CPSC 340: Machine Learning and Data Mining

Linear Regression

Fall 2022

Admin

- Assignment 2:
  - 1 late day to hand in tonight, 2 for Friday.
- Assignment 3 is up:
  - Due October 17th (minor updates since Monday, see Piazza thread).
  - Start early, this is usually the longest assignment.
- We're going to start using calculus and linear algebra a lot.
  - You should start reviewing these ASAP if you are rusty.
  - A review of relevant calculus concepts is here.
  - A review of relevant linear algebra concepts is here.

Supervised Learning Round 2: Regression

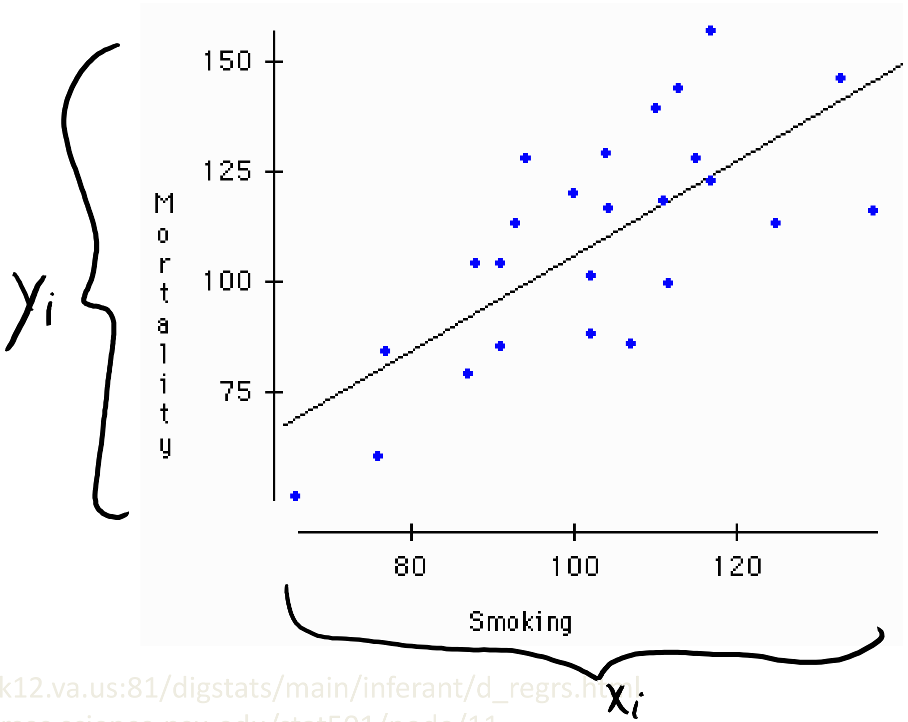
- We're going to revisit supervised learning:

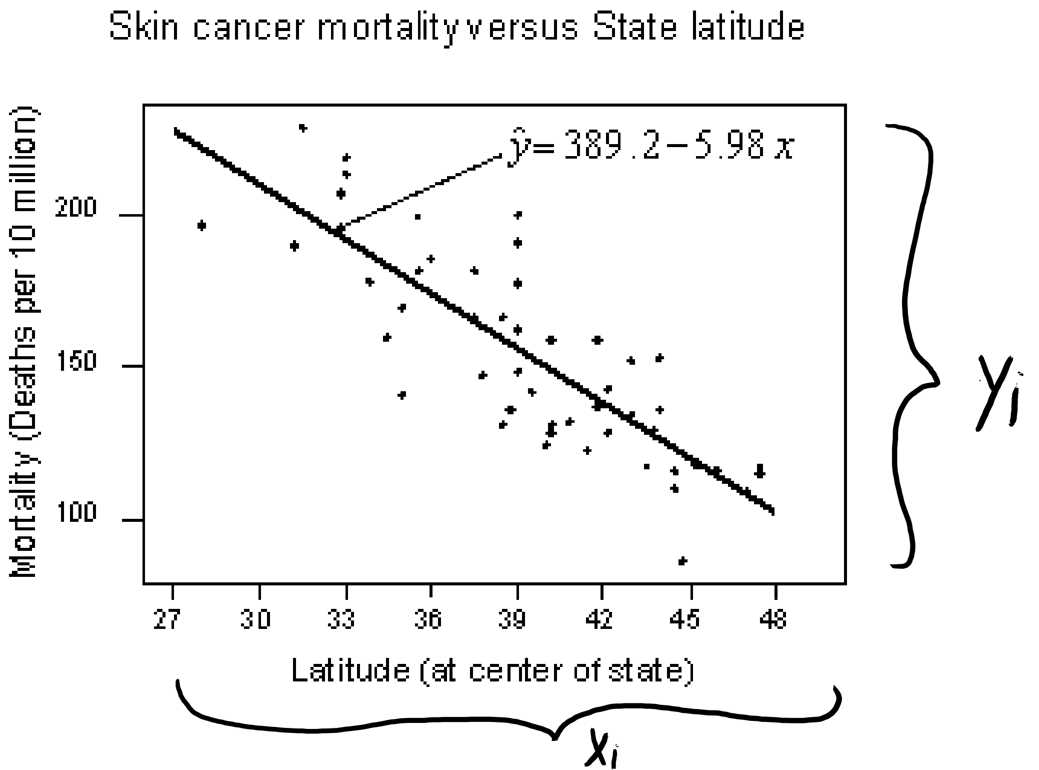
$$X = \begin{bmatrix} \quad & \quad & \quad \end{bmatrix} \qquad y = \begin{bmatrix} \; \end{bmatrix}$$

- Previously, we considered classification:
  - We assumed y_i was categorical: y_i = 'spam' or y_i = 'not spam'.
- Now we are going to consider regression:
  - We allow y_i to be numerical: y_i = 10.34cm.

Example: Dependent vs. Explanatory Variables

- We want to predict a numerical value given features:
  - Does number of lung cancer deaths change with number of cigarettes?
  - Does number of skin cancer deaths change with latitude?



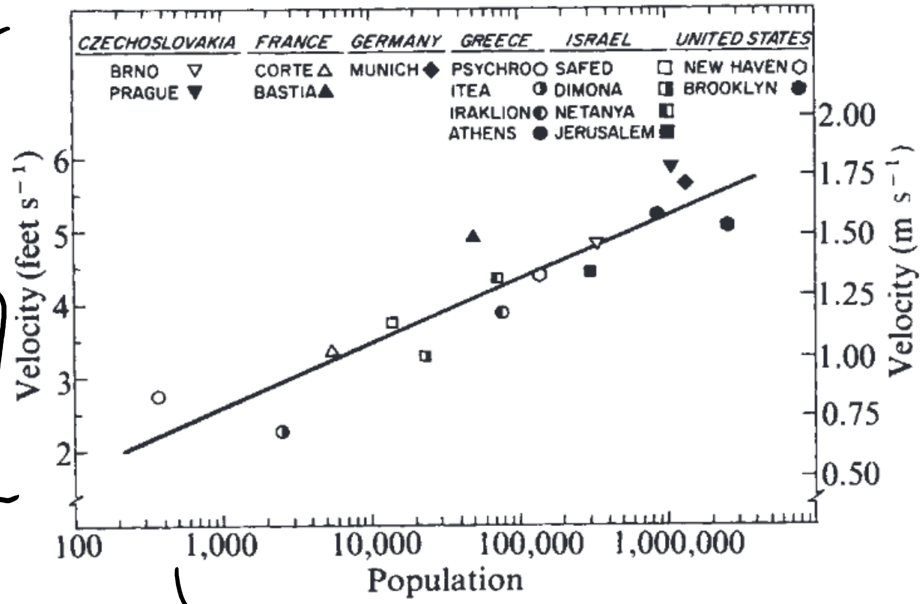


http://www.cvgs.k12.va.us:81/digstats/main/inferant/d_regrs.html
https://onlinecourses.science.psu.edu/stat501/node/11

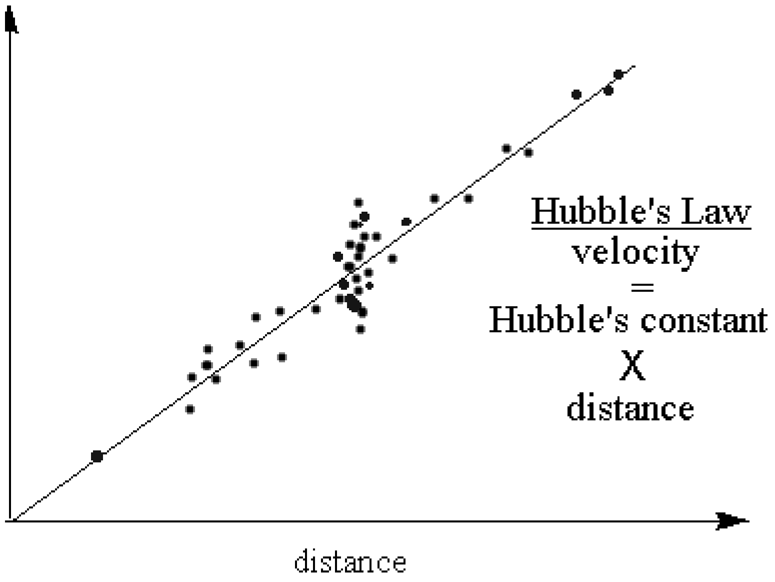
Example: Dependent vs. Explanatory Variables

