Root Finding

- Basic methods can be understood by looking at the function graphically.

- Function $f(x)$ has a zero at $x_\star$.
- Note the sign of $f(x)$ changes at the root.
Bisection

- Simplest method: bisection

- Evaluate at $x_1$ and $x_2$: $f(x_1)$ and $f(x_2)$
- If these are different signs, then the root lies between them
- Evaluate at the midpoint: $x_m = (x_1 + x_2)/2$ getting $f(x_m)$
- The root lies in one of the two intervals—repeat the process
Bisection

- Need two initial points (guesses) that you believe bound the root
  - If there are two roots in-between, then you are in trouble
  - Some pathological cases: e.g. \( f(x) = x^2 \)
- Convergence can be slow—each iteration reduces the error by a factor of 2
Bisection

root approx = 0.0
If we know $d f / dx$ we can do better

- Start with an initial guess, $x_0$, that is “close” to the root
- Taylor expansion:
  
  $f(x_0 + \delta) \approx f(x_0) + f'(x_0)\delta + \ldots$

- If we are close, then

  $f(x_0 + \delta) \approx 0 \quad \rightarrow \quad \delta = -\frac{f(x_0)}{f'(x_0)}$

- Update

  $x_1 = x_0 + \delta$

- We can continue, iterating again and again, until the change in the root is $< \varepsilon$

- Converges fast: usually only a few iterations are needed
Newton-Raphson

- Requirements for good convergence:
  - Derivative must exist and be non-zero in the interval near the root
  - Second derivative must be finite
  - $x_0$ must be close to the root
- Can be used with systems (we'll see this later)
- Multiple roots?
  - Generally: try to start with a good estimate

*not a guarantee
• Basins

- Consider \( q(x) = x^3 - 2x^2 - 11x + 12 \) (example from Wikipedia / Dence, T. 1997)

<table>
<thead>
<tr>
<th>( x_0 )</th>
<th>root</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.35287527</td>
<td>4.0</td>
</tr>
<tr>
<td>2.35284172</td>
<td>-3.0</td>
</tr>
<tr>
<td>2.35283735</td>
<td>4.0</td>
</tr>
<tr>
<td>2.352836327</td>
<td>-3.0</td>
</tr>
<tr>
<td>2.352836323</td>
<td>1.0</td>
</tr>
</tbody>
</table>
• Consider $f(x) = x^3 - 2x + 2$
  
  – Start with $0 \rightarrow 1 \rightarrow 0 \rightarrow 1 \rightarrow 0 \ldots$
  
  – Cycle
Secant Method

- If we don't know $df/dx$, we can still use the same ideas
  - We need to initial guesses: $x_{-1}$ and $x_0$
  - Use approximate derivative
    \[
    x_1 = x_0 - \frac{f(x_0)}{[f(x_0) - f(x_{-1})]/(x_0 - x_{-1})}
    \]
  - Used when an analytic derivative is unavailable, or too expensive to compute (e.g. EOS)
Practical Notes

- N-R is used successfully with equations of state
  - Function takes $\rho$, $T$ and we want to come in with $P$, $\rho$
  - Requires well-behaved derivatives and an initial guess
- Secant method is used, for example, in Riemann solvers in hydrodynamics, where EOS evaluations can be expensive or the derivative may not be known