Data, Environment and Society:
Lecture 13: Gradient Descent

* a bit of EJ?

Instructor: Duncan Callaway
GSI: Seigi Karasaki

October 4, 2018

Announcements

Today

- Gradient descent
- Environmental Justice

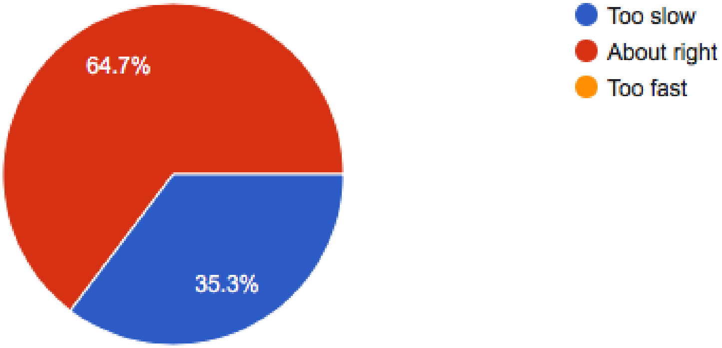
Reading

- Today: Ch 11 DS100
- Next *thursday:* Clark *et al* (using LUR data for EJ questions)

Survey results

Lecture pace is

17 responses



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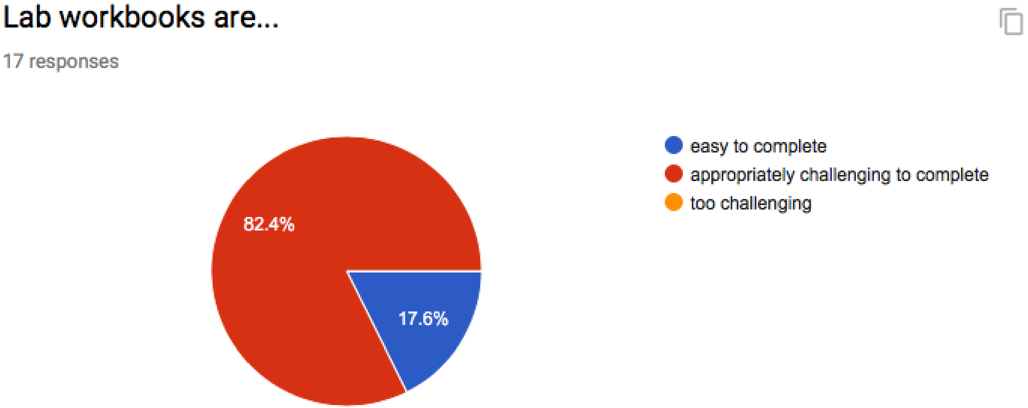

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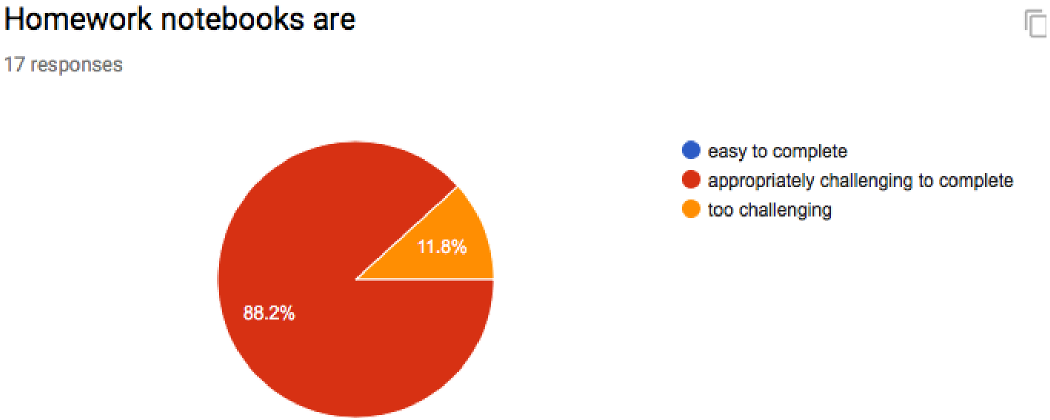

