# COMP 543: Tools & Models for Data Science

## Optimization–Newton's Method

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# Gradient Descent

1. Find the best direction to go in
2. Take a [sized] step in that best direction
3. 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
- Comes from Newton's method for finding zero of a function $F()$
- Recall that the "zeroes" of a function are the roots / solutions

# 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

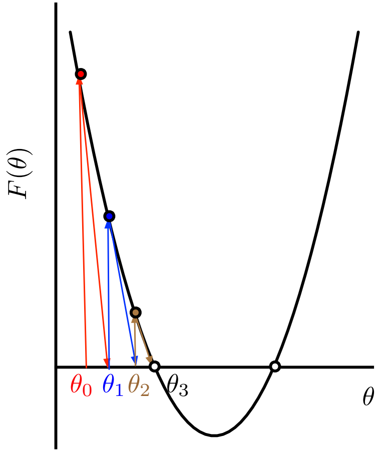
$\theta \leftarrow$ `intial guess;`
`while` $\theta$ `keeps changing, do:`
    $\theta \leftarrow \theta - \frac{F(\theta)}{F'(\theta)}$ `;`

- $\theta$ is the value of the model parameter

- Make an initial guess
- Approximate $F(\theta)$ with a line
- Update $\theta$

# Newton's Method Intuition

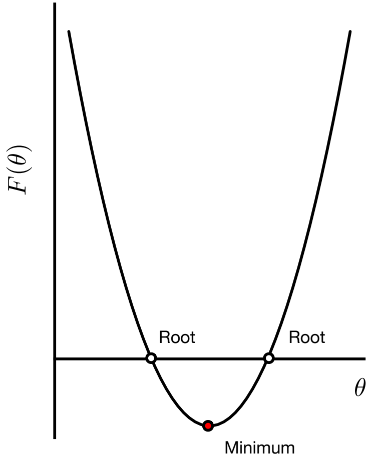
1. Pick a value for $\theta$
2. Evaluate $F(\theta)$
3. Evaluate the derivative of the function at $\theta$, $F'(\theta)$
4. Revise $\theta$ based on these values
5. Repeat until convergence of $\theta$



# 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` $\theta$ `keeps changing, do:`
  $\theta \leftarrow \theta - \frac{L'(\theta)}{L''(\theta)}$`;`

# Multi-Variate Newton's Method

- Say we have a multi-variate function $F : \mathbb{R}^d \rightarrow \mathbb{R}^d$, where $d$ is the number of dimensions
  - The $i$th 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)
  - Recall (from Linear Algebra) that a Jacobian Matrix contains all the partial first derivatives of a function
  - Here, $F_i$ is the function that governs the $i$th 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 Function value 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` $\Theta$ `keeps changing, do:`
  $\quad \Theta \leftarrow \Theta - J_F^{-1}(\Theta) F(\Theta)$;

- Update each model parameter using the inverse of the Jacobian evaluated at the current values of the model parameters, $\Theta$, 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 $\Theta$ 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 $\Theta$ 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` $\Theta$ `keeps changing, do:`
  $\Theta \leftarrow \Theta - J_F^{-1}(\Theta)F(\Theta)$;

Becomes this:

$\Theta \leftarrow$ `intial guess;`
`while` $\Theta$ `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:

```
Θ ← intial guess;
while Θ keeps changing, do:
    Θ ← Θ − J_{∇L}^{-1}(Θ)∇L(Θ);
```

- 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, $\Theta$

# 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?