25: Linear Regression and Gradient Ascent

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Linear Regression

Today's goals

We are going to learn linear regression.

- Informally known as "fitting data to a straight line"
- Linear models, however, are too simple for more complex datasets.
- Furthermore, many tasks in CS deal with classification (categorical data), not regression.

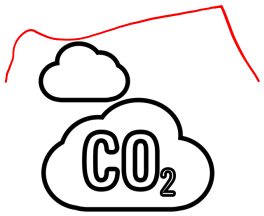
We cover this topic anyway so we can learn ***important techniques*** that will help us design and understand more complicated ML algorithms:

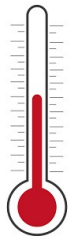
1. How to model likelihood of training data $\left(\boldsymbol{x}^{(i)}, y^{(i)}\right)$
2. What rules of argmax and calculus are important to remember
3. What **gradient ascent** is and why it is useful

Regression: Predicting real numbers

Review

Training data: $(\boldsymbol{x}^{(1)}, y^{(1)}), (\boldsymbol{x}^{(2)}, y^{(2)}), \ldots, (\boldsymbol{x}^{(n)}, y^{(n)})$





Global Land-Ocean temperature

	CO2 levels	Output
Year 1	338.8	0.26
Year 2	340.0	0.32
...		⋮
Year n	340.76	0.14

$\boldsymbol{X} = (X_1)$
(assume one feature)

$Y \in \mathbb{R}$

Model:

real number

composed of mix of real and discrete

$$\hat{Y} = g(\boldsymbol{X}),$$

for some parametric function g

Linear Regression

Assume linear model (and $\boldsymbol{X}$ is 1-D):

$$\hat{Y} = g(\boldsymbol{X}) = aX + b$$

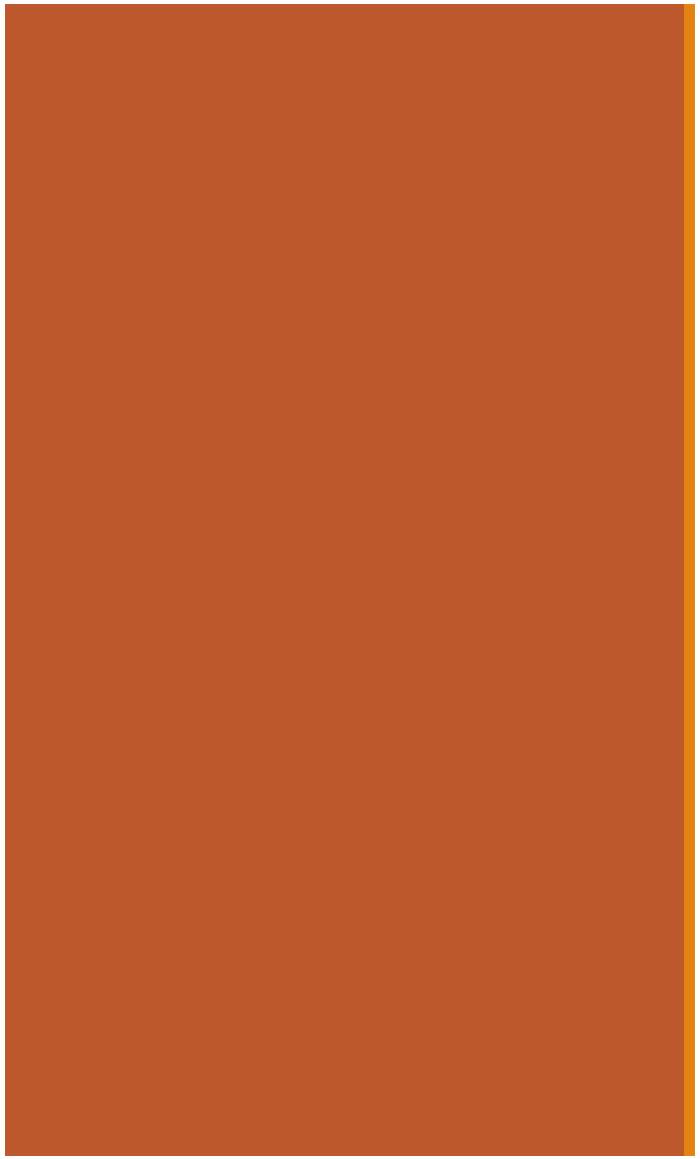
Training

Training data: $(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(n)}, y^{(n)})$

Learn parameters $\theta = (a, b)$

Two approaches:

- Analytical solution via mean squared error
- Iterative solution via MLE and gradient ascent



Linear Regression: MSE

Mean Squared Error (MSE)

For regression tasks, we want to choose a $g(X)$ that minimizes MSE:

$$\theta_{MSE} = \arg\min_{\theta} E\left[\left(Y - \hat{Y}\right)^2\right] = \arg\min_{\theta} E\left[\left(Y - g(X)\right)^2\right]$$

- Y and $\hat{Y} = g(X)$ are both random variables
- Intuitively: Choose parameter θ that minimizes the expected squared deviation ("error") of your prediction $\hat{Y}$ from the true Y

For **linear** regression, where $\hat{Y} = aX + b$ (so that $\theta = (a, b)$):

$$E[(Y - aX - b)^2]$$

Don't make me get non-linear!

$$\theta_{MSE} = \arg\min_{\theta=(a,b)} E[(Y - aX - b)^2]$$

$$a_{MSE} = \rho(X,Y)\frac{\sigma_Y}{\sigma_X}, \quad b_{MSE} = \mu_Y - a_{MSE}\,\mu_X$$

(Derivation included at the end of slides)

Can we compute these statistics for X and Y from our training data?

