Introduction to Matlab

Lesson 03 — Basics of Root Finding, Numerical Differentiation, and Integration

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Basics of Root Finding

Root Finding — The Problem

Say we want to find all x such that f(x) = 0. If:

- o $f(x)=ax^2+bx+c \Rightarrow x=\frac{-b\pm\sqrt{b^2-4ac}}{2a}$ solves the problem for any $\{a,b,c\}\in\mathbb{R}$ (and $a\neq 0$).
- \circ Sometimes, we cannot solve explicitly for x even in the realm of polynomials!
- o If $f(x) = ax^5 + bx^4 + cx^3 + dx^2 + ex + f$ where $\{a, b, c, d, e, f\} \in \mathbb{R}$ we do not have an explicit formula to solve for f(x) = 0. Neither for polynomials of order ≥ 5 . But we know **such roots do exist!** see Fundamental Theorem of Algebra
- Then... what should we do?

Root Finding — Intuition

Say we have a nonlinear f(x) for which we know at least one root exists.

- Suppose we know the root is somewhere around x_0 .
- Starting from x_0 construct a sequence of $\{x_k\}$ hoping it converges to a root x^* such that $f(x^*) = 0$.

This highlights two important features of root finding algorithms:

- **Convergence:** is the sequence $\{f(x_k)\}$ getting *closer* to $f(x^*) = 0$?
- Stopping criteria: how do we know we are close enough?

We can discuss convergence and stopping criteria in each method studied.



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 - 3. Open by the middle, check if G is left or right. Discard one half. Repeat until you find it.

Consider $f: \mathbb{R} \to \mathbb{R}$ where the problem is $f(x^*) = 0$. Suppose f(x) is continuous in [a,b] and we know $\exists x^* \in [a,b]$ (The ideas presented generalize to n dimensions)

- **Bisect** the interval [a,b] and take the middle point $c=\frac{a+b}{2}$. If f(c)=0 we are done. Otherwise, x^* must be in either [a,c] or [c,b].
- Find the one that contains x^* and bisect again. How?!?
- Continue until the interval is as small as the accuracy desired.

Theorem 1 (The Intermediate Value Theorem (IVT))

Suppose f(x) is continuous on $[a,b] \subseteq \mathbb{R}$ and M in between f(a) and f(b). Then, there is at least one $c \in (a,b)$ such that f(c) = M. If f(a) < 0 < f(b) then, there is a root x = c such that f(c) = 0.

- If f(c) < 0, by the IVT, the root of f(x) must be in [c,b]
- Otherwise, if f(c) > 0, by the IVT, the root must be in [a, c]
- Note that this algorithm finds a zero, not all zeros of f(x)

Bisection Method — the Algorithm

- 1. Initialize and bracket a zero. (Initial guess)
 - Find $x^L < x^R$ such that $f(x^L)f(x^R) < 0$
 - Choose stopping rule parameters
- 2. Compute $x^M = \frac{x^L + x^R}{2}$
- 3. Test if x^M is a root. If so, stop. (Test if it is an acceptable solution)
- 4. If x^M is not a root, refine interval. (Iterate)

 o If $f(x^M)f(x^L) < 0$ let $x^R = x^M$ and leave x^L unchanged.
 - Else, $x^L = x^M$ and leave x^R unchanged.
- 5. Repeat until the stopping rule tells us to stop.

Bisection Method — Remarks

- The algorithm always converges (we always find a solution).
- Convergence can be very slow but it is a very reliable method.
- We have not yet defined proper stopping criteria.

Stopping Criteria:

- 1. The value of the function is lower than or equal to the tolerance $|f(x^M)| \leq \delta$.
- 2. The length of the interval is very small. $(x^R x^L)/(1 + |x^L| + |x^R|) \le \varepsilon$.
- 3. The number of iterations is larger than a predetermined number N.



Newton-Raphson Method — Intuition

- When using bisection, we have only assumed continuity of f(x)
- However, bisection can be slow. Newton-Raphson's method uses properties of smooth functions.
- This method is faster but may not always converge.
- **Key idea:** approximate f(x) by a succession of linear functions. Approximate zeros with the zeros of the linear approximations.

Newton-Raphson — Preliminaries

Definition 1

A number c is a **fixed point** of g(x) if g(c) = c.