- We want to predict a numerical value given features:
  - Do people in big cities walk faster?
  - Is the universe expanding or shrinking or staying the same size?

y_i



x_i



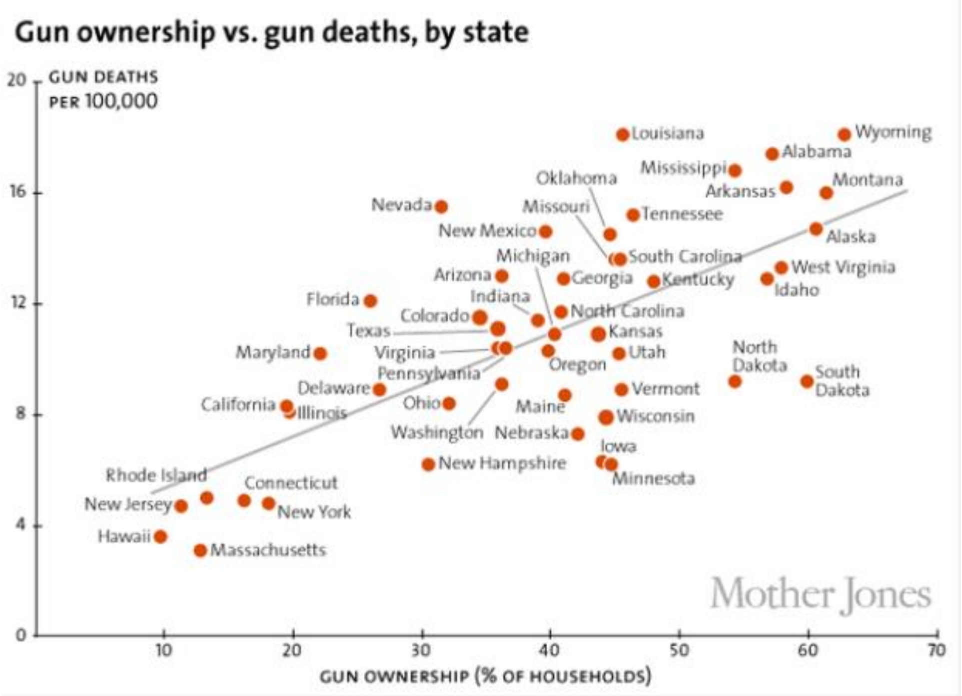
y_i

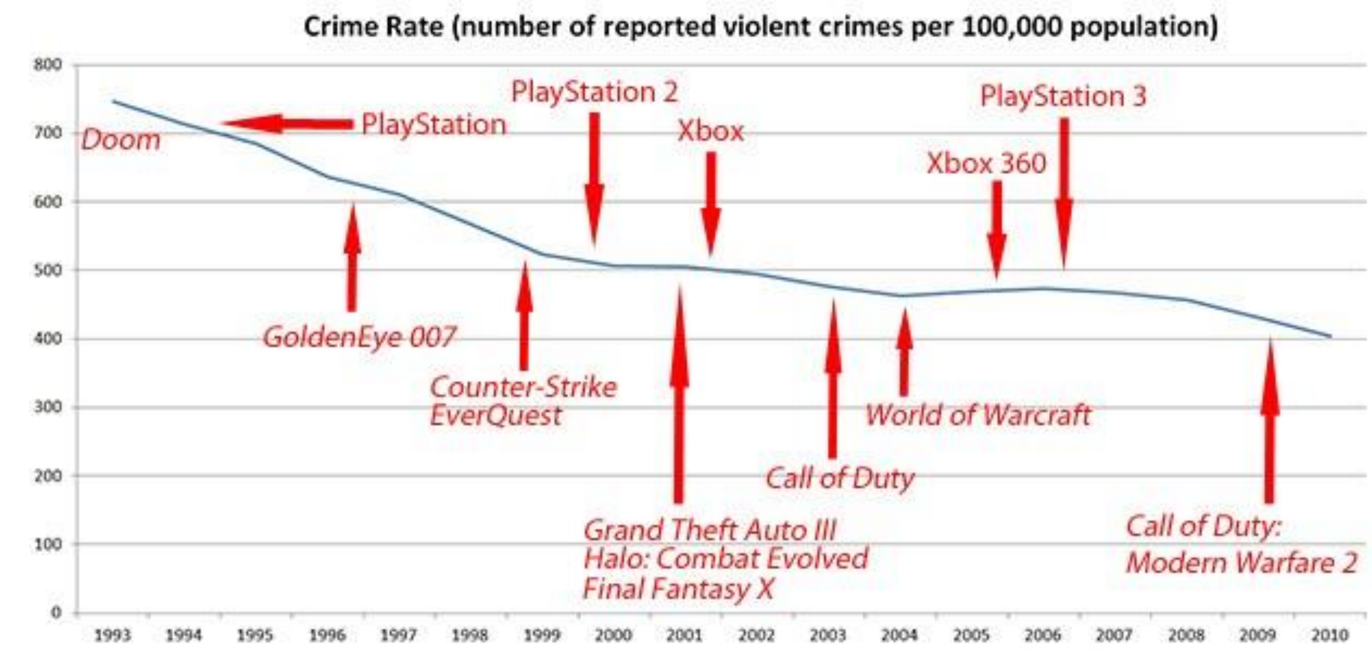
x_i

http://hosting.astro.cornell.edu/academics/courses/astro201/hubbles_law.htm
https://www.nature.com/articles/259557a0.pdf

Example: Dependent vs. Explanatory Variables

- We want to predict a numerical value given features:
  - Does number of gun deaths change with gun ownership?
  - Does number violent crimes change with violent video games?





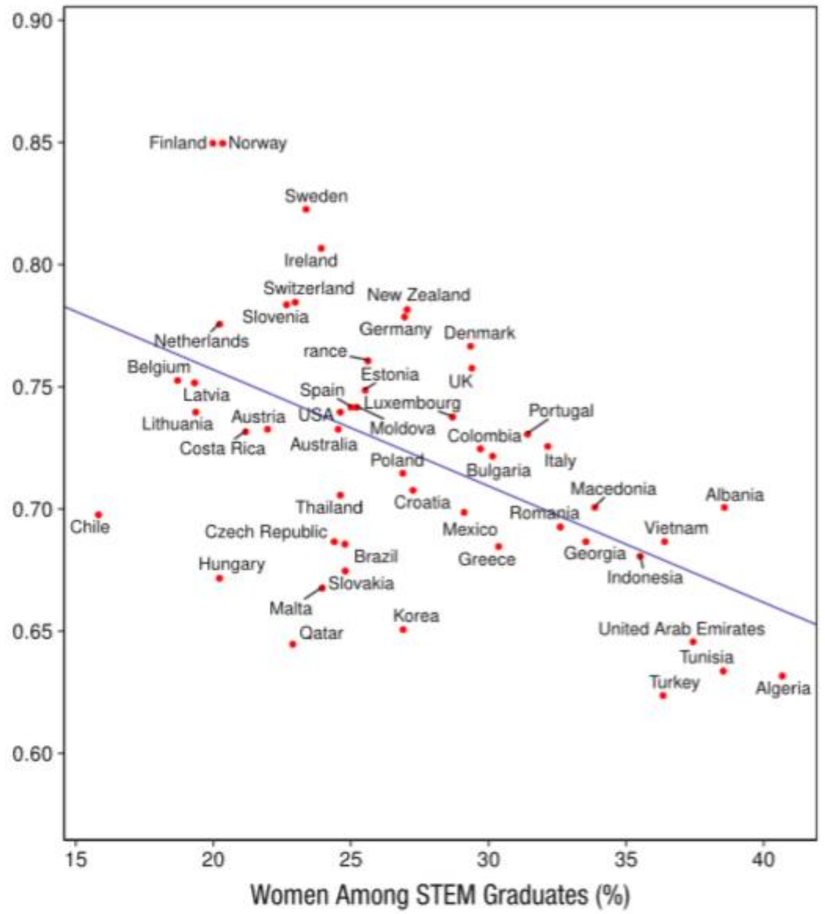
http://www.vox.com/2015/10/3/9444417/gun-violence-united-states-america
https://www.soundandvision.com/content/violence-and-video-games

Example: Dependent vs. Explanatory Variables

- We want to predict a numerical value given features:
  - Does higher gender equality index lead to more women STEM grads?

