18-661 Introduction to Machine Learning

Linear Regression – Part I

Spring 2025

ECE – Carnegie Mellon University

Outline

Recap of MLE/MAP

Dogecoin

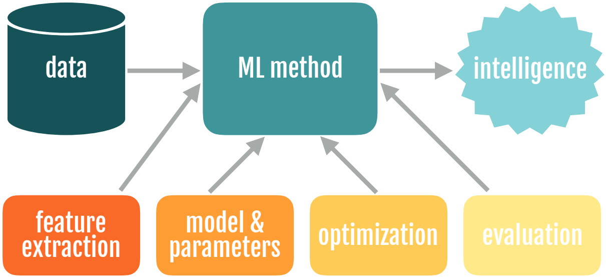
- Scenario: You find a coin on the ground.

- *You ask yourself: Is this a fair or biased coin? What is the probability that I will flip a heads?*

- You flip the coin 10 times ...
- It comes up as 'H' 8 times and 'T' 2 times

- Can we learn the bias of the coin from this data?

Recall: Machine Learning Pipeline



Two approaches that we discussed:

- Maximum likelihood Estimation (MLE)
- Maximum a posteriori Estimation (MAP)

Maximum Likelihood Estimation (MLE)

- **Data**: Observed set D of n_H heads and n_T tails
- **Model**: Each flip follows a Bernoulli distribution

$$P(H) = \theta,\ P(T) = 1 - \theta,\ \theta \in [0, 1]$$

Thus, the likelihood of observing sequence D is

$$P(D \mid \theta) = \theta^{n_H}(1-\theta)^{n_T}$$

- Question: Given this model and the data we've observed, can we calculate an estimate of θ?
- **MLE**: Choose θ that maximizes the *likelihood* of the observed data

$$\begin{aligned} \hat{\theta}_{MLE} &= \arg\max_{\theta} P(D \mid \theta) \\ &= \arg\max_{\theta} \log P(D \mid \theta) \\ &= \frac{n_H}{n_H + n_T} \end{aligned}$$

MAP for Dogecoin

$$\hat{\theta}_{MAP} = \arg\max_{\theta} P(D \mid \theta)P(\theta) = \arg\max_{\theta} P(\theta \mid D)$$

- Recall that $P(D \mid \theta) = \theta^{n_H}(1-\theta)^{n_T}$
- How should we set the prior, $P(\theta)$?
- Common choice for a binomial likelihood is to use the Beta distribution, $\theta \sim Beta(\alpha, \beta)$:

$$P(\theta) = \frac{1}{B(\alpha,\beta)}\,\theta^{\alpha-1}(1-\theta)^{\beta-1}, \text{where } B(\alpha,\beta) = \int_0^1 \theta^{\alpha-1}(1-\theta)^{\beta-1}d\theta$$

- Interpretation: α = number of expected heads, β = number of expected tails. Larger value of $\alpha + \beta$ denotes more confidence (and smaller variance).

Putting It All Together

$$\hat{\theta}_{MLE} = \frac{n_H}{n_H + n_T}$$

$$\hat{\theta}_{MAP} = \frac{\alpha + n_H - 1}{\alpha + \beta + n_H + n_T - 2}$$

Learning involves:

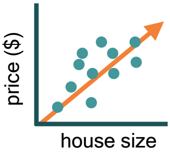
- Collect some data
  - e.g., coin flips
- Set up the problem: Choose a model / loss function
  - e.g., Bernoulli model, data likelihood, prior distribution
- Solve the problem: Choose an optimization procedure
  - e.g., set derivative of log to zero and solve to find MLE/MAP

Key idea: these are *choices*. It's important to understand the implications of these choices and evaluate their trade-offs for the problem at hand.