• Note then that $f(x) = 0 \Rightarrow f(x) = x - g(x) = 0$ and any fixed point c of g(x) is a root of f(x) because

$$f(c) = c - g(c) = c - c = 0$$

- Finding a root of $f(x) \equiv$ find a fixed point of x = g(x) such that f(x) = 0
- **Problem:** How to rewrite f(x) = 0 as x = g(x)?

Newton-Raphson — Preliminaries

- We can know existence, uniqueness, and convergence (see Theorem 3).
 However, verifying Assumption 1 is not easy.
- This method chooses g(x) as $g(x) = x \frac{f(x)}{f'(x)}$ and the iteration scheme is:

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} \tag{1}$$

For this choice, we can state sufficient conditions for convergence.

Theorem 2

Suppose f(x) is C^2 and that $f(x^*) = 0$. If x_0 is sufficiently close to x^* , $f'(x) \neq 0$, and $|f''(x)/f'(x)| < \infty$, the iteration scheme defined by (1) converges to x^* .

Newton-Raphson — Preliminaries

Where does the choice for g(x) come from? Recall Taylor's Theorem and linearly approximate f(x) around x_k :

$$p(x) = f(x_k) + (x - x_k)f'(x_k)$$

- \circ p(x) and f(x) are tangent at x_k and close in the neighborhood of x_k
- Solving for a zero of $p(x) \Rightarrow x = x_k \frac{f(x_k)}{f'(x_k)}$ which is the iteration scheme (1)
- Which yields our new guess for x_{k+1}

Newton-Raphson — The Algorithm

- 1. Choose stopping criterion parameters $\{\varepsilon, \delta, N\}$, and a starting point x_0 . Set the iteration counter k = 0.
- 2. Compute next iteration using (1)
- 3. Test for convergence. If either one of the following:

$$|x_k - x_{k+1}| \le \varepsilon (1 + |x_{k+1}|)$$

$$\circ |f(x_{k+1})| \le \delta$$

$$\circ$$
 $k > N$

Stop

4. Repeat until one of the convergence criteria is satisfied.

Newton-Raphson — Remarks

- The method is not guaranteed to converge. If after *N* iterations we have not found a root, the method failed.
- Note that we rely on our initial guess being close to the root. If we are far, we may very well fail.
- For some functions and starting points, we may enter an infinite loop. The sequence of iterations will oscillate without converging to any value.
- \circ Even when passing both ε and δ tests, we may not have found a zero.

Newton-Raphson — Some Issues

• Consider
$$f(x) = x^6$$

$$x_{k+1} = (5/6)x_k$$

Still far after 100 iterations!

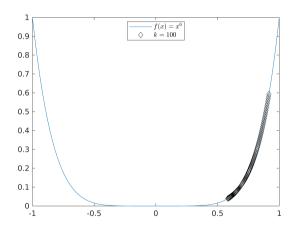


Figure 1: Convergence Issues with Newton-Raphson

Root Finding in Matlab

- We have learned two very powerful methods to find roots
- Matlab has implemented fzero for such problems.
- This function combines bisection with secant and inverse quadratic interpolation (we have not seen this but many ideas apply).
- Another function is **roots** which finds the roots of polynomials.
- Familiarize yourselves with these functions and compare them with the methods we have implemented.



 Say we have two agents A and B, and two goods 1 and 2. The preferences of the agents are

$$u_A(x_{1,A}, x_{2,A}) = (x_{1,A})^{\alpha} (x_{2,A})^{1-\alpha} \qquad u_B(x_{1,B}, x_{2,B}) = (x_{1,B})^{\beta} (x_{2,B})^{1-\beta}$$

- Their initial endowments are $\{\omega_{1,i}, \omega_{2,i}\}$
- In equilibrium, it must be that $m_i = p_1 \omega_{1,i} + p_2 \omega_{2,i}$.

• The demand functions are given by:

$$x_{1,A}(p_1, p_2, m_A) = \alpha \frac{m_A}{p_1}$$

$$x_{2,A}(p_1, p_2, m_A) = (1 - \alpha) \frac{m_A}{p_2}$$

$$x_{1,B}(p_1, p_2, m_B) = \beta \frac{m_B}{p_1}$$

$$x_{2,B}(p_1, p_2, m_B) = (1 - \beta) \frac{m_B}{p_2}$$
(5)

