Computational Astrophysics

ASTR 660, Spring 2021
計算天文物理

Lecture 6

Nonlinear equations / Integration / Differentiation / Random numbers

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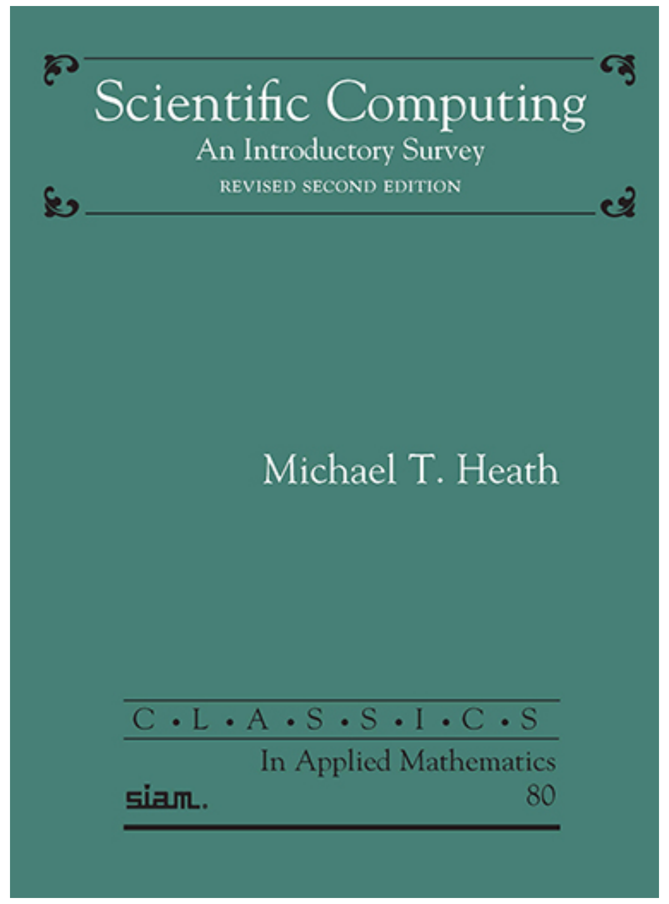
Class website

https://kuochuanpan.github.io/courses/109ASTR660_CA/

Plan for today

- Nonlinear equations
- Numerical Integration
- Random numbers
- Numerical differentiation



Reference:

“Scientific Computing: An introductory survey”, Michael Heath

Chapter 5, chapter 8, and chapter 13

https://books.google.com.tw/books?id=f6Z8DwAAQBAJ&hl=zh-TW

Nonlinear equations

Nonlinear equations

In astrophysical environments, often the relevant system of equations is not linear in the unknowns

Thus, the system cannot be approximated by $\boldsymbol{A} \cdot \boldsymbol{x} = (b)$

In stead, we could write it as:

$$f(x) = 0 \quad \text{1D}$$

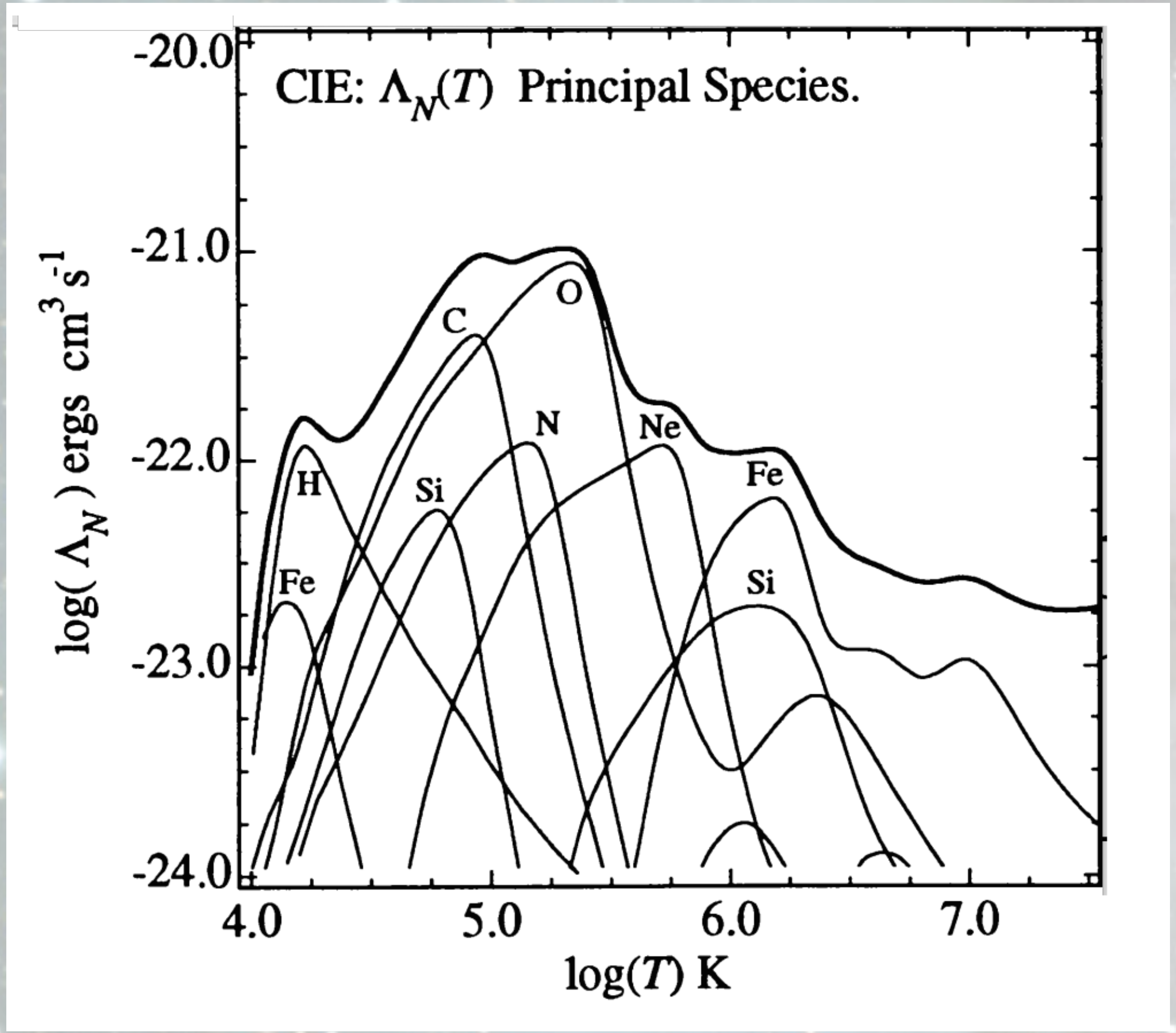
$$\boldsymbol{f}(\boldsymbol{x}) = 0 \quad \text{nD}$$