Bayesians vs. Frequentists

Linear Algebra Review

Data Can Be Compactly Represented by Matrices



- Learn parameters (w_1, w_0) of the orange line $y = w_1 x + w_0$

Sq.ft

$$\text{House 1: } 1000 \times w_1 + w_0 = 200,000$$

$$\text{House 2: } 2000 \times w_1 + w_0 = 350,000$$

- Can represent compactly in matrix notation

$$\begin{bmatrix} 1000 & 1 \\ 2000 & 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_0 \end{bmatrix} = \begin{bmatrix} 200,000 \\ 350,000 \end{bmatrix}$$

Matrix Inverse

The inverse of a matrix $A \in \mathbb{R}^{n \times n}$ is a matrix $A^{-1} \in \mathbb{R}^{n \times n}$ such that:

$$AA^{-1} = A^{-1}A = I_n$$

.

- If A^{-1} exists, then A is called invertible or non-singular
- Matrix A is invertible iff $\det(A) \neq 0$
- If A^{-1} exists, then it is unique
- Can be used to solve the house-price prediction problem:

$$\begin{bmatrix} 1000 & 1 \\ 2000 & 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_0 \end{bmatrix} = \begin{bmatrix} 200,000 \\ 350,000 \end{bmatrix} \tag{1}$$

$$\begin{bmatrix} w_1 \\ w_0 \end{bmatrix} = \left(\begin{bmatrix} 1000 & 1 \\ 2000 & 1 \end{bmatrix} \right)^{-1} \begin{bmatrix} 200,000 \\ 350,000 \end{bmatrix} \tag{2}$$

$$\begin{bmatrix} w_1 \\ w_0 \end{bmatrix} = \begin{bmatrix} 150 \\ 50,000 \end{bmatrix} \tag{3}$$

Norms and Loss Functions

- You could have data from many houses

$$\begin{bmatrix} 1000 & 1 \\ 2000 & 1 \\ 1500 & 1 \\ \vdots & \vdots \\ 2500 & 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_0 \end{bmatrix} = \begin{bmatrix} 200,000 \\ 350,000 \\ 300,000 \\ \vdots \\ 450,000 \end{bmatrix}$$

$$A \quad \times \quad w = \quad y$$

- There isn't a $w = [w_1, w_0]^T$ that will satisfy all equations
- Want to find w that minimizes the difference between Aw, y
- But since this a vector, we need an operator that can map the vector $y - Aw$ to a scalar

Norms and Loss Functions

- A vector norm is any function $f : \mathbb{R}^n \to \mathbb{R}$ with
  - $f(x) \geq 0$ and $f(x) = 0 \iff x = 0$
  - $f(ax) = |a| f(x)$ for $a \in \mathbb{R}$
  - $f(x + y) \leq f(x) + f(y)$
- e.g., ℓ_2 norm: $\|x\|_2 = \sqrt{x^\top x} = \sqrt{\sum_{i=1}^n x_i^2}$
- e.g., ℓ_1 norm: $\|x\|_1 = \sum_{i=1}^n |x_i|$
- Question: What is the ℓ_1 norm of $y - Aw$ for the following problem?

$$\underbrace{\begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 1.5 & 1 \\ 2.5 & 1 \end{bmatrix}}_{A} \times \underbrace{\begin{bmatrix} 1.5 \\ 0.5 \end{bmatrix}}_{w} = \underbrace{\begin{bmatrix} 2 \\ 3.5 \\ 3 \\ 4.5 \end{bmatrix}}_{y}$$

- Answer: $\|y - Aw\|_1 = 0.5$

Eigenvalues and Eigenvectors

- For $A \in \mathbb{R}^{n\times n}$, λ is an eigenvalue and $x \neq 0$ is an eigenvector if $Ax = \lambda x$.
- Eigenvalues are the roots of $\det(A - \lambda I_n) = 0$
- Eigenvectors are non-zero solutions of $Ax = \lambda x$
- Viewing A as a linear transformation
  - The vectors that remain unchanged and only get re-scaled are the eigenvectors.
  - Their scaling factors are the eigenvalues!
- Question: Find the eigenvalues and eigenvectors of

$$\begin{bmatrix} 1 & 2 \\ 4 & 3 \end{bmatrix}$$

Eigenvalue Decomposition

- Group the eigenvectors and eigenvalues into the following matrices.

