Tools & Models for Data Science

Optimization–Newton's Method

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Gradient Descent

1. Goal: Find the parameter values for a model that best fit our data
2. Find the best direction to go in
3. Take a [sized] step in that best direction
4. Repeat until convergence

Alternatives to Gradient Descent

- Gradient descent is great
  - Easy to use
  - Widely applicable
  - But convergence can be slow
- Can we do better? Sure!

Second-Order Methods

- Class of iterative optimization methods
  - Use not only first partial derivatives
  - But second as well
  - Speeds convergence
  - Cost: more complexity
  - Cost: quadratic in number of variables

Newton's Method

- Classic second order method for optimization[1]
- Comes from Newton's method for finding zero of a function $F()$
- Recall that the "zeroes" of a function are the roots / solutions
- Use this approach to keep finding better approximations to the zeros of a function

[1] second order method means it uses the second derivative

Roadmap

1. Review of Newton's method for finding the root of a **1 variable function**
2. Introduce method for finding the root of a **1 variable gradient of a Loss function**
3. Review of Newton's method for finding the root of a **multi-variable function**
4. Introduce method for finding the root of a **multi-variable gradient of a Loss function**

Newton's Method - Refresher

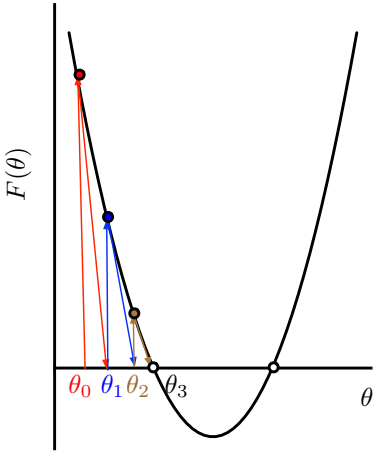
$\theta \leftarrow$ `intial guess;`
`while` θ `keeps changing, do:`
  $\theta \leftarrow \theta - F'(\theta)^{-1}F(\theta)$`;`

- θ is the value of the model parameter

- Make an initial guess
- Approximate $F(\theta)$ with a line (tangent to $F()$ at that guess)
- Update θ

Newton's Method Intuition

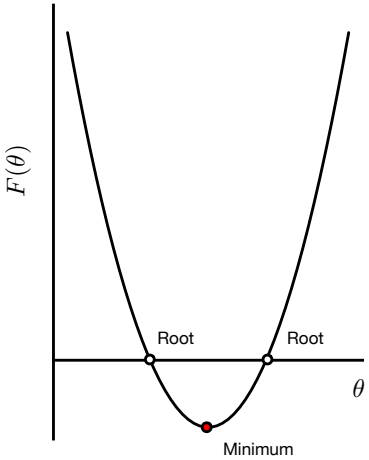
1. Pick a value for θ
2. Evaluate $F(\theta)$
3. Evaluate the derivative of the function at θ, $F'(\theta)$
4. Revise θ based on these values
5. Repeat until convergence of θ



Isn't that what we did in Gradient Descent?

Key difference:

- Root finding, not minimum finding
- Want the zero of the **function**
- Not the zero of the **derivative**



Netwon's Method for Optimization

- In data science, don't want a zero
  - We want a max/min of loss function $L()$
  - So, just find the root (zero) of the derivative $L'()$
  - So, $F(\theta) \rightarrow L'(\theta)$
- Algorithm becomes:

$\theta \leftarrow$ `intial guess;`
`while` θ `keeps changing, do:`
  $\theta \leftarrow \theta - \frac{L'(\theta)}{L''(\theta)}$`;`

Multi-Variate Newton's Method

- Say we have a multi-variate function $F : \mathbb{R}^d \to \mathbb{R}^d$, where d is the number of dimensions
  - The ith output of F is given by the function F_i
  - So $F(\Theta) = \langle F_1(\Theta), F_2(\Theta), ..., F_d(\Theta) \rangle$
- We want to find a zero of F; that is, find $\Theta = \langle \theta_1, \theta_2, ..., \theta_d \rangle$ such that:

$$
\begin{aligned}
F_1(\theta_1, \theta_2, ..., \theta_d) &= 0 \\
F_2(\theta_1, \theta_2, ..., \theta_d) &= 0 \\
&... \\
F_d(\theta_1, \theta_2, ..., \theta_d) &= 0
\end{aligned}
$$

- How to do this?