- Note that we are doing supervised learning:
  - Trying to predict value of 1 variable (the ‘y_i’ values). (instead of measuring correlation between 2).

- Supervised learning does not give causality:
  - OK: “Higher index is correlated with lower grad %”.
  - OK: “Higher index helps predict lower grad %”.
  - BAD: “Higher index leads to lower grads %”.
    - People/media get these confused all the time, be careful!
    - There are lots of potential reasons for this correlation.



https://www.weforum.org/agenda/2018/02/does-gender-equality-result-in-fewer-female-stem-grads/

Handling Numerical Labels

- One way to handle numerical y_i: discretize.
  - E.g., for ‘age’ could we use {‘age ≤ 20’, ‘20 < age ≤ 30’, ‘age > 30’}.
  - Now we can apply methods for classification to do regression.
  - But coarse discretization loses resolution.
  - And fine discretization requires lots of data (“coupon collecting”).
- There exist regression versions of classification methods:
  - Regression trees, neighbour-based methods, and so on.
- Today: one of oldest, but still most popular/important methods:
  - Linear regression based on squared error.
  - Interpretable and the building block for more-complex methods.

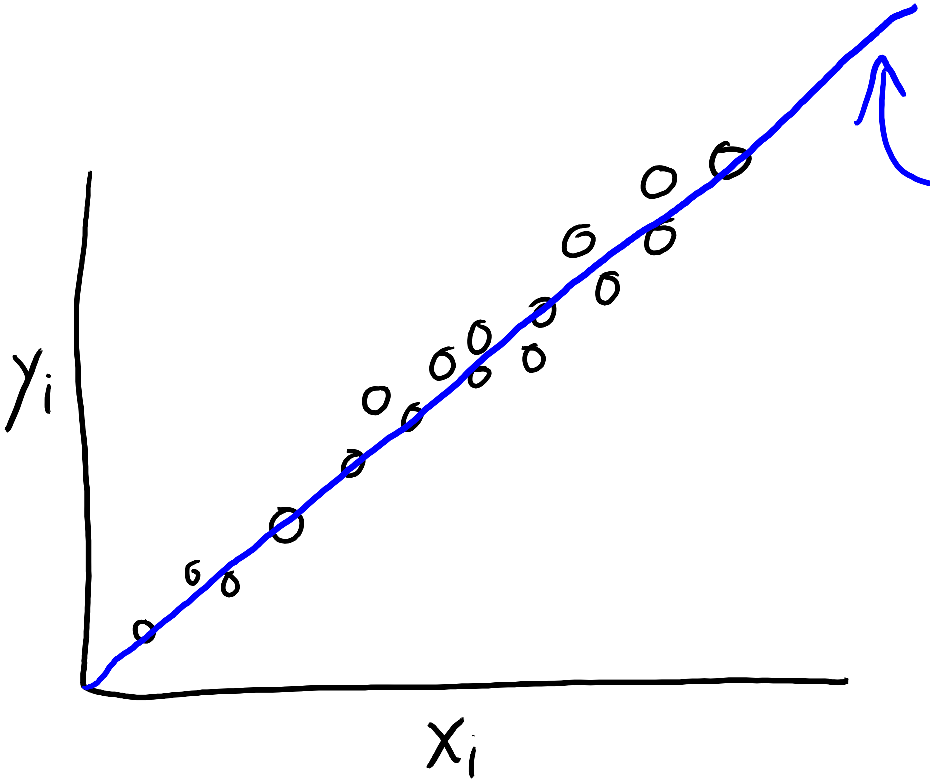
Linear Regression in 1 Dimension

- Assume we only have 1 feature (d = 1):
  - E.g., x_i is number of cigarettes and y_i is number of lung cancer deaths.
- Linear regression makes predictions $\hat{y}_i$ using a linear function of x_i:

$$\hat{y}_i = w x_i$$

- The parameter 'w' is the weight or regression coefficient of x_i.
  - We are temporarily ignoring the y-intercept.
- As x_i changes, slope 'w' affects the rate that $\hat{y}_i$ increases/decreases:
  - Positive 'w': $\hat{y}_i$ increase as x_i increases.
  - Negative 'w': $\hat{y}_i$ decreases as x_i increases.

Linear Regression in 1 Dimension



line $\hat{y}_i = wx_i$ for a particular slope 'w'.

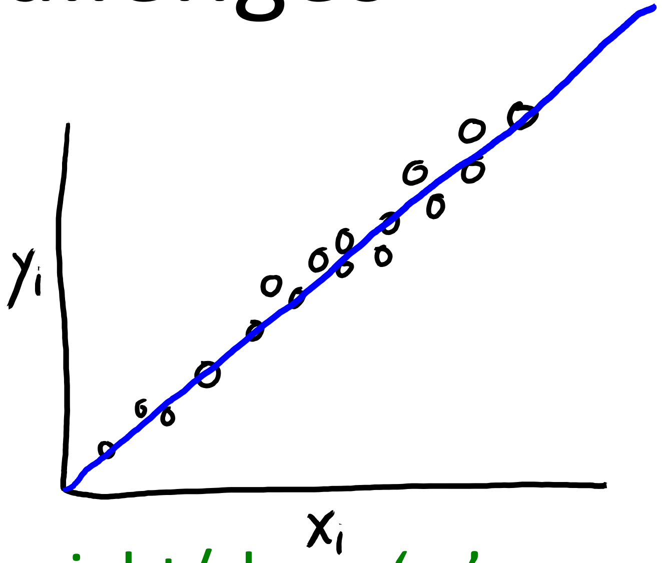
Aside: terminology woes

- Different fields use different terminology and symbols.
  - Data points 'i' = **objects** = **examples** = rows = observations.
  - **Inputs** x_i = predictors = **features** = explanatory variables= regressors = independent variables = covariates = columns.
  - **Outputs** y_i = outcomes = targets = response variables = dependent variables (also called a "label" if it's categorical).
  - Regression coefficients 'w' = **weights** = parameters = betas.
- With linear regression, the symbols are inconsistent too:
  - In ML, the data is X and y, and the weights are w.
  - In statistics, the data is X and y, and the weights are β.
  - In optimization, the data is A and b, and the weights are x.

Linear Regression Training Challenges

- Linear regression makes predictions by using:

$$\hat{y}_i = w\tilde{x}_i$$



- To train a linear regression model, we need to find weight/slope 'w'.
- Challenges in finding 'w' compared to fitting a decision stump:
  – Cannot enumerate all possible values of 'w' (could be any real number).
    - Instead, we will use calculus to find the best 'w'.
  – It is unlikely that a line will go exactly through many data points.
    - Due to noise, relationship not being quite linear or just floating-point issues.
    - So it does not make sense to find the 'w' minimizing how many times $\hat{y}_i \neq y_i$.

Residuals and Sum of Squared Residuals

- The residual is the difference between our prediction and true value:

$$r_i = \hat{y}_i - y_i$$

  - This can be positive or negative.
  - If this is close to zero, then our prediction is close to the true value.

- We typically look for a ‘w’ that makes residuals close to zero.
  - For example, many models minimize the sum of the squared residuals:

$$(\hat{y}_1 - y_1)^2 + (\hat{y}_2 - y_2)^2 + \cdots + (\hat{y}_n - y_n)^2$$

    - The smaller we make this, the smaller the distance between our predictions and targets.
  - Plugging in $\hat{y}_i = wx_i$ for the case of linear regression, we get:

$$(wx_1 - y_1)^2 + (wx_2 - y_2)^2 + \cdots + (wx_n - y_n)^2$$

    - The linear least squares model minimizes this function to choose the slope ‘w’.

Linear Least Squares Objective Function

- Linear least squares sets 'w' is to minimize sum of squared residuals:

$$f(w) = \sum_{i=1}^{n} (wx_i - y_i)^2$$

True value of y_i

Our prediction $\hat{y}_i$

Sum up the squared differences over all training examples.

