

# Bonus Lecture: Solving Systems of Equations

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Grad IO

Often we are interested in solving a problem like this:

**Root Finding**  $f(x) = 0$

**Optimization**  $\arg \min_x f(x)$ .

These problems are related because we find the minimum by setting:  $f'(x) = 0$

# Root Finding

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# Newton's Method for Root Finding

Consider the Taylor series for  $f(x)$  approximated around  $f(x_0)$ :

$$f(x) \approx f(x_0) + f'(x_0) \cdot (x - x_0) + f''(x_0) \cdot (x - x_0)^2 + o_p(3)$$

Suppose we wanted to find a **root** of the equation where  $f(x^*) = 0$  and solve for  $x$ :

$$\begin{aligned} 0 &= f(x_0) + f'(x_0) \cdot (x - x_0) \\ x_1 &= x_0 - \frac{f(x_0)}{f'(x_0)} \end{aligned}$$

This gives us an **iterative** scheme to find  $x^*$ :

1. Start with some  $x_k$ . Calculate  $f(x_k), f'(x_k)$
2. Update using  $x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$
3. Stop when  $|x_{k+1} - x_k| < \epsilon_{tol}$ .

# Halley's Method for Root Finding

Consider the Taylor series for  $f(x)$  approximated around  $f(x_0)$ :

$$f(x) \approx f(x_0) + f'(x_0) \cdot (x - x_0) + f''(x_0) \cdot (x - x_0)^2 + o_p(3)$$

Now let's consider the second-order approximation:

$$\begin{aligned} x_{n+1} &= x_n - \frac{2f(x_n)f'(x_n)}{2[f'(x_n)]^2 - f(x_n)f''(x_n)} = x_n - \frac{f(x_n)}{f'(x_n) - \frac{f(x_n)}{f'(x_n)} \frac{f''(x_n)}{2}} \\ &= x_n - \frac{f(x_n)}{f'(x_n)} \left[ 1 - \frac{f(x_n)}{f'(x_n)} \cdot \frac{f''(x_n)}{2f'(x_n)} \right]^{-1} \end{aligned}$$

- Last equation is useful because we only need to know  $f(x_n)/f'(x_n)$  and  $f''(x_n)/f'(x_n)$
- If we are lucky  $f''(x_n)/f'(x_n)$  is easy to compute or  $\approx 0$  (Newton's method).

# Root Finding: Convergence

How many iterations do we need? This is a tough question to answer.

- However we can consider convergence where  $f(a) = 0$ :

$$|x_{n+1} - a| \leq K_d * |x_n - a|^d$$

- $d = 2$  (Newton's Method) **quadratic convergence** (we need  $f'(x)$ )
- $d = 3$  (Halley's Method) **cubic convergence** (but we need  $f''(x)$ )

## Root Finding: Fixed Points

Some (not all) equations can be written as  $f(x) = x$  or  $g(x) = 0 : f(x) - x = 0$ .

- In this case we can iterate on the **fixed point** directly

$$x_{n+1} = f(x_n)$$

- Advantage: we only need to calculate  $f(x)$ .
- There need not be a unique solution to  $f(x) = x$ .
- But... this may or may not actually work.

# Contraction Mapping Theorem/ Banach Fixed Point

Consider a set  $D \subset \mathbb{R}^n$  and a function  $f : D \rightarrow \mathbb{R}^n$ . Assume

1.  $D$  is closed (i.e., it contains all limit points of sequences in  $D$ )
2.  $x \in D \implies f(x) \in D$
3. The mapping  $g$  is a contraction on  $D$  : There exists  $q < 1$  such that

$$\forall x, y \in D : \quad \|f(x) - f(y)\| \leq q\|x - y\|$$

Then

1. There exists a unique  $x^* \in D$  with  $f(x^*) = x^*$
2. For any  $x^{(0)} \in D$  the fixed point iterates given by  $x^{(k+1)} := f(x^{(k)})$  converge to  $x^*$  as  $k \rightarrow \infty$
3.  $x^{(k)}$  satisfies the **a-priori error** estimate  $\|x^{(k)} - x^*\| \leq \frac{q^k}{1-q} \|x^{(1)} - x^{(0)}\|$
4.  $x^{(k)}$  satisfies the **a-posteriori error** estimate  $\|x^{(k)} - x^*\| \leq \frac{q}{1-q} \|x^{(k)} - x^{(k-1)}\|$



- Not every fixed point relationship is a contraction.
- Iterating on  $x_{n+1} = f(x_n)$  will not always lead to  $f(x) = x$  or  $g(x) = 0$ .
- Convergence rate of fixed point iteration is **slow** or  $q$ -linear.
- When  $q$  is small this will be faster.
- $q$  is sometimes called **modulus** of contraction mapping.
- A key example of a contraction: **value function iteration**!

