

2072U Computational Science I

Winter 2022

Week	Topic
1	Introduction
1–2	Solving nonlinear equations in one variable
3–4	Solving systems of (non)linear equations
5–6	Computational complexity
6–8	Interpolation and least squares
8–10	Integration & differentiation
10–12	Additional Topics

1. Error plotting
2. Recursion
3. Newton-Raphson iteration

Bisection

Bisection

- ▶ Evaluate function only.

Bisection

- ▶ Evaluate function only.
- ▶ Need to find a and b such that f is continuous and has unique zero on $[a, b]$.

Bisection

- ▶ Evaluate function only.
- ▶ Need to find a and b such that f is continuous and has unique zero on $[a, b]$.
- ▶ Upper bound for error:

$$|x^{(k)} - x^*| \leq \epsilon^{(k)} = |b^{(k)} - a^{(k)}|$$

Bisection

- ▶ Evaluate function only.
- ▶ Need to find a and b such that f is continuous and has unique zero on $[a, b]$.
- ▶ Upper bound for error:

$$|x^{(k)} - x^*| \leq \epsilon^{(k)} = |b^{(k)} - a^{(k)}|$$
- ▶ Decreases as

$$\epsilon^{(k+1)} = \epsilon^{(k)} / 2 \dots$$

Bisection

- ▶ Evaluate function only.
- ▶ Need to find a and b such that f is continuous and has unique zero on $[a, b]$.
- ▶ Upper bound for error:

$$|x^{(k)} - x^*| \leq \epsilon^{(k)} = |b^{(k)} - a^{(k)}|$$
- ▶ Decreases as

$$\epsilon^{(k+1)} = \epsilon^{(k)} / 2 \dots$$
- ▶ ... so that $\epsilon^{(k)} = \epsilon^{(0)} / 2^k$.
 aka **linear** convergence.

Bisection

- ▶ Evaluate function only.
- ▶ Need to find a and b such that f is continuous and has unique zero on $[a, b]$.
- ▶ Upper bound for error:
 $|x^{(k)} - x^*| \leq \epsilon^{(k)} = |b^{(k)} - a^{(k)}|$
- ▶ Decreases as
 $\epsilon^{(k+1)} = \epsilon^{(k)} / 2 \dots$
- ▶ ... so that $\epsilon^{(k)} = \epsilon^{(0)} / 2^k$.
 aka **linear** convergence.
- ▶ Straight line on semilog plot.

Bisection

- ▶ Evaluate function only.
- ▶ Need to find a and b such that f is continuous and has unique zero on $[a, b]$.
- ▶ Upper bound for error:
 $|x^{(k)} - x^*| \leq \epsilon^{(k)} = |b^{(k)} - a^{(k)}|$
- ▶ Decreases as
 $\epsilon^{(k+1)} = \epsilon^{(k)} / 2 \dots$
- ▶ ... so that $\epsilon^{(k)} = \epsilon^{(0)} / 2^k$.
 aka **linear** convergence.
- ▶ Straight line on semilog plot.
- ▶ Works only for one unknown.

Bisection

- ▶ Evaluate function only.
- ▶ Need to find a and b such that f is continuous and has unique zero on $[a, b]$.
- ▶ Upper bound for error:
 $|x^{(k)} - x^*| \leq \epsilon^{(k)} = |b^{(k)} - a^{(k)}|$
- ▶ Decreases as
 $\epsilon^{(k+1)} = \epsilon^{(k)} / 2 \dots$
- ▶ ... so that $\epsilon^{(k)} = \epsilon^{(0)} / 2^k$.
 aka **linear** convergence.
- ▶ Straight line on semilog plot.
- ▶ Works only for one unknown.

Newton/secant

Bisection

- ▶ Evaluate function only.
- ▶ Need to find a and b such that f is continuous and has unique zero on $[a, b]$.
- ▶ Upper bound for error:
 $|x^{(k)} - x^*| \leq \epsilon^{(k)} = |b^{(k)} - a^{(k)}|$
- ▶ Decreases as
 $\epsilon^{(k+1)} = \epsilon^{(k)} / 2 \dots$
- ▶ ... so that $\epsilon^{(k)} = \epsilon^{(0)} / 2^k$.
 aka **linear** convergence.
- ▶ Straight line on semilog plot.
- ▶ Works only for one unknown.

Newton/secant

- ▶ Uses function *and* derivative/two initial points.

