Physics 331
Introduction to Numerical Techniques in Physics

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So far:

- Number representation
- Sources of error
- Introductory MATLAB: command line, functions, programs
- Instructions for turning in homework
- Round-off errors in practice
- Root-finding algorithms: Bisection, Secant, False-position, Newton-Raphson, Fixed-point
Today:

- Quick review
- Discussion of results
- A bit about convergence
- Higher dimensions
Root-finding: Newton-Raphson

Algorithm

1. Choose a point and compute the derivative of the function
2. Calculate the first estimate of the solution by extrapolating to the x axis
3. Calculate the value of the function
4. Update the point and go back to step 1.

Tangent line equation:

\[ y = f'(x_0)(x - x_0) + f(x_0) \]

Setting \( y = 0 \):

\[ x = x_0 - \frac{f(x_0)}{f'(x_0)} \]

\( x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \)
## Root-finding: Summary of 1D methods

<table>
<thead>
<tr>
<th>Bisection</th>
<th>False Position</th>
<th>Secant</th>
<th>Newton-Raphson</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x_{new} = \frac{(a + b)}{2} )</td>
<td>( x_{n+2} = x_{n+1} - \frac{f(x_{n+1})}{f(x_n) - f(x_{n+1})} (x_n - x_{n+1}) )</td>
<td>( x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} )</td>
<td></td>
</tr>
</tbody>
</table>

(a) Midpoint of the interval is new guess. Choose new interval **bracketing root**.

(b) Conditions: Starting points bracketing root.

(c) Failure: touching root.

(d) Convergence: linear

(a) Draw secant through most recent points **bracketing root**.

(b) Conditions: Starting points bracketing root.

(c) Failure: extrema.

(d) Convergence: one-sided, about linear.

(a) Draw secant through most recent points.

(b) Conditions: Starting points within convergence radius.

(c) Failure: extrema.

(d) Convergence: Golden Mean, except at multiple roots.

(a) Draw **tangent** through most recent point.

(b) Conditions: Starting points within convergence radius.

(c) Failure: extrema.

(d) Convergence: quadratic, except at multiple roots.
Root-finding: Fixed-point method

Algorithm

Rewrite the problem:

\[ f(x) = 0 \quad \Rightarrow \quad x = g(x) \]

Iterate on “fixed point”:

\[ x_{new} = g(x_{old}) \]
Root-finding: Fixed-point method

Convergence

Notice that a problem can be re-written as

\[ x = g(x) \]

potentially in many different ways!

**Theorem:** The fixed-point method converges if, in the *neighborhood* of the fixed point,

\[ |g'(x)| < 1 \]

(the iterating function \( g \) is then said to be Lipschitz continuous in that neighborhood)
Root-finding: Fixed-point method

Geometry/Example

\[ f(x) = x - \cos x \quad g(x) = \cos x \]
Root-finding: Fixed-point method

Example

\[ f(x) = x^2 - 2x - 3 \]

Step 1: Work out the three possible fixed-point methods \( x = g(x) \)

\[
\begin{align*}
g_1 &= \frac{x^2 - 3}{2} \\
g_2 &= \sqrt{2x + 3} \\
g_3 &= \frac{3}{x - 2}
\end{align*}
\]

Step 2: Each group 1,2,3 work out the following:

(a) Calculate the derivative of \( g \)
(b) Determine the convergence radius
(c) Solve the equation graphically starting at \( x=4 \)
(d) Find a root! (if possible)
Root-finding: Fixed-point method

Discussion

\[ f(x) = x^2 - 2x - 3 \quad \quad x = g(x) \]

Option \( g_1 \): Convergence region: \(|x| < 1\)
    Starting point is not in that region - expect divergence!

\[ g_1 = \frac{x^2 - 3}{2} \]
\[ g_2 = \sqrt{2x + 3} \]
\[ g_3 = \frac{3}{x - 2} \]
**Root-finding: Fixed-point method**

**Discussion**

\[ f(x) = x^2 - 2x - 3 \quad x = g(x) \]

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Root-finding: Fixed-point method

Discussion

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Root-finding: Fixed-point method

Discussion

\[ f(x) = x^2 - 2x - 3 \quad x = g(x) \]

Option \( g_2 \): Convergence region: \( x > -1 \)
Starting point is in the region - expect convergence!

