I3344
Numerical Simulation & Modeling

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Tentative Syllabus

- ✓ Interpolation and extrapolation
  - ✓ Linear: linear regression y = ax + b; correlation, standard deviation, etc.
  - ✓ Non-linear: k nearest neighbors (KNN)
  - ✓ Validation of two models: k-fold cross validation method.
- ✓ Multiple Linear Regression
- ✓ Solving a linear equation
  - ✓ Direct methods: Gauss and LU
  - ✓ Iterative methods: Jacobi and Gauss-Seidel
- ✓ Derivation
  - ✓ Finite difference method (FDM): Euler and Runge-kutta
- Integration: surface estimation
  - Monte Carlo method.
  - Finite Element Method (FEM).
- Non-linear problems
  - Bisection method
- Introduction to the notion of parallel computing and underlying algorithms

Outline

- Introduction
- Intermediate Value Theorem
- Bisection Method
- Error Analysis

Introduction

- Linear equations are of the form: *find x such that* $ax+b=0$ and are easy to solve.
- Some non-linear problems are also easy to solve, e.g., *find x such that* $ax^2 + bx + c = 0$.
- <u>Cubic and quartic equations</u> also have solutions for which we can obtain a formula.
- But **most equations to not have simple formulae for their solutions**, so **numerical methods are needed.**

Introduction (cont'd)

- Our generic problem is:

Let f be a continuous function on the interval [a, b].

Find τ = [a, b] such that $f(\tau) = 0$.

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f is some specified function, and τ is the solution to f(x)=0.

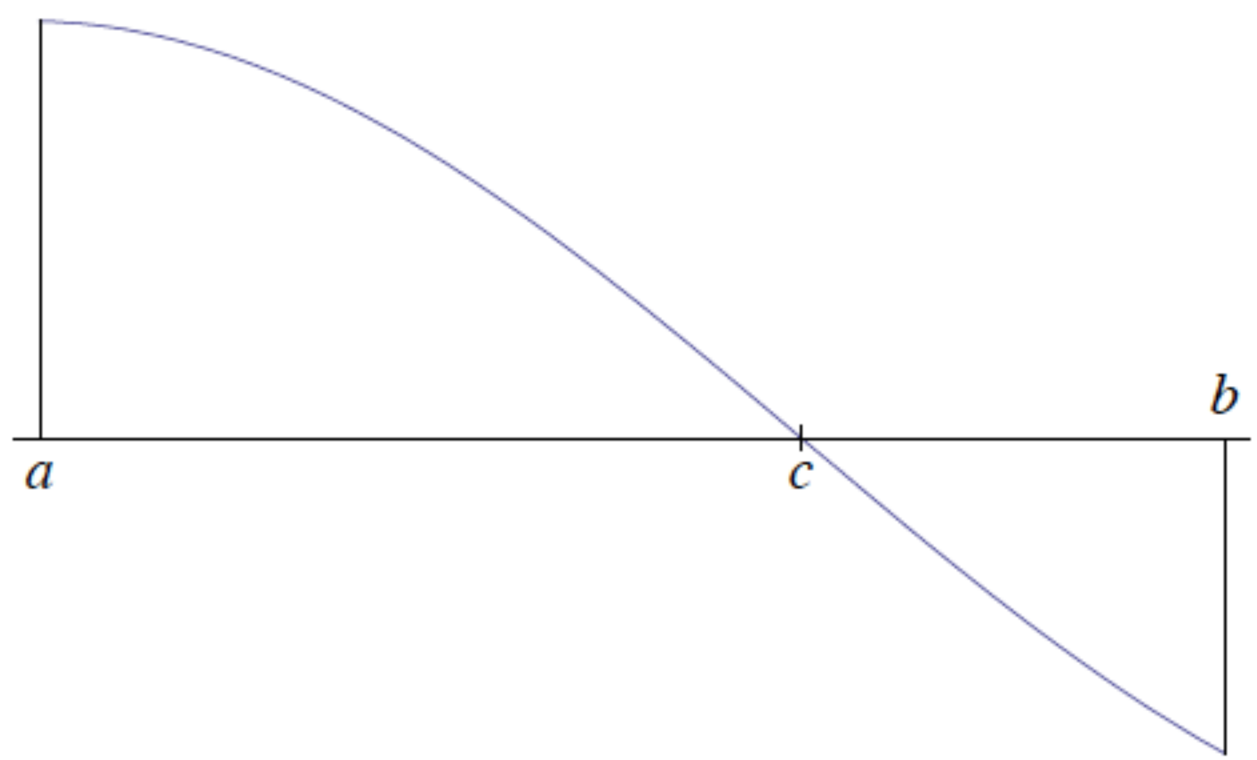
- This leads to two natural questions:

    1. **How do we know there is a solution?**
    2. **How do we find it?**

Intermediate Value Theorem

- Sufficient conditions for the existence of a solution:

Let f be a real-valued function that is ***defined and continuous*** *on a bounded closed interval [a, b] ⊂ R. Suppose that* ***f(a)*f(b) ≤ 0,***
Then ***there exists τ ∈ [a, b] such that f (τ) = 0.***



Bisection Method

- The most elementary algorithm
- Also known as "Interval Bisection"
- Suppose that we know that f changes sign on the interval $[a,b] = [x_0,x_1]$ and, thus, $f(x) = 0$ has a solution, τ, in $[a, b]$.
- Proceed as follows
  - Set x_2 to be the **midpoint of the interval** $[x_0,x_1]$.
  - Choose one of the sub-intervals $[x_0, x_2]$ and $[x_2, x_1]$ **where f changes sign**
  - **Repeat Steps 1–2** on that sub-interval, **until f sufficiently small** at the end points of the interval.

Bisection Method - Algorithm

Set ***<u>eps</u>*** *to be the stopping criterion.*

If $|f(a)| \leq eps$, *return a. Exit.*

If $|f(b)| \leq eps$, *return b. Exit.*

Set $x_0 = a$ *and* $x_1 = b$.

Set $x_L = x_0$ *and* $x_R = x_1$. *Set* $k = 1$

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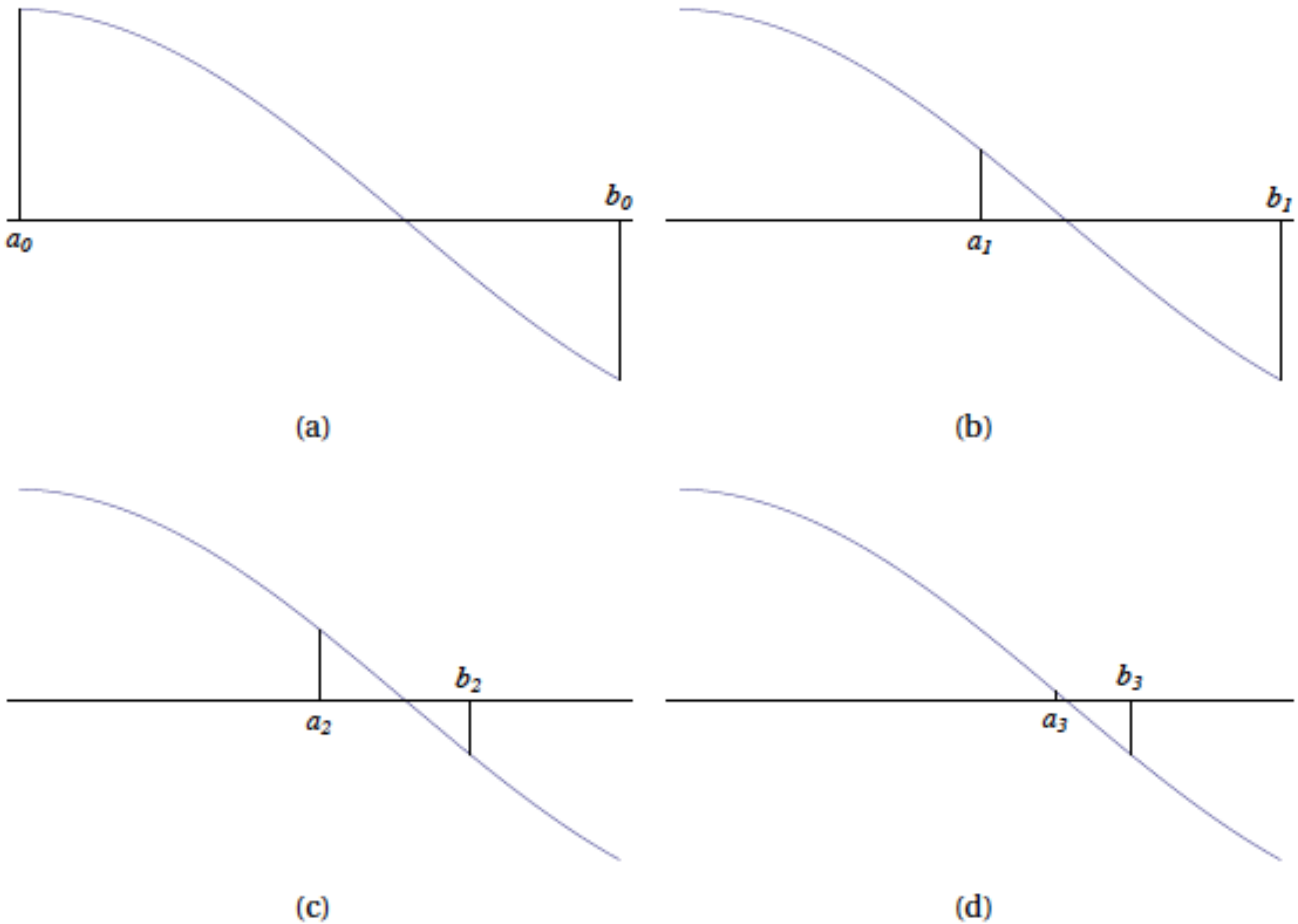
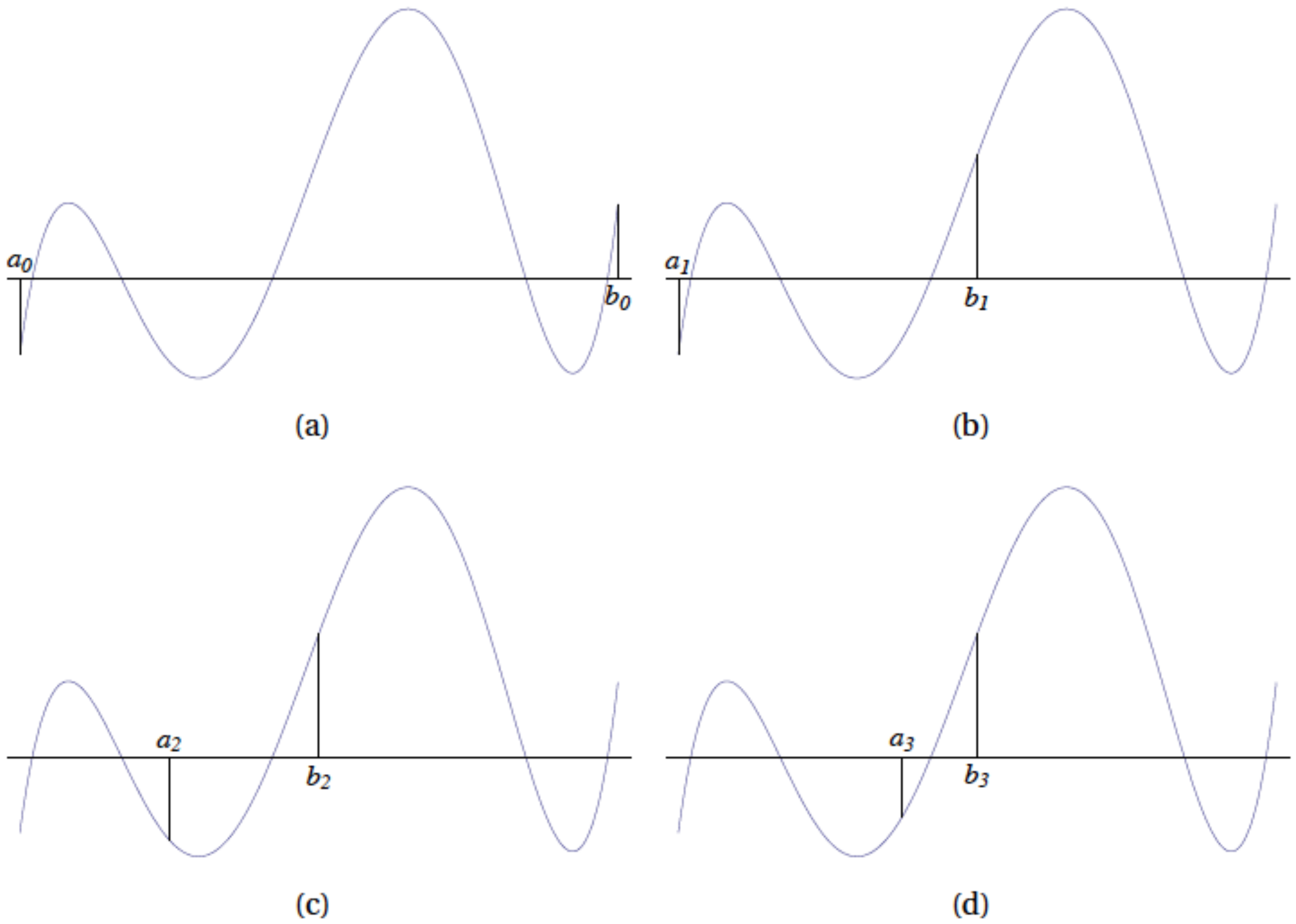
while( |f(x_k)| > eps )
  x_{k+1} = (x_L + x_R)/2;
  if (f(x_L) f(x_{k+1}) < 0)
    x_R = x_{k+1};
  else
    x_L = x_{k+1}
  end if;
  k = k+1
end while;
```

Bisection Method - Examples



Bisection Method - Examples



Error Analysis

- Suppose f is a function with a zero c in the interval [a, b] . If the midpoint $x_2 = (a + b)/2$ of [a, b] is used as an approximation to c, the error is bounded by

$$|c - x_2| \leq \frac{a-b}{2}$$

- Repeating the algorithm for N iterations will result in the following error

$$|c - x_{N+2}| \leq \frac{a-b}{2^{N+1}}$$

- Number of steps necessary to achieve a certain error $\in$

$$|c - x_{N+2}| \leq \frac{a-b}{2^{N+1}} \leq \epsilon$$

$$N \geq \frac{ln(b-a) - ln\epsilon}{ln2} - 1$$

Lab 6