

Lecture 10 – Regression via Linear Algebra



Winter 24

DSC 40A, Spring 2023

Announcements

- ▶ Homework 3 is due **today at 11:59pm.**
 - ▶ Last homework before Midterm 1
 - ▶ Please come to office hours!
- ▶ Midterm 1 on Friday, Feb. 9th
 - ▶ A cheat sheet will be provided, no calculator
 - ▶ Topics cover up to and include lecture 12
 - ▶ Problem will be similar to those in HW and **mock exams**
 - ▶ Review session in next Monday's discussion

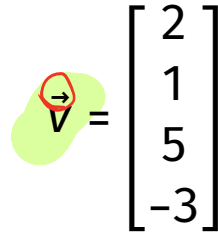
Agenda

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

Linear algebra review

Vectors

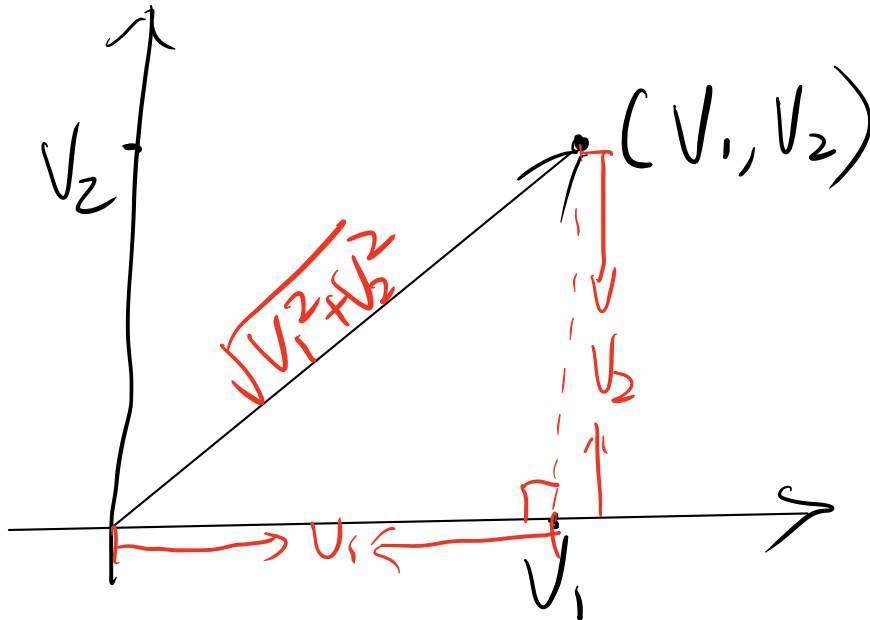
- ▶ An **vector** in \mathbb{R}^n is an $n \times 1$ matrix.
- ▶ We use lower-case letters for vectors.


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

- ▶ 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:

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

- ▶ Definition:

$$\begin{pmatrix} v_1 & v_2 & \dots & v_n \end{pmatrix}_{1 \times n} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix}_{n \times 1} = v_1 u_1 + v_2 u_2 + \dots + v_n u_n$$
$$\vec{u} \cdot \vec{v} = \sum_{i=1}^n u_i v_i = u_1 v_1 + u_2 v_2 + \dots + u_n v_n$$

- ▶ The result is a **scalar**!

$$\cancel{(1 \times n)} \cancel{(n \times 1)} \rightarrow \cancel{(1 \times 1)} \rightarrow \text{Scalar}$$

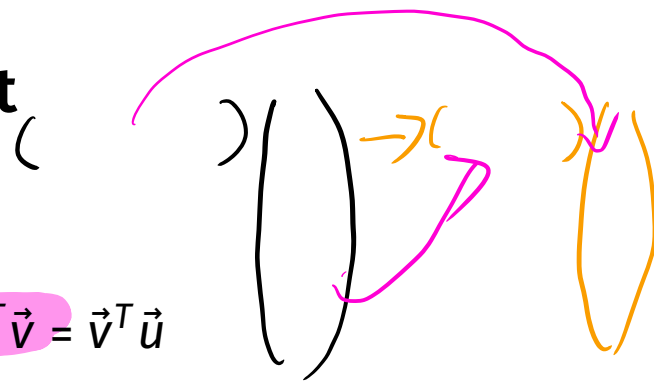
Properties of the dot product

- ▶ 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.

$$\begin{bmatrix} 1 & 2 & 1 \\ 3 & 4 & 5 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} = 2 \begin{bmatrix} 1 \\ 3 \end{bmatrix} + 1 \cdot \begin{bmatrix} 2 \\ 4 \end{bmatrix} + 0 \begin{bmatrix} 1 \\ 5 \end{bmatrix}$$

- ▶ One view: a “mixture” of the columns.