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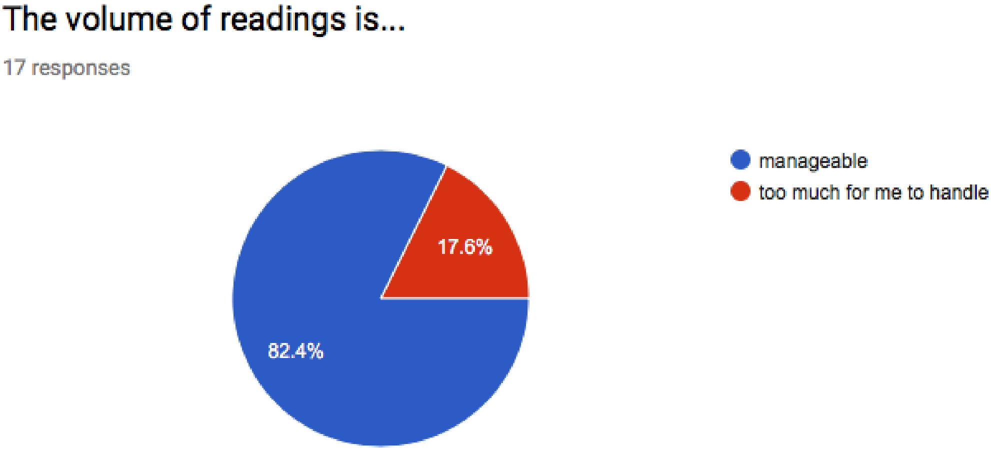

Survey results: A few key takeaways

- Students asked for more time for discussion and interaction
- A few students suggested I assume background reading is done...
- Request for more board work
- Requests for more energy-enviro applications
- Students are struggling to find a way to take notes
- Grading rubric, more clarity on questions in HW and Labs
- Lots of positive feedback for Seigi

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- Lots of positive feedback for Seigi
  - Your GSI rocks!

Basic estimation process, so far

1. Define a loss function
2. Set derivatives of loss function equal to zero and solve for parameters

The challenge:

- Setting loss function derivatives to zero not always easy.
- This doesn't scale well for big problems (e.g. many different nonlinear transformations of the Novotny data)

The loss function

Mean squared error, aka the 'L2' norm

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

constant model $\Rightarrow \quad \hat{y}_i = \theta \quad \Rightarrow \quad MSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \theta)^2$

Mean absolute error, aka the 'L1' norm

$$MAE = \frac{1}{n} \sum_{i=1}^{n} | y_i - \theta |$$

The loss function

Mean squared error, aka the ‘L2’ norm

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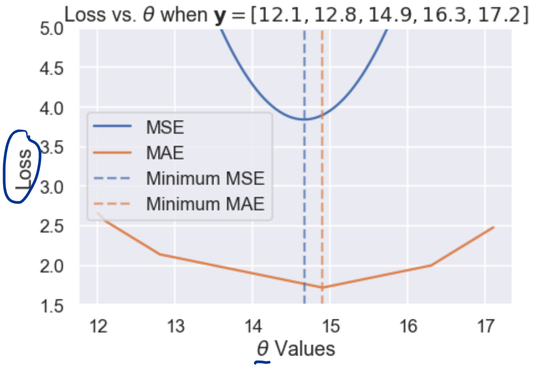
$$\text{Constant model,} \hat{y} = \theta \rightarrow \text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \theta)^2$$

Mean absolute error, aka the ‘L1’ norm

$$\begin{aligned}\text{MAE} &= \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| \\ &= \frac{1}{n}\sum_{i=1}^{n}|y_i - \theta|\end{aligned}$$

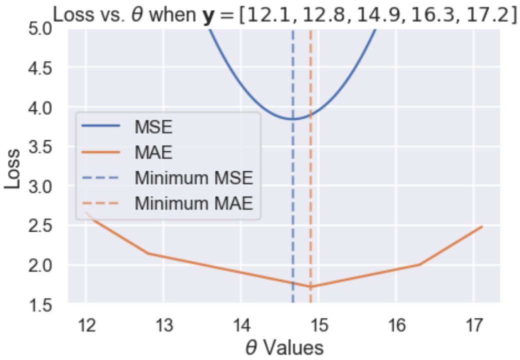
Advantages and disadvantages to MAE and MSE?



← data set

MSE : Continuously dif'able

Advantages and disadvantages to MAE and MSE?



