

Project 1

Dan Kolbman

September 22, 2014

$$f(x) = x \left(1 + \sum_{j=1}^M \frac{k_j \eta_j}{1 + k_j x} \right) - \xi \quad (1)$$

Define some test cases to user later:

Case 1:

$M = 1, k = 1, \eta = 10, \xi = 1$

$x_r = 0.099020$

Case 2:

$M = 2, k_1 = 5, k_2 = 3, \eta_1 = 4, \eta_2 = 2, \xi = 5$

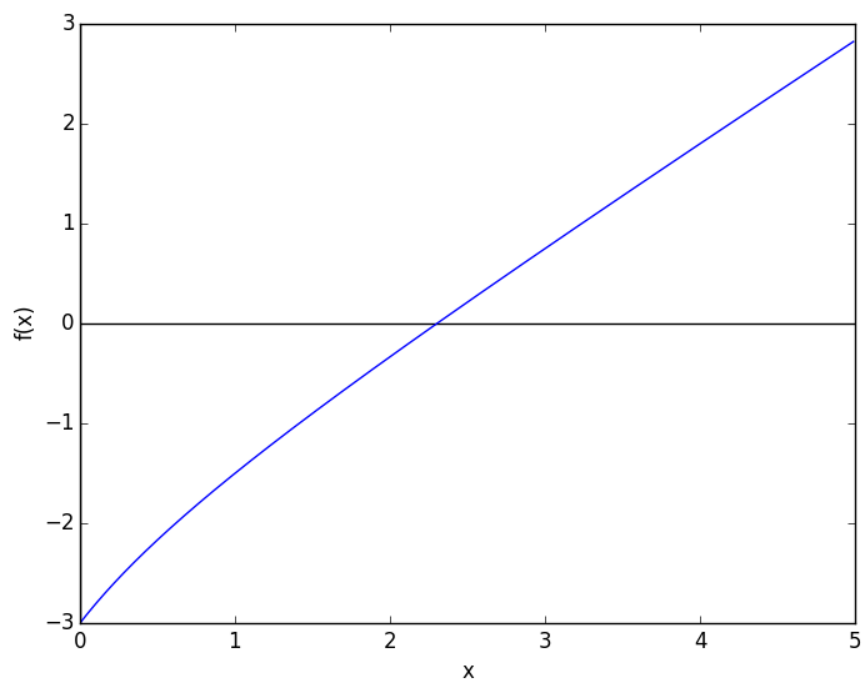
$x_r = 0.63905$

Case 3:

$M = 3, k_1 = 1, k_2 = 2, k_3 = 6, \eta_1 = 2, \eta_2 = 3, \eta_3 = 1, \xi = 9$

$x_r = 3.8064$

Plot for $M = 1, k = 1, \eta = 1, \xi = 3$



Show that Eq. 1 is Negative for $x = 0$

If $x = 0$:

$$f(0) = x \left(1 + \sum_{j=1}^M \frac{k_j \eta_j}{1 + k_j 0} \right) - \xi$$

$$f(0) = -\xi$$

Where $\xi > 0$, as the concentration can not be negative. Thus,

$$f(0) < 0 \tag{2}$$

Eq. 1 is Strictly Increasing for $x > 0$

We can show that $f(x)$ is constantly increasing by observing that the derivative is positive for $x > 0$:

$$\frac{df(x)}{dx} = 1 + \frac{d}{dx} \left(\sum_{j=1}^M \frac{x k_j \eta_j}{1 + k_j x} \right)$$

$$\frac{df(x)}{dx} = 1 + \sum_{j=1}^M \frac{k_j \eta_j}{(1 + k_j x)^2}$$

$$\frac{df(x)}{dx} > 0 \quad \forall (x > 0) \in \Re \tag{3}$$

Eq. 1 is Positive for for large x

Given that the derivative is always positive, there must be some point at which,

$$f(x) > 0, x \rightarrow \infty \tag{4}$$

Eq. 1 Always has one Positive Solution

Given conditions 2, 3, and 4, there must exist one value of $x > 0$ for which $f(x) = 0$.

