Broyden's Method

Outline

What is Broyden's method? → How is it used? → Newton's method algorithm

→ Broyden's method algorithm → Comparison of both methods → Application of Broyden's method

Broyden's Method

- Broyden's Method is a method for solving $\mathbf{F}(\mathbf{x})=\mathbf{0}$.
- $\mathbf{F}(\mathbf{x})$ could be one function or a set of functions.
- Instead of computing the Jacobian (derivative), it is updated to save computation time.
- Newton's method also solves $\mathbf{F}(\mathbf{x})=\mathbf{0}$, however it computes the Jacobian (derivative) at every iteration.

Newton's Method

$f(x) = (x-2)^2 = 0$

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

Guess x_0.

Evaluate $f(x_0)$.

Evaluate $f'(x_0)$.

Solve for x_1.

Evaluate $f(x_1)$....

Until $f(x_n) \approx 0$

$f'(x_0) = 2(x-2)$

$x_0 = 1$

$f(x_0) = 1$

$f'(x_0) = -2$

$x_1 = 1.5$

....

Newton's Method

$f(x) = (x-2)^2$

$f'(x_0) = 2(x-2)$

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

n	x_n	$f(x_n)$	$f'(x_n)$	x_{n+1}
0	1	1	-2	1.5
1	1.5	0.25	-1	1.75
2	1.75	0.0625	-0.5	1.875
3	1.875	0.015625	-0.25	1.9375
4	1.9375	0.0039063	-0.125	1.96875
5	1.96875	0.0009766	-0.0625	1.984375
6	1.984375	0.0002441	-0.03125	1.9921875

Newton's Method

In one dimension, we have $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$

In multiple dimensions, we have $x_{n+1} = x_n - J^{-1}(x_n) f(x_n)$

$f_1(x_1,x_2) = (x_1 - 2)^2 + (x_2 + 3)^2$ $f_2(x_1,x_2) = (x_1 - 2) + (x_2 + 3)^2$

$$J(x_n) = \begin{matrix} \frac{\partial F_1}{\partial x_1} & \frac{\partial F_1}{\partial x_2} \\ \frac{\partial F_2}{\partial x_1} & \frac{\partial F_2}{\partial x_2} \end{matrix} \qquad J(x_n) = \begin{matrix} 2(x_1 - 2) & 2(x_2 + 3) \\ 1 & 2(x_2 + 3) \end{matrix}$$

In one dimension, f'(x) was evaluated in each step.
In multiple dimensions, **J**(**x**) is evaluated.

Broyden's Method

As before, we have $x_{n+1} = x_n - J^{-1}(x_n) f(x_n)$

We do not want to evaluate **J**(**x**) at every iteration – it takes too much time!

Instead, we will update the Jacobian with the following formula:

$$J_n = J_{n-1} + \frac{\Delta F_n - J_{n-1} \Delta x_n}{\| x_n \|^2} \Delta x_n^T$$

$$\Delta x_n = x_n - x_{n-1}$$

$$\Delta F_n = F_n - F_{n-1}$$

Broyden's Method

1. Start with a guess $\mathbf{x}_0$.
2. Evaluate $\mathbf{J}(\mathbf{x}_0)$ and $\mathbf{f}(\mathbf{x}_0)$.
3. Calculate $\mathbf{J}^{-1}(\mathbf{x}_0)$.
4. Calculate $\mathbf{x}_1$.