Nonlinear equations

- In 1D, the problem is reduced to solving for root(s) of the function f.
- In 1D, it is usually possible to trap or bracket the physical solution and hunt them down
- Not guaranteed to have any real solutions, but generally do for astrophysical problems
- All root-finding methods proceed by iteration, improving from a trial solution until converged

Example: Temperature of ISM

Example: Temperature of ISM



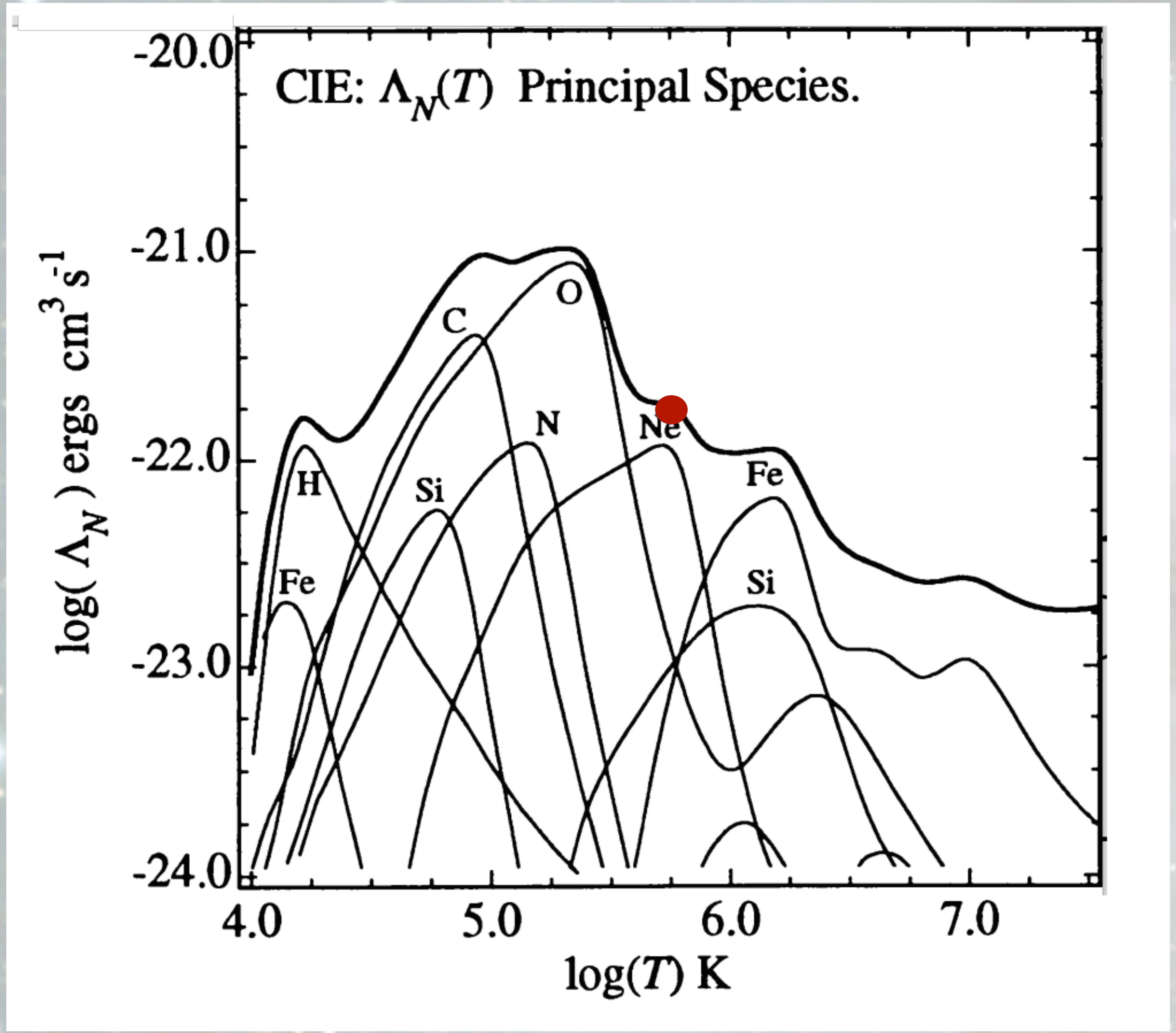
Cooling:

- Bremsstrahlung: collision between electrons and ions
- Radiative cooling: atom-electron collisions
- Thermal radiation from dust grains

Heating:

- Heating from nearby stars
- Heating from cosmic-rays

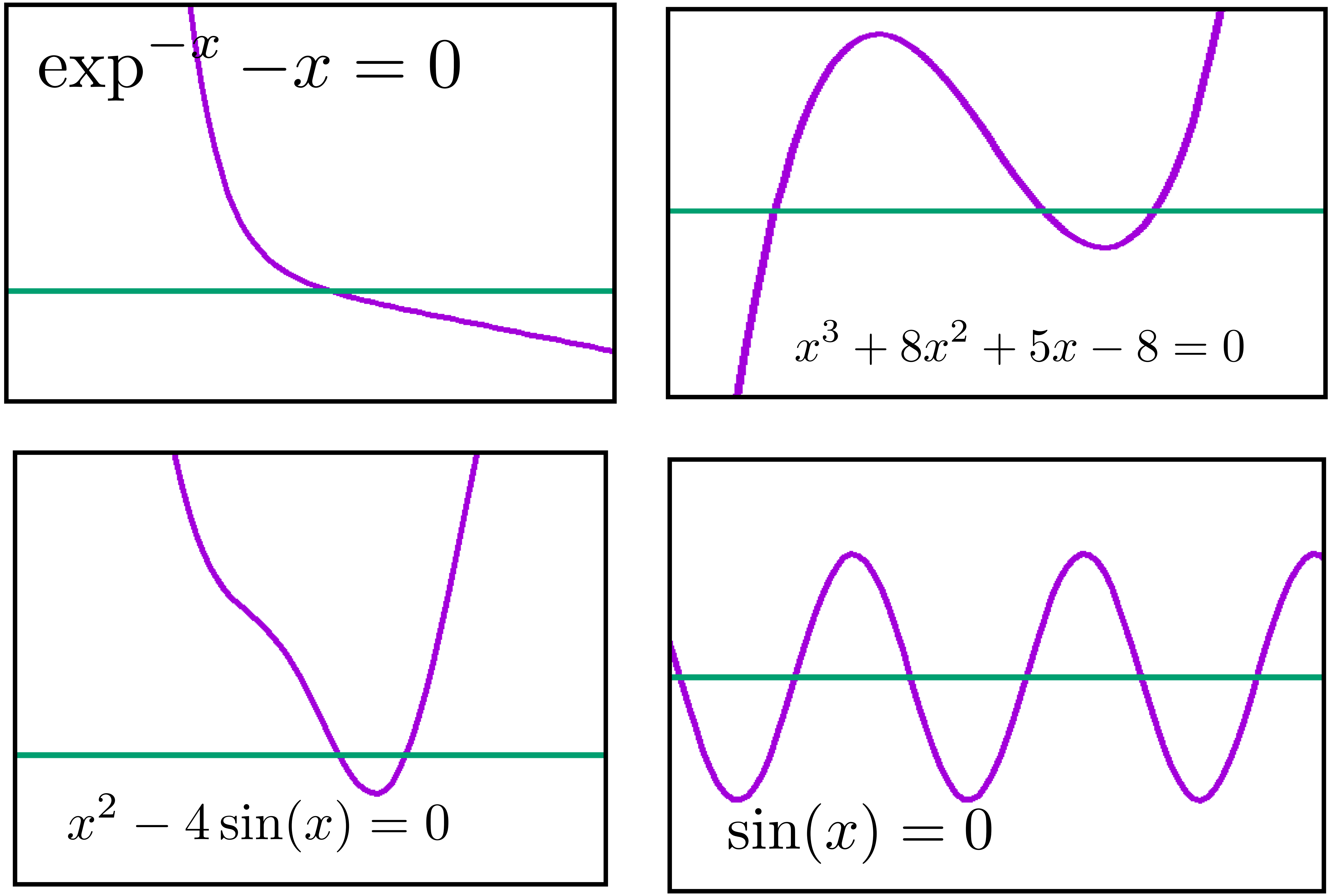