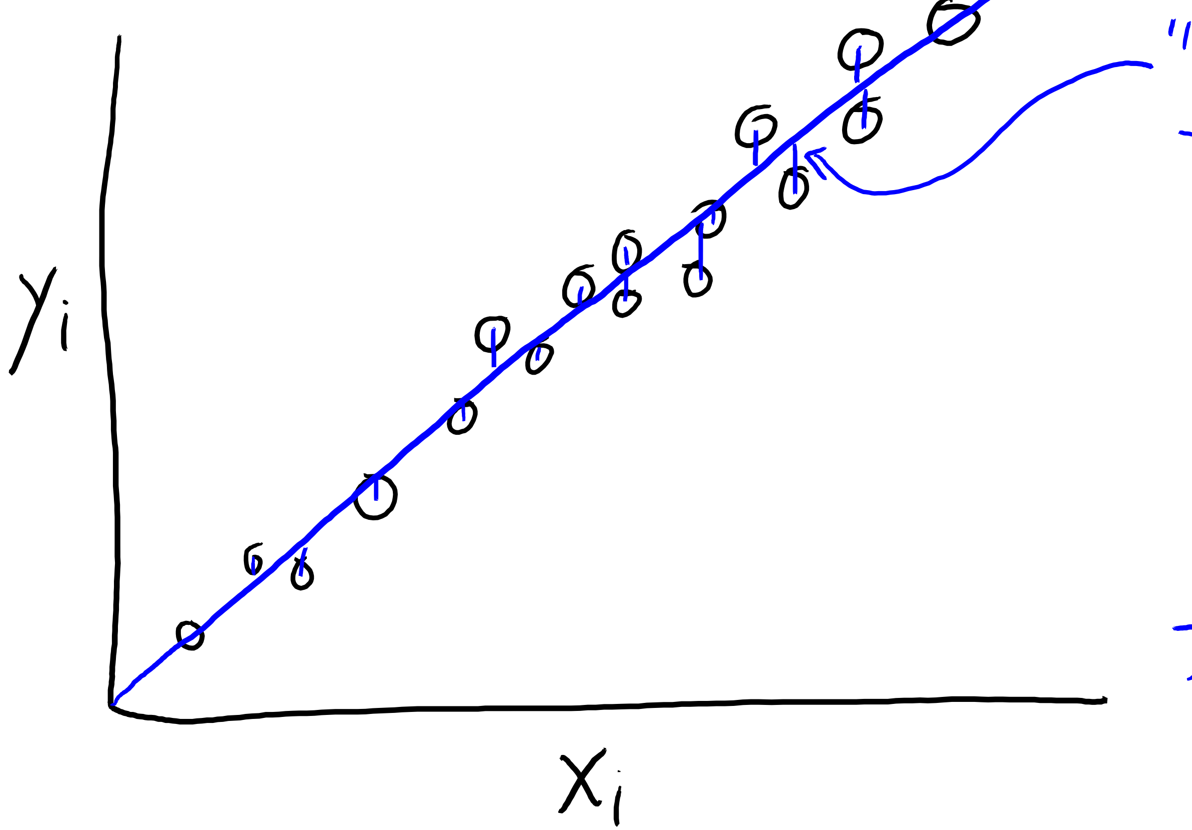
Difference between prediction and true value for example 'i'. (residual)

- If this is zero, we exactly fit data. If this small, line is "close" to data.
- There are some justifications for choosing this function 'f'.
  - A probabilistic interpretation is coming later in the course.
- But usually, we choose this 'f' because it is easy to minimize.

Linear Least Squares Objective Function

- Linear least squares sets ‘w’ is to minimize sum of squared residuals:

$$f(w) = \sum_{i=1}^{n} (w x_i - y_i)^2$$



"Error" is the sum of the squared values of these vertical distances between the line ($w x_i$) and the targets (y_i)

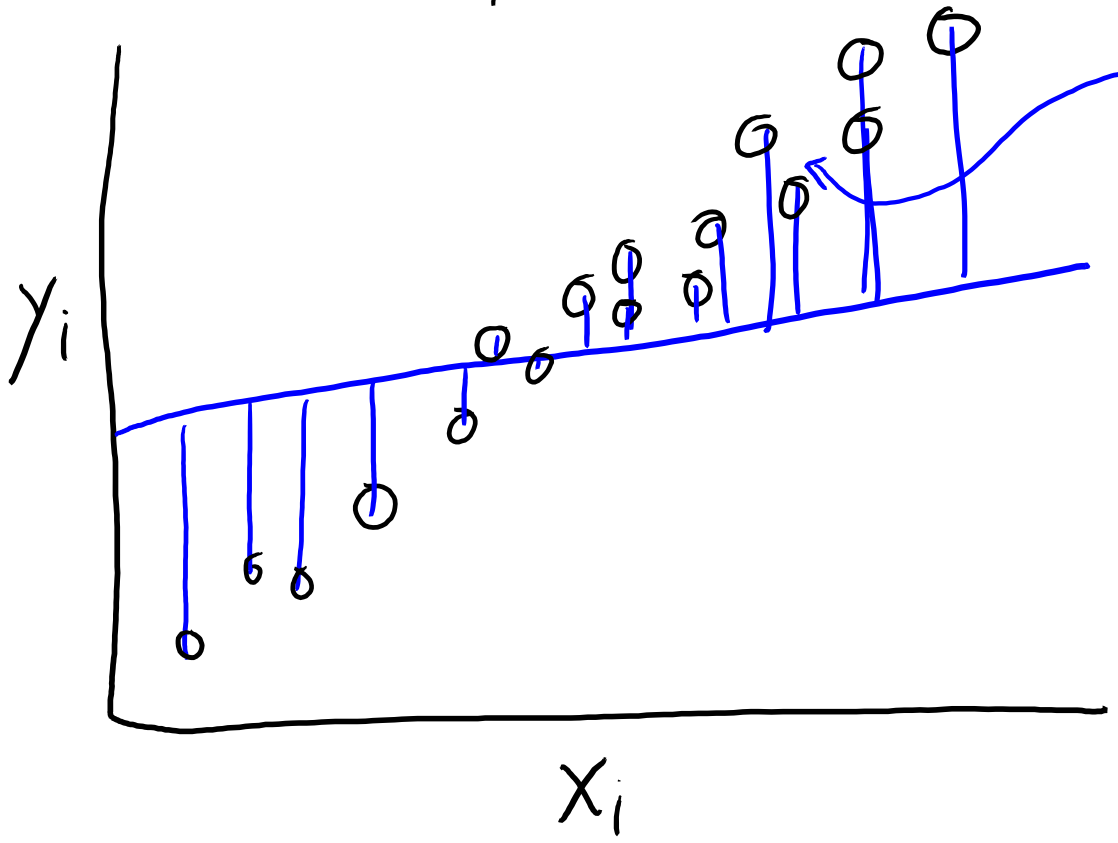
$\downarrow$

If this error is small, then our predictions are close to the targets.

Linear Least Squares Objective Function

- Linear least squares sets ‘w’ is to minimize sum of squared residuals:

$$f(w) = \sum_{i=1}^{n} (wx_i - y_i)^2$$

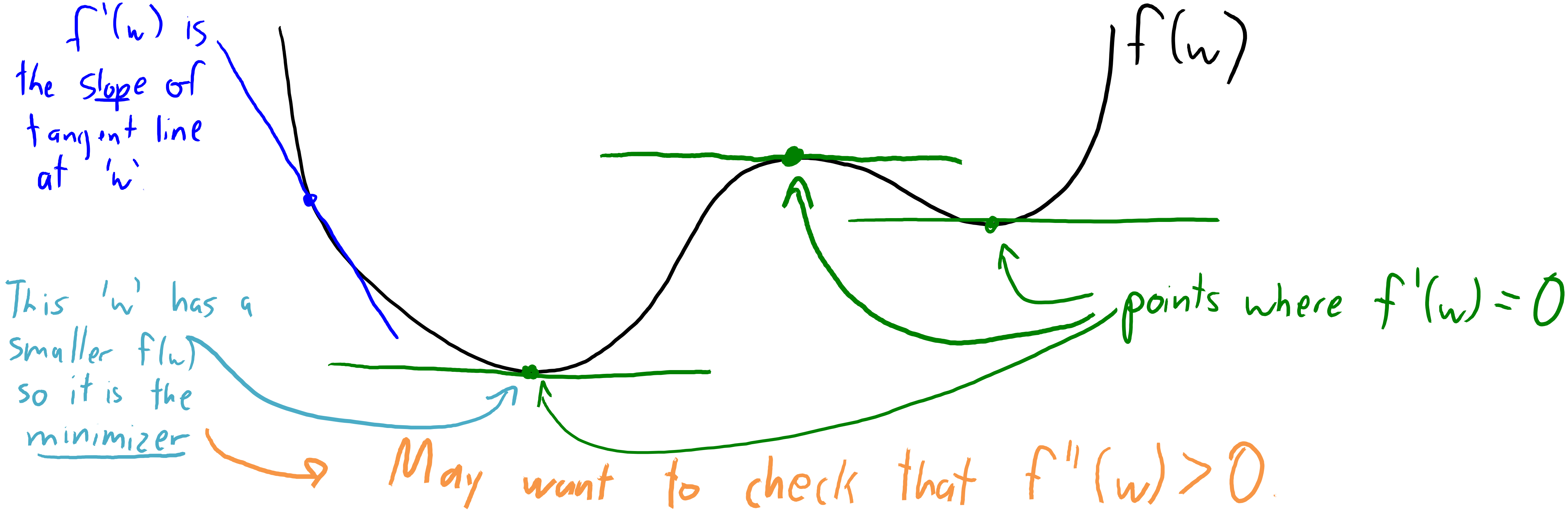


"Error" is the sum of the squared values of these vertical distances between the line (wx_i) and the targets (y_i)

If this error is large, then our predictions are far from the targets.

