COMP 543: Tools & Models for Data Science

Optimization–Gradient Descent

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Optimization

- At the heart of all “learning” frameworks discussed
  - Is optimization!
- Why?
  - Well, it’s explicit in case of loss functions, MLE
  - Implicitly in case of Bayesian
- Means we need to ask: how to solve optimization problems?
  - Fundamental question in data science!!

Desired Properties

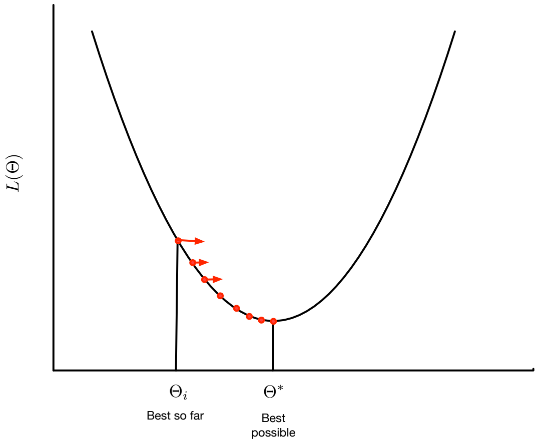
- To be useful for data science, an optimization framework should be
  - Easily applied to many types of optimization problems
  - Scalable (easily built in Spark, for example)
  - Fast (quick convergence)

Most Widely Used Optimization Framework Is...

- For (big) data science, at least...
  - Gradient descent!
- What's the idea?
  - GD is an iterative algorithm
  - Goal: choose Θ^* to minimize/maximize the Loss function $L(\Theta)$
  - Tries to incrementally improve current solution
  - At step i, Θ_i is current guess for Θ^*

Gradient Descent Intuition

- Look at the slope of L
- Go in the direction of steepest descent
- Don't go too far!
- Stop when your parameter values aren't changing much
- Can end up oscillating if your step size is too big



Gradient Descent

- Basic algorithm:

$\Theta_1 \leftarrow$ non-stupid guess for Θ^*;
$i \leftarrow 1$;
repeat {
  $\Theta_{i+1} \leftarrow \Theta_i - \lambda \nabla L(\Theta_i)$;
  $i \leftarrow i+1$;
} while $(||\Theta_i - \Theta_{i-1}||_1 > \varepsilon)$

- $\lambda \nabla L(\Theta_i)$ is some distance along the direction of steepest descent
- $||\Theta_i - \Theta_{i-1}||_1$ is the absolute value of the change in parameter value(s)

Gradient Descent

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  - λ is the "learning rate"
    - how far you go a each step in the direction of steepest descent
    - Controls speed of convergence
    - If too big, algorithm will oscillate
    - If too small, algorithm will take a very long time to run
  - $\nabla L(\Theta_i)$ is the gradient of L evaluated at Θ_i

Stopping Condition

- Here we use

`while` $(||\Theta_i - \Theta_{i-1}||_1 > \varepsilon)$

  - Easy to compute
  - Efficient because it just requires checking for small changes in **model**
  - Serves as a proxy for the change in the **loss function**
  - But does not always make sense (big change in model can mean small change in accuracy)

Stopping Condition

- If feasible, instead use

`while` $(|L(\Theta_i) - L(\Theta_{i-1})| > \varepsilon)$

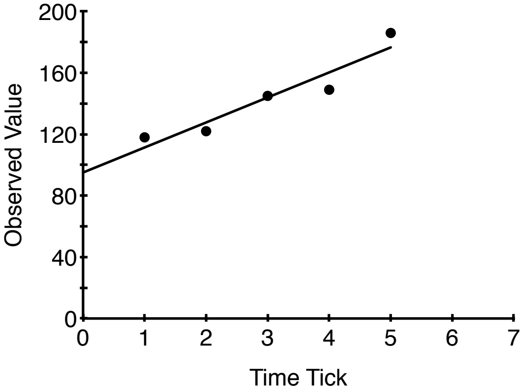
- Drawback: requires loss computation... can be expensive
- Can be more expensive than another iteration
- Alternative: Stochastic Gradient Descent or Minibatch
  - Use a small sample of the dataset
  - Note: the parameters (Θ) will never stop changing, due to different data points used each time
  - Much more difficult to decide when to stop

A Gradient

- What's a "gradient"?
- Gradient is the multi-dimensional analog to a derivative
  - If $L(.)$ accepts a vector
  - ∇L is a vector-valued function
    - That is, accepts a vector Θ
    - Returns a vector, Θ'
    - whose ith entry is ith partial derivative evaluated at Θ

Example

- Returning to linear regression...
  - Want a line to fit points $\langle 118, 122, 145, 149, 186 \rangle$
  - At time ticks t in $\langle 1, 2, 3, 4, 5 \rangle$
  - Prediction $f(t|b,m) = b + m \times t$
  - Loss $L(c,m) = \sum_i (f(t_i|b,m) - x_i)^2$
  - Model parameters: {b,m} {intercept, slope}
  - Use L_2 loss: Least Squares