## Accelerated Fixed Points: Secant Method

Start with Newton's method and use the finite difference approximation

$$f'(x_{n-1}) \approx \frac{f(x_{n-1}) - f(x_{n-2})}{x_{n-1} - x_{n-2}}$$
$$x_n = x_{n-1} - f(x_{n-1}) \frac{x_{n-1} - x_{n-2}}{f(x_{n-1}) - f(x_{n-2})}$$

- This doesn't have the actual  $f'(x_n)$  so it isn't quadratically convergent
- Instead is superlinear with rate  $q = \frac{1+\sqrt{5}}{2} = 1.618 < 2$  (Golden Ratio)
- Faster than fixed-point iteration but doesn't require computing  $f'(x_n)$ .
- Idea: can use past iterations to approximate derivatives and accelerate fixed points.

## Accelerated Fixed Points: Anderson (1965) Mixing

Define the residual  $r(x_n) = f(x_n) - x_n$ . Find weights on previous  $k$  residuals:

$$\widehat{\alpha}^n = \arg \min_{\alpha} \left\| \sum_{k=0}^m \alpha_k^n \cdot r_{n-k} \right\| \quad \text{subject to} \quad \sum_{k=0}^m \alpha_k^n = 1$$
$$x_{n+1} = (1 - \lambda) \sum_{j=0}^m \widehat{\alpha}_j^n \cdot x_{n-k} + \lambda \sum_{j=0}^m \widehat{\alpha}_j^n \cdot f(x_{n-k})$$

- Convex combination of weighted average of: lagged  $x_{n-k}$  and lagged  $f(x_{n-k})$ .
- Variants on this are known as **Anderson Mixing** or **Anderson Acceleration**.

## Accelerated Fixed Points: SQUAREM (Varadhan and Roland 2008)

Define the residual  $r(x_n) = f(x_n) - x_n$  and  $v(x_n) = f \circ f(x_n) - f(x_n)$ .

$$\begin{aligned} x_{n+1} &= x_n - 2s[f(x_n) - x_n] + s^2[f \circ f(x_n) - 2f(x_n) + x_n] \\ &= x_n - 2sr + s^2(v - r) \end{aligned}$$

Three versions of stepsize:

$$s_1 = \frac{r^t r}{r^t(v - r)}, \quad s_2 = \frac{r^t(v - r)}{(v - r)^t(v - r)}, \quad s_3 = -\sqrt{\frac{r^t r}{(v - r)^t(v - r)}}$$

Idea: use two iterations to construct something more like the quadratic/Halley method.

Note: I am hand-waving, don't try to derive this.

# Newton-Raphson for Minimization

We can re-write **optimization** as **root finding**;

- We want to know  $\hat{\theta} = \arg \max_{\theta} \ell(\theta)$ .
- Construct the FOCs  $\frac{\partial \ell}{\partial \theta} = 0 \rightarrow$  and find the zeros.
- How? using Newton's method! Set  $f(\theta) = \frac{\partial \ell}{\partial \theta}$

$$\theta_{k+1} = \theta_k - \left[ \frac{\partial^2 \ell}{\partial \theta^2}(\theta_k) \right]^{-1} \cdot \frac{\partial \ell}{\partial \theta}(\theta_k)$$

The SOC is that  $\frac{\partial^2 \ell}{\partial \theta^2} > 0$ . Ideally at all  $\theta_k$ .

This is all for a **single variable** but the **multivariate** version is basically the same.

# Newton's Method: Multivariate

Start with the objective  $Q(\theta) = -l(\theta)$ :

- Approximate  $Q(\theta)$  around some initial guess  $\theta_0$  with a quadratic function
- Minimize the quadratic function (because that is easy) call that  $\theta_1$
- Update the approximation and repeat.

$$\theta_{k+1} = \theta_k - \left[ \frac{\partial^2 Q}{\partial \theta \partial \theta'} \right]^{-1} \frac{\partial Q}{\partial \theta}(\theta_k)$$

- The equivalent SOC is that the Hessian Matrix is **positive semi-definite** (ideally at all  $\theta$ ).
- In that case the problem is **globally convex** and has a **unique maximum** that is easy to find.