Define the excess demand for goods 1 and 2 as

$$z_{1}(p_{1}, p_{2}) = x_{1,A}(p_{1}, p_{2}, m_{A}) + x_{1,B}(p_{1}, p_{2}, m_{B}) - \omega_{1,A} - \omega_{1,B}$$

$$z_{2}(p_{2}, p_{2}) = x_{2,A}(p_{2}, p_{2}, m_{A}) + x_{2,B}(p_{2}, p_{2}, m_{B}) - \omega_{2,A} - \omega_{2,B}$$
(6)
$$z_{2}(p_{2}, p_{2}) = x_{2,A}(p_{2}, p_{2}, m_{A}) + x_{2,B}(p_{2}, p_{2}, m_{B}) - \omega_{2,A} - \omega_{2,B}$$

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$$z_2(p_2, p_2) = x_{2,A}(p_2, p_2, m_A) + x_{2,B}(p_2, p_2, m_B) - \omega_{2,A} - \omega_{2,B}$$

• Substituting the demand functions (2)-(5) and dividing by p_2 (we only care about relative prices, check Walras' Law if you don't see this).

$$z_{1}(p_{1},1) = \alpha \frac{p_{1}\omega_{1,A} + \omega_{2,A}}{p_{1}} + \beta \frac{p_{1}\omega_{1,B} + \omega_{2,B}}{p_{1}} - \omega_{1,A} - \omega_{1,B}$$

$$z_{2}(p_{1},1) = (1-\alpha)(p_{1}\omega_{1,A} + \omega_{2,A}) + (1-\beta)(p_{1}\omega_{1,B} + \omega_{2,B}) - \omega_{2,A} - \omega_{2,B}$$

$$z_{1}(p_{1},1) = \alpha \frac{p_{1}\omega_{1,A} + \omega_{2,A}}{p_{1}} + \beta \frac{p_{1}\omega_{1,B} + \omega_{2,B}}{p_{1}} - \omega_{1,A} - \omega_{1,B}$$
(8)
$$z_{2}(p_{1},1) = (1-\alpha) \left(p_{1}\omega_{1,A} + \omega_{2,A} \right) + (1-\beta) \left(p_{1}\omega_{1,B} + \omega_{2,B} \right) - \omega_{2,A} - \omega_{2,B}$$
(9)

- An equilibrium is then a price p_1 such that $z_1(p_1,1)=z_2(p_2,1)=0$.
- We can use any of the two to get the solution for p_1 .
- The analytical solution is

$$p_1^* = \frac{\alpha \omega_{2,A} + \beta \omega_{2,B}}{(1 - \alpha)\omega_{1,A} + (1 - \beta)\omega_{1,B}}$$

Exercise 1

Let's find the equilibrium price of the Arrow-Debreu model in Matlab using $z_1(p_1, 1)$. Use the following values for the parameters:

$$\alpha = 0.6$$
 $\beta = 0.4$ $\omega_{1,A} = 10$ $\omega_{2,A} = 15$ $\omega_{1,B} = 15$ $\omega_{2,B} = 10$

Basics of Numerical Differentiation

Numerical Differentiation — Why?

- Numerical evaluation of the derivatives in economics is crucial!
 - Newton-Raphson, optimization, ODEs ...
- Sometimes, it is difficult or cumbersome to compute derivatives analytically. In those cases, we turn to *numerical* evaluation of derivatives.
- Recall the definition of the derivative of a function

$$f'(x) = \lim_{h o 0} rac{f(x+h) - f(x)}{h}$$
 (can recall why?)

we can approximate f'(x) by choosing a step size h.

• That is called, finite differences.

Numerical Differentiation — An Example

Take the function

$$f(x) = x^3 - 6x^2 + 11x - 6$$

The analytical derivative is

$$f'(x) = 3x^2 - 12x + 11$$

- Let's approximate the derivative by using finite differences in Matlab with on $x \in [-5,5]$
- Compute dy as f(x+h) f(x) for a fixed h and dx = h.
- The numerical derivative is given by $f'(x) = \frac{dy}{dx}$.

Numerical Differentiation — An Example

As $h \to 0$, the derivative converges.

```
1 N = 10;
2 x = linspace(-5,5,N);
3 h = 1;
4 % Numerical derivative
5 dy = myf(x+h) - myf(x);
6 dx = h.*ones(size(dy));
7 fp_num = dy./dx;
```

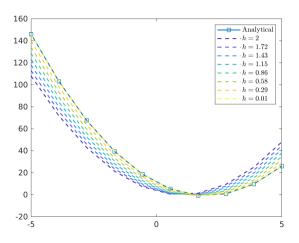


Figure 2: Accuracy of Finite Difference

Numerical Differentiation — An Application to ODEs

 The Solow-Swan growth model finds an equilibrium solution by solving the ODE

$$\dot{k} = \frac{dk}{dt} = sf(k) - \delta k \tag{10}$$

where k is physical capital, f(k) is the production function, s is an exogenous savings rate, and δ is the depreciation rate of capital.