Training data: $(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(n)}, y^{(n)})$

Technically no, but *we can estimate* them!

Don't make me get non-linear!

$$\theta_{MSE} = \arg\min_{\theta=(a,b)} E[(Y - aX - b)^2]$$

$$a_{MSE} = \rho(X,Y)\frac{\sigma_Y}{\sigma_X}, \qquad b_{MSE} = \mu_Y - a_{MSE}\,\mu_X$$

(Derivation included at the end of slides)

Can we compute these statistics for X and Y from our training data?

Training data: $\left(x^{(1)}, y^{(1)}\right), \left(x^{(2)}, y^{(2)}\right), \ldots, \left(x^{(n)}, y^{(n)}\right)$

Estimate parameters based on observed training data:

$$\hat{a}_{MSE} = \hat{\rho}(X,Y)\frac{S_Y}{S_X}, \qquad \hat{b}_{MSE} = \bar{Y} - \hat{a}_{MSE}\bar{X}$$

$\hat{\rho}(X,Y)$: Sample correlation (Wikipedia)

Linear Regression

Review

Assume linear model (and $\boldsymbol{X}$ is 1-D):

$$\hat{Y} = g(\boldsymbol{X}) = aX + b$$

Training

Training data: $\left(x^{(1)}, y^{(1)}\right), \left(x^{(2)}, y^{(2)}\right), \ldots, \left(x^{(n)}, y^{(n)}\right)$

Learn parameters $\theta = (a, b)$

If we want to minimize the mean squared error of our prediction,

$$\hat{a}_{MSE} = \hat{\rho}(X, Y)\frac{S_Y}{S_X}, \qquad \hat{b}_{MSE} = \bar{Y} - \hat{a}_{MSE}\bar{X}$$

Linear Regression: MLE

Linear Regression

Review

Assume linear model (and $\boldsymbol{X}$ is 1-D, i.e. $\boldsymbol{X} = X$):

$$\hat{Y} = g(\boldsymbol{X}) = aX + b$$

Training

Learn parameters $\theta = (a, b)$

Training data: $\left(x^{(1)}, y^{(1)}\right), \left(x^{(2)}, y^{(2)}\right), \ldots, \left(x^{(n)}, y^{(n)}\right)$

We've seen which parameters—that is, what choices of a and b—minimize mean squared error: a_{MSE} and b_{MSE}, estimated by $\hat{a}_{MSE}$ and $\hat{b}_{MSE}$.

What if we want parameters that maximize the likelihood of the training data?

Note: Maximizing likelihood is typically an objective for classification models.

Likelihood, it's been a minute

Review

Consider a sample of n iid random variables $X_1, X_2, \ldots, X_n$.

- X_i was drawn from some distribution with density function $f(X_i|\theta)$.
- Observed sample: $(X_1, X_2, \ldots, X_n)$

Likelihood question:

How likely is the observed sample $(X_1, X_2, \ldots, X_n)$ given parameter θ?

Likelihood function, $L(\theta)$:

$$L(\theta) = f(X_1, X_2, \ldots, X_n|\theta) = \prod_{i=1}^{n} f(X_i|\theta)$$

This is just a product, since X_i are i.i.d.

Likelihood of the training data

Training data (n datapoints):

- $(x^{(i)}, y^{(i)})$ drawn iid from a distribution $f(X = x^{(i)}, Y = y^{(i)}|\theta) = f(x^{(i)}, y^{(i)}|\theta)$ (shorthand)
- $\hat{Y} = g(X)$, where g is a function on (X) and parameter θ

We can show that θ_{MLE} maximizes the **log conditional likelihood** function:

$$\theta_{MLE} = \arg\max_{\theta} \sum_{i=1}^{n} \log f(y^{(i)} | x^{(i)}, \theta)$$

Linear Regression, MLE

1. Assume linear model (and $\boldsymbol{X}$ is 1-D):

$$\hat{Y} = g(\boldsymbol{X}) = aX + b$$

2. Define maximum likelihood estimator:

$$\theta_{MLE} = \arg\max_{\theta} \sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$$

⚠ Drama: We have a model for $\hat{Y}$, not Y

- Remember the MSE approach, where we minimize the squared **error** between $\hat{Y}$ and Y?
- Here we **model this error** directly!

$$Y = \hat{Y} + Z$$
$$= aX + b + Z$$

error/noise (also random)