# Newton's Method

We can generalize to Quasi-Newton methods:

$$\theta_{k+1} = \theta_k - \lambda_k \underbrace{\left[ \frac{\partial^2 Q}{\partial \theta \partial \theta'} \right]^{-1}}_{A_k} \frac{\partial Q}{\partial \theta}(\theta_k)$$

Two Choices:

- Step length  $\lambda_k$
- Step direction  $d_k = A_k \frac{\partial Q}{\partial \theta}(\theta_k)$
- Often rescale the direction to be unit length  $\frac{d_k}{\|d_k\|}$ .
- If we use  $A_k$  as the true Hessian and  $\lambda_k = 1$  this is a **full Newton step**.

# Newton's Method: Alternatives

Choices for  $A_k$

- $A_k = I_k$  (Identity) is known as **gradient descent** or **steepest descent**
- BHHH. Specific to MLE. Exploits the **Fisher Information**.

$$\begin{aligned} A_k &= \left[ \frac{1}{N} \sum_{i=1}^N \frac{\partial \ln f}{\partial \theta} (\theta_k) \frac{\partial \ln f}{\partial \theta'} (\theta_k) \right]^{-1} \\ &= -\mathbb{E} \left[ \frac{\partial^2 \ln f}{\partial \theta \partial \theta'} (Z, \theta^*) \right] = \mathbb{E} \left[ \frac{\partial \ln f}{\partial \theta} (Z, \theta^*) \frac{\partial \ln f}{\partial \theta'} (Z, \theta^*) \right] \end{aligned}$$

- Alternatives **SR1** and **DFP** rely on an initial estimate of the Hessian matrix and then approximate an update to  $A_k$ .
- Usually updating the Hessian is the costly step.
- Non invertible Hessians are bad news.



## Extended Example: Binary Choice

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# Binary Choice: Overview

Many problems we are interested in look at discrete rather than continuous outcomes:

- Entering a Market/Opening a Store
- Working or a not
- Being married or not
- Exporting to another country or not
- Going to college or not
- Smoking or not
- etc.

## Simplest Example: Flipping a Coin

Suppose we flip a coin which yields heads ( $Y = 1$ ) and tails ( $Y = 0$ ). We want to estimate the probability  $p$  of heads:

$$Y_i = \begin{cases} 1 & \text{with probability } p \\ 0 & \text{with probability } 1 - p \end{cases}$$

We see some data  $Y_1, \dots, Y_N$  which are (i.i.d.)

We know that  $Y_i \sim \text{Bernoulli}(p)$ .

## Simplest Example: Flipping a Coin

We can write the likelihood of  $N$  Bernoulli trials as

$$Pr(Y_1 = y_1, Y_2 = y_2, \dots, Y_N = y_N) = f(y_1, y_2, \dots, y_N | p)$$

$$\begin{aligned} &= \prod_{i=1}^N p^{y_i} (1-p)^{1-y_i} \\ &= p^{\sum_{i=1}^N y_i} (1-p)^{N - \sum_{i=1}^N y_i} \end{aligned}$$

And then take logs to get the **log likelihood**:

$$\ln f(y_1, y_2, \dots, y_N | p) = \left( \sum_{i=1}^N y_i \right) \ln p + \left( N - \sum_{i=1}^N y_i \right) \ln (1-p)$$

## Simplest Example: Flipping a Coin

Differentiate the log-likelihood to find the maximum:

$$\begin{aligned}\ln f(y_1, y_2, \dots, y_N | p) &= \left( \sum_{i=1}^N y_i \right) \ln p + \left( N - \sum_{i=1}^N y_i \right) \ln(1 - p) \\ \rightarrow 0 &= \frac{1}{\hat{p}} \left( \sum_{i=1}^N y_i \right) + \frac{-1}{1 - \hat{p}} \left( N - \sum_{i=1}^N y_i \right) \\ \frac{\hat{p}}{1 - \hat{p}} &= \frac{\sum_{i=1}^N y_i}{N - \sum_{i=1}^N y_i} = \frac{\bar{Y}}{1 - \bar{Y}} \\ \hat{p}^{MLE} &= \bar{Y}\end{aligned}$$

That was a lot of work to get the obvious answer: **fraction of heads**.

## More Complicated Example: Adding Covariates

We probably are interested in more complicated cases where  $p$  is not the same for all observations but rather  $p(X)$  depends on some covariates. Here is an example from the Boston HMDA Dataset:

- 2380 observations from 1990 in the greater Boston area.
- Data on: individual Characteristics, Property Characteristics, Loan Denial/Acceptance (1/0).
- Mortgage Application process circa 1990-1991:
  - Go to bank
  - Fill out an application (personal+financial info)
  - Meet with loan officer
  - Loan officer makes decision
    - Legally in race blind way (discrimination is illegal but rampant)
    - Wants to maximize profits (ie: loan to people who don't end up defaulting!)