- Approximate k(t) at N discrete points in the time dimension $t^n, n = 1, ..., N$ and denote the distance between the points by h.
- Approximate \dot{k} using finite differences $\dot{k}(t^n) \approx \frac{k^{n+1}-k^n}{h}$
- \circ We can compute $k(t^{n+1})$ recursively given h and $k(0)=k_0$

$$k(t^{n+1}) = k(t^n) + h\left(sf(k^n) - \delta k^n\right)$$

Numerical Differentiation — An Application to ODEs

- Horizon T = 70
- \circ N = 10 points.
- Compare with ode45 and analytical solution.

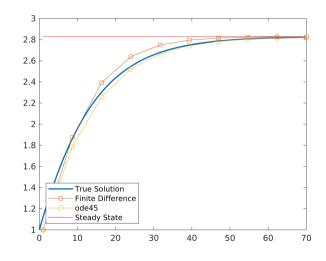


Figure 3: Trajectory for k(t)

Symbolic and Automatic Differentiation

- Symbolic differentiation applies the rules of derivatives to symbolic expressions. What we humans do.
- Automatic differentiation breaks codes into smaller sections and applies the chain rule [Kwon 2019, See Chapter 4].
- The advantage of automatic differentiation is that computes analytical derivatives at the same cost. No error!
- Automatic differentiation evaluates expressions numerically early, symbolic differentiation at the end.
- Thus, symbolic is more costly. Check Matlab's documentation

Basics of Numerical Integration

Numerical Integration — Why?

- Numerical evaluation of integrals in economics is ubiquitous.
 - Expectations, posteriors in Bayesian statistics, ODEs (again...)
- Again, sometimes it is computationally expensive to compute integrals.
- The definite integral of f(x) is the area under its graph.
- Furthermore, the definition of the definite integral involves an infinte sum (Riemann Sum).
- We will approximate integrals by computing sums in particular ways.

Numerical Integration — Preliminaries

Definition 2

Let $f:[a,b]\mapsto \mathbb{R}$. Let \mathcal{P} and \mathcal{T} be a **partition pair** such that $\mathcal{P},\mathcal{T}\subset [a,b]$ where $\mathcal{P}=\{x_0,\ldots,x_n\},\,\mathcal{T}=\{t_1,\ldots,t_n\}$ and

$$a = x_0 \le t_1 \le x_1 \le t_2 \le x_2 \le \cdots \le t_n \le x_n = b$$

where we assume the points $\{x_0, \ldots, x_n\}$ are distinct. The **Riemann sum** corresponding to $f, \mathcal{P}, \mathcal{T}$ is

$$\mathcal{R}(f,\mathcal{P},\mathcal{T}) = \sum_{i=1}^{n} f(t_i) \Delta x_i = f(t_1) \Delta x_1 + f(t_2) \Delta x_2 + \ldots + f(t_n) \Delta x_n$$

and $\Delta x_i = x_i - x_{i-1}$.

Notice this is just the area of the rectangles of base Δx_i under the curve of f.

Numerical Integration — Preliminaries

Definition 3

The **mesh** of the partition \mathcal{P} is the length of the largest subinterval $[x_{i-1}, x_i]$.

Definition 4

A real number I is the **Riemann Integral** of f over [a,b] if it satisfies $\forall \epsilon > 0, \exists \delta > 0$ such that if \mathcal{P}, \mathcal{T} is any partition pair, then

$$\operatorname{mesh}(\mathcal{P}) < \delta \Rightarrow |\mathcal{R}(f, \mathcal{P}, \mathcal{T}) - I| < \epsilon$$

If such an I exists it is unique and we denote it by

$$\int_{a}^{b} f(x)dx = I = \lim_{\mathsf{mesh}(\mathcal{P}) \to 0} \mathcal{R}(f, \mathcal{P}, \mathcal{T})$$

and we say that f is **Riemann integrable** with Riemann integral I.