Multi-Variate Newton's Method

- Turns out it's not so difficult...
  - Won't do the derivation (relies on multi-variate Taylor expansion)
  - From Linear Algebra: a Jacobian Matrix contains all the partial first derivatives of a function
  - Here, F_i is the function that governs the ith dimension
  - Define the "Jacobian" of F to be:

$$J_F = \begin{pmatrix} \frac{\partial F_1}{\partial \theta_1} & \frac{\partial F_1}{\partial \theta_2} & \frac{\partial F_1}{\partial \theta_3} & \cdots \\ \frac{\partial F_2}{\partial \theta_1} & \frac{\partial F_2}{\partial \theta_2} & \frac{\partial F_2}{\partial \theta_3} & \cdots \\ \frac{\partial F_3}{\partial \theta_1} & \frac{\partial F_3}{\partial \theta_2} & \frac{\partial F_3}{\partial \theta_3} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

  - Note: this is a $d \times d$ matrix of functions!
  - Rows cover the different parameters for a single dimension
  - Columns cover the value of F for each dimension for a single parameter
  - We can evaluate it at any set of parameter values
  - So $J_F(\Theta)$ is a matrix of scalars

Multi-Variate Newton's Method

- Multi-Variate Newton's is simply:

$\Theta \leftarrow$ `intial guess;`
`while` Θ `keeps changing, do:`
  $\Theta \leftarrow \Theta - J_F^{-1}(\Theta)F(\Theta)$`;`

- Update each model parameter using the inverse of the Jacobian evaluated at the current values of the model parameters, Θ, and the value of the function using the same parameters

What About Multi-Variate Optimization?

- Again, we want to solve an optimization problem, not find function roots
- Difference: we don't have a system of equations to solve
- In multidimensional space, this is equivalent to standing at the top of a mountain or bottom of a valley
  - Just have a loss function $L()$, which we want to minimize (or maximize)
  - Min/max is at Θ such that:

$$\frac{\partial L}{\partial \theta_1}(\Theta) = 0$$
$$\frac{\partial L}{\partial \theta_2}(\Theta) = 0$$
$$\ldots$$
$$\frac{\partial L}{\partial \theta_d}(\Theta) = 0$$

  - That is, we want Θ such that $\nabla L(\Theta) = \langle 0, 0, ..., 0 \rangle$
  - Can then use exactly the same algorithm as before [MV Newton's Method] to find root of $\nabla L(\Theta)$

Multi-Variate Optimization

To find max/min, then this:

$\Theta \leftarrow$ intial guess;
while Θ keeps changing, do:
  $\Theta \leftarrow \Theta - J_F^{-1}(\Theta) F(\Theta)$;

Becomes this:

$\Theta \leftarrow$ intial guess;
while Θ keeps changing, do:
  $\Theta \leftarrow \Theta - J_{\nabla L}^{-1}(\Theta) \nabla L(\Theta)$;

- We are taking the Jacobian over the gradient instead of over a system of equations, F_i

One Last Thing

We have:

$\Theta \leftarrow$ `intial guess;`
`while` Θ `keeps changing, do:`
  $\Theta \leftarrow \Theta - J_{\nabla L}^{-1}(\Theta)\nabla L(\Theta)$;

- The matrix of functions $J_{\nabla L}$ is typically called the "Hessian" of L
- Entries are:

$$H_L = \begin{pmatrix} \frac{\partial L}{\partial \theta_1^2} & \frac{\partial L}{\partial \theta_1 \partial \theta_2} & \frac{\partial L}{\partial \theta_1 \partial \theta_3} & \cdots \\ \frac{\partial L}{\partial \theta_1 \partial \theta_2} & \frac{\partial L}{\partial \theta_2^2} & \frac{\partial L}{\partial \theta_2 \partial \theta_3} & \cdots \\ \frac{\partial L}{\partial \theta_1 \partial \theta_3} & \frac{\partial L}{\partial \theta_2 \partial \theta_3} & \frac{\partial L}{\partial \theta_3^2} & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

- Each entry is the 2nd derivative of the loss function with respect to each parameter
- Each row is the Jacobian given a set of model parameters, Θ

Pros and Cons of Newton's

- Pro: Convergence is quadratic; that is, error decreases quadratically
- Pro: Hundreds/thousands of iterations (gradient descent) becomes tens
- Pro: No learning rate to set
- Pro: Doesn't require $F(\Theta)$ to be convex

- Con: More complicated than gradient descent!
- Con: quadratic cost each iteration (linear gradient descent)
  The Hessian is quadratic in the number of variables
- Actually, the cost is worse than quadratic, since the matrix has to be inverted
- Con: The second derivative has to exist

In Practice

- Not used much in practice since in high dimensions, $d \times d$ is too big
- Usable for < 100K parameters, really hard at 1M
- Quasi-Newton methods are used instead
- Typically use just a portion or estimation of the Hessian matrix
- E.g. Limited-memory BFGS

Questions?

? What do we know now that we didn't know before?

? How can we use what we learned today?

Questions?

- What do we know now that we didn't know before?
  - We have another numerical method to find the parameters of a loss function
  - We understand how we can handle multi-dimensional data
- How can we use what we learned today?
  - We can find the model parameters using a different approach