$$P = \begin{bmatrix} 1 & -1 \\ 2 & 1 \end{bmatrix}$$
$$\Lambda = \begin{bmatrix} 5 & 0 \\ 0 & -1 \end{bmatrix}$$

- If the eigenvectors are linearly independent, we can express A as

$$\begin{aligned} A &= P\Lambda P^{-1} \\ &= \begin{bmatrix} 1 & -1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 5 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 2 & 1 \end{bmatrix}^{-1} \end{aligned}$$

Eigenvalue Decomposition

- Why is this useful?
- Suppose we want to find powers of A, eg. A^4
- One option, that is quite tedious is:

$$A^4 = \begin{bmatrix} 1 & 2 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 4 & 3 \end{bmatrix}$$

- Instead we could use the eigenvalue decomposition

$$\begin{aligned} A^4 &= P\Lambda P^{-1} P\Lambda P^{-1} P\Lambda P^{-1} P\Lambda P^{-1} \\ &= P\Lambda^4 P^{-1} \\ &= \begin{bmatrix} 1 & -1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 5^4 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 2 & 1 \end{bmatrix}^{-1} \end{aligned}$$

Singular value decomposition (SVD)

- EVD only works for square, diagonalizable matrices
- SVD works for matrices of any size! It decomposes $A \in \mathbb{R}^{m \times n}$ as follows.

$$A = U \Sigma V^\top,$$

- $U \in \mathbb{R}^{m \times m}$, $V \in \mathbb{R}^{n \times n}$ are orthogonal matrices (*i.e.* $U^\top = U^{-1}$)
- $\Sigma \in \mathbb{R}^{m \times n}$ is a diagonal matrix with *singular values* of A denoted by σ_i appearing by non-increasing order: $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{\min(m,n)} \geq 0$.
- The squared singular values of A are the eigenvalues of the matrix $AA^\top$ or $A^\top A$, i.e., $\sigma_i(A) = \sqrt{\lambda_i(AA^\top)} = \sqrt{\lambda_i(A^\top A)}$
- V is the matrix of eigenvectors of $A^T A$
- U is the matrix of eigenvectors of AA^T

Linear Regression

Outline

Recap of MLE/MAP

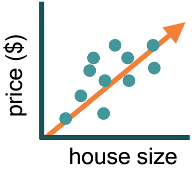
Linear Algebra Review

Linear Regression

- Formulation
- Univariate Solution
- Multivariate Solution
- Probabilistic Interpretation

Task 1: Regression

How much should you sell your house for?



input: houses & features **learn**: $x \to y$ relationship **predict**: y (*continuous*)

Course Covers: Linear/Ridge Regression, Loss Function, SGD, Feature Scaling, Regularization, Cross Validation

Supervised Learning

Supervised learning

In a supervised learning problem, you have access to input variables (X) and outputs (Y), and the goal is to predict an output given an input

- Examples:
  - **Housing prices (Regression)**: predict the price of a house based on features (size, location, etc)
  - **Cat vs. Dog (Classification)**: predict whether a picture is of a cat or a dog

Regression

Predicting a continuous outcome variable:

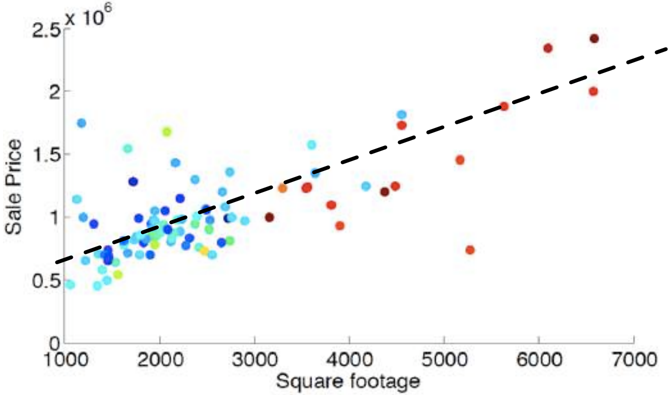
- Predicting a company's future stock price using its profit and other financial info
- Predicting annual rainfall based on local flora and fauna
- Predicting distance from a traffic light using LIDAR measurements