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

5. Calculate the terms in (ΔF_n, Δx_n, Δx_n^T, and $||x_n||^2$)

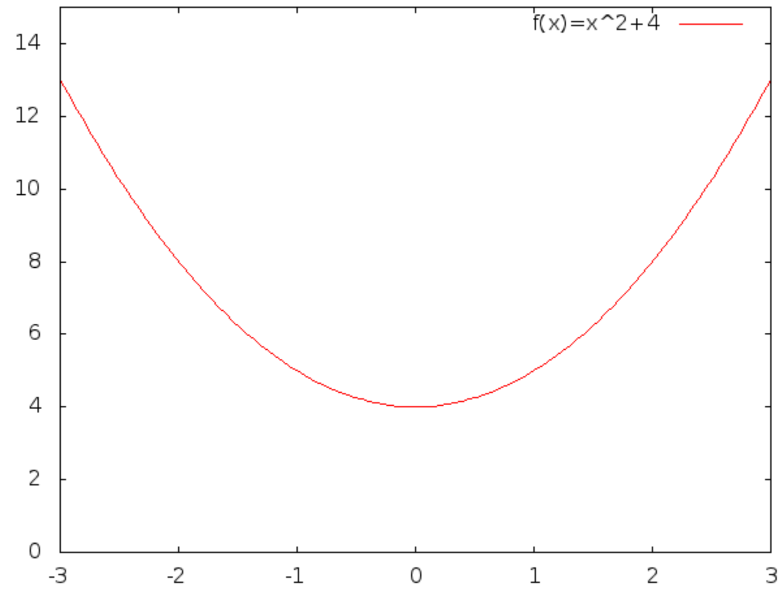
$$J_n = J_{n-1} + \frac{\Delta F_n - J_{n-1} \Delta x_n}{\| x_n \|^2} \Delta x_n^T$$

6. Update the Jacobian and find its inverse.
7. Go to step 4, but calculate $\mathbf{x}_{n+1}$. Repeat until $\mathbf{f}(\mathbf{x}_n) \approx 0$.

Comparison of Newton's Method and Broyden's Method

Application of Broyden's Method

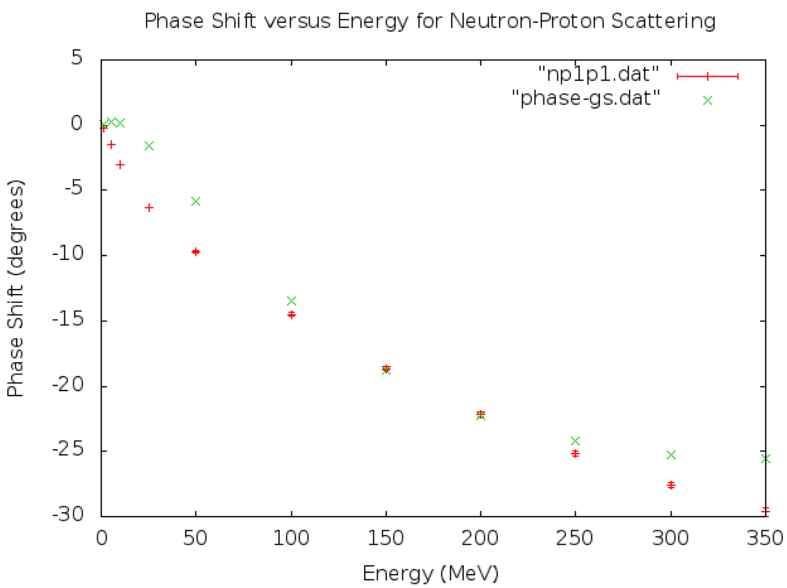
The function may not have a root, however it can have minima.



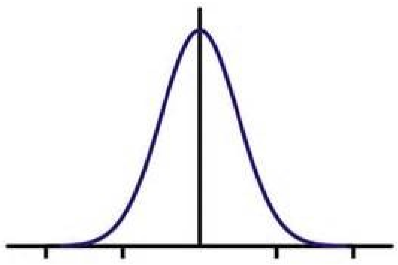
Instead of **F**(**x**)=0, d**F**(**x**)/d**x**=0.

$x_{n+1} = x_n - J^{-1}(x_n) f(x_n)$ becomes $x_{n+1} = x_n - H^{-1}(x_n) \nabla f(x_n)$

Application of Broyden's Method



Gaussian



My x values are my parameters of the potential (4 parameters).

One for the width of the Gaussian and one for the height.

There are two Gaussians.

My f(x) values are the reduced chi-square.

By mimizing the reduced chi-square, I can find the best parameters to fit to scattering data.

Application of Broyden's Method

Newton's method and Broyden's method appeared to take the same time.

The time it takes to evaluate a function in my case is around 40 seconds.

To calculate the Hessian, this means four evaluations per element and there are sixteen elements total.

For Newton's method, the derivative of F must be calculated as well (two evaluations per element and four elements).

Newton's method requires evaluating the function 72 times and takes 48 minutes total.

To update the Hessian using Broyden's method, the function is evaluated eight times, and it takes around five minutes and twenty seconds.