- MSE is differentiable $\rightarrow$ can solve directly for coefficients
- MAE is less impacted by extreme values

Aside: what do these cost functions provide with the "constant" model?

What well-known values minimize these loss functions?

$$\theta^*_{\text{MSE}} = \arg\min_\theta \frac{1}{n}\sum_{i=1}^{n}(y_i - \theta)^2$$

$$\theta^*_{\text{MAE}} = \arg\min_\theta \frac{1}{n}\sum_{i=1}^{n}|y_i - \theta|$$

$$\rightarrow \frac{\partial}{\partial\theta}\frac{1}{n}\sum(y_i-\theta)^2 = 0$$

$$\frac{1}{n}2(y_i-\theta)\frac{\partial(-\theta)}{\partial\theta} = 0$$

$$-\frac{2}{n}\sum(y_i-\theta) = 0$$

$$-\frac{2}{n}\left[\sum_{i=1}^{n}y_i - \sum_{i=1}^{n}\theta\right] = 0$$

$$\sum_{i=1}^{n}y_i = \sum_{i=1}^{n}\theta$$

$$\sum_{i=1}^{n}y_i = n\theta$$

$$\Rightarrow \theta = \frac{1}{n}\sum_{i=1}^{n}y_i$$

$\Rightarrow$ Mean!

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$$\theta^*_{\text{MAE}} = \arg\min_{\theta} \frac{1}{n}\sum_{i=1}^{n}|y_i - \theta|$$

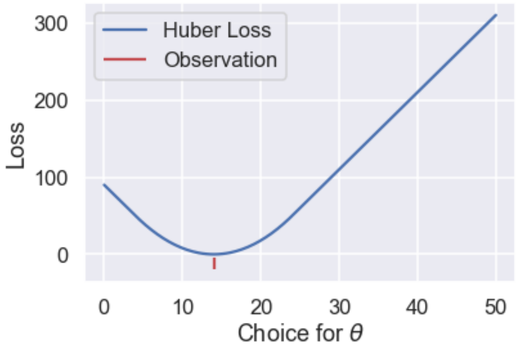
- MSE returns the mean value of a sequence
- MAE returns the *median*

Huber loss

What does this buy us?

$$L_\delta(\theta, \mathbf{y}) = \frac{1}{n}\sum_{i=1}^{n} \begin{cases} \frac{1}{2}(y_i - \theta)^2 & |y_i - \theta| \le \delta \\ \delta(|y_i - \theta| - \frac{1}{2}\delta) & \text{otherwise} \end{cases}$$

Huber loss



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- Differentiable
- Absolute value at extremes – not dominated by outlier.

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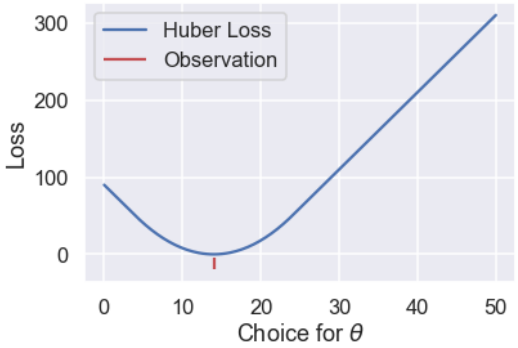

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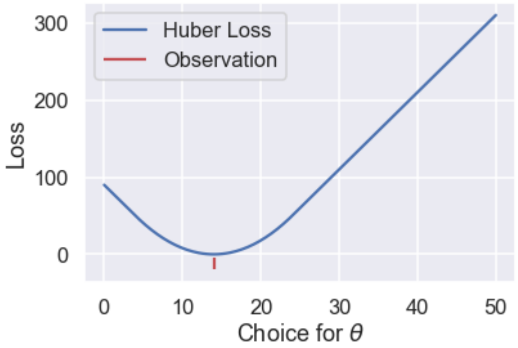

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What does this cost us?

- Optimal solution requires derivative w.r.t. θ *and* derivative w.r.t. δ equal zero.
- That can be tricky.

Estimation takeaway # 1:

Analytical solutions for parameters (e.g. by setting partial derivatives equal to zero) not always available for some of the types of loss functions we'd like to use.