Example: Temperature of ISM



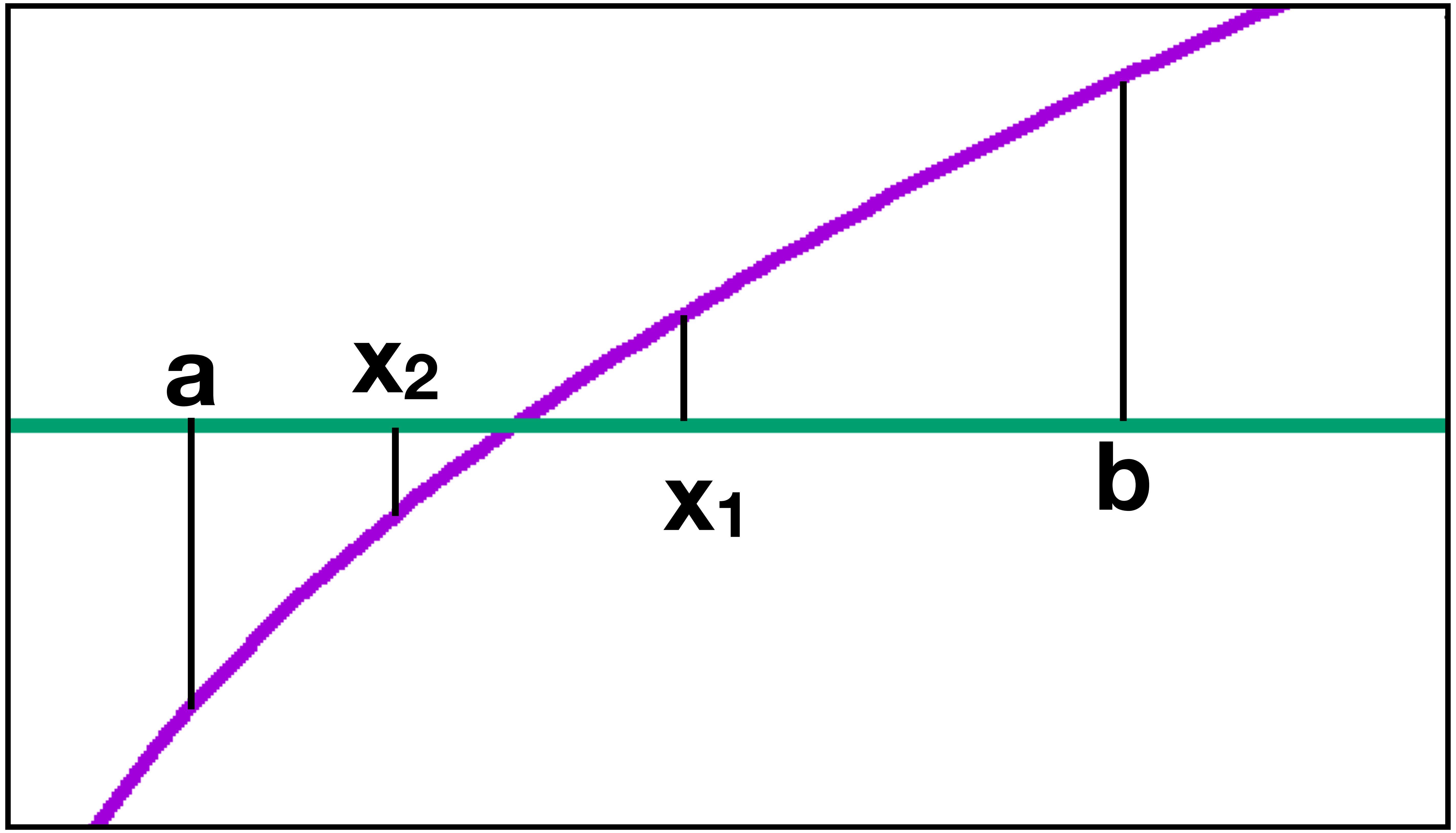
Question:

Find T, such that H - C(T) = 0

Graphical Search



Bisection method



If f(a) and f(x) have different sign, update b.

If f(a) and f(x) have the same sign, update a.

