Module 10 – Regression via Linear Algebra

DSC 40A, Summer 2023

Agenda

- Finish linear algebra review.
- Formulate mean squared error in terms of linear algebra.
- Minimize mean squared error using linear algebra.

Linear algebra review

Vectors

- An **vector** in $\mathbb{R}^n$ is an $n \times 1$ matrix.
- We use lower-case letters for vectors.

$$\vec{v} = \begin{bmatrix} 2 \\ 1 \\ 5 \\ -3 \end{bmatrix}$$

- Vector addition and scalar multiplication occur elementwise.

Geometric meaning of vectors

- A vector $\vec{v} = (v_1, \dots, v_n)^T$ is an arrow to the point $(v_1, \dots, v_n)$ from the origin.

- The **length**, or **norm**, of $\vec{v}$ is $\|\vec{v}\| = \sqrt{v_1^2 + v_2^2 + \dots + v_n^2}$.

Dot products

- The **dot product** of two vectors $\vec{u}$ and $\vec{v}$ in $\mathbb{R}^n$ is denoted by:

$$\vec{u} \cdot \vec{v} = \vec{u}^T \vec{v}$$

- Definition:

$$\vec{u} \cdot \vec{v} = \sum_{i=1}^{n} u_i v_i = u_1 v_1 + u_2 v_2 + \ldots + u_n v_n$$

- The result is a **scalar**!

Properties of the dot product

- Commutative:

$$\vec{u} \cdot \vec{v} = \vec{v} \cdot \vec{u} = \vec{u}^T \vec{v} = \vec{v}^T \vec{u}$$

- Distributive:

$$\vec{u} \cdot (\vec{v} + \vec{w}) = \vec{u} \cdot \vec{v} + \vec{u} \cdot \vec{w}$$

Matrix-vector multiplication

- Special case of matrix-matrix multiplication.
- The result is always a vector with the same number of rows as the matrix.
- One view: a "mixture" of the columns.

$$\begin{bmatrix} 1 & 2 & 1 \\ 3 & 4 & 5 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = a_1 \begin{bmatrix} 1 \\ 3 \end{bmatrix} + a_2 \begin{bmatrix} 2 \\ 4 \end{bmatrix} + a_3 \begin{bmatrix} 1 \\ 5 \end{bmatrix}$$

- Another view: a dot product with the rows.

Discussion Question

If A is an $m \times n$ matrix and $\vec{v}$ is a vector in $\mathbb{R}^n$, what are the dimensions of the product $\vec{v}^T A^T A\vec{v}$?

a) $m \times n$ (matrix)

b) $n \times 1$ (vector)

c) 1×1 (scalar)

d) The product is undefined.

Matrices and functions

- Suppose A is an $m \times n$ matrix and $\vec{x}$ is a vector in $\mathbb{R}^n$.

- Then, the function $f(\vec{x}) = Ax$ is a linear function that maps elements in $\mathbb{R}^n$ to elements in $\mathbb{R}^m$.
  - The input to f is a vector, and so is the output.

- **Key idea:** matrix-vector multiplication can be thought of as applying a linear function to a vector.

Mean squared error, revisited

Wait... why do we need linear algebra?

- Soon, we'll want to make predictions using more than one feature (e.g. predicting salary using years of experience and GPA).
  - If the intermediate steps get confusing, think back to this overarching goal.
- Thinking about linear regression in terms of **linear algebra** will allow us to find prediction rules that
  - use multiple features.
  - are non-linear.
- **Let's start by expressing R_{sq} in terms of matrices and vectors.**

Regression and linear algebra

- We chose the parameters for our prediction rule

$$H(x) = w_0 + w_1 x$$

by finding the w_0^* and w_1^* that minimized mean squared error:

$$R_{\text{sq}}(H) = \frac{1}{n} \sum_{i=1}^{n} (y_i - H(x_i))^2.$$

- This is *kind of* like the formula for the length of a vector:

$$\|\vec{v}\| = \sqrt{v_1^2 + v_2^2 + \ldots + v_n^2}$$

Regression and linear algebra

Let's define a few new terms:

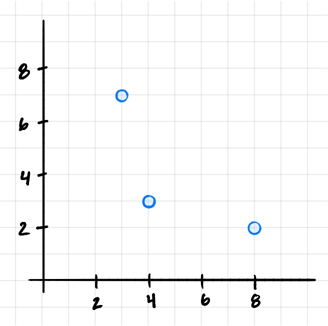
- The **observation vector** is the vector $\vec{y} \in \mathbb{R}^n$ with components y_i. This is the vector of observed/"actual" values.