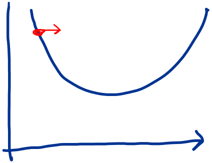
Estimation takeaway # 2:

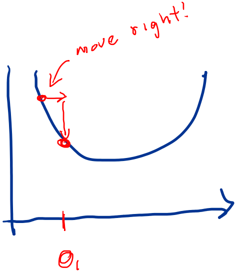
A separate issue: In situations where the normal equations (or something like them) can be used to solve for parameters:

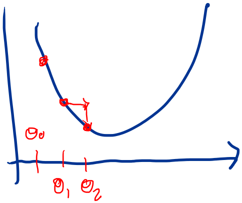
$$\Theta = (X^T X)^{-1} X^T Y$$

It can be very difficult computationally to invert a large $X^T X$ (I crashed my computer with 50,000 by 50,000).

Gradient descent – sketch

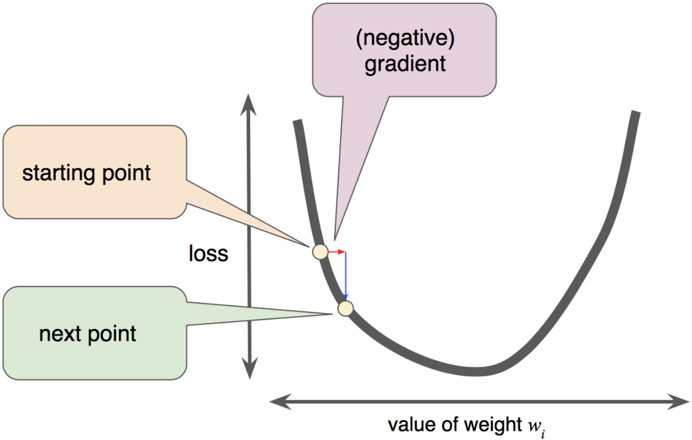






How big should the move be?

Gradient descent – sketch



https://developers.google.com/machine-learning/crash-course/reducing-loss/gradient-descent

Gradient descent – math

What's the gradient? For our purposes, it is the slope of the loss function at a given point *with respect to a particular parameter.*

The gradient is $\nabla_\theta L(\theta, \mathbf{y}) =$ $\frac{\partial}{\partial \theta} L(\theta, y)$

Gradient descent process:

1. Choose a value for the "learning rate", α
2. Choose a starting value of θ (0 is a common choice).
3. Compute $\theta - \alpha \cdot \frac{\partial}{\partial \theta} L(\theta, \mathbf{y})$ and store this as the new value of θ.
4. Repeat until θ doesn't change (much) between iterations.

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Gradient descent for quadratic loss

Let's derive the gradient:

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$$L = \sum_{i=1}^{n} (y_i - \theta)^2$$

$$\frac{\partial L}{\partial \theta} = -2 \sum_{i=1}^{n} (y_i - \theta)$$

...and then write a few iterations:

$$\theta_0 = 0$$

$$\theta_1 = \theta_0 - \alpha \left(-2 \sum_{i=1}^{n} (y_i - \theta_0)\right)$$

$$\theta_2 = \theta_1 - \alpha \left(-2 \sum_{i=1}^{n} (y_i - \theta_1)\right)$$

$$\vdots$$

$$\theta_{t+1} = \theta_t - \alpha \left(-2 \sum (y_i - \theta_t)\right)$$

$$|\theta_{t+1} - \theta_t| < \text{tolerance}$$

$\Rightarrow$ stop!

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$$\vdots$$

$$\theta_{t+1} = \theta_t - \alpha\left(-2 \sum_{i=1}^{n} (y_i - \theta_t)\right)$$

Stop when $|\theta_{t+1} - \theta_t| < \text{tol}$, where "tol" is a small tolerance parameter.

Gradient descent, in code

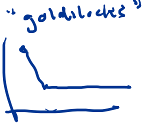
```
def minimize(loss_fn, grad_loss_fn, dataset, alpha=0.2, progress=True):
    '''
    Uses gradient descent to minimize loss_fn. Returns the minimizing value of
    theta_hat once theta_hat changes less than 0.001 between iterations.
    '''
    theta = 0
    while True:
        if progress:
            print(f'theta: {theta:.2f} | loss: {loss_fn(theta, dataset):.2f}')
        gradient = grad_loss_fn(theta, dataset)
        new_theta = theta - alpha * gradient

        if abs(new_theta - theta) < 0.001:
            return new_theta

        theta = new_theta
```

https://www.textbook.ds100.org/ch/11/gradient_descent_define.html

Gradient descent – what does the learning rate do?