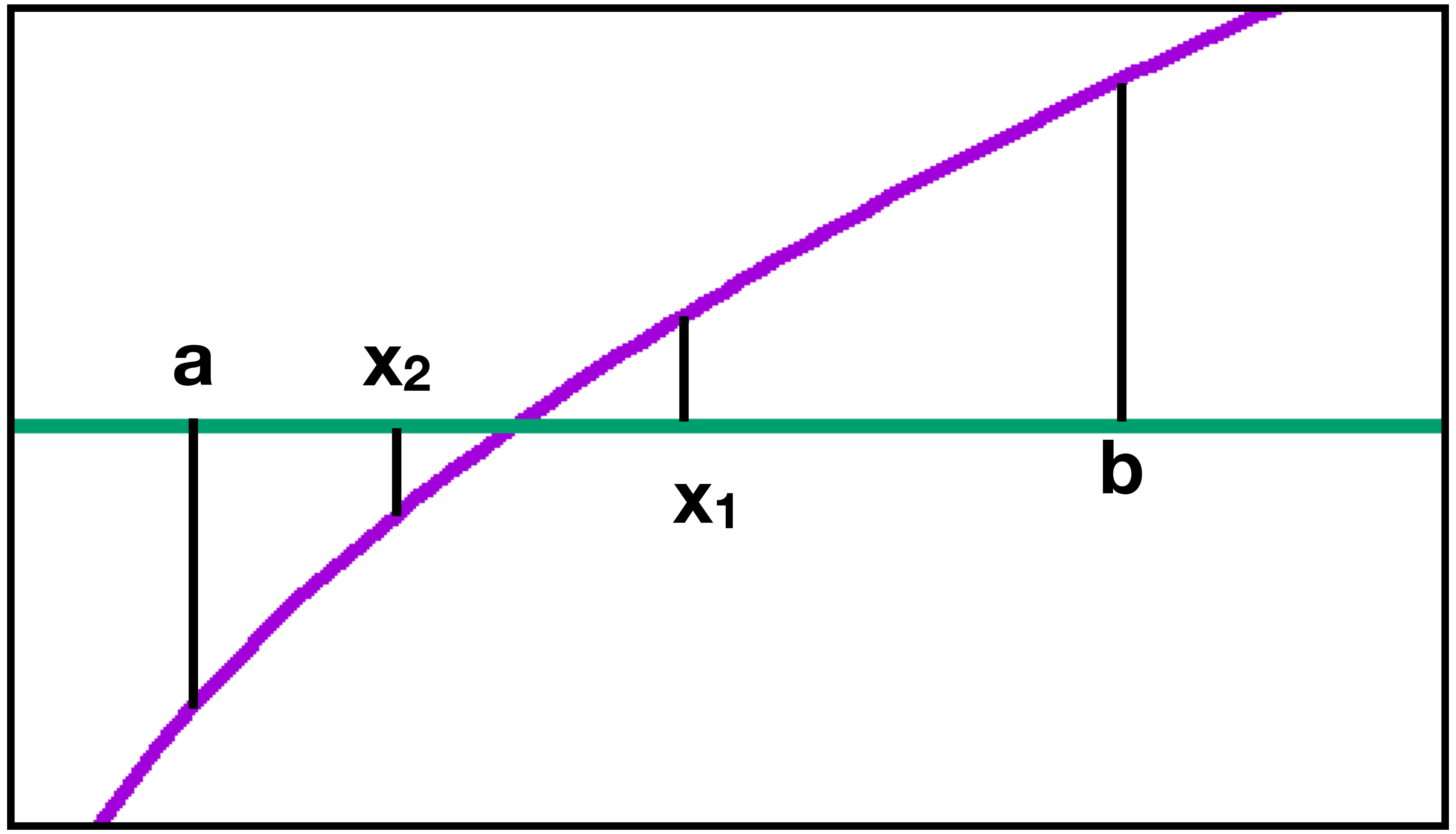
x =(a+b)/2

Bisection is robust, but slow converging

The length of bracket after k iteration is $(b-a)/2^k$

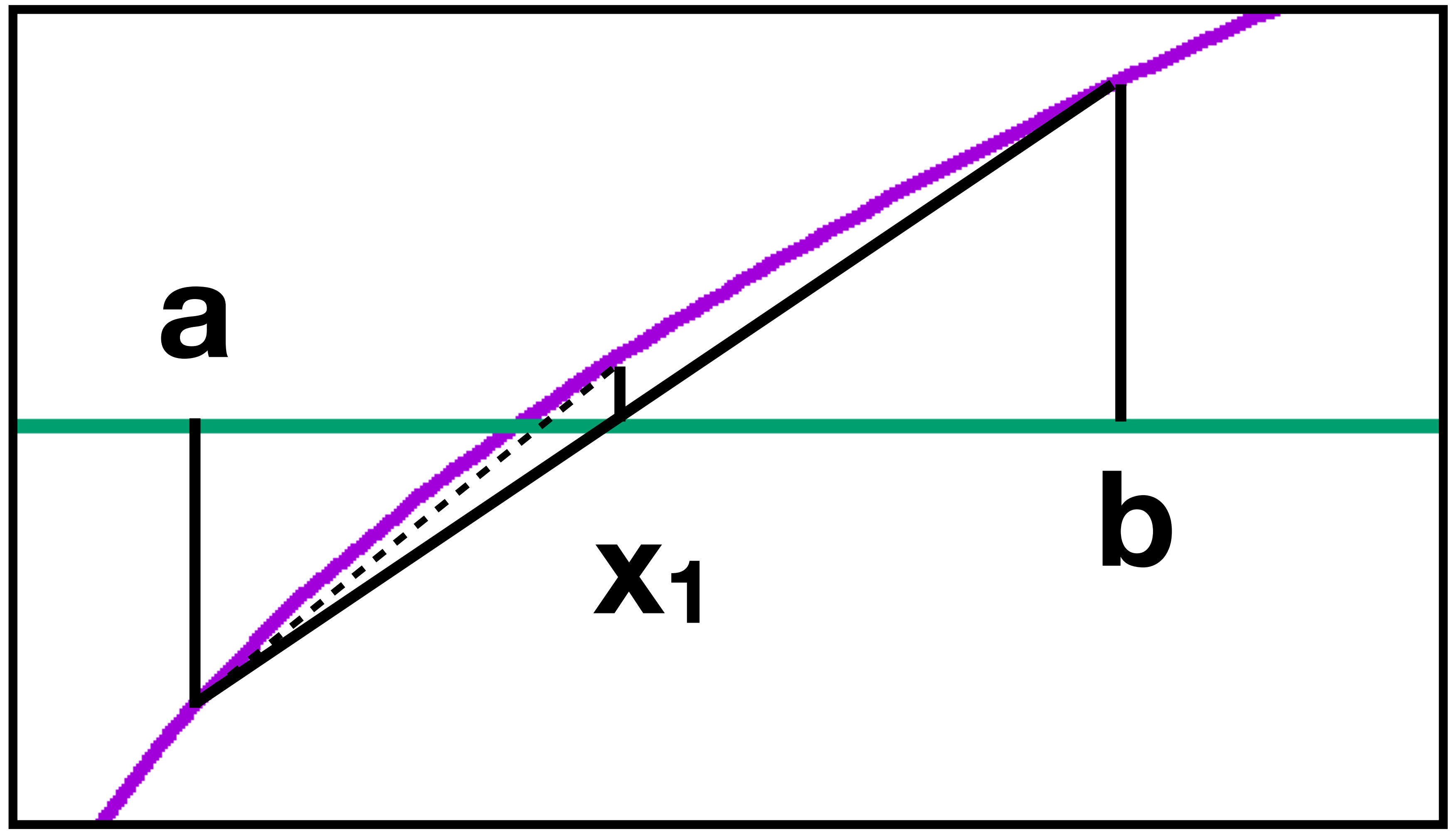
Exercise Bisection method

$$f(x) = x^2 - 4\sin(x) = 0$$



- If f(a) and f(x) have different sign, update b.
- If f(a) and f(x) have the same sign, update a.
- x =(a+b)/2

