)$ ** $2)$
)

Bias-Variance Decomposition

Bias-Variance Decomposition

For training, we choose datapoints by sampling i.i.d. from some data distribution. This introduces randomness into the outputs of the model.

- Consider the squared error loss between outputs and targets, $(y - t)^2$.
- Treat both y and t as random variables.
- We saw in lecture that the expected loss can be decomposed into the bias and variance of y, the outputs.
- Recall that bias is the deviation of a random variable from its expectation.

Bias-Variance Decomposition

Let's revisit the proof.

- Let $y_* = \mathbb{E}[t]$.
- From lecture, we have

$$\mathbb{E}\left[(y-t)^2\right] = \mathbb{E}\left[(y-y_*)^2\right] + \mathrm{Var}(t)$$

- Here, $\mathrm{Var}(t)$ is called the Bayes error.

Bias-Variance Decomposition

- We expand the first term and use linearity of expectation:

$$\mathbb{E}\left[(y - y^*)^2\right] = y_*^2 - 2y_*\mathbb{E}\left[y\right] + \mathbb{E}\left[y^2\right]$$

Bias-Variance Decomposition

- Next, recall the definition of

$$\mathrm{Var}(y) = \mathbb{E}\left[y^2\right] - \mathbb{E}\left[y\right]^2$$

to get

$$\mathbb{E}\left[(y - y^*)^2\right] = y_*^2 - 2y_*\mathbb{E}\left[y\right] + \mathbb{E}\left[y\right]^2 + \mathrm{Var}(y)$$

Bias-Variance Decomposition

- Note that
$$(y_* - \mathbb{E}[y])^2 = y_*^2 - 2y_*\mathbb{E}[y] + \mathbb{E}[y]^2$$
- Putting all this together, we have
$$\mathbb{E}\left[(y - t)^2\right] = (y_* - \mathbb{E}[y])^2 + \mathrm{Var}(y) + \mathrm{Var}(t)$$
- In words, *expected loss* = *bias* + *variance* + *Bayes error*.

Exercise: Bias, Variance and Bayes Error

Assume we have N scalar-valued observations $\{x^{(i)}\}_{i=1}^{N}$ sampled independently from some distribution with known variance 2 and unknown mean μ.
We'd like to estimate the mean parameter μ, or equivalently, choose a $\hat{\mu}$ which minimizes the squared error risk $\mathbb{E}\left[(x - \hat{\mu})^2\right]$.
We will estimate the unknown mean parameter μ by taking the empirical mean, or average, of the observations:

$$\hat{\mu} = \frac{1}{N}\sum_{i=1}^{N} x^{(i)}$$

Compute the different terms from the bias-variance decomposition.

Exercise: Bias, Variance and Bayes Error

Bayes Error: $\mathbb{E}\left[(x-\mu)^2\right]$

(Solution: Bayes error = $\mathrm{Var}(x) = 2$)

Exercise: Bias, Variance and Bayes Error

Bias: $(\mathbb{E}[\hat{\mu}] - \mu)^2$

(Solution: $\mathbb{E}\left[\frac{1}{N}\sum_{i=1}^{N} x^{(i)}\right] = \frac{1}{N}\sum_{i=1}^{N} \mathbb{E}\left[x^{(i)}\right] = \frac{N\mu}{N} = \mu$
Bias = $\mu - \mu = 0$
)

Exercise: Bias, Variance and Bayes Error

Variance: $\mathrm{Var}(\hat{\mu})$

(Solution: $\mathrm{Var}(\frac{1}{N}\sum_{i=1}^{N} x^{(i)}) = \frac{1}{N^2}\sum_{i=1}^{N}\mathrm{Var}(x^{(i)}) = \frac{2N}{N^2} = \frac{2}{N}$
)