Get in small groups and play with this Google tool: https://goo.gl/JNPhUv.

Set α to a higher value than the default – it'll take forever at $\alpha = 0.01$.

Questions to answer together: How does the rate change on each iteration...

1. ...when the learning rate is really small?
2. ...when the learning rate is really big?

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There are four qualitatively different behaviors:

1. Monotonically decreasing loss
2. One step to optimal parameter
3. Loss declines in periodic oscillations
4. Loss grows out of control

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Basic idea: Start with a big learning rate, then make it smaller and smaller as you approach the optimal value

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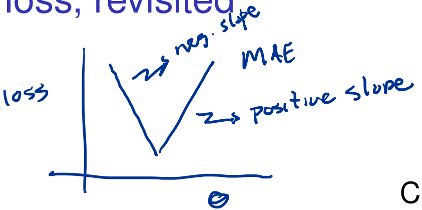
Basic idea: Start with a big learning rate, then make it smaller and smaller as you approach the optimal value

Advantages:

- cover a lot of ground when you’re far from the optimal value
- refined steps when you get close, so you don’t miss the optimal value.

Absolute deviation loss, revisited



$$L = \frac{1}{n}\sum_{i=1}^{n} |y_i - \theta|$$

$$= \frac{1}{n}\left(\sum_{y_i<\theta} |y_i - \theta| + \sum_{y_i=\theta} |y_i - \theta| + \sum_{y_i>\theta} |y_i - \theta|\right)$$

$$\frac{\partial L}{\partial \theta} = \frac{1}{n}\left(\sum_{y_i<\theta}(-1) + \sum_{y_i=\theta}(0) + \sum_{y_i>\theta}(1)\right)$$

Can you see why the optimal value is the median?

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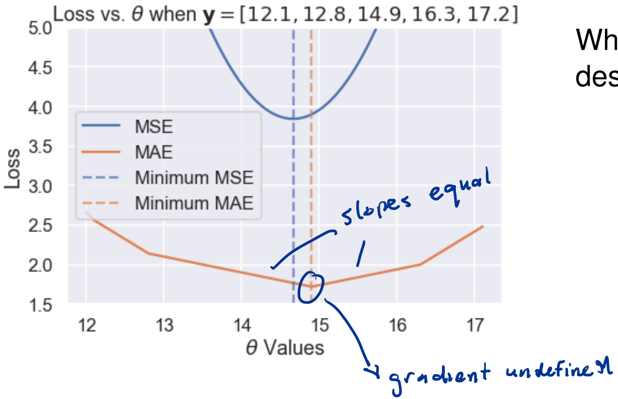
The right solution just “counts” the number of observations on each side of the optimal value

Gradient descent – absolute deviation loss, ctd.



What's the problem with doing gradient descent here?

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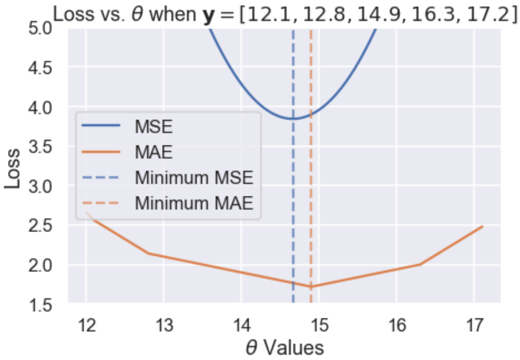

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So once the solution is close, it won't converge, unless...

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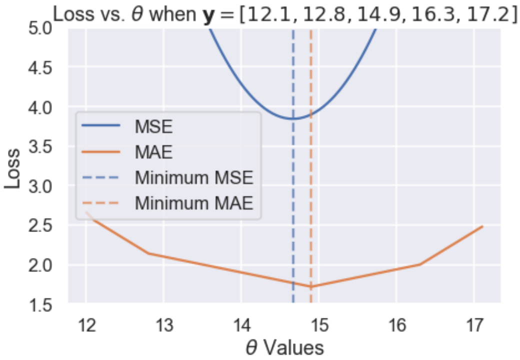

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