Magnitude of the error matters:

- We can measure 'closeness' of prediction and labels, leading to different ways to evaluate prediction errors.
    - Predicting stock price: better to be off by 1$ than by 20$
    - Predicting distance from a traffic light: better to be off 1 m than by 10 m
- We should choose learning models and algorithms accordingly.

Predicting House Prices: Collecting Data

Correlation between Square Footage and Sale Price



- Sale price $\approx$ price_per_sqft $\times$ square_footage $+$ fixed_expense
- Learn parameters (w_0, w_1) of the dotted line $y = w_1 x + w_0$

Reduce Prediction Error

How to measure prediction errors?

sqft	sale price	prediction	abs error	squared error
2000	810K	720K	90K	8100
2100	907K	800K	107K	107^2
1100	312K	350K	38K	38^2
5500	2,600K	2,600K	0	0
...	...			

- absolute difference (ℓ_1 norm): $|\text{prediction} - \text{sale price}|$.
- squared difference (ℓ_2 norm): $(\text{prediction} - \text{sale price})^2$ [differentiable!].

Minimize Squared Errors

Our model:

Sale_price =

price_per_sqft $\times$ square_footage + fixed_expense + unexplainable_stuff

Training data:

sqft	sale price	prediction	error	squared error
2000	810K	720K	90K	8100
2100	907K	800K	107K	107^2
1100	312K	350K	38K	38^2
5500	2,600K	2,600K	0	0
...	...			
Total				$8100 + 107^2 + 38^2 + 0 + \cdots$

Aim:

Adjust price_per_sqft and fixed_expense such that the sum of the squared error is minimized — i.e., the unexplainable_stuff is minimized.

Linear Regression

Setup:

- **Input**: $\mathbf{x} \in \mathbb{R}^D$ (covariates, predictors, features, etc)
- **Output**: $y \in \mathbb{R}$ (responses, targets, outcomes, outputs, etc)
- **Model**: $f : \mathbf{x} \to y$, with $f(\mathbf{x}) = w_0 + \sum_{d=1}^{D} w_d x_d = w_0 + \mathbf{w}^\top \mathbf{x}$.
  - $\mathbf{w} = [w_1 \; w_2 \; \cdots \; w_D]^\top$: *weights*, *parameters*, or *parameter vector*
  - w_0 is called *bias*.
  - Sometimes, we also call $\tilde{\mathbf{w}} = [w_0 \; w_1 \; w_2 \; \cdots \; w_D]^\top$ parameters.
- **Training data**: $\mathcal{D} = \{(\mathbf{x}_n, y_n), n = 1, 2, \ldots, N\}$

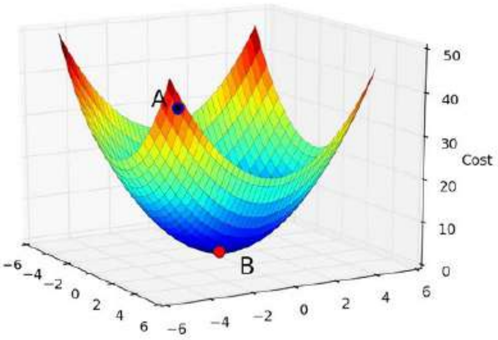
Minimize the Residual Sum of Squares:

$$RSS(\tilde{\mathbf{w}}) = \sum_{n=1}^{N} [y_n - f(\mathbf{x}_n)]^2 = \sum_{n=1}^{N} [y_n - (w_0 + \sum_{d=1}^{D} w_d x_{nd})]^2$$