Minimizing a Differential Function

- Math 101 approach to minimizing a differentiable function ‘f’:
  1. Take the derivative of ‘f’.
  2. Find points ‘w’ where the derivative f’(w) is equal to 0.
  3. Choose the smallest one (and check that f’’(w) is positive).



Digression: Multiplying by a Positive Constant

- Note that this problem: $$f(w) = \sum_{i=1}^{n}(wx_i - y_i)^2$$
- Has the same set of minimizers as this problem: $$f(w) = \frac{1}{2}\sum_{i=1}^{n}(wx_i - y_i)^2$$
- And these also have the same minimizers: $$f(w) = \frac{1}{n}\sum_{i=1}^{n}(wx_i - y_i)^2 \qquad f(w) = \frac{1}{2n}\sum_{i=1}^{n}(wx_i - y_i)^2 + 1000$$
- I can multiply 'f' by any positive constant and not change solution.
  - Derivative will still be zero at the same locations.
  - We will use this trick a lot!

(Quora trolling on ethics of this)

Deriving Least Squares Solution

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(wx_i - y_i)^2 = \frac{1}{2}\sum_{i=1}^{n}\left[w^2x_i^2 - 2wx_iy_i + y_i^2\right]$$ (expand square)

$$= \frac{1}{2}\sum_{i=1}^{n} w^2x_i^2 - \frac{1}{2}\sum_{i=1}^{n} 2wx_iy_i + \frac{1}{2}\sum_{i=1}^{n} y_i^2$$ (split sum up into different terms)

$$= \frac{w^2}{2}\underbrace{\sum_{i=1}^{n} x_i^2}_{\text{constant 'a'}} - w\underbrace{\sum_{i=1}^{n} x_iy_i}_{\text{constant 'b'}} + \underbrace{\frac{1}{2}\sum_{i=1}^{n} y_i^2}_{\text{constant 'c'}}$$ (remove factors from sums that do not depend on example 'i')

$$= \frac{w^2}{2}a - wb + c$$

Take derivative: $f'(w) = wa - b + 0$

Setting $f'(w) = 0$ and solving gives $w = \frac{b}{a} = \frac{\sum_{i=1}^{n} x_iy_i}{\sum_{i=1}^{n} x_i^2}$ (exists if we have a non-zero feature)

Finding Least Squares Solution

- Finding 'w' that minimizes sum of squared errors:

Setting $f'(w) = 0$ and solving gives $w = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}$ (exists if we have one non-zero x_{ij})

- Let's check that this is a minimizer by checking second derivative:

$$f'(w) = w \sum_{i=1}^{n} x_i^2 - \sum_{i=1}^{n} x_i y_i$$

$$f''(w) = \sum_{i=1}^{n} x_i^2$$

  - Since $(\text{anything})^2$ is non-negative, we have $f''(w) \geq 0$.
  - If at least one feature is not zero, then $f''(w) > 0$ and 'w' is a minimizer.

Next Topic: Least Squares in d-Dimensions

Motivation: Combining Explanatory Variables

- Smoking is not the only contributor to lung cancer.
  - For example, there environmental factors like exposure to asbestos.
- How can we model the combined effect of smoking and asbestos?
- A simple way is with a 2-dimensional linear function:

$$\hat{y}_i = w_1 x_{i1} + w_2 x_{i2}$$

Value of feature 2 in example 'i'

"weight" on feature 2.

"weight" of feature 1

Value of feature 1 in example 'i'

- We have a weight w_1 for feature '1' and w_2 for feature '2':

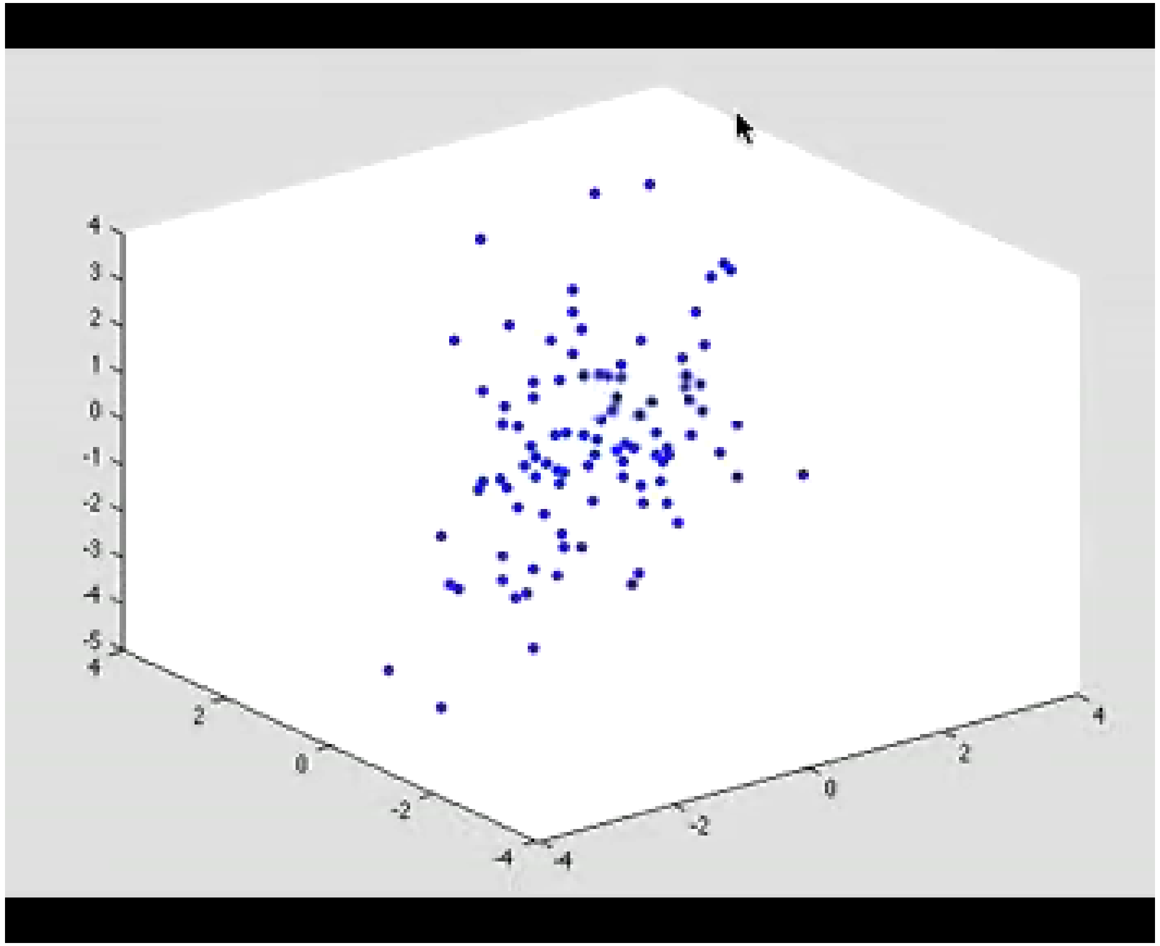
$$\hat{y}_i = 10(\#\text{cigarettes}) + 25(\#\text{asbetos})$$

Linear Regression in 2-Dimensions

- Linear model:

$$\hat{y}_i = w_1 x_{i1} + w_2 x_{i2}$$

- This defines a two-dimensional plane.