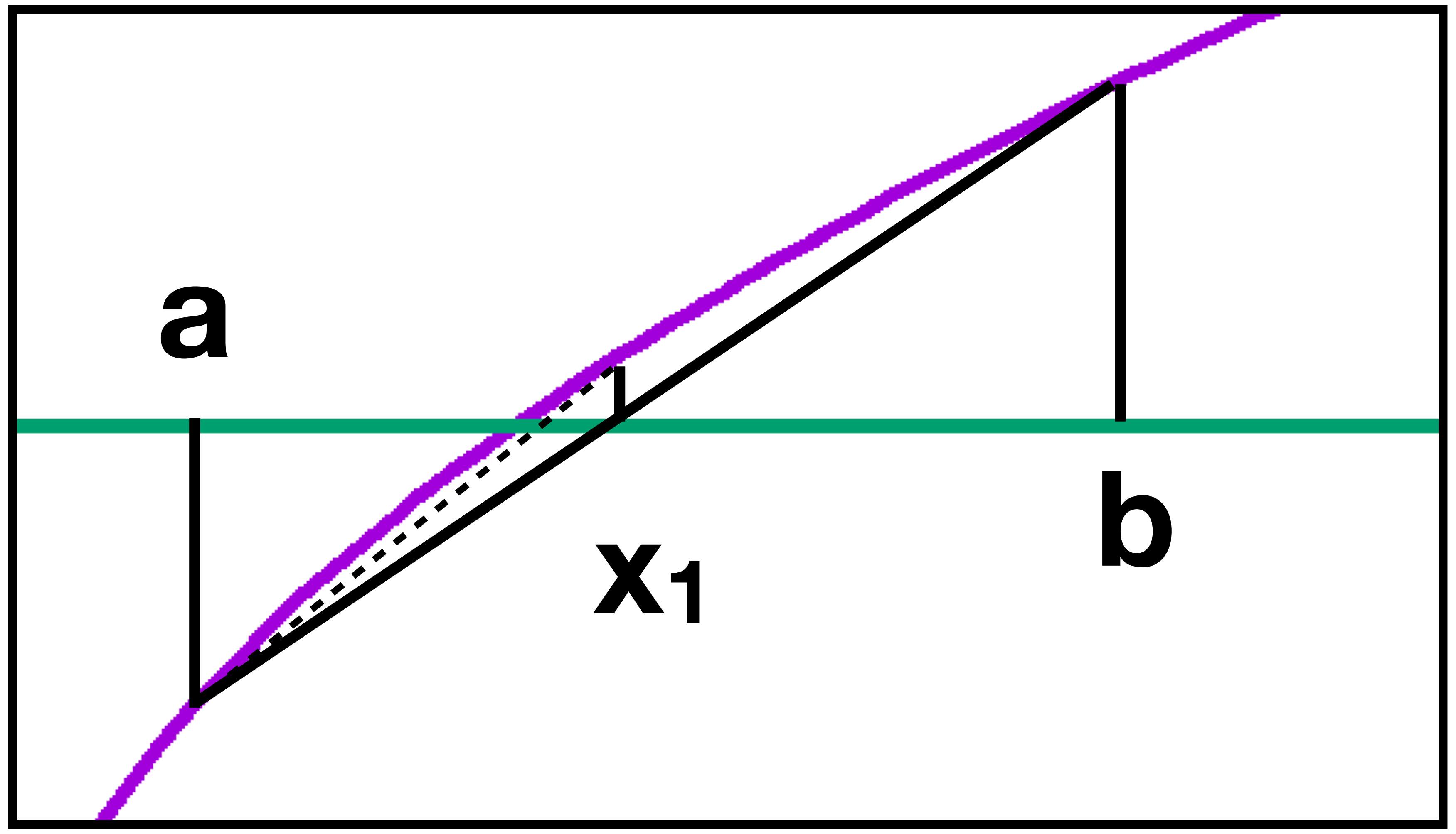
False position method



- If f(a) and f(x) have different sign, update b.
- If f(a) and f(x) have the same sign, update a.
- $x = a - f(a)\,(b-a)/(f(b) - f(a))$

Exercise: False position method

$$f(x) = x^2 - 4\sin(x) = 0$$

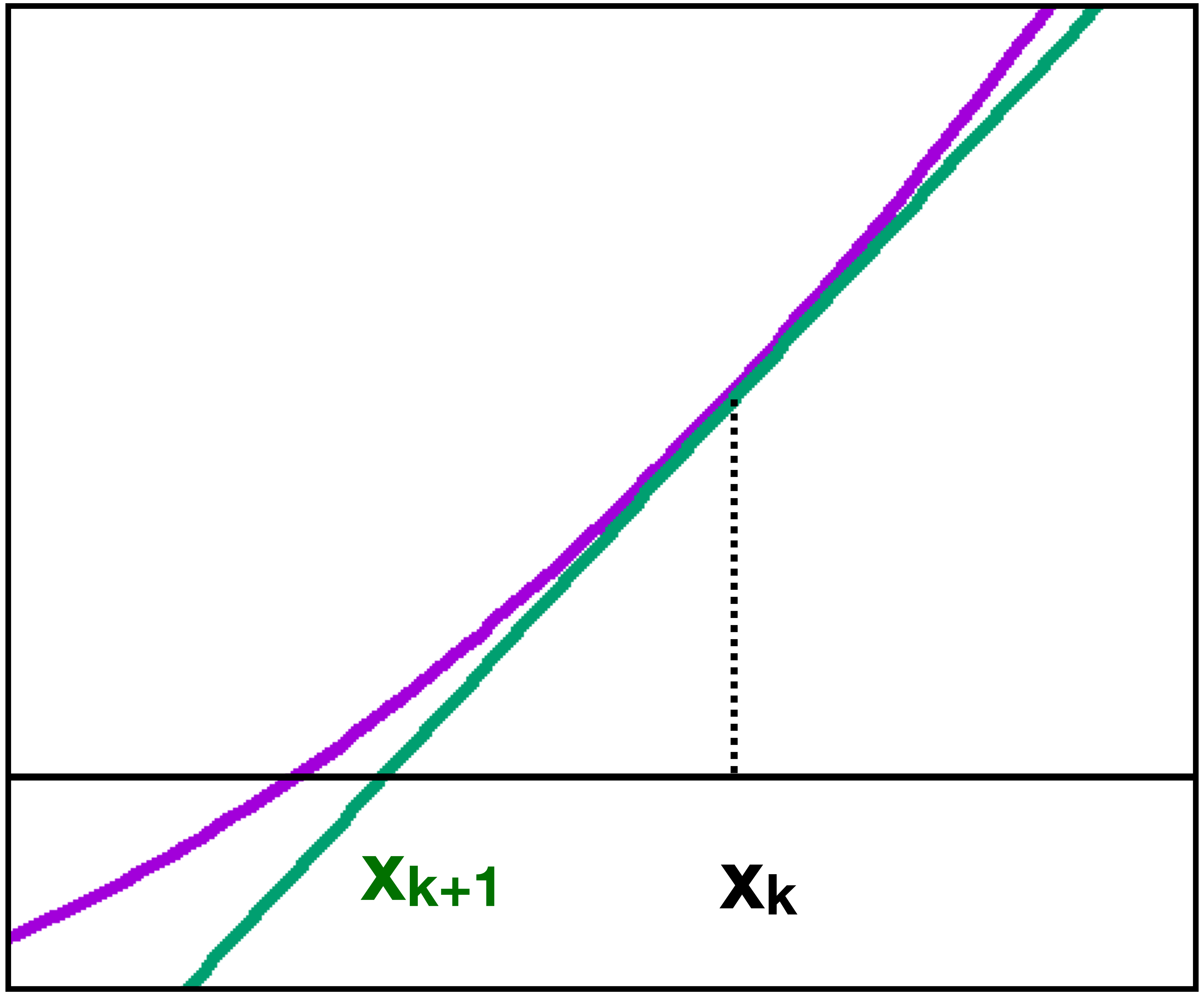


If f(a) and f(x) have different sign, update b.

