Lecture 10 – Regression via Linear Algebra

DSC 40A, Spring 2023

Announcements

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

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

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:

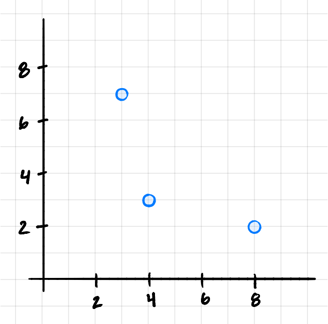
- The **observation vector** is the vector $\vec{y} \in \mathbb{R}^n$ with components y_i. This is the vector of observed/"actual" values.

- 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

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

- 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^TX is invertible

Minimizing mean squared error, again

Some key linear algebra facts

If A and B are matrices, and $\vec{u}, \vec{v}, \vec{w}, \vec{z}$ are vectors:

- $(A + B)^T = A^T + B^T$
- $(AB)^T = B^T A^T$
- $\vec{u} \cdot \vec{v} = \vec{v} \cdot \vec{u} = \vec{u}^T \vec{v} = \vec{v}^T \vec{u}$
- $\|\vec{u}\|^2 = \vec{u} \cdot \vec{u}$
- $(\vec{u} + \vec{v}) \cdot (\vec{w} + \vec{z}) = \vec{u} \cdot \vec{w} + \vec{u} \cdot \vec{z} + \vec{v} \cdot \vec{w} + \vec{v} \cdot \vec{z}$

Goal

- We want to minimize the mean squared error:

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

- Strategy: Calculus.

- **Problem:** This is a *function of a vector*. What does it even mean to take the derivative of $R_{\text{sq}}(\vec{w})$ with respect to a vector $\vec{w}$?

A function of a vector

- **Solution:** A function *of a vector* is really just a function *of multiple variables*, which are the components of the vector. In other words,

$$R_{\text{sq}}(\vec{w}) = R_{\text{sq}}(w_0, w_1, \dots, w_d)$$

  where $w_0, w_1, \dots, w_d$ are the entries of the vector $\vec{w}$.[2]

- We know how to deal with derivatives of multivariable functions: the gradient!

[2] In our case, $\vec{w}$ has just two components, w_0 and w_1. We'll be more general since we eventually want to use prediction rules with even more parameters.

The gradient with respect to a vector

- The **gradient of $R_{\text{sq}}(\vec{w})$ with respect to $\vec{w}$** is the vector of partial derivatives:

$$\nabla_{\vec{w}} R_{\text{sq}}(\vec{w}) = \frac{dR_{\text{sq}}}{d\vec{w}} = \begin{bmatrix} \frac{\partial R_{\text{sq}}}{\partial w_0} \\ \frac{\partial R_{\text{sq}}}{\partial w_1} \\ \vdots \\ \frac{\partial R_{\text{sq}}}{\partial w_d} \end{bmatrix}$$

where $w_0, w_1, \dots, w_d$ are the entries of the vector $\vec{w}$.

Example gradient calculation

Example: Suppose $f(\vec{x}) = \vec{a} \cdot \vec{x}$, where $\vec{a}$ and $\vec{x}$ are vectors in $\mathbb{R}^n$. What is $\frac{d}{d\vec{x}} f(\vec{x})$?

Goal

- We want to minimize the mean squared error:

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

- Strategy:
  1. Compute the gradient of $R_{\text{sq}}(\vec{w})$.
  2. Set it to zero and solve for $\vec{w}$.
     - The result is called $\vec{w}^*$.

- Let's start by rewriting the mean squared error in a way that will make it easier to compute its gradient.

Rewriting mean squared error

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

Discussion Question

Which of the following is equivalent to $R_{\text{sq}}(\vec{w})$?

a) $\frac{1}{n}(\vec{y} - X\vec{w}) \cdot (X\vec{w} - y)$

b) $\frac{1}{n}\sqrt{(\vec{y} - X\vec{w}) \cdot (y - X\vec{w})}$

c) $\frac{1}{n}(\vec{y} - X\vec{w})^T(y - X\vec{w})$

d) $\frac{1}{n}(\vec{y} - X\vec{w})(y - X\vec{w})^T$

Rewriting mean squared error

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

Rewriting mean squared error

$R_{\text{sq}}(\vec{w}) =$

Compute the gradient

$$
\begin{aligned}
\frac{dR_{\text{sq}}}{d\vec{w}} &= \frac{d}{d\vec{w}}\left(\frac{1}{n}\left[\vec{y}\cdot\vec{y} - 2X^T\vec{y}\cdot\vec{w} + \vec{w}^T X^T X\vec{w}\right]\right) \\
&= \frac{1}{n}\left[\frac{d}{d\vec{w}}\left(\vec{y}\cdot\vec{y}\right) - \frac{d}{d\vec{w}}\left(2X^T\vec{y}\cdot\vec{w}\right) + \frac{d}{d\vec{w}}\left(\vec{w}^T X^T X\vec{w}\right)\right]
\end{aligned}
$$