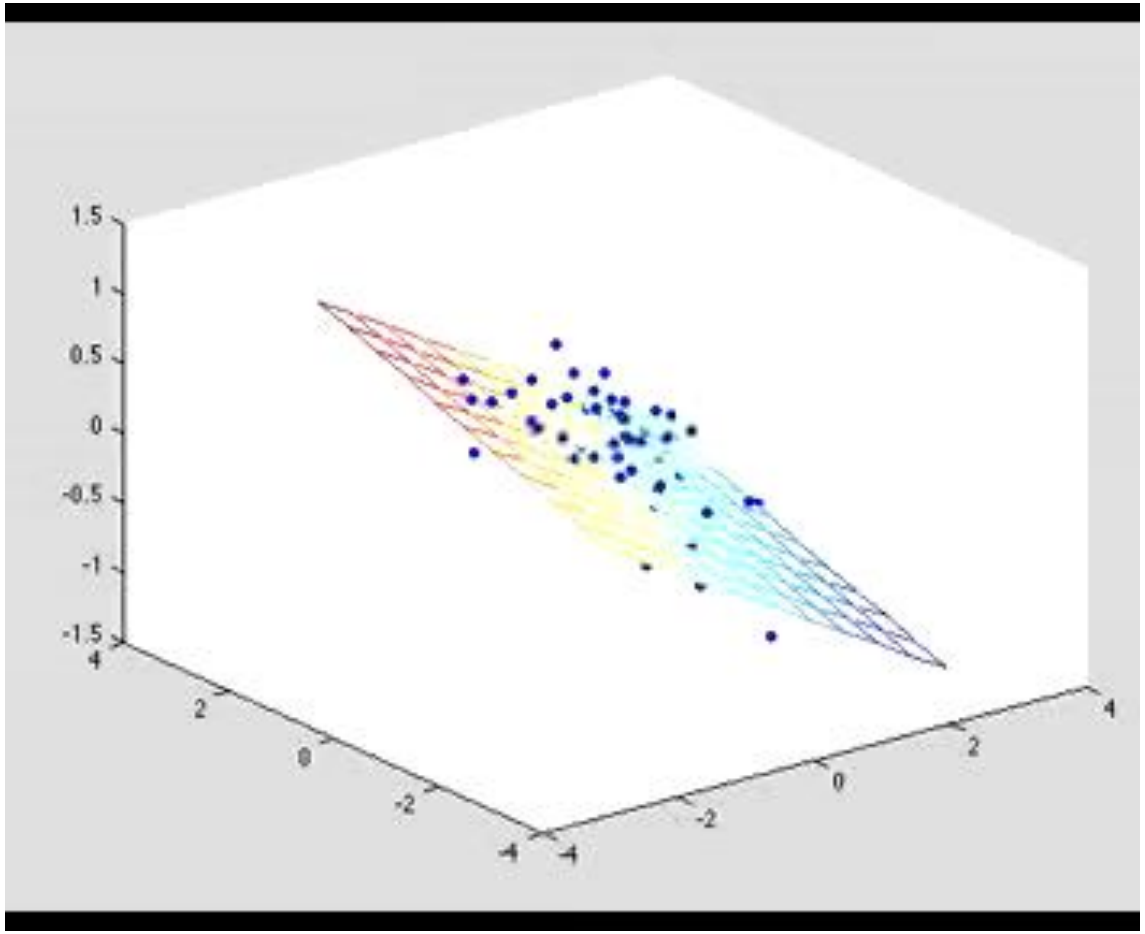
Linear Regression in 2-Dimensions

- Linear model:

$$\hat{y}_i = w_1 x_{i1} + w_2 x_{i2}$$

- This defines a two-dimensional plane.

- Not just a line!



Linear Regression in d-Dimensions

- If we have 'd' features, the d-dimensional linear model is:

$$\hat{y}_i = w_1 x_{i1} + w_2 x_{i2} + w_3 x_{i3} + \cdots + w_d x_{id}$$

  - In words, prediction is a weighted sum of the features.
- We can re-write this using summation notation as:

$$\hat{y}_i = \sum_{j=1}^{d} w_j x_{ij}$$

- We can again choose 'w' to minimize the sum of squared residuals:

$$f(w_1, w_2, \dots, w_d) = \frac{1}{2} \sum_{i=1}^{n} \Big(\underbrace{\sum_{j=1}^{d} w_j x_{ij}}_{\hat{y}_i} - y_i \Big)^2$$

  - Dates back to 1801: Gauss used it to predict location of the asteroid Ceres.
  - We can use multi-variable calculus to minimize 'f' with respect to the parameters w_1, w_2,…, w_d.

Minimizing Multi-Variable Differentiable Function

- With one variable, we "find 'w' where the derivative is equal to 0".
- The generalization of this idea to when we have 'd' variables:
  - "Find 'w' where the gradient vector is equal to the zero vector".

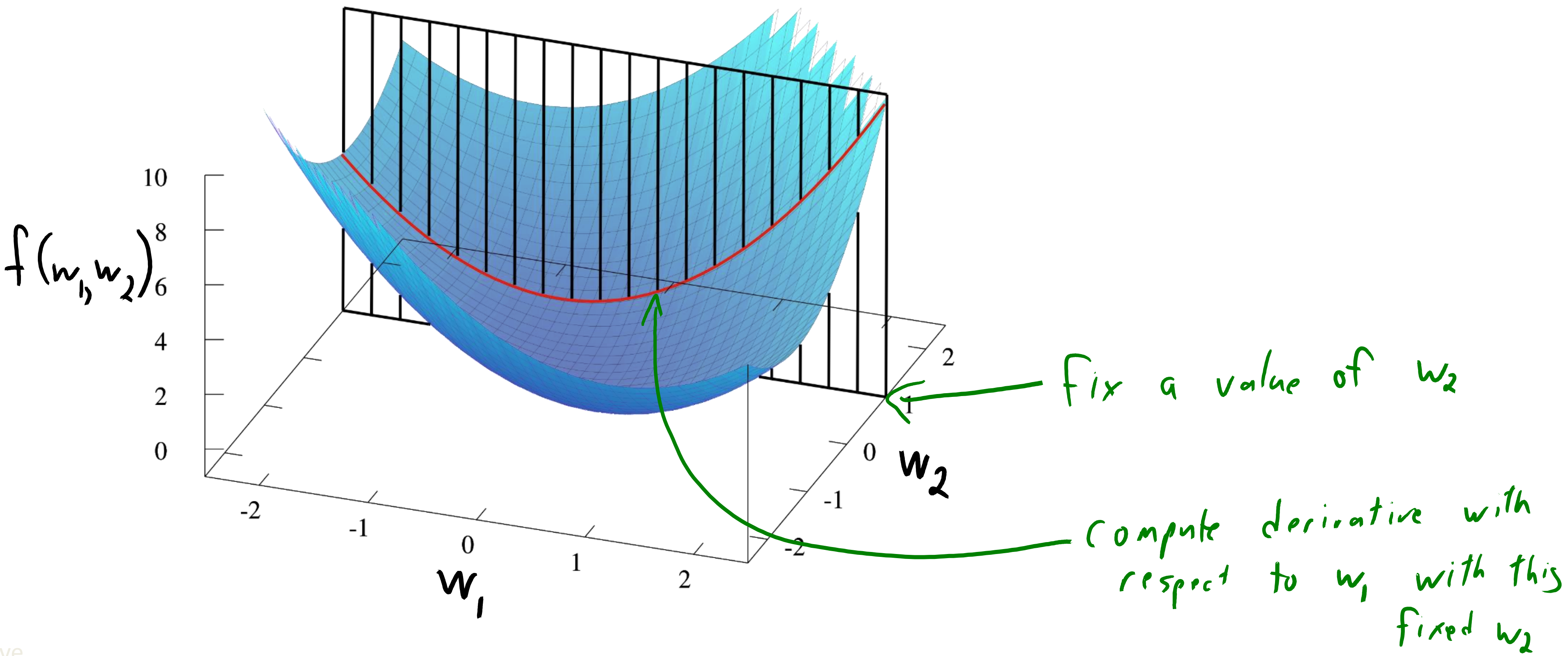
- Gradient is a vector with partial derivative 'j' in position 'j'.

$$\underbrace{\nabla f(w)}_{\text{gradient vector}} = \begin{bmatrix} \frac{\partial f}{\partial w_1} \\ \frac{\partial f}{\partial w_2} \\ \vdots \\ \frac{\partial f}{\partial w_d} \end{bmatrix}$$

partial derivative of 'f' with respect to variable w_2

Review: Partial Derivative

- Partial derivative with respect to w_j (written $\frac{\partial f}{\partial w_j}$).
  - Derivative with respect to w_j, keeping all others variables fixed.



https://en.wikipedia.org/wiki/Partial_derivative

Partial Derivative for Least Squares

- Partial derivative with respect to w_1 for least squares with n=1:

$$f(w_1, w_2, \dots, w_d) = \frac{1}{2}\left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)^2$$

$$\frac{\partial f}{\partial w_1} = \left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right) x_{i1}$$

$$\sum_{j=1}^{d} w_j x_{ij} = \underbrace{w_1 x_{i1}}_{\text{only one term involving } w_1} + w_2 x_{i2} + \dots + w_d x_{id}$$

$$\frac{\partial}{\partial w_1}\left[\underbrace{\frac{1}{2}\left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)^2}_{\frac{\partial}{\partial w_1} \frac{1}{2} g(w_1, w_2, \dots, w_d)^2 = g(w_1, w_2, \dots, w_d)\frac{\partial}{\partial w_1}[g(w_1, w_2, \dots, w_d)]}\right] = \left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)\frac{\partial}{\partial w_1}\left[\underbrace{\sum_{j=1}^{d} w_j x_{ij} - y_i}_{\frac{\partial}{\partial w_1}\left[w_1 x_{i1} + \text{terms with no } w_1\right]}\right]$$

$$= x_{i1} + 0$$

Partial Derivative for Least Squares

- Partial derivative with respect to w_j for least squares with n=1:

$$f(w_1, w_2, \dots, w_d) = \frac{1}{2}\left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)^2$$

$$\frac{\partial f}{\partial w_j} = \left(\underbrace{\sum_{j'=1}^{d}}_{} w_{j'} x_{ij'} - y_i\right) x_{ij}$$

We use j' to distinguish the summation index from the variable w_j we are differentiating