A Simple Case: x Is One-dimensional (D=1)

Residual sum of squares:

$$RSS(\tilde{\mathbf{w}}) = \sum_n [y_n - f(\mathbf{x}_n)]^2 = \sum_n [y_n - (w_0 + w_1 x_n)]^2$$



What kind of function is this? CONVEX (has a unique global minimum)

A Simple Case: x Is One-dimensional (D=1)

Residual sum of squares:

$$RSS(\mathbf{w}) = \sum_n [y_n - f(\mathbf{x}_n)]^2 = \sum_n [y_n - (w_0 + w_1 x_n)]^2$$

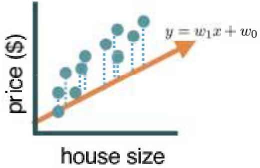


Figure 2: RSS is the sum of squares of the dotted lines

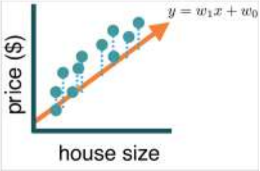


Figure 3: Adjust (w_0, w_1) to reduce RSS

Figure 4: RSS minimized at (w_o^*, w_1^*)

A Simple Case: x Is One-dimensional (D=1)

Residual sum of squares:

$$RSS(\tilde{\mathbf{w}}) = \sum_n [y_n - f(\mathbf{x}_n)]^2 = \sum_n [y_n - (w_0 + w_1 x_n)]^2$$

Stationary points:
Take derivative with respect to parameters and set it to zero

$$\frac{\partial RSS(\tilde{\mathbf{w}})}{\partial w_0} = 0 \Rightarrow -2 \sum_n [y_n - (w_0 + w_1 x_n)] = 0,$$

$$\frac{\partial RSS(\tilde{\mathbf{w}})}{\partial w_1} = 0 \Rightarrow -2 \sum_n [y_n - (w_0 + w_1 x_n)] x_n = 0.$$

A Simple Case: x Is One-dimensional (D=1)

$$\frac{\partial RSS(\tilde{\mathbf{w}})}{\partial w_0} = 0 \Rightarrow -2\sum_n [y_n - (w_0 + w_1 x_n)] = 0$$

$$\frac{\partial RSS(\tilde{\mathbf{w}})}{\partial w_1} = 0 \Rightarrow -2\sum_n [y_n - (w_0 + w_1 x_n)]x_n = 0$$

Simplify these expressions to get the "Normal Equations":

$$\sum y_n = Nw_0 + w_1 \sum x_n$$

$$\sum x_n y_n = w_0 \sum x_n + w_1 \sum x_n^2$$

Solving the system we obtain the least squares coefficient estimates:

$$w_1 = \frac{\sum (x_n - \bar{x})(y_n - \bar{y})}{\sum (x_i - \bar{x})^2} \qquad \text{and} \qquad w_0 = \bar{y} - w_1 \bar{x}$$

where $\bar{x} = \frac{1}{N}\sum_n x_n$ and $\bar{y} = \frac{1}{N}\sum_n y_n$.

Least Mean Squares: x Is D-dimensional

sqft (1000's)	bedrooms	bathrooms	sale price (100k)
1	2	1	2
2	2	2	3.5
1.5	3	2	3
2.5	4	2.5	4.5

$RSS(\tilde{\mathbf{w}})$ in matrix form:

$$RSS(\tilde{\mathbf{w}}) = \sum_n [y_n - (w_0 + \sum_d w_d x_{nd})]^2 = \sum_n [y_n - \tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_n]^2,$$

where we have redefined some variables (by augmenting)

$$\tilde{\mathbf{x}} \leftarrow [1 \ x_1 \ x_2 \ \ldots \ x_D]^\top, \quad \tilde{\mathbf{w}} \leftarrow [w_0 \ w_1 \ w_2 \ \ldots \ w_D]^\top$$