- The **hypothesis vector** is the vector $\vec{h} \in \mathbb{R}^n$ with components $H(x_i)$. This is the vector of predicted values.

- The **error vector** is the vector $\vec{e} \in \mathbb{R}^n$ with components $e_i = y_i - H(x_i)$. This is the vector of (signed) errors.

Example

Consider $H(x) = \frac{1}{2}x + 2$.



$\vec{y} =$

$\vec{h} =$

$\vec{e} = \vec{y} - \vec{h} =$

$$R_{\text{sq}}(H) = \frac{1}{n}\sum_{i=1}^{n}(y_i - H(x_i))^2 =$$

Regression and linear algebra

- The **observation vector** is the vector $\vec{y} \in \mathbb{R}^n$ with components y_i. This is the vector of observed/“actual” values.

- The **hypothesis vector** is the vector $\vec{h} \in \mathbb{R}^n$ with components $H(x_i)$. This is the vector of predicted values.

- The **error vector** is the vector $\vec{e} \in \mathbb{R}^n$ with components $e_i = y_i - H(x_i)$. This is the vector of (signed) errors.

- We can rewrite the mean squared error as:

$$R_{\text{sq}}(H) = \frac{1}{n}\sum_{i=1}^{n}(y_i - H(x_i))^2 = \frac{1}{n}||\vec{e}||^2 = \frac{1}{n}||\vec{y} - \vec{h}||^2.$$

The hypothesis vector

- The **hypothesis vector** is the vector $\vec{h} \in \mathbb{R}^n$ with components $H(x_i)$. This is the vector of predicted values.

- For the linear prediction rule $H(x) = w_0 + w_1 x$, the hypothesis vector $\vec{h}$ can be written

$$\vec{h} = \begin{bmatrix} H(x_1) \\ H(x_2) \\ \vdots \\ H(x_n) \end{bmatrix} = \begin{bmatrix} w_0 + w_1 x_1 \\ w_0 + w_1 x_2 \\ \vdots \\ w_0 + w_1 x_n \end{bmatrix} =$$

Rewriting the mean squared error

- Define the **design matrix** X to be the $n \times 2$ matrix

$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}.$$

- Define the **parameter vector** $\vec{w} \in \mathbb{R}^2$ to be $\vec{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$.

- Then $\vec{h} = X\vec{w}$, so the mean squared error becomes:

$$R_{\text{sq}}(H) = \frac{1}{n} ||\vec{y} - \vec{h}||^2$$

$$R_{\text{sq}}(\vec{w}) = \frac{1}{n} ||\vec{y} - X\vec{w}||^2$$

Mean squared error, reformulated

- Before, we found the values of w_0 and w_1 that minimized

$$R_{sq}(w_0, w_1) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - (w_0 + w_1 x_i)\right)^2$$

  - The results:

$$w_1^* = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} = r\frac{\sigma_y}{\sigma_x} \qquad w_0^* = \bar{y} - w_1^*\bar{x}$$

- **Now**, our goal is to find the vector $\vec{w}$ that minimizes

$$R_{sq}(\vec{w}) = \frac{1}{n}||\vec{y} - X\vec{w}||^2$$

- **Both versions of R_{sq} are equivalent. The results will also be equivalent.**

Spoiler alert...

- Goal: find the vector $\vec{w}$ that minimizes

$$R_{sq}(\vec{w}) = \frac{1}{n}||\vec{y} - X\vec{w}||^2$$

- Spoiler alert: the answer[1] is

$$\vec{w}^* = (X^T X)^{-1} X^T \vec{y}$$

- Let's look at this formula in action in a notebook. Follow along here.

- Then we'll prove it ourselves by hand.

---

[1]assuming $X^T X$ is invertible