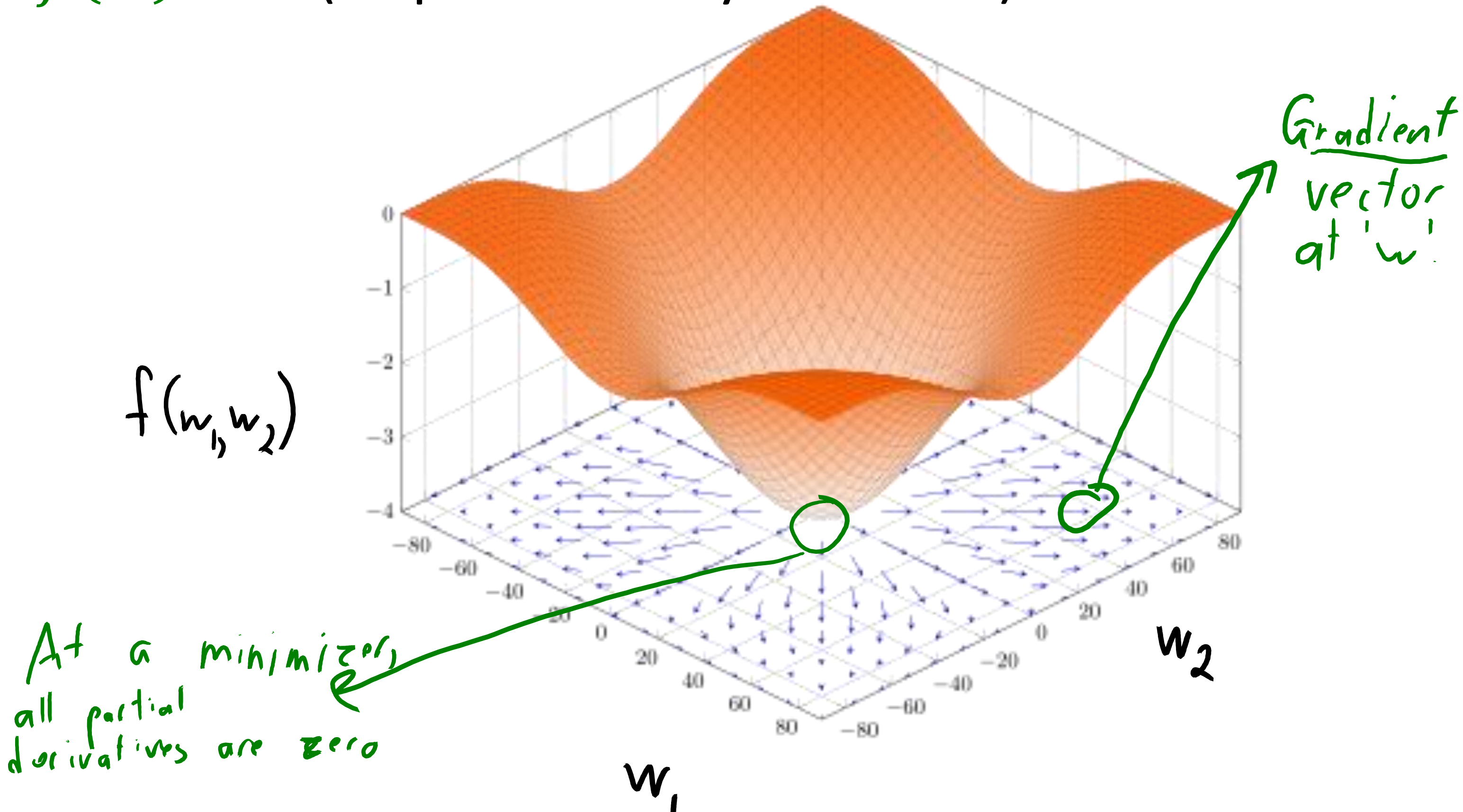
- Partial derivative with respect to w_j for least squares for general 'n':

$$f(w_1, w_2, \dots, w_d) = \frac{1}{2}\sum_{i=1}^{n}\left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)^2$$

$$\frac{\partial f}{\partial w_j} = \sum_{i=1}^{n}\left(\sum_{j'=1}^{d} w_{j'} x_{ij'} - y_i\right) x_{ij}$$

Gradient Vector for Least Squares

- The gradient vector is the concatenation of all partial derivatives:
  - At ‘w’, $\nabla f(w)$ is in the direction with most-positive slope.
  - At minimizers we have $\nabla f(w) = 0$ (slope is 0 every direction).



https://en.wikipedia.org/wiki/Gradient

Gradient Vector for Least Squares

- The gradient vector is the concatenation of all partial derivatives:
  - At ‘w’, $\nabla f(w)$ is in the direction with most-positive slope.
  - At minimizers we have $\nabla f(w) = 0$ (slope is 0 every direction).
- For linear least squares we have:

$$\nabla f(w) = \begin{bmatrix} \frac{\partial f}{\partial w_1} \\ \frac{\partial f}{\partial w_2} \\ \vdots \\ \frac{\partial f}{\partial w_d} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n}\left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)x_{i1} \\ \sum_{i=1}^{n}\left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)x_{i2} \\ \vdots \\ \sum_{i=1}^{n}\left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)x_{id} \end{bmatrix}$$

  - So to train a least squares model, we need this to equal the zero vector.

Fitting a Linear Least Squares Model

- Setting gradient to equal 0 vector for linear least squares gives:

$$\nabla f(w) = 0 \iff \begin{aligned} \sum_{i=1}^{n}\left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)x_{i1} &= 0 \\ \sum_{i=1}^{n}\left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)x_{i2} &= 0 \\ &\vdots \\ \sum_{i=1}^{n}\left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)x_{id} &= 0 \end{aligned}$$

  – This is a set of ‘d’ linear equations, with ‘d’ unknowns (w_1, w_2,…, w_d).
    - You can solve these equations using Gaussian elimination (linear algebra).

  – Claim: all ‘w’ with $\nabla f(w) = 0$ are minimizers (we will discuss why later).
    - There may be more than ‘w’ satisfying this, but all have the same minimum error.

Next Topic: Matrix Notation

Matrix Notation: Motivation

- We have expressed linear least squares with summation notation:

$$f(w_1, w_2, \dots, w_d) = \sum_{i=1}^{n}\left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)^2$$

- But you often see it equivalently expressed using matrix notation:

$$f(w) = \|Xw - y\|^2$$

- Why do people use matrix notation?
  - Can be easier to understand and lead to "nicer" code (once you are used to it).
  - Makes it easier to see some properties (like the connection to norms above).
    - Or derive properties, like showing that all 'w' with $\nabla f(w) = 0$ are minimizers.
  - Can lead to code with fewer bugs.
    - Since you can use existing implementations of standard operations.
  - Can lead to faster code.
    - If we are using packages that implement fast matrix operations.

Matrix Notation (MEMORIZE/STUDY THIS)

- In this course, all vectors are assumed to be column-vectors:

$$w = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \end{bmatrix} \qquad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \qquad x_i = \begin{bmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{id} \end{bmatrix}$$

- So rows of 'X' are actually transposes of the column-vectors x_i:

$$X = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1d} \\ x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nd} \end{bmatrix} = \begin{bmatrix} \text{---} & x_1^T & \text{---} \\ \text{---} & x_2^T & \text{---} \\ & \vdots & \\ \text{---} & x_n^T & \text{---} \end{bmatrix}$$

Matrix Notation (MEMORIZE/STUDY THIS)

- Linear regression prediction for one example in matrix notation:

$$\hat{y}_i = w^T x_i$$

- Why?

$$\hat{y}_i = w_1 x_{i1} + w_2 x_{i2} + \cdots + w_d x_{id} = \underbrace{\begin{bmatrix} w_1 & w_2 & \cdots & w_d \end{bmatrix}}_{w^T} \underbrace{\begin{bmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{id} \end{bmatrix}}_{x_i} = w^T x_i$$

- Using $\hat{y}_i = w^T x_i$, we can re-write sum of squared residuals as:

$$\sum_{i=1}^{n} (\hat{y}_i - y_i)^2 = \sum_{i=1}^{n} (w^T x_i - y_i)^2$$

Matrix Notation (MEMORIZE/STUDY THIS)

- Linear regression prediction for all 'n' example in matrix notation:

$$\underbrace{\hat{y}}_{\substack{n \times 1 \text{ vector} \\ \text{of predictions}}} = \underbrace{X}_{\substack{n \times d \text{ matrix} \\ \text{of features}}} \underbrace{w}_{\substack{d \times 1 \text{ vector} \\ \text{of parameters.}}}$$

- Why?

$$Xw = \underbrace{\begin{bmatrix} — & x_1^T & — \\ — & x_2^T & — \\ & \vdots & \\ — & x_n^T & — \end{bmatrix}}_{X} \underbrace{\begin{bmatrix} | \\ w \\ | \end{bmatrix}}_{w} = \begin{bmatrix} x_1^T w \\ x_2^T w \\ \vdots \\ x_n^T w \end{bmatrix} = \begin{bmatrix} w^T x_1 \\ w^T x_2 \\ \vdots \\ w^T x_n \end{bmatrix} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \hat{y}$$