Bisection

Fixed Point Iteration

$$x = \xi - x \sum_{j=1}^M \frac{k_j \eta_j}{1 + k_j x} = g(x) \quad (5)$$

The root of

$$x(1 + \frac{1}{1+x}) - 3 = 0$$

Using FPI and Eq. 5 to obtain a $g(x)$:

$$g(x) = 3 - \frac{x}{1+x}$$

which correctly converges to 2.30277.

However, using the form of Eq. 5 to find the root of

$$x(1 + \frac{5}{1+x}) - 3 = 0$$

with a $g(x)$:

$$g(x) = 3 - \frac{5x}{1+x}$$

By inspecting $|g'(x)|$ at the desired root we see, for the second case, that:

$$g'(0.79129) = |\frac{5}{(x+1)^2}| = 1.558$$

Which indicates that it diverges since it is greater than one. Compare with the first case where we see that:

$$g'(2.30277) = |\frac{1}{(x+1)^2}| = 0.0918$$

Thus implying convergence (which it does) as it is less than one.

Now using a definition of $g_\alpha(x)$:

$$g_\alpha(x) = \frac{1}{1+\alpha} \left[\xi + x \left(\alpha - \sum_{j=1}^M \frac{k_j \eta_j}{1 + k_j x} \right) \right] = x \quad (6)$$

We can find an α such that $|g'_\alpha(r)| < 1$ so that we will have convergence:

$$g_\alpha(x) = \frac{1}{1+\alpha} \left[3 + x\left(\alpha - \frac{5}{1+x}\right) \right]$$

$$g'_\alpha(x) = \frac{1}{1+\alpha} \frac{\alpha(x+1)^2 - 5}{(x+1)^2}$$

$$g'_\alpha(2.30277) = \frac{\alpha - 0.45836}{1+\alpha}$$

Thus, to guarantee convergence, we find that $\alpha > 0.27$ (by finding the root of $g'_\alpha(2.30277) - 1 = 0$). With a value of $\alpha = 1$, the root for the second case correctly converges to $x = 0.79128$.

Newton's Method

Consider Eq. 1 for $M = 1$, $k = 1$, $\eta = 1$, and $\xi = 3$:

For an initial guess $x_0 = 1.6$, Newton's Method will converge on a root, however, it is the root at $x = -10.099$ rather than the root closer to the initial guess at $x = 0.099$.

When choosing $x_0 = 1.4999$, the next guess still overestimates the root, but not badly enough to jump over the asymptote and converge on a different root.

When starting from $x_0 = 1.5$, the next guess will land very close to the asymptote and many small steps are spent moving down the steep slope until it eventually reaches the root.

The guess following $x_0 = 1$ lies closest to the root due to the down concavity as the function approaches the root. This results in the following guesses being close to the root where there is no extreme slopes and will quickly converge.