\[
\begin{align*}
g_1 & = \frac{x^2 - 3}{2} \\
g_2 & = \sqrt{2x + 3} \\
g_3 & = \frac{3}{x - 2}
\end{align*}
\]
Root-finding: Fixed-point method

Discussion

\[ f(x) = x^2 - 2x - 3 \quad x = g(x) \]

Option \( g_3 \): Convergence region: \( x > 3.73 \ldots \) or \( x < 0.268 \ldots \)
Starting point is in the region, but root is not!
Expect divergence!

\[ g_1 = \frac{x^2 - 3}{2} \]
\[ g_2 = \sqrt{2x + 3} \]
\[ g_3 = \frac{3}{x - 2} \]
Root-finding: Fixed-point method

Discussion

\[ f(x) = x^2 - 2x - 3 \quad \quad \quad x = g(x) \]

Option \( g_3 \): Convergence region: \( x > 3.73 \ldots \) or \( x < 0.268 \ldots \)
Starting point is in the region, but root is not!
Expect divergence!

What’s going to happen next?
Root-finding: Fixed-point method

Discussion

\[ f(x) = x^2 - 2x - 3 \quad \Rightarrow \quad x = g(x) \]

Option \( g_3 \): Convergence region: \( x > 3.73 \ldots \) or \( x < 0.268 \ldots \)
Starting point is in the region, but root is not!
Expect divergence!

We do diverge from one of the roots, but end up at the other one by chance!
Root-finding: Fixed-point method

Discussion

\[ f(x) = x^2 - 2x - 3 \]

\[ x = g(x) \]

Option \( g_3 \): Convergence region: \( x > 3.73\ldots \) or \( x < 0.268\ldots \)
Starting point is in the region, but root is not!
Expect divergence!

We do diverge from one of the roots, but end up at the other one by chance!
Root-finding: convergence

Fixed-point method

$$x_{\text{new}} = g(x_{\text{old}})$$

We know that convergence is guaranteed if $$|g'(x)| < 1$$ in the interval of interest.

Knowing this, how fast does this method converge to the answer?
Root-finding: convergence

Newton-Raphson method

\[ x_{new} = x_{old} - \frac{f(x_{old})}{f'(x_{old})} \]

We know that convergence is guaranteed if \( |g'(x)| < 1 \) in the interval of interest.
Root-finding: convergence

Newton-Raphson method

\[ x_{\text{new}} = x_{\text{old}} - \frac{f(x_{\text{old}})}{f'(x_{\text{old}})} \]

We know that convergence is guaranteed if \( |g'(x)| < 1 \) in the interval of interest.

\[ |g'(x)| = \left| \frac{f(x) f''(x)}{[f'(x)]^2} \right| < 1 \]

Check it!
Root-finding: convergence

Newton-Raphson method

\[ x_{new} = x_{old} - \frac{f(x_{old})}{f'(x_{old})} \]

We know that convergence is guaranteed if \( |g'(x)| < 1 \) in the interval of interest.

\[ |g'(x)| = \left| \frac{f(x)f''(x)}{[f'(x)]^2} \right| < 1 \]

Knowing this, how fast does this method converge to the answer?
Root-finding: Systems of equations

Now we have

\[ F_1(x_1, x_2, \ldots) = 0 \]
\[ F_2(x_1, x_2, \ldots) = 0 \]
\[ \vdots \]

We need to generalize our methods to higher dimensions!

We may expand the functions in a Taylor series

\[ F_i(x + \delta x) = F_i(x) + \sum_{j=1}^{n} \frac{\partial F_i}{\partial x_j} \delta x_j + O(\delta x^2) \]

...and if we are really approaching the root we will have

\[ F_i(x + \delta x) = 0 \]

...this means that our new point should be, in the linear approximation, given by

\[ x_{new} = x_{old} + \delta x \]

where \[ J \cdot \delta x = -F \]
Construct your own Newton-Raphson root finder for the function

\[ f(z) = z^3 - 1 \]

where \( z = x + iy \) is a complex variable.
Root-finding: build your own Newton-Raphson!

Exercise:
Construct your own Newton-Raphson root finder for the function

\[ f(z) = z^3 - 1 \]

where \( z = x + iy \) is a complex variable.

Split the problem at each table:

Group 1: Write the function as two real-valued functions of two variables \( x, y \)
Group 2: Calculate the Jacobian and its inverse (need to communicate with group 1!)
Group 3: Write a pseudo-code, including convergence conditions.