Prediction for example 'i' in row 'i'

We have $w^T x_i = x_i^T w$ because it is a scalar. (For example, $[5]^T = [5]$)

Matrix Notation (MEMORIZE/STUDY THIS)

- Linear regression residual vector in matrix notation:

$$\underbrace{r}_{n\times 1 \text{ vector of residuals } r_i = \hat{y}_i - y_i} = Xw - y$$

- Why?

$$r = \begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_n \end{bmatrix} = \begin{bmatrix} \hat{y}_1 - y_1 \\ \hat{y}_2 - y_2 \\ \vdots \\ \hat{y}_n - y_n \end{bmatrix} = \underbrace{\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix}}_{\hat{y}} - \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}}_{y} = \hat{y} - y = Xw - y$$

$\hat{y} = Xw$ (last slide)

Matrix Notation (MEMORIZE/STUDY THIS)

- Different ways to write sum of residuals squared in linear regression model:

$$f(w) = \sum_{i=1}^{n}\left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)^2$$

$$= \sum_{i=1}^{n}\left(w^T x_i - y_i\right)^2$$

$$= \sum_{i=1}^{n} r_i^2$$

$$= \|r\|^2$$

$$= \|Xw - y\|^2$$

Can also write $\|r\|^2 = r^T r$

Can also write $\|Xw - y\|^2$
$= (Xw - y)^T (Xw - y)$
or $\|\hat{y} - y\|^2$

- So least squares minimizes L2-norm between target and predictions.

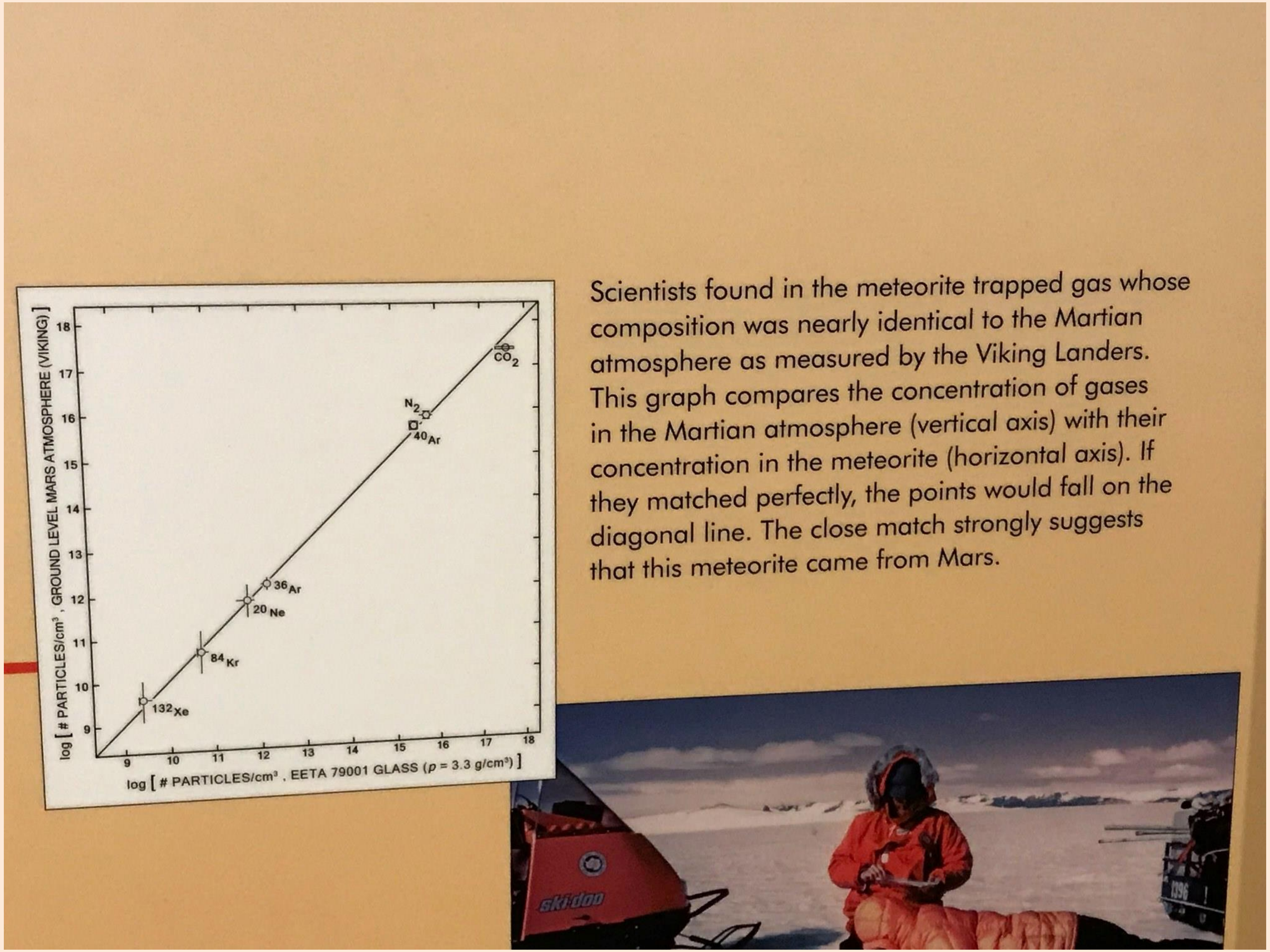
Summary

- Regression considers the case of a numerical y_i.
- Least squares is a classic method for fitting linear models.
  - Minimizes sum of squared residuals (prediction and true value difference).
  - With 1 feature, it has a simple closed-form solution.
  - Can be generalized to 'd' features, taking linear weighting of features.
- Gradient is vector containing partial derivatives of all variables.
- Matrix notation for expressing least squares problem: $||Xw - y||^2$.
- Next time:

minimizing $\frac{1}{2}\sum_{i=1}^{n}(w^T x_i - y_i)^2$ in terms of 'w' is: $w = (X'X)\backslash(X'y)$

(in Julia)

- In Smithsonian National Air and Space Museum (Washington, DC):



Causality, Interventions, and RCTs

- What if you want to assess causality?
- You can sometimes do this by collecting data in specific ways.
  - You need to set the values of the features “by intervention”.
    - You do not passively observe, you *set* them and then watch the effect.
  - Most common way this is done is with a randomized control trial.
    - Say you want to evaluate the effectiveness of a pill for a certain disease.
    - You get a bunch of people with the disease for training data.
    - You randomly decide which of the people will take the pill, and which won’t.
    - If the people who got the pill did better/worse on average, it was caused by the pill.
      - The randomness takes away the possibility that certain groups are more/less likely to take the pill.
      - Group not taking the pill often given placebo, removing effect of “feel like you are being treated”.
      - Often the researchers do not even get to know who took the pills until after the study is over.
        - » “Double blind”, to avoid the researchers giving hints about who got the pill.

Converting Partial Derivative to Matrix Notation

- Re-writing linear least squares partial derivative in matrix notation:

$$\frac{\partial f}{\partial w_j} = \sum_{i=1}^{n}\left(\sum_{j'=1}^{d} w_{j'} x_{ij'} - y_i\right)x_{ij} \quad \text{(from earlier)}$$

$$= \sum_{i=1}^{n}(w^T x_i - y_i)x_{ij} \quad \text{(no need for } j'\text{)}$$

$$= \sum_{i=1}^{n} r_i x_{ij} \quad \text{(definition of } r_i\text{)}$$

$$= \underbrace{r}_{\text{residual vector}}{}^T \underbrace{x^j}_{\text{column 'j' of 'X'}}$$

Converting Gradient to Matrix Notation

- Re-writing linear least squares gradient in matrix notation:

$$\nabla f(w) = \begin{bmatrix} \frac{\partial f}{\partial w_1} \\ \frac{\partial f}{\partial w_2} \\ \vdots \\ \frac{\partial f}{\partial w_d} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n}\left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)x_{i1} \\ \sum_{i=1}^{n}\left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)x_{i2} \\ \vdots \\ \sum_{i=1}^{n}\left(\sum_{j=1}^{d} w_j x_{ij} - y_i\right)x_{id} \end{bmatrix} = \begin{bmatrix} r^T x^1 \\ r^T x^2 \\ \vdots \\ r^T x^d \end{bmatrix}$$

(from last slide)

$$= \underbrace{\begin{bmatrix} \text{---} & x^1 & \text{---} \\ \text{---} & x^2 & \text{---} \\ & \vdots & \\ \text{---} & x^d & \text{---} \end{bmatrix}}_{X^T} r = \underbrace{X^T r}$$

Transpose of 'X' multiplied by residual vector