Bisection

- ▶ Evaluate function only.
- ▶ Need to find a and b such that f is continuous and has unique zero on $[a, b]$.
- ▶ Upper bound for error:
 $|x^{(k)} - x^*| \leq \epsilon^{(k)} = |b^{(k)} - a^{(k)}|$
- ▶ Decreases as
 $\epsilon^{(k+1)} = \epsilon^{(k)} / 2 \dots$
- ▶ ... so that $\epsilon^{(k)} = \epsilon^{(0)} / 2^k$.
 aka **linear** convergence.
- ▶ Straight line on semilog plot.
- ▶ Works only for one unknown.

Newton/secant

- ▶ Uses function *and* derivative/two initial points.
- ▶ Function must be *continuously differentiable* /continuous around x^* .

Bisection

- ▶ Evaluate function only.
- ▶ Need to find a and b such that f is continuous and has unique zero on $[a, b]$.
- ▶ Upper bound for error:
 $|x^{(k)} - x^*| \leq \epsilon^{(k)} = |b^{(k)} - a^{(k)}|$
- ▶ Decreases as
 $\epsilon^{(k+1)} = \epsilon^{(k)} / 2 \dots$
- ▶ ... so that $\epsilon^{(k)} = \epsilon^{(0)} / 2^k$.
 aka **linear** convergence.
- ▶ Straight line on semilog plot.
- ▶ Works only for one unknown.

Newton/secant

- ▶ Uses function *and* derivative/two initial points.
- ▶ Function must be *continuously differentiable* /continuous around x^* .
- ▶ Need one/two initial guesses.

Bisection

- ▶ Evaluate function only.
- ▶ Need to find a and b such that f is continuous and has unique zero on $[a, b]$.
- ▶ Upper bound for error:
 $|x^{(k)} - x^*| \leq \epsilon^{(k)} = |b^{(k)} - a^{(k)}|$
- ▶ Decreases as
 $\epsilon^{(k+1)} = \epsilon^{(k)} / 2 \dots$
- ▶ ... so that $\epsilon^{(k)} = \epsilon^{(0)} / 2^k$.
 aka **linear** convergence.
- ▶ Straight line on semilog plot.
- ▶ Works only for one unknown.

Newton/secant

- ▶ Uses function *and* derivative/two initial points.
- ▶ Function must be *continuously differentiable* /continuous around x^* .
- ▶ Need one/two initial guesses.
- ▶ Error estimate: $\epsilon^{(k)} \approx |\delta x^{(k)}|$.

Bisection

- ▶ Evaluate function only.
- ▶ Need to find a and b such that f is continuous and has unique zero on $[a, b]$.
- ▶ Upper bound for error:
 $|x^{(k)} - x^*| \leq \epsilon^{(k)} = |b^{(k)} - a^{(k)}|$
- ▶ Decreases as
 $\epsilon^{(k+1)} = \epsilon^{(k)} / 2 \dots$
- ▶ ... so that $\epsilon^{(k)} = \epsilon^{(0)} / 2^k$.
 aka **linear** convergence.
- ▶ Straight line on semilog plot.
- ▶ Works only for one unknown.

Newton/secant

- ▶ Uses function *and* derivative/two initial points.
- ▶ Function must be *continuously differentiable* /continuous around x^* .
- ▶ Need one/two initial guesses.
- ▶ Error estimate: $\epsilon^{(k)} \approx |\delta x^{(k)}|$.
- ▶ Decreases as
 $\epsilon^{(k+1)} \approx (\epsilon^{(k)})^2 \dots$

Bisection

- ▶ Evaluate function only.
- ▶ Need to find a and b such that f is continuous and has unique zero on $[a, b]$.
- ▶ Upper bound for error:
 $|x^{(k)} - x^*| \leq \epsilon^{(k)} = |b^{(k)} - a^{(k)}|$
- ▶ Decreases as
 $\epsilon^{(k+1)} = \epsilon^{(k)} / 2 \dots$
- ▶ ... so that $\epsilon^{(k)} = \epsilon^{(0)} / 2^k$.
 aka **linear** convergence.
- ▶ Straight line on semilog plot.
- ▶ Works only for one unknown.