Comparison: MSE vs MLE

$$\hat{Y} = g(\boldsymbol{X}) = aX + b$$

Minimum Mean Squared Error

$$\theta_{MSE} = \arg\min_{\theta} E\left[\left(Y - g(X)\right)^2\right]$$

- Don't directly model Y (or any errors)
- Parameters are estimates of statistics from training data:

$$\hat{a}_{MSE} = \hat{\rho}(X, Y)\frac{S_Y}{S_X}$$

$$\hat{b}_{MSE} = \bar{Y} - \hat{a}_{MSE}\bar{X}$$

Maximum Likelihood Estimation

$$\theta_{MLE} = \arg\max_{\theta} \sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$$

- Directly model error between predicted $\hat{Y}$ and Y as an RV Z

$$Y = \hat{Y} + Z = aX + b + Z$$

If we assume error $Z \sim \mathcal{N}(0, \sigma^2)$, then these two estimators are **equivalent.**

$$\theta_{MSE} = \theta_{MLE}!$$

Linear Regression, MLE (next steps)

1. Assume linear model (and $\boldsymbol{X}$ is 1-D):

$$\hat{Y} = g(\boldsymbol{X}) = aX + b$$

2. Define maximum likelihood estimator:

$$\theta_{MLE} = \arg\max_{\theta} \sum_{i=1}^{n} \log f\left(y^{(i)} | \, x^{(i)}, \theta\right)$$

3. Model error, Z:

$$Y = aX + b + Z, \text{ where } Z \sim \mathcal{N}(0, \sigma^2)$$

4. Pick $\theta = (a, b)$ that maximizes likelihood of training data

We won't find a solution analytically. Instead, we'll leverage **gradient ascent**, an **iterative optimization algorithm.**

Gradient Ascent

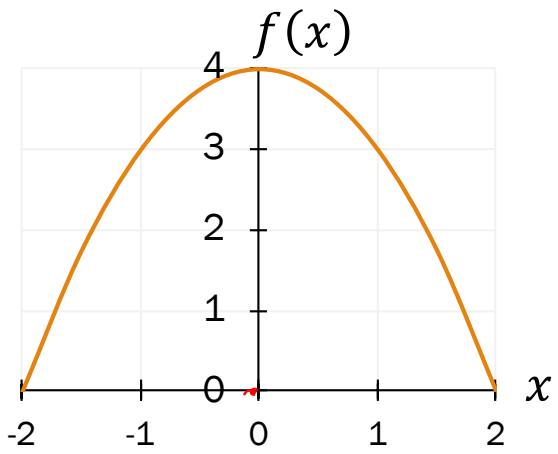
Multiple ways to calculate argmax

Let $f(x) = -x^2 + 4$, where $-2 < x < 2$.

What is $\arg\max_x f(x)$?