Numerical Integration — Intuition

- Notice the definition of the **Riemann integral** is just a weighted sum of the values of *f* at certain points.
- If the subintervals $[x_{i-1}, x_i]$ are all the same length, the weights are all equal. But we do not need to choose equal weights.
- The problem of numerical integration is also called *cuadrature*.
- There are many cuadrature methods, we will only study a couple of Newton-Cotes formulas. But the general idea is to use a formula such as (11)

$$\int_{a}^{b} f(x)dx \approx \sum_{i=1}^{n} \omega_{i} f(x_{i})$$
(11)

where ω_i are the weights, and x_i the points.

Numerical Integration — Newton-Cotes Quadratures

General Idea:

- Evaluate f(x) at a finite number of points.
- \circ Construct a piece-wise polynomial approximation of f based on those points.
- Integrate the approximation of f to approximate $\int_a^b f(x)dx$

Numerical Integration — Newton-Cotes Quadratures

- aUQVb ⇒ midpoint rule.
- $aPRb \Rightarrow trapezoid$ rule.
- Parabola *PQSR*

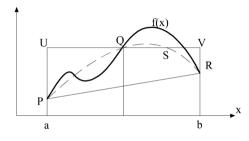


Figure 4: See Judd 1998

Numerical Integration — Newton Cotes Quadratures

Midpoint Rule:

• The simplest quadrature formula with one point given by

$$\int_{a}^{b} f(x)dx = \underbrace{(b-a)f\left(\frac{a+b}{2}\right)}_{Rule} + \underbrace{\frac{(b-a)^{3}}{24}f''(\xi)}_{Error}$$

for some $\xi \in [a,b]$. Based on Taylor's theorem and the IVT.

• Let $n \ge 1$ be the number of subintervals, h = (b-a)/n, and $x_j = a + (j-\frac{1}{2})h$, $j = 1, 2, \ldots, n$. The **composite midpoint rule** (omitting the error) is given by

$$\int_a^b f(x)dx = h \sum_{i=1}^n f(x_i) \Rightarrow$$
 Same as the Riemann Sum!!

Numerical Integration — Newton-Cotes Quadratures

Example 1 Compute $\int_1^5 x^2 dx = \frac{124}{3} \approx 41.333$. Errors decline with the number of points n.

```
1 function [value] =
    midpoint_rule(a,b,n,myfunc)
   % Numerical integration with
       midpoint rule
   xpts = zeros(n,1);
   h = (b-a)/n;
   for ii=1:n
       xpts(jj,1) = a + (jj -
           1/2)*h:
   end
   value = h*sum(myfunc(xpts));
9 end
```

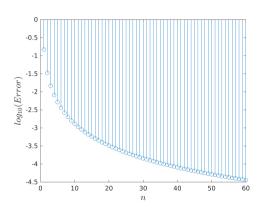


Figure 5: Relative errors in log_{10} units

Numerical Integration — Newton-Cotes Quadratures

Trapezoid Rule:

- \circ Use linear approximations of f using the end-points of [a, b].
- The rule is

$$\int_{a}^{b} f(x)dx = \frac{b-a}{2}(f(a)+f(b)) - \frac{(b-a)^{3}}{12}f''(\xi)$$

for some $\xi \in [a, b]$.

o Composite trapezoid rule letting h = (b - a)/n and $x_i = a + ih$

$$\int_{a}^{b} f(x)dx = \frac{h}{2} \left(f(x_0) + 2f(x_1) + \dots + 2f(x_{n-1}) + f(x_n) \right)$$

Numerical Integration in Matlab

- As with root finding, Matlab has routines for numerical integration.
- The trapezoid rule is implemented in trapz (you'll work with this on the Problem Set).
- Another routine is integral.
- The latter uses adaptive quadratures. Basically, adapts the subintervals refining the process. But the quadrature rules can still be Newton-Cotes.
- For double and triple integrals, Matlab has integral2 and integral3 respectively.

Details on Solution Methods



Bisection Method — Stopping Criteria

Criterion 1:

- Parameter δ controls the "acceptable error".
- Sometimes, computing f(x) involves other numerical operations that add errors to the computation of f.
- \circ We should take that into account when choosing a value for δ

Bisection Method — Stopping Criteria

Criterion 2:

The size of the interval is too small whenever

$$\frac{x^R - x^L}{(1 + |x^L| + |x^R|)} \le \varepsilon$$

- No sense in choosing $\varepsilon=0$, unachievable. Same for $\varepsilon=10^{-130}$, computers store finite digits.
- Bear in mind the sizes of x^L and x^R . If x^L and x^R are of the order 10^{10} , convergence of $x^R x^L < 10^{-5}$ is infeasible.
- o Note that adding 1 avoids problems when $x^R pprox x^L pprox 0$