What is $\tilde{\mathbf{x}}$ for the first house? $[1, 1, 2, 1]^\top$

Least Mean Squares: $\mathbf{x}$ Is D-dimensional

$RSS(\tilde{\mathbf{w}})$ in matrix form:

$$RSS(\tilde{\mathbf{w}}) = \sum_n [y_n - (w_0 + \sum_d w_d x_{nd})]^2 = \sum_n [y_n - \tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_n]^2,$$

where we have redefined some variables (by augmenting)

$$\tilde{\mathbf{x}} \leftarrow [1 \ x_1 \ x_2 \ \ldots \ x_D]^\top, \quad \tilde{\mathbf{w}} \leftarrow [w_0 \ w_1 \ w_2 \ \ldots \ w_D]^\top$$

which leads to

$$\begin{aligned} RSS(\tilde{\mathbf{w}}) &= \sum_n (y_n - \tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_n)(y_n - \tilde{\mathbf{x}}_n^\top \tilde{\mathbf{w}}) \\ &= \sum_n \tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_n \tilde{\mathbf{x}}_n^\top \tilde{\mathbf{w}} - 2 y_n \tilde{\mathbf{x}}_n^\top \tilde{\mathbf{w}} + \text{const.} \\ &= \left\{ \tilde{\mathbf{w}}^\top \left(\sum_n \tilde{\mathbf{x}}_n \tilde{\mathbf{x}}_n^\top \right) \tilde{\mathbf{w}} - 2 \left(\sum_n y_n \tilde{\mathbf{x}}_n^\top \right) \tilde{\mathbf{w}} \right\} + \text{const.} \end{aligned}$$

$RSS(\tilde{\mathbf{w}})$ in New Notations

From previous slide:

$$RSS(\tilde{\mathbf{w}}) = \left\{ \tilde{\mathbf{w}}^\top \left(\sum_n \tilde{\mathbf{x}}_n \tilde{\mathbf{x}}_n^\top \right) \tilde{\mathbf{w}} - 2 \left(\sum_n y_n \tilde{\mathbf{x}}_n^\top \right) \tilde{\mathbf{w}} \right\} + \text{const.}$$

Design matrix and target vector:

$$\tilde{\mathbf{X}} = \begin{pmatrix} \tilde{\mathbf{x}}_1^\top \\ \tilde{\mathbf{x}}_2^\top \\ \vdots \\ \tilde{\mathbf{x}}_N^\top \end{pmatrix} \in \mathbb{R}^{N \times (D+1)}, \quad \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} \in \mathbb{R}^N$$

Compact expression:

$$RSS(\tilde{\mathbf{w}}) = \|\tilde{\mathbf{X}}\tilde{\mathbf{w}} - \mathbf{y}\|_2^2 = \left\{ \tilde{\mathbf{w}}^\top \tilde{\mathbf{X}}^\top \tilde{\mathbf{X}} \tilde{\mathbf{w}} - 2 \left(\tilde{\mathbf{X}}^\top \mathbf{y} \right)^\top \tilde{\mathbf{w}} \right\} + \text{const}$$

Example: $RSS(\tilde{\mathbf{w}})$ in Compact Form

sqft (1000's)	bedrooms	bathrooms	sale price (100k)
1	2	1	2
2	2	2	3.5
1.5	3	2	3
2.5	4	2.5	4.5

Design matrix and target vector:

$$\tilde{\mathbf{X}} = \begin{pmatrix} \tilde{\mathbf{x}}_1^\top \\ \tilde{\mathbf{x}}_2^\top \\ \vdots \\ \tilde{\mathbf{x}}_N^\top \end{pmatrix} = \begin{bmatrix} 1 & 1 & 2 & 1 \\ 1 & 2 & 2 & 2 \\ 1 & 1.5 & 3 & 2 \\ 1 & 2.5 & 4 & 2.5 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 2 \\ 3.5 \\ 3 \\ 4.5 \end{bmatrix}$$