objective function

A. Graph and guess

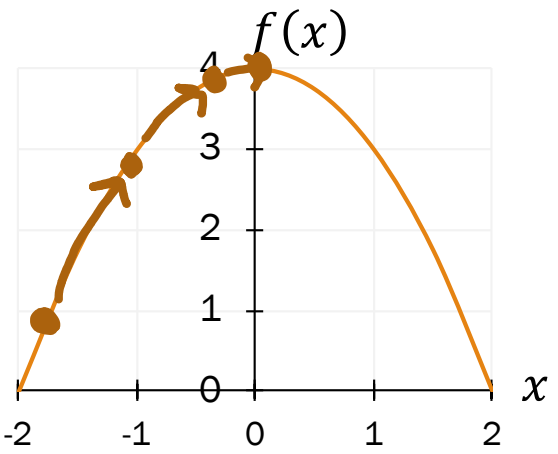


B. Differentiate, set derivative to 0, and solve

$$\frac{df}{dx} = -2x = 0$$

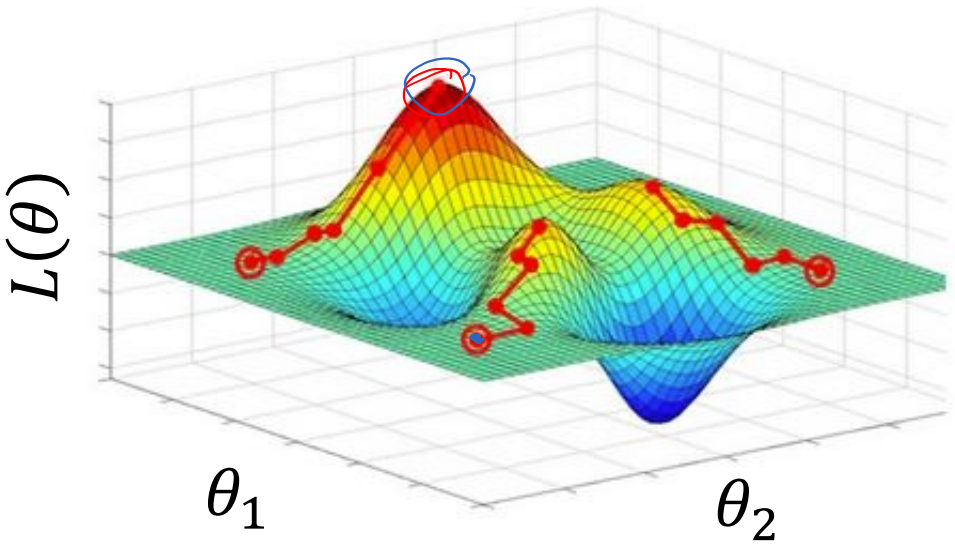
$$x = 0$$

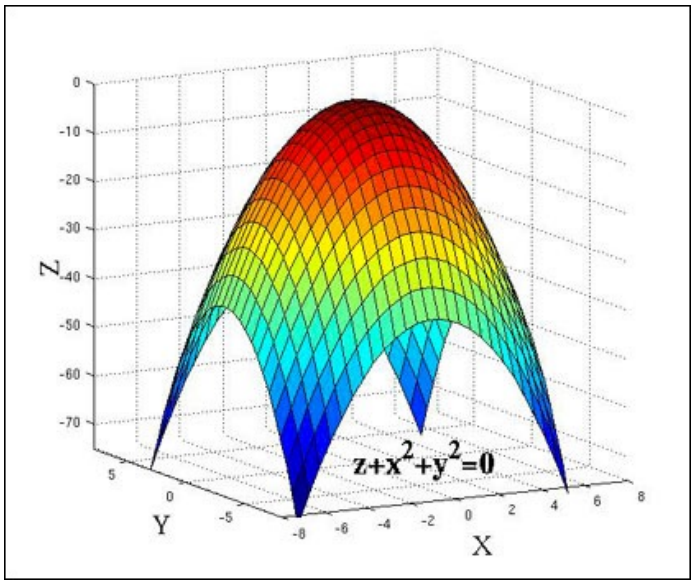
C. Gradient ascent: educated guess & iteratively update



Gradient ascent

Walk uphill and you'll find a local maxima
(if your step is small enough).



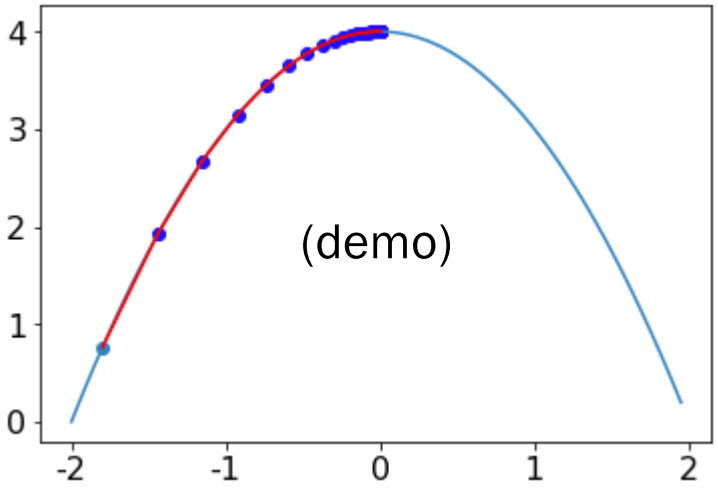


If your function is concave,
Local maxima = global maxima

Gradient ascent algorithm

Walk uphill and you'll find a local maxima
(if your step is small enough).

Let $f(x) = -x^2 + 4$,
where $-2 < x < 2$.



1. $\frac{df}{dx} = -2x$ Gradient at x

2. Gradient ascent algorithm:

```
initialize x
repeat many times:
  compute gradient
  x += η * gradient
```

learning rate

Computing the MLE

Review

General approach for finding $\theta_{MLE} = \arg\max_{\theta} LL(\theta)$:

1. Determine formula for $LL(\theta)$

$$LL(\theta) = \sum_{i=1}^{n} \log f(X_i|\theta)$$

2. Differentiate $LL(\theta)$ w.r.t. (each) θ

$$\frac{\partial LL(\theta)}{\partial \theta}$$

To maximize: $\frac{\partial LL(\theta)}{\partial \theta} = 0$

3. Solve resulting (simultaneous) equations

(algebra or **computer**)

If algebra is intractable or otherwise cumbersome, find a maximum using gradient ascent.