Bisection Method — Stopping Criteria

Criterion 3:

- \circ We can compute the minimum number of iterations N to achieve accuracy δ
- \circ We want the length of the interval after N iterations lower than δ

$$\frac{x^R - x^L}{2^N} \le \delta \Rightarrow 2^N \ge \frac{x^R - x^L}{\delta}$$

taking logs on both sides and simplifying

$$N \ge \frac{\log(x^R - x^L) - \log(\delta)}{\log(2)}$$

which depends on the length of the interval $[x^L, x^R]$ and the value of δ

Bisection Method — Example

Compute the positive root of $f(x) = x^3 - 6x^2 + 11x - 6$

- 1. Find the interval $[x^L, x^R]$
- 2. The function has three positive roots, let's focus on the one on the interval [2.5,4]
- 3. Note $f(2.5)f(4) = -2.25 < 0 \Rightarrow$ by IVT there is a root in [2.5,4]
- 4. Choose $\delta=10^{-4}$ and $\varepsilon=10^{-8}$
- 5. The minimum number of iterations needed to achieve accuracy δ is $N^{min}=13.8$, choose $N=N^{min}+50$

Bisection Method — The Actual Code

• Initialize with a while loop with three conditionals

```
while (error_f > delta) && (error_i > epsil) && (it < maxit
)
% Actual algorithm in here
end</pre>
```

Middle steps

```
1 % Compute xm
2 xm = xl + (xr - xl) / 2; % Slightly improves performance
3
4 % Compute value of f at xm
5 fxm = myf(xm);
6
7 % Compute bounds values of f
8 fxl = myf(xl);
9 fxr = myf(xr);
```

Bisection Method — The Actual Code

Compute errors

```
1 % Compute errors
2 error_f = abs(fxm);
3 error_i = (xr - xl)./(1 + abs(xl) + abs(xr));
```

Update iteration counter and refine interval

```
1 % Update iteration counter
2 it = it + 1;
3
4 % Update if necessary
5 if fxm*fxl < 0
6     xr = xm;
7 else
8     xl = xm;
9 end</pre>
```



Newton-Raphson — Existence, Uniqueness, and Convergence

Theorem 3 (Fixed-Point Iteration Theorem)

Let f(x) = 0 be written as x = g(x). Let g(x) satisfy:

- 1. $\forall x \in [a,b], g(x) \in [a,b]$
- 2. $g'(x) \in (a,b)$ and, for $q \in (0,1)$, g'(x) satisfies |g'(x)| < q for all $x \in (a,b)$ then
 - 1. $\exists ! c \in (a, b) : g(c) = c$ (Existence of a unique solution)
 - 2. For any $x_0 \in [a,b]$, the sequence $\{x_k\}$ defined by

$$x_{k+1} = g(x_k)$$
, $k = 0, 1, ...$

converges to the fixed point c = g(c), that is to the root c of f(x) = 0.

Newton-Raphson Method — Example

As with the bisection method, let's compute the root of $f(x) = x^3 - 6x^2 + 11x - 6$ in the interval [2.5, 4]. Keep the same stopping criteria parameters.

- 1. Choose N=64, $\delta=10^{-4}$, and $\varepsilon=10^{-8}$
- 2. Choose $x_0 = 2.65$.

Newton-Raphson Method — The Actual Code

• Initialize with a while loop with three conditionals as in bisection

```
while (error_f > delta) && (error_i > epsil) && (it < maxit
)
Actual algorithm in here
end</pre>
```

Middle steps

```
1 % Compute next guess
2 xkp = xk - myf(xk) ./ fprime(xk);
3
4 % Compute the errors at current guess
5 error_f = abs(myf(xk));
6 error_i = abs(xk - xkp) ./ (1 + abs(xkp));
7
8 % Update iteration counter and guess
9 it = it+1;
10 xk = xkp;
```

Newton-Raphson vs Bisection

- In previous example, it took 14 iterations for the bisection method to find a solution.
- o It took Newton-Raphson half of those. In 7 iterations it was done.
- Both achieved the same solution.
- Note that the first guess for bisection yields $x^M=3.25$. If we start Newton-Raphson with that guess, only 4 iterations are needed.
- If we give Newton-Raphson $x_0 = 2.5$, we end up in the root $x^* = 1$.
- Both methods have pros and cons. It depends on the problem which one to choose.