Newton/secant

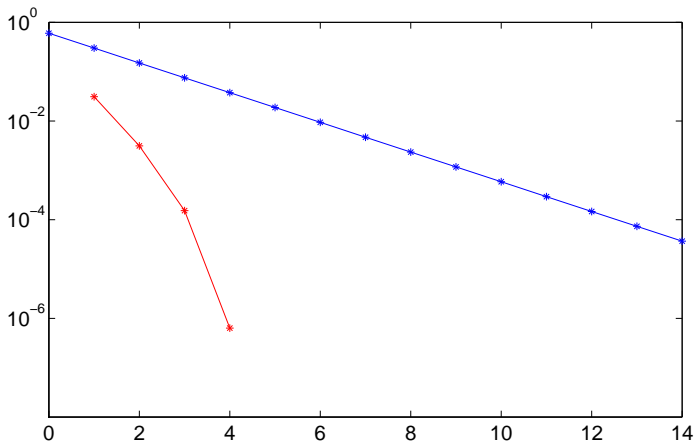
- ▶ Uses function *and* derivative/two initial points.
- ▶ Function must be *continuously differentiable* /continuous around x^* .
- ▶ Need one/two initial guesses.
- ▶ Error estimate: $\epsilon^{(k)} \approx |\delta x^{(k)}|$.
- ▶ Decreases as
 $\epsilon^{(k+1)} \approx (\epsilon^{(k)})^2 \dots$
- ▶ ... so that $\epsilon^{(k)} \approx (\epsilon^{(0)})^{2^k}$.
 aka **quadratic** convergence.

Bisection

- ▶ Evaluate function only.
- ▶ Need to find a and b such that f is continuous and has unique zero on $[a, b]$.
- ▶ Upper bound for error:
 $|x^{(k)} - x^*| \leq \epsilon^{(k)} = |b^{(k)} - a^{(k)}|$
- ▶ Decreases as
 $\epsilon^{(k+1)} = \epsilon^{(k)} / 2 \dots$
- ▶ ... so that $\epsilon^{(k)} = \epsilon^{(0)} / 2^k$.
 aka **linear** convergence.
- ▶ Straight line on semilog plot.
- ▶ Works only for one unknown.

Newton/secant

- ▶ Uses function *and* derivative/two initial points.
- ▶ Function must be *continuously differentiable* /continuous around x^* .
- ▶ Need one/two initial guesses.
- ▶ Error estimate: $\epsilon^{(k)} \approx |\delta x^{(k)}|$.
- ▶ Decreases as
 $\epsilon^{(k+1)} \approx (\epsilon^{(k)})^2 \dots$
- ▶ ... so that $\epsilon^{(k)} \approx (\epsilon^{(0)})^{2^k}$.
 aka **quadratic** convergence.
- ▶ Steeper than linear on semilog plot.



Simple example of *recursive* programming:

```
def bisection(a, b, kMax, epsX, epsF):
    mid = (a+b)/2 ; x = mid
    err = abs(a-b)/2
    fm = func(mid)
    res = abs(fm)
    if (kMax > 0):
        if err > epsX or res > epsF:
            fa = func(a)
            if (fm*fa > 0):
                a = mid
            else:
                b = mid
            x,err,res = bisection(a, b, kMax-1, epsX
                                ,epsF)
    else:
        print("Warning: no convergence...")
    return x,err,res
```

Pros:

Pros:

- ▶ clean, concise, elegant code;
- ▶ conceptually clear.

Cons:

Pros:

- ▶ clean, concise, elegant code;
- ▶ conceptually clear.

Cons:

- ▶ code harder to follow;
- ▶ uses more memory;
- ▶ small mistake can give bad crash!

Newton iteration can be generalized to n equations with n unknowns.

Alternative derivation in 1D:

$$f(x + \delta x) \approx f(x) + f'(x)\delta x = 0 \Rightarrow \delta x = -\frac{f(x)}{f'(x)}$$

Now in 2D. We want to find x_1 and x_2 such that

$$f_1(x_1, x_2) = 0$$

$$f_1(x_1, x_2) = 0$$

Note that, in general, we need **the same number of equations and unknowns** to find (isolated) solutions...

$$f_1(x_1 + \delta x_1, x_2 + \delta x_2) \approx f_1(x_1, x_2) + \frac{\partial f_1}{\partial x_1}(x_1, x_2)\delta x_1 + \frac{\partial f_1}{\partial x_2}(x_1, x_2)\delta x_2$$

$$f_2(x_1 + \delta x_1, x_2 + \delta x_2) \approx f_2(x_1, x_2) + \frac{\partial f_2}{\partial x_1}(x_1, x_2)\delta x_1 + \frac{\partial f_2}{\partial x_2}(x_1, x_2)\delta x_2$$

which gives:

$$\begin{pmatrix} \frac{\partial f_1}{\partial x_1}(x_1, x_2) & \frac{\partial f_1}{\partial x_2}(x_1, x_2) \\ \frac{\partial f_2}{\partial x_1}(x_1, x_2) & \frac{\partial f_2}{\partial x_2}(x_1, x_2) \end{pmatrix} \begin{pmatrix} \delta x_1 \\ \delta x_2 \end{pmatrix} = - \begin{pmatrix} f_1(x_1, x_2) \\ f_2(x_1, x_2) \end{pmatrix}$$