Linear Regression, MLE (so far)

Assume linear model (and $\boldsymbol{X}$ is 1-D):

$$\hat{Y} = g(\boldsymbol{X}) = aX + b$$

Model Y as $\hat{Y} + Z$:

$$Y = aX + b + Z, \text{ where } Z \sim \mathcal{N}(0, \sigma^2)$$

Pick $\theta = (a, b)$ that maximizes likelihood of training data

$$\theta_{MLE} = \arg\max_{\theta} LL(\theta)$$

$$= \arg\max_{\theta} \sum_{i=1}^{n} \log f\left(x^{(i)}, y^{(i)}, |\theta\right)$$

(θ_{MLE} also maximizes log conditional likelihood)

$$= \arg\max_{\theta} \sum_{i=1}^{n} \log f\left(y^{(i)} | \, x^{(i)}, \theta\right)$$

Computing the MLE with gradient ascent

General approach for finding θ_{MLE} , the MLE of θ:

1. Determine formula for $LL(\theta)$

   log conditional likelihood

   $$\sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$$

2. Differentiate $LL(\theta)$ w.r.t. (each) θ

   $$\frac{\partial}{\partial \theta_j} \sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$$

3. Solve resulting equations

   (computer) Gradient Ascent

1. Determine formula for log conditional likelihood

Model: $\theta = (a, b)$

$Y = aX + b + Z$

$Z \sim \mathcal{N}(0, \sigma^2)$

$\hat{Y} = aX + b$

Optimization problem: $\arg\max_{\theta} \sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$

Over the next few slides, we will show that our MLE linear regression θ_{MLE} reduces to

$$\arg\max_{\theta} \left[-\sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b\right)^2 \right]$$

objective function

1. Determine formula for log conditional likelihood

Model: $\theta = (a, b)$
$Y = aX + b + Z$
$Z \sim \mathcal{N}(0, \sigma^2)$

Optimization problem: $\arg\max_{\theta} \sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$

goal $\arg\max_{\theta} \left[-\sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b\right)^2 \right]$

1. What is the conditional distribution, $Y|X, \theta$?

2. Substitute 1. into objective fn.

3. Use argmax properties to simplify objective fn.

1. Determine formula for log conditional likelihood

Model: $\theta = (a, b)$
$Y = aX + b + Z$
$Z \sim \mathcal{N}(0, \sigma^2)$

Optimization problem: $\arg\max_{\theta} \sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$

1. What is the conditional distribution, $Y|X, \theta$?

$$Y|X, \theta \sim \mathcal{N}(aX + b, \sigma^2)$$

$$f\left(y^{(i)} | x^{(i)}, \theta\right) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\left(y^{(i)} - (ax^{(i)} + b)\right)^2 / (2\sigma^2)}$$

2. Substitute 1. into objective fn.

$$\arg\max_{\theta} \sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right) = \arg\max_{\theta} \sum_{i=1}^{n} \log \left[\frac{1}{\sqrt{2\pi}\sigma} e^{-\left(y^{(i)} - ax^{(i)} - b\right)^2 / (2\sigma^2)}\right]$$

using natural log

$$= \arg\max_{\theta} \left[\sum_{i=1}^{n} -\log\sqrt{2\pi}\sigma - \frac{1}{2\sigma^2} \sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b\right)^2\right]$$

1. Determine formula for log conditional likelihood

Model: $\theta = (a, b)$
$Y = aX + b + Z$
$Z \sim \mathcal{N}(0, \sigma^2)$

Optimization problem: $\arg\max_{\theta} \sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$

3. Use argmax properties to simplify objective fn.

$$\arg\max_{\theta} \left[\sum_{i=1}^{n} -\log\sqrt{2\pi}\sigma - \frac{1}{2\sigma^2} \sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b\right)^2 \right]$$

(from previous slide)

$$= \arg\max_{\theta} \left[-\frac{1}{2\sigma^2} \sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b\right)^2 \right]$$

Argmax refresher #1:
Invariant to additive constants

$$= \arg\max_{\theta} \left[-\sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b\right)^2 \right]$$

Argmax refresher #2:
Invariant to positive constant scalars

1. Determine formula for log conditional likelihood

Model: $\theta = (a, b)$
$Y = aX + b + Z$
$Z \sim \mathcal{N}(0, \sigma^2)$

Optimization problem: $\arg\max_{\theta} \sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$

4. Celebrate!

$$\arg\max_{\theta} \left[-\sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b\right)^2 \right]$$

Computing the MLE with gradient ascent

General approach for finding θ_{MLE} , the MLE of θ:

1. Determine formula for $LL(\theta)$

   log conditional likelihood

$$\sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$$

$$h(\theta) = -\sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b\right)^2$$

2. Differentiate $LL(\theta)$ w.r.t. (each) θ

$$\frac{\partial}{\partial \theta_j} \sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$$

2-D gradient:

$$\left(\frac{\partial h(\theta)}{\partial a}, \frac{\partial h(\theta)}{\partial b}\right)$$

3. Solve resulting (simultaneous) equations

(computer) Gradient Ascent

2. Compute gradient

Model: $\theta = (a, b)$

$Y = aX + b + Z$

$Z \sim \mathcal{N}(0, \sigma^2)$

Optimization problem: $\arg\max_{\theta} \left[-\sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b \right)^2 \right]$

$\frac{\partial}{\partial a}\left(y^{(i)} - ax^{(i)} - b\right)^2$ ←x

1. What is the derivative of the objective function w.r.t. a?

$$\frac{\partial}{\partial a}\left[-\sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b \right)^2 \right] =$$

