18-661 Introduction to Machine Learning

Linear Regression – Part I

Spring 2023

ECE – Carnegie Mellon University

Linear Regression

Outline

Recap of MLE/MAP

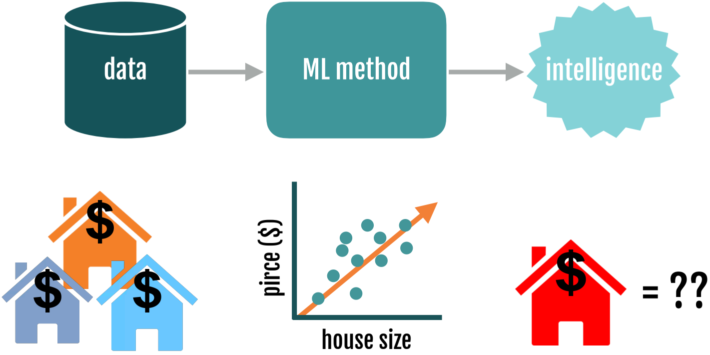
Linear Algebra Review

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

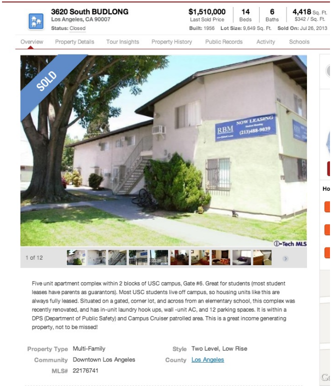
Predicting a continuous outcome variable:

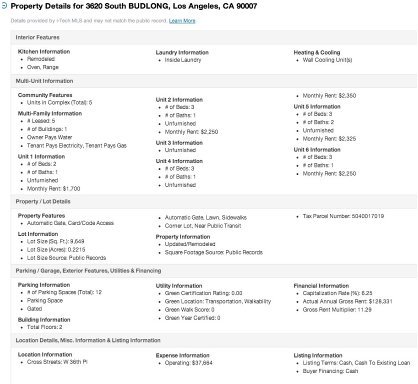
- Predicting a company's future stock price using its profit and other financial info
- Predicting annual rainfall based on local flora and fauna
- Predicting distance from a traffic light using LIDAR measurements

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





Property Details for 3620 South BUDLONG, Los Angeles, CA 90007

Details provided by i-Tech MLS and may not match the public record. Learn More

Interior Features

Kitchen Information
- Remodeled
- Oven, Range

Laundry Information
- Inside Laundry

Heating & Cooling
- Wall Cooling Unit(s)

Multi-Unit Information

Community Features
- Units in Complex (Total): 5

Multi-Family Information
- # Leased: 5
- # of Buildings: 1
- Owner Pays Water
- Tenant Pays Electricity, Tenant Pays Gas

Unit 1 Information
- # of Beds: 2
- # of Baths: 1
- Unfurnished
- Monthly Rent: $1,700

Unit 2 Information
- # of Beds: 3
- # of Baths: 1
- Unfurnished
- Monthly Rent: $2,250

Unit 3 Information
- Unfurnished

Unit 4 Information
- # of Beds: 3
- # of Baths: 1
- Unfurnished

- Monthly Rent: $2,350

Unit 5 Information
- # of Beds: 3
- # of Baths: 2
- Unfurnished
- Monthly Rent: $2,325

Unit 6 Information
- # of Beds: 3
- # of Baths: 1
- Monthly Rent: $2,250

Property / Lot Details

Property Features
- Automatic Gate, Card/Code Access

Lot Information
- Lot Size (Sq. Ft.): 9,649
- Lot Size (Acres): 0.2215
- Lot Size Source: Public Records

- Automatic Gate, Lawn, Sidewalks
- Corner Lot, Near Public Transit

Property Information
- Updated/Remodeled
- Square Footage Source: Public Records

- Tax Parcel Number: 5040017019

Parking / Garage, Exterior Features, Utilities & Financing

Parking Information
- # of Parking Spaces (Total): 12
- Parking Space
- Gated

Building Information
- Total Floors: 2

Utility Information
- Green Certification Rating: 0.00
- Green Location: Transportation, Walkability
- Green Walk Score: 0
- Green Year Certified: 0