Compute the gradient

$$\begin{aligned}\frac{dR_{\text{sq}}}{d\vec{w}} &= \frac{d}{d\vec{w}}\left(\frac{1}{n}\left[\vec{y}\cdot\vec{y} - 2X^T\vec{y}\cdot\vec{w} + \vec{w}^TX^TX\vec{w}\right]\right)\\ &= \frac{1}{n}\left[\frac{d}{d\vec{w}}\left(\vec{y}\cdot\vec{y}\right) - \frac{d}{d\vec{w}}\left(2X^T\vec{y}\cdot\vec{w}\right) + \frac{d}{d\vec{w}}\left(\vec{w}^TX^TX\vec{w}\right)\right]\end{aligned}$$

- $\frac{d}{d\vec{w}}\left(\vec{y}\cdot\vec{y}\right) = 0.$
  - Why? $\vec{y}$ is a constant with respect to $\vec{w}$.
- $\frac{d}{d\vec{w}}\left(\vec{2}X^T\vec{y}\cdot\vec{w}\right) = 2X^Ty.$
  - Why? We already showed $\frac{d}{d\vec{x}}\vec{a}\cdot\vec{x} = \vec{a}$.
- $\frac{d}{d\vec{w}}\left(\vec{w}^TX^TX\vec{w}\right) = 2X^TX\vec{w}.$
  - Why? See Homework 4.

Compute the gradient

$$
\begin{aligned}
\frac{dR_{\text{sq}}}{d\vec{w}} &= \frac{d}{d\vec{w}}\left(\frac{1}{n}\left[\vec{y}\cdot\vec{y} - 2X^T\vec{y}\cdot\vec{w} + \vec{w}^T X^T X\vec{w}\right]\right) \\
&= \frac{1}{n}\left[\frac{d}{d\vec{w}}\left(\vec{y}\cdot\vec{y}\right) - \frac{d}{d\vec{w}}\left(2X^T\vec{y}\cdot\vec{w}\right) + \frac{d}{d\vec{w}}\left(\vec{w}^T X^T X\vec{w}\right)\right]
\end{aligned}
$$

The normal equations

- To minimize $R_{\text{sq}}(\vec{w})$, set its gradient to zero and solve for $\vec{w}$:

$$\begin{aligned} -2X^T\vec{y} + 2X^TX\vec{w} &= 0 \\ \implies \quad X^TX\vec{w} &= X^T\vec{y} \end{aligned}$$

- This is a system of equations in matrix form, called the **normal equations**.

- If X^TX is invertible, the solution is

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

- This is equivalent to the formulas for w_0^* and w_1^* we saw before!
    - Benefit – this can be easily extended to more complex prediction rules.

Summary

Summary

- We used linear algebra to rewrite the mean squared error for the prediction rule $H(x) = w_0 + w_1 x$ as

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

  - X is called the **design matrix**, $\vec{w}$ is called the **parameter vector**, $\vec{y}$ is called the **observation vector**, and $\vec{h} = X\vec{w}$ is called the **hypothesis vector**.

- We minimized $R_{sq}(\vec{w})$ using multivariable calculus and found that the minimizing $\vec{w}$ satisfies the **normal equations**, $X^T X\vec{w} = X^T y$.
  - If $X^T X$ is invertible, the solution is:

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

What's next?

- The whole point of reformulating linear regression in terms of linear algebra was so that we could generalize our work to more sophisticated prediction rules.
  - Note that when deriving the normal equations, we didn't assume that there was just one feature.
- Examples of the types of prediction rules we'll be able to fit soon:
  - $H(x) = w_0 + w_1 x + w_2 x^2$.
  - $H(x) = w_0 + w_1 \cos(x) + w_2 e^x$.
  - $H(x^{(1)}, x^{(2)}) = w_0 + w_1 x^{(1)} + w_2 x^{(2)}$.
    - e.g. Predicted Salary = $w_0 + w_1$(Years of Experience) + w_2(GPA).