2. What is the derivative of the objective function w.r.t. b?

Calculus refresher #1:
Derivative(sum) = sum(derivative)

Calculus refresher #2:
Chain rule ⭐ ⭐ ⭐

2. Compute gradient

Model: $\theta = (a, b)$
$Y = aX + b + Z$
$Z \sim \mathcal{N}(0, \sigma^2)$

Optimization problem: $\arg\max_{\theta} \left[-\sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b \right)^2 \right]$

1. What is the derivative of the objective function w.r.t. a?

$$\frac{\partial}{\partial a} \left[-\sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b \right)^2 \right] =$$

Calculus refresher #1:
Derivative(sum) = sum(derivative)

Calculus refresher #2:
Chain rule 🌟 🌟 🌟

2. Compute gradient

Model: $\theta = (a, b)$
$Y = aX + b + Z$
$Z \sim \mathcal{N}(0, \sigma^2)$

Optimization problem: $\arg\max_{\theta} \left[-\sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b \right)^2 \right]$

1. What is the derivative of the objective function w.r.t. a?

$$\sum_{i=1}^{n} 2\left(y^{(i)} - ax^{(i)} - b \right)\left(x^{(i)} \right)$$

2. What is the derivative of the objective function w.r.t. b?

$$\sum_{i=1}^{n} 2\left(y^{(i)} - ax^{(i)} - b \right)$$

analytical solution for a_{MLE}, b_{MLE}: Set to 0 and solve simultaneous equations

Next up: We will reach the same solution **computationally** with **gradient ascent.**

Computing the MLE with gradient ascent

General approach for finding θ_{MLE} , the MLE of θ:

1. Determine formula for $LL(\theta)$

   log conditional likelihood

$$\sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$$

$$h(\theta) = -\sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b\right)^2$$

2. Differentiate $LL(\theta)$ w.r.t. (each) θ

$$\frac{\partial}{\partial \theta_j} \sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$$

$$\frac{\partial h(\theta)}{\partial a} = \sum_{i=1}^{n} 2\left(y^{(i)} - ax^{(i)} - b\right)\left(x^{(i)}\right)$$

$$\frac{\partial h(\theta)}{\partial b} = \sum_{i=1}^{n} 2\left(y^{(i)} - ax^{(i)} - b\right)$$

3. Solve resulting (simultaneous) equations

   (computer) Gradient Ascent

3. Gradient ascent with multiple parameters (if time)

Optimization problem:

$$\arg\max_{\theta}\left[-\sum_{i=1}^{n}\left(y^{(i)}-ax^{(i)}-b\right)^2\right]$$

$$=\arg\max_{\theta} h(\theta)$$

Gradient:

$$\frac{\partial h(\theta)}{\partial a}=\sum_{i=1}^{n}2\left(y^{(i)}-ax^{(i)}-b\right)\left(x^{(i)}\right)$$

$$\frac{\partial h(\theta)}{\partial b}=\sum_{i=1}^{n}2\left(y^{(i)}-ax^{(i)}-b\right)$$

```
initialize θ
repeat many times:
  compute gradient
  θ += η * gradient
```

step size / learning rate

How does this work for multiple parameters?

3. Gradient ascent with multiple parameters

Optimization problem:

$$\arg\max_{\theta}\left[-\sum_{i=1}^{n}\left(y^{(i)}-ax^{(i)}-b\right)^2\right]$$

$$=\arg\max_{\theta} h(\theta)$$

Gradient:

$$\frac{\partial h(\theta)}{\partial a}=\sum_{i=1}^{n}2\left(y^{(i)}-ax^{(i)}-b\right)\left(x^{(i)}\right)$$

$$\frac{\partial h(\theta)}{\partial b}=\sum_{i=1}^{n}2\left(y^{(i)}-ax^{(i)}-b\right)$$

```
a, b = 0, 0                          # initialize θ
repeat many times:
    gradient_a, gradient_b = 0, 0
    # TODO: fill in

    a += η * gradient_a              # θ += η * gradient
    b += η * gradient_b
```

How do we pseudocode the gradients we derived?

3. Gradient ascent with multiple parameters

Optimization problem: $\arg\max_\theta \left[-\sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b\right)^2 \right]$

$= \arg\max_\theta h(\theta)$

Gradient: $\frac{\partial h(\theta)}{\partial a} = \sum_{i=1}^{n} 2\left(y^{(i)} - ax^{(i)} - b\right)\left(x^{(i)}\right)$

$\frac{\partial h(\theta)}{\partial b} = \sum_{i=1}^{n} 2\left(y^{(i)} - ax^{(i)} - b\right)$

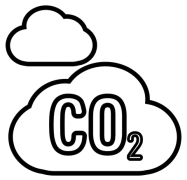
```
a, b = 0, 0                    # initialize θ
repeat many times:
  gradient_a, gradient_b = 0, 0
  for each training example (x, y):
    diff = y - (a * x + b)
    gradient_a += 2 * diff * x
    gradient_b += 2 * diff
  a += η * gradient_a          # θ += η * gradient
  b += η * gradient_b
```

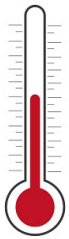
Finish computing gradient before updating any part of θ.