$$= \begin{bmatrix} 2 \\ 6 \end{bmatrix} + \begin{bmatrix} 2 \\ 4 \end{bmatrix} = \begin{bmatrix} 4 \\ 10 \end{bmatrix}$$

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

- ▶ Another view: a dot product with the rows.

$$\begin{bmatrix} 1 & 2 & 1 \\ 3 & 4 & 5 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 4 \\ 10 \end{bmatrix}$$

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.

$$\vec{v}^T A^T A \vec{v} = (A\vec{v})^T (A\vec{v}) = (A\vec{v}) \cdot (A\vec{v})$$

$$A \rightarrow (m \times n) \quad \vec{v} \rightarrow (n \times 1)$$

$$A\vec{v} \rightarrow (m \times 1)$$

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.

$$A\vec{v} \Rightarrow (m \times n)(n \times 1) \rightarrow (m \times 1)$$

The diagram illustrates the dimensions of matrix-vector multiplication. On the left, a matrix A is represented by a rectangle with an orange horizontal bar at the top and a green horizontal bar below it, labeled $m \times n$. To its right is a vector \vec{v} represented by a vertical oval with a green vertical bar on the left and an orange vertical bar on the right, labeled $n \times 1$. An equals sign follows, leading to a resulting vector of size $m \times 1$, shown as a vertical oval with an orange horizontal bar at the top and a green horizontal bar below it, labeled $m \times 1$.

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:

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

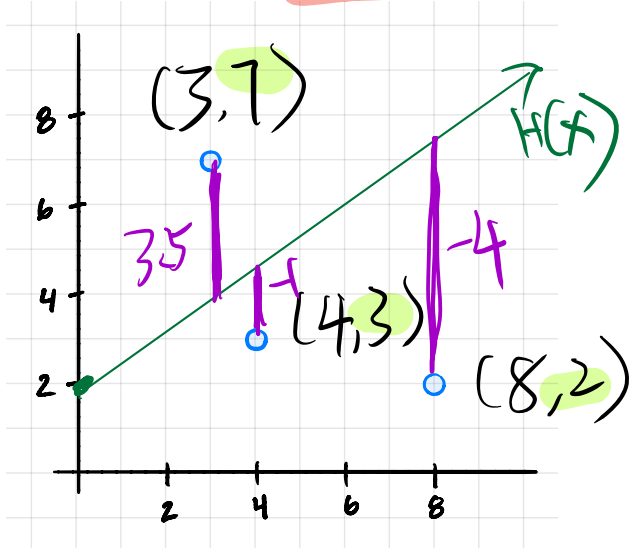
Regression and linear algebra

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



$$\vec{y} = \begin{pmatrix} 7 \\ 3 \\ 2 \end{pmatrix}$$

$$\vec{h} = \begin{pmatrix} 3.5 \\ 4 \\ 6 \end{pmatrix} \begin{array}{l} \leftarrow \frac{1}{2} \cdot 3 + 2 = H(3) \\ \leftarrow \frac{1}{2} \cdot 4 + 2 = H(4) \\ \leftarrow \frac{1}{2} \cdot 8 + 2 = H(8) \end{array}$$

$$\vec{e} = \vec{y} - \vec{h} = \begin{pmatrix} 7 \\ 3 \\ 2 \end{pmatrix} - \begin{pmatrix} 3.5 \\ 4 \\ 6 \end{pmatrix} = \begin{pmatrix} 3.5 \\ -1 \\ -4 \end{pmatrix}$$

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

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

$$\vec{h} = \begin{bmatrix} H(x_1) \\ H(x_2) \\ \vdots \\ H(x_n) \end{bmatrix} = \begin{bmatrix} w_0 + w_1 x_1 \\ w_0 + w_1 x_2 \\ \vdots \\ w_0 + w_1 x_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$$

$(n \times 2)$

$\vec{h} = \underbrace{\text{Matrix}}_X \underbrace{\text{Vector}}_W$

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

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

- ▶ The results:

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

- ▶ **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 answer¹ 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.

¹assuming $X^T X$ 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:

▶ $(A + B)^T = A^T + B^T$

▶ $(AB)^T = B^T A^T$

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

▶ $\|\vec{u}\|^2 = \vec{u} \cdot \vec{u}$

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

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

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!

²In 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 $R_{sq}(\vec{w})$ with respect to \vec{w}** is the vector of partial derivatives:

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

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

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

Compute the gradient

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

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

Compute the gradient

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

The normal equations

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

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

- ▶ This is a system of equations in matrix form, called the **normal equations**.
- ▶ If $X^T X$ is invertible, the solution is

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

- ▶ 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 $H(x) = w_0 + w_1x$ 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**, $X^T X \vec{w} = X^T \vec{y}$.
 - ▶ 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 = $w_0 + w_1(\text{Years of Experience}) + w_2(\text{GPA})$.