. Compact expression:

$$RSS(\tilde{\mathbf{w}}) = \|\tilde{\mathbf{X}}\tilde{\mathbf{w}} - \mathbf{y}\|_2^2 = \left\{ \tilde{\mathbf{w}}^\top \tilde{\mathbf{X}}^\top \tilde{\mathbf{X}} \tilde{\mathbf{w}} - 2 \left(\tilde{\mathbf{X}}^\top \mathbf{y} \right)^\top \tilde{\mathbf{w}} \right\} + \text{const}$$

Solution in Matrix Form

Compact expression

$$RSS(\tilde{\mathbf{w}}) = ||\tilde{\mathbf{X}}\tilde{\mathbf{w}} - \mathbf{y}||_2^2 = \left\{\tilde{\mathbf{w}}^\top \tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}\tilde{\mathbf{w}} - 2\left(\tilde{\mathbf{X}}^\top \mathbf{y}\right)^\top \tilde{\mathbf{w}}\right\} + \text{const}$$

Gradients of Linear and Quadratic Functions

- $\nabla_{\mathbf{x}}(\mathbf{b}^\top \mathbf{x}) = \mathbf{b}$
- $\nabla_{\mathbf{x}}(\mathbf{x}^\top \mathbf{A}\mathbf{x}) = 2\mathbf{A}\mathbf{x}$ (symmetric $\mathbf{A}$)

Normal equation

$$\nabla_{\tilde{\mathbf{w}}} RSS(\tilde{\mathbf{w}}) = 2\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}\tilde{\mathbf{w}} - 2\tilde{\mathbf{X}}^\top \mathbf{y} = 0$$

This leads to the least-mean-squares (LMS) solution

$$\tilde{\mathbf{w}}^{LMS} = \left(\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}\right)^{-1} \tilde{\mathbf{X}}^\top \mathbf{y}$$

Example: $RSS(\tilde{\mathbf{w}})$ in Compact Form

sqft (1000's)	bedrooms	bathrooms	sale price (100k)
1	2	1	2
2	2	2	3.5
1.5	3	2	3
2.5	4	2.5	4.5

Write the least-mean-squares (LMS) solution

$$\tilde{\mathbf{w}}^{LMS} = \left(\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}\right)^{-1} \tilde{\mathbf{X}}^\top \mathbf{y}$$

Can use solvers in Matlab, Python etc., to compute this for any given $\tilde{\mathbf{X}}$ and $\mathbf{y}$.

Exercise: $RSS(\tilde{\mathbf{w}})$ in Compact Form

Using the general least-mean-squares (LMS) solution

$$\tilde{\mathbf{w}}^{LMS} = \left(\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}\right)^{-1} \tilde{\mathbf{X}}^\top \mathbf{y}$$

recover the uni-variate solution that we had computed earlier:

$$w_1 = \frac{\sum (x_n - \bar{x})(y_n - \bar{y})}{\sum (x_i - \bar{x})^2} \qquad \text{and} \qquad w_0 = \bar{y} - w_1 \bar{x}$$

where $\bar{x} = \frac{1}{N} \sum_n x_n$ and $\bar{y} = \frac{1}{N} \sum_n y_n$.

Exercise: $RSS(\tilde{\mathbf{w}})$ in Compact Form

For the 1-D case, the least-mean-squares solution is

$$
\begin{aligned}
\tilde{\mathbf{w}}^{LMS} &= \left(\tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}\right)^{-1} \tilde{\mathbf{X}}^\top \mathbf{y} \\
&= \left(\begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_N \end{bmatrix} \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & \dots \\ 1 & x_N \end{bmatrix} \right)^{-1} \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_N \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_N \end{bmatrix} \\
&= \left(\begin{bmatrix} N & N\bar{x} \\ N\bar{x} & \sum_n x_n^2 \end{bmatrix} \right)^{-1} \begin{bmatrix} \sum_n y_n \\ \sum_n x_n y_n \end{bmatrix} \\
\begin{bmatrix} w_0 \\ w_1 \end{bmatrix} &= \frac{1}{\sum (x_i - \bar{x})^2)} \begin{bmatrix} \bar{y} \sum (x_i - \bar{x})^2 - \bar{x} \sum (x_n - \bar{x})(y_n - \bar{y}) \\ \sum (x_n - \bar{x})(y_n - \bar{y}) \end{bmatrix}
\end{aligned}
$$