(Spring 2022 demo)

Global land-ocean temperature prediction

Training data: $(\boldsymbol{x}^{(1)}, y^{(1)}), (\boldsymbol{x}^{(2)}, y^{(2)}), \ldots, (\boldsymbol{x}^{(n)}, y^{(n)})$





	CO2 levels	Output
Year 1	338.8	0.26
Year 2	340.0	0.32
...		⋮
Year n	340.76	0.14

$\boldsymbol{X} = (X_1)$
(assume one feature)

$Y \in \mathbb{R}$

Review

Minimizing Mean Square Error

$$\theta_{MSE} = \arg\min_{\theta} E\left[\left(Y - g(X)\right)^2\right]$$

$$\hat{Y} = \hat{\rho}(X, Y)\frac{S_Y}{S_X}(X - \bar{X}) + \bar{Y}$$

$$a_{MSE} = 0.01452$$

$$b_{MSE} = 0.17511$$

3b. Interpret

Optimization problem:

$$\arg\max_{\theta}\left[-\sum_{i=1}^{n}\left(y^{(i)}-ax^{(i)}-b\right)^2\right]$$

$$=\arg\max_{\theta} h(\theta)$$

Gradient:

$$\frac{\partial h(\theta)}{\partial a}=\sum_{i=1}^{n}2\left(y^{(i)}-ax^{(i)}-b\right)\left(x^{(i)}\right)$$

$$\frac{\partial h(\theta)}{\partial b}=\sum_{i=1}^{n}2\left(y^{(i)}-ax^{(i)}-b\right)$$

```
a, b = 0, 0                    # initialize θ
repeat many times:
  gradient_a, gradient_b = 0, 0
  for each training example (x, y):
    diff = y - (a * x + b)
    gradient_a += 2 * diff * x
    gradient_b += 2 * diff
  a += η * gradient_a          # θ += η * gradient
  b += η * gradient_b
```

Updates to a and b should include information from all n training datapoints

3b. Interpret

Optimization problem:

$$\arg\max_{\theta}\left[-\sum_{i=1}^{n}\left(y^{(i)}-ax^{(i)}-b\right)^2\right]$$

$$=\arg\max_{\theta} h(\theta)$$

Gradient:

$$\frac{\partial h(\theta)}{\partial a}=\sum_{i=1}^{n}2\left(y^{(i)}-ax^{(i)}-b\right)\left(x^{(i)}\right)$$

$$\frac{\partial h(\theta)}{\partial b}=\sum_{i=1}^{n}2\left(y^{(i)}-ax^{(i)}-b\right)$$

```
a, b = 0, 0                    # initialize θ
repeat many times:
    gradient_a, gradient_b = 0, 0
    for each training example (x, y):
        diff = y - (a * x + b)
        gradient_a += 2 * diff * x
        gradient_b += 2 * diff
    a += η * gradient_a        # θ += η * gradient
    b += η * gradient_b
```

How do we interpret the contribution of the i-th training datapoint?

3b. Interpret

Optimization problem: $\arg\max_{\theta} \left[-\sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b \right)^2 \right]$

$= \arg\max_{\theta} h(\theta)$

Gradient: $\frac{\partial h(\theta)}{\partial a} = \sum_{i=1}^{n} 2\left(y^{(i)} - ax^{(i)} - b \right)\left(x^{(i)} \right)$

$\frac{\partial h(\theta)}{\partial b} = \sum_{i=1}^{n} 2\left(y^{(i)} - ax^{(i)} - b \right)$

```
a, b = 0, 0                    # initialize θ
repeat many times:
  gradient_a, gradient_b = 0, 0
  for each training example (x, y):
    diff = y - (a * x + b)
    gradient_a += 2 * diff * x
    gradient_b += 2 * diff
  a += η * gradient_a          # θ += η * gradient
  b += η * gradient_b
```

Prediction error!

$y^{(i)} - \hat{y}^{(i)}$

3b. Interpret

Optimization problem:

$$\arg\max_{\theta}\left[-\sum_{i=1}^{n}\left(y^{(i)}-ax^{(i)}-b\right)^2\right]$$

$$=\arg\max_{\theta} h(\theta)$$

Gradient:

$$\frac{\partial h(\theta)}{\partial a}=\sum_{i=1}^{n}2\left(y^{(i)}-ax^{(i)}-b\right)\left(x^{(i)}\right)$$

$$\frac{\partial h(\theta)}{\partial b}=\sum_{i=1}^{n}2\left(y^{(i)}-ax^{(i)}-b\right)$$

```
a, b = 0, 0                    # initialize θ
repeat many times:
  gradient_a, gradient_b = 0, 0
  for each training example (x, y):
    prediction_error = y − (a * x + b)
    gradient_a += 2 * prediction_error * x
    gradient_b += 2 * prediction_error
  a += η * gradient_a          # θ += η * gradient
  b += η * gradient_b
```