Example

- Prediction $f(t|b,m) = b + m \times t$
- Loss $L(b,m) = \sum_i (f(t_i|b,m) - x_i)^2$
- First we deal with b and then with m:

$$\frac{\partial L}{\partial b} = \frac{\partial \sum_i (f(t_i|b,m) - x_i)^2}{\partial b}$$
$$= \sum_i 2(f(t_i|b,m) - x_i) \frac{\partial\, (f(t_i|b,m) - x_i)}{\partial b}$$
$$= \sum_i 2(f(t_i|b,m) - x_i)$$
$$\frac{\partial L}{\partial m} = \frac{\partial \sum_i (f(t_i|b,m) - x_i)^2}{\partial m}$$
$$= \sum_i 2(f(t_i|b,m) - x_i) \frac{\partial\, (f(t_i|b,m) - x_i)}{\partial m}$$
$$= \sum_i 2t_i(f(t_i|b,m) - x_i)$$

Grad Descent and Big Data

- So $\nabla L(b,m) =$
$$\langle \sum_i 2(f(t_i|b,m) - x_i), \sum_i 2t_i(f(t_i|b,m) - x_i) \rangle$$
- Gradient of this form (summing up values over all the data points) is very common

? Why is this so good for “big data”, MapReduce/Spark?

Grad Descent and Big Data

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$$\langle \sum_i 2(f(t_i|b,m) - x_i), \sum_i 2t_i(f(t_i|b,m) - x_i) \rangle$$
- Gradient of this form (summing up values over all the data points) is very common
- Why is this so good for “big data”, MapReduce/Spark?
  - Sums are easily parallelized

The Learning Rate

- Reconsider the algorithm:

$\Theta_1 \leftarrow$ non-stupid guess for Θ^*;
$i \leftarrow 1$;
repeat {
  $\Theta_{i+1} \leftarrow \Theta_i - \lambda \nabla L(\Theta_i)$;
  $i \leftarrow i+1$;
} while $(||\Theta_i - \Theta_{i-1}||_1 > \varepsilon)$

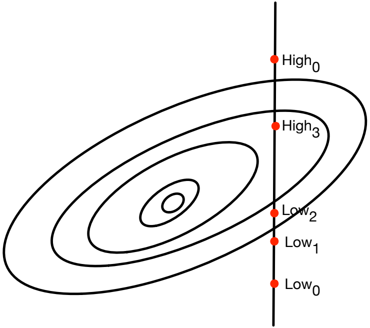
- How to choose λ?
- Super important
  - Too small: many, many passes thru the data to converge
  - Too large: oscillate into oblivion
- There are two classic approaches

Line Search

- Best option (in terms of results) but most expensive:
  - Solve another mini-optimization problem at each iteration
  - That is, choose λ so as to minimize $L(\Theta_{i+1})$
  - At lest now, it's a 1-dimensional optimization problem!
  - Called a "line search"

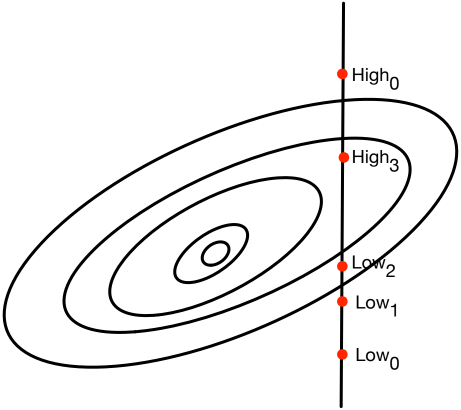
Line Search

- Sort of like a binary search
- But try to find a minimum, not a specific value
  - Always have two bounds l and h on λ
  - At each iteration, choose two l', h' within $[l, h]$
  - Breaks line segment between l and h three ways (two ends and a middle)
  - Evaluate loss at l', h'
  - Cut off the worse of the two ends



Line Search

$l \leftarrow 0$;
$h \leftarrow 999999$;
while $(h - l > \varepsilon)$ do {
  $h' \leftarrow l + \frac{1}{c}(h-l)$;
  $l' \leftarrow h - \frac{1}{c}(h-l)$;
  $\mathtt{loss}_h \leftarrow L(\Theta_i - h'\nabla L(\Theta_i))$;
  $\mathtt{loss}_l \leftarrow L(\Theta_i - l'\nabla L(\Theta_i))$;
  if ($\mathtt{loss}_h$ < $\mathtt{loss}_l$) {
    $l \leftarrow l'$;
  else
    $h \leftarrow h'$;
  }
}



- "Golden section search": $c = \frac{1}{2}(1+\sqrt{5}) = 1.618$

Problems with Line Search

- Line search is costly!
  - We have to keep recalculating the value of the loss function
  - This is not feasible for big data!

Other Ways To Choose Learning Rate

- Other standard method is "Bold Driver"
  - Widely used approach
- Approach
  - Make a very conservative initial guess for λ
  - At each iteration, compute $L(\Theta_i)$
  - Better than last time? Increment λ just a little bit: $\lambda \leftarrow \lambda \times 1.05$
  - Worse than last time? Reduce λ by a lot: $\lambda \leftarrow \lambda \times 0.5$
  - Just one eval of loss function per iteration!

Bold Driver Intuition

- Increase λ slowly so we don't miss a divergence
- At first sign of a divergence, back up massively
- Theory says that if you choose reasonable increment and decrement factors, the algorithm is guaranteed to converge

Questions?