Financial Information
- Capitalization Rate (%): 6.25
- Actual Annual Gross Rent: $128,331
- Gross Rent Multiplier: 11.29

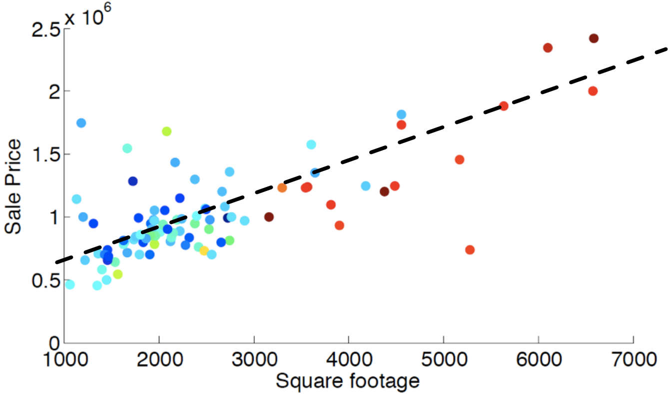
Location Details, Misc. Information & Listing Information

Location Information
- Cross Streets: W 36th Pl

Expense Information
- Operating: $37,664

Listing Information
- Listing Terms: Cash, Cash To Existing Loan
- Buyer Financing: Cash

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 $y = w_1 x + w_0$

Data from Many Houses?

- Sale_price = price_per_sqft × square_footage + fixed_expense + unexplainable_stuff
- Want to learn the price_per_sqft and fixed_expense
- Training data: past sales records

sqft	sale price
2000	800K
2100	907K
1100	312K
5500	2,600K
...	...

Problem: there isn't a $\mathbf{w} = [w_1, w_0]^T$ that will satisfy all equations

Reduce Prediction Error

How to measure 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
$\cdots$	$\cdots$			

- 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**: $f : \mathbf{x} \rightarrow y$, 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**: $\mathcal{D} = \{(\mathbf{x}_n, y_n), n = 1, 2, \ldots, N\}$

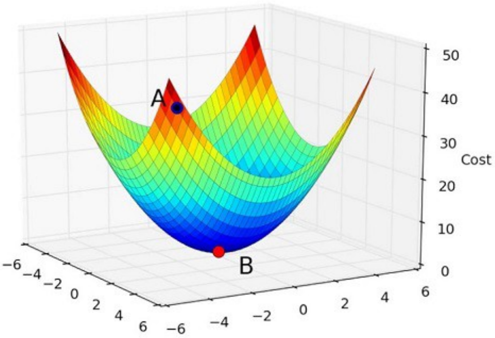
Minimize the Residual Sum of Squares:

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

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:

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

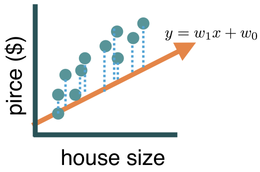


Figure 2: RSS is the sum of squares of the dotted lines

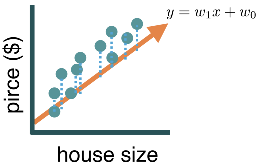


Figure 3: Adjust (w_0, w_1) to reduce RSS

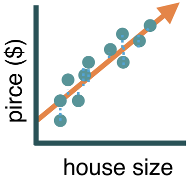


Figure 4: RSS minimized at (w_o^*, w_1^*)

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":

$$\sum y_n = N w_0 + w_1 \sum x_n$$

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

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 $\bar{y} = \frac{1}{N}\sum_n y_n$.

Example

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

Residual sum of squares:

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

The w_1 and w_0 that minimize this are given by:

$$w_1 \approx 1.6$$

$$w_0 \approx 0.45$$

Least Mean Squares: $\mathbf{x}$ 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

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

$$
\begin{bmatrix} w_0 \\ w_1 \end{bmatrix} = \frac{1}{\sum(x_i - \bar{x})^2)} \begin{bmatrix} \bar{y} \sum(x_i - \bar{x})^2 - \bar{x} \sum(x_n - \bar{x})(y_n - \bar{y}) \\ \sum(x_n - \bar{x})(y_n - \bar{y}) \end{bmatrix}
$$

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 $\mathrm{RSS}(\tilde{\mathbf{w}})$ 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