3b. Interpret

Optimization problem: $\arg\max_\theta \left[-\sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b\right)^2 \right]$

$= \arg\max_\theta h(\theta)$

Gradient: $\frac{\partial h(\theta)}{\partial a} = \sum_{i=1}^{n} 2\left(y^{(i)} - ax^{(i)} - b\right)\left(x^{(i)}\right)$

$\frac{\partial h(\theta)}{\partial b} = \sum_{i=1}^{n} 2\left(y^{(i)} - ax^{(i)} - b\right)$

```
a, b = 0, 0                          # initialize θ
repeat many times:
  gradient_a, gradient_b = 0, 0
  for each training example (x, y):
    prediction_error = y - (a * x + b)
    gradient_a += 2 * prediction_error * x
    gradient_b += 2 * prediction_error
  a += η * gradient_a                # θ += η * gradient
  b += η * gradient_b
```

$\hat{Y} = aX + b$, so update to a should also scale by $x^{(i)}$

3b. Interpret

Optimization problem: $\arg\max_\theta \left[-\sum_{i=1}^{n} \left(y^{(i)} - ax^{(i)} - b\right)^2 \right]$

$= \arg\max_\theta h(\theta)$

Gradient: $\frac{\partial h(\theta)}{\partial a} = \sum_{i=1}^{n} 2\left(y^{(i)} - ax^{(i)} - b\right)\left(x^{(i)}\right)$

$\frac{\partial h(\theta)}{\partial b} = \sum_{i=1}^{n} 2\left(y^{(i)} - ax^{(i)} - b\right)$

```
a, b = 0, 0                    # initialize θ
repeat many times:
  gradient_a, gradient_b = 0, 0
  for each training example (x, y):
    prediction_error = y − (a ∗ x + b)
    gradient_a += 2 ∗ prediction_error ∗ x
    gradient_b += 2 ∗ prediction_error ∗ 1
  a += η ∗ gradient_a          # θ += η ∗ gradient
  b += η ∗ gradient_b
```

$\hat{Y} = aX + b$, so update to b just scales by 1, not $x^{(i)}$

Reflecting on today

We did a lot today!

- Learned gradient ascent
- Modeled likelihood of training dataset
- Thanked argmax for its convenience
- Remembered calculus
- Implemented gradient ascent with multiple parameters to optimize for

Next up, we will use all these skills and more to tackle the final prediction model of CS109:

Logistic Regression

Extra: Derivations

Don't make me get non-linear!

$$\theta_{MSE} = \arg\min_{\theta=(a,b)} E[(Y - aX - b)^2]$$

1. Differentiate w.r.t. (each) θ, set to 0

$$\frac{\partial}{\partial a} E[(Y - aX - b)^2] = E\left[\frac{\partial}{\partial a}(Y - aX - b)^2\right]$$
$$= E[-2(Y - aX - b)X]$$
$$= -2E[XY] + 2aE[X^2] + 2bE[X]$$

($E[\cdot]$ is a linear function w.r.t. a)

$$\frac{\partial}{\partial b} E[(Y - aX - b)^2] = E[-2(Y - aX - b)]$$
$$= -2E[Y] + 2aE[X] + 2b$$

2. Solve resulting simultaneous equations

$$a_{MSE} = \frac{E[XY] - E[X]E[Y]}{E[X^2] - (E[X])^2} = \frac{\text{Cov}(X,Y)}{\text{Var}(X)} = \rho(X,Y)\frac{\sigma_Y}{\sigma_X}$$

$$b_{MSE} = E[Y] - a_{MSE}E[X] = \mu_Y - \rho(X,Y)\frac{\sigma_Y}{\sigma_X}\mu_X$$

Log conditional likelihood, a derivation

$\hat{Y} = g(X)$, where $g(\cdot)$ is a function with parameter θ

Show that θ_{MLE} maximizes the **log conditional likelihood** function:

$$\theta_{MLE} = \arg\max_{\theta} \sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$$

Proof:

$$\theta_{MLE} = \arg\max_{\theta} \prod_{i=1}^{n} f\left(x^{(i)}, y^{(i)} | \theta\right) = \arg\max_{\theta} \sum_{i=1}^{n} \log f\left(x^{(i)}, y^{(i)} | \theta\right)$$

(θ_{MLE} also maximizes $LL(\theta)$)

$f(x, y|\theta) = f(x|\theta) f(y|x, \theta)$

$$= \arg\max_{\theta} \sum_{i=1}^{n} \log f\left(x^{(i)} | \theta\right) + \sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$$

(chain rule, log of product = sum of logs)

$$= \arg\max_{\theta} \sum_{i=1}^{n} \log f\left(x^{(i)}\right) + \sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$$

($x^{(i)}$ indep. of θ)

$$= \arg\max_{\theta} \sum_{i=1}^{n} \log f\left(y^{(i)} | x^{(i)}, \theta\right)$$

($f\left(x^{(i)}\right)$ constant w.r.t. θ)