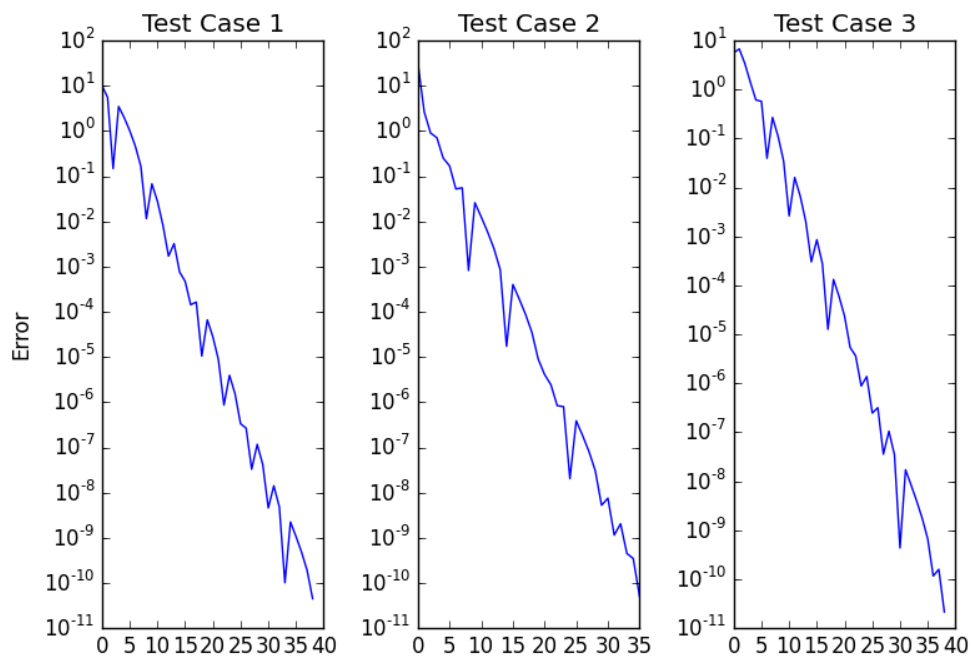
Consider Eq. 1 for $M = 3$, $\xi = 9$, $k_1 = 1, k_2 = 2, k_3 = 6$ $\eta_1 = 2, \eta_2 = 3, \eta_3 = 1$:

The function is nearly linear for values of $x > 0$ so Newton's Method converges very quickly. For initial values of $x_0 < 0$ but greater than the asymptote, more iterations will be needed, but the function will still converge on $x = 3.086$.

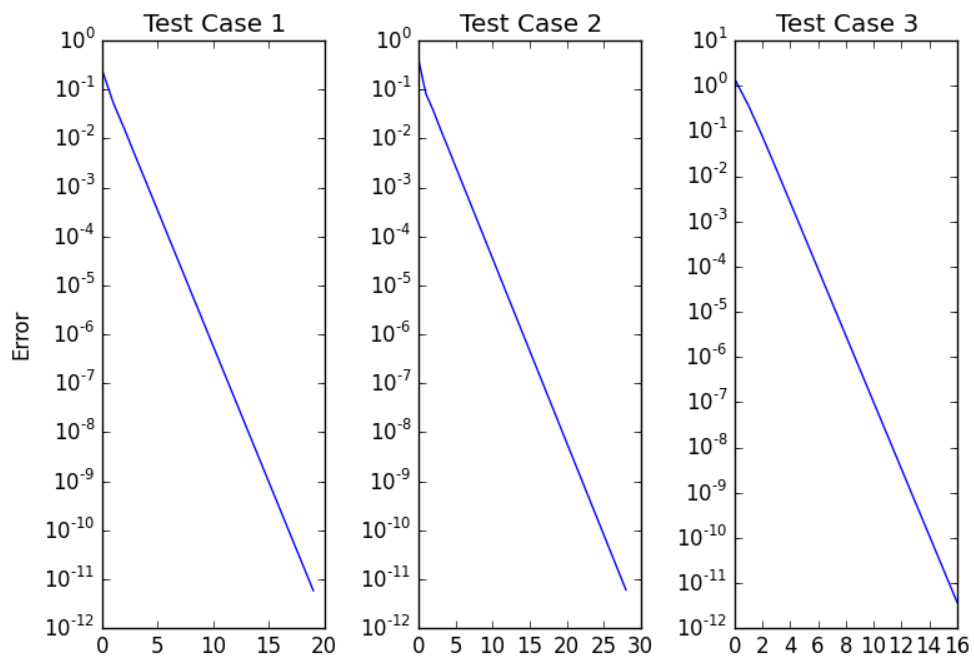
Comparison Between Methods

Bisection, FPI, and Newton's Method were applied to each of the three test cases listed at the beginning. Bisection and FPI methods both converged linearly on the roots. Bisection took about 40 steps to converge on the roots, while FPI took between 15-25. Newton's method converged quadratically never taking more than 5 steps to converge within tolerance.

Convergence for Bisection



Convergence for FPI



Convergence for Newton's Method