where $\bar{x} = \frac{1}{N} \sum_n x_n$ and $\bar{y} = \frac{1}{N} \sum_n y_n$.

Why Minimize the RSS?

Probabilistic interpretation

- **Noisy observation model** for generating the dataset:

$$Y = w_0 + w_1 X + \eta$$

  where $\eta \sim N(0, \sigma^2)$ is a Gaussian random variable

- Conditional likelihood of one training sample:

$$p(y_n|x_n) = N(w_0 + w_1 x_n, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{[y_n - (w_0 + w_1 x_n)]^2}{2\sigma^2}}$$

Probabilistic Interpretation (cont'd)

Log-likelihood of the training data $\mathcal{D}$ (assuming i.i.d):

$$
\begin{aligned}
\log P(\mathcal{D}) &= \log \prod_{n=1}^{N} p(y_n|x_n) = \sum_n \log p(y_n|x_n) \\
&= \sum_n \left\{ -\frac{[y_n - (w_0 + w_1 x_n)]^2}{2\sigma^2} - \log \sqrt{2\pi}\sigma \right\} \\
&= -\frac{1}{2\sigma^2} \sum_n [y_n - (w_0 + w_1 x_n)]^2 - \frac{N}{2} \log \sigma^2 - N \log \sqrt{2\pi} \\
&= -\frac{1}{2} \left\{ \frac{1}{\sigma^2} \sum_n [y_n - (w_0 + w_1 x_n)]^2 + N \log \sigma^2 \right\} + \text{const}
\end{aligned}
$$

What is the relationship between minimizing RSS and maximizing the log-likelihood?

Maximum Likelihood Estimation

$$\log P(\mathcal{D}) = -\frac{1}{2}\left\{\frac{1}{\sigma^2}\sum_n [y_n - (w_0 + w_1 x_n)]^2 + N \log \sigma^2\right\} + \text{const}$$

Estimating σ, w_0 and w_1 can be done in two steps

- Maximize over w_0 and w_1:

$$\max \ \log P(\mathcal{D}) \Leftrightarrow \min \ \sum_n [y_n - (w_0 + w_1 x_n)]^2 \leftarrow \text{This is RSS}(\tilde{\mathbf{w}})!$$

- Maximize over $s = \sigma^2$:

$$\frac{\partial \log P(\mathcal{D})}{\partial s} = -\frac{1}{2}\left\{-\frac{1}{s^2}\sum_n [y_n - (w_0 + w_1 x_n)]^2 + N\frac{1}{s}\right\} = 0$$

$$\rightarrow \sigma^{*2} = s^* = \frac{1}{N}\sum_n [y_n - (w_0 + w_1 x_n)]^2$$

Why Is This Interpretation Useful?

- It gives a solid footing to our intuition: minimizing $\text{RSS}(\tilde{\mathbf{w}})$ is a sensible thing based on reasonable modeling assumptions.
- Estimating σ^* tells us how much noise there is in our predictions. For example, it allows us to place confidence intervals around our predictions.

You Should Know

- Linear regression is the linear combination of features $f : \boldsymbol{x} \rightarrow y$, with $f(\boldsymbol{x}) = w_0 + \sum_d w_d x_d = w_0 + \boldsymbol{w}^\top \boldsymbol{x}$
- If we minimize residual sum of squares as our learning objective, we get a closed-form solution of parameters
- Probabilistic interpretation: maximum likelihood if assuming residual is Gaussian distributed