If f(a) and f(x) have the same sign, update a.

x = a - f(a) (b-a)/(f(b) - f(a))

Newton-Raphson Method



$$f(x+h) \sim f(x) + f'(x)h$$

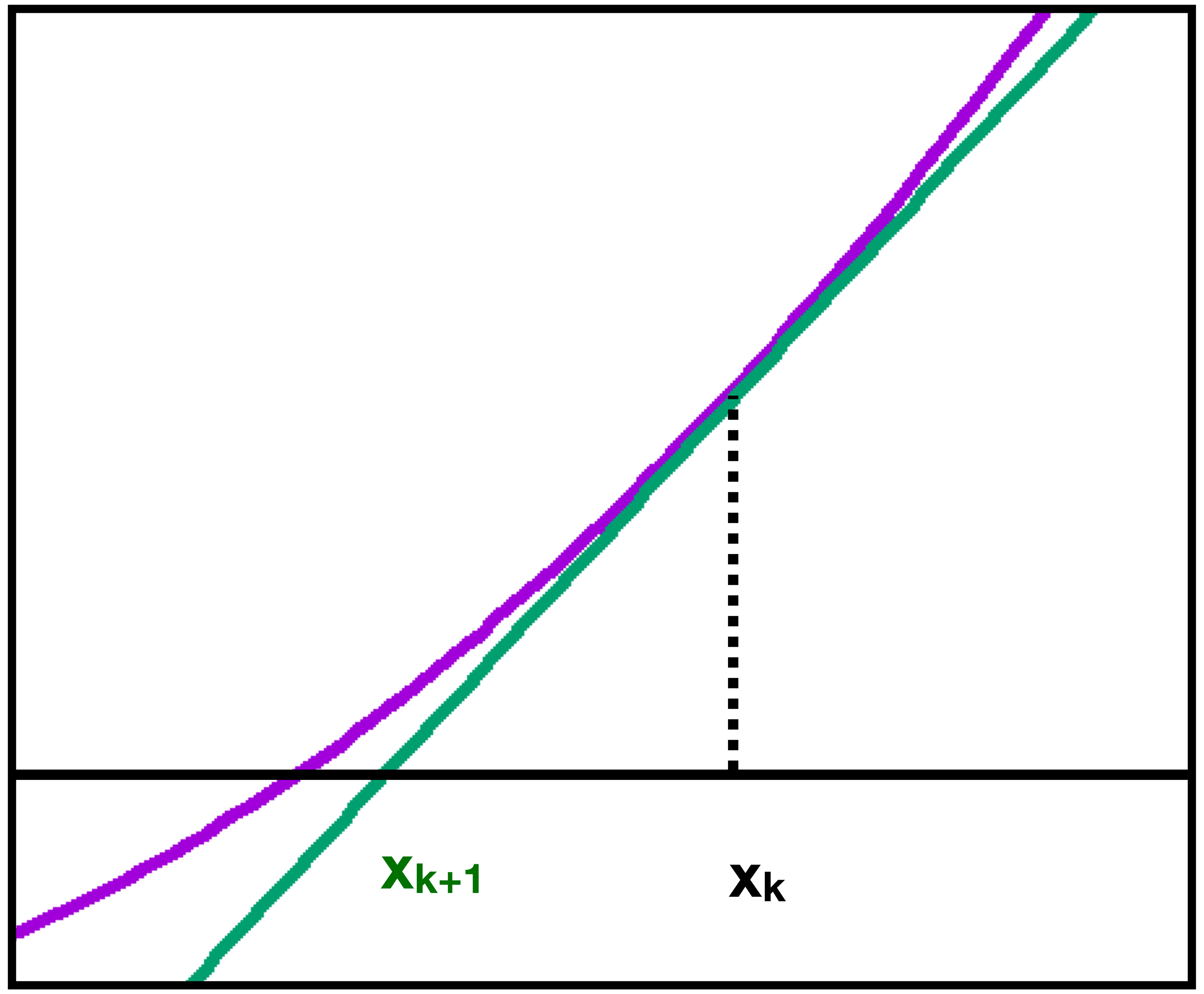
$$f(x) + f'(x)h = 0$$

$$h = x_{k+1} - x_k$$

$$x_{k+1} = x_k - f(x_k)/f'(x_k)$$

Exercise: Newton-Raphson Method

$$f(x) = x^2 - 4\sin(x) = 0$$



$$f(x+h) \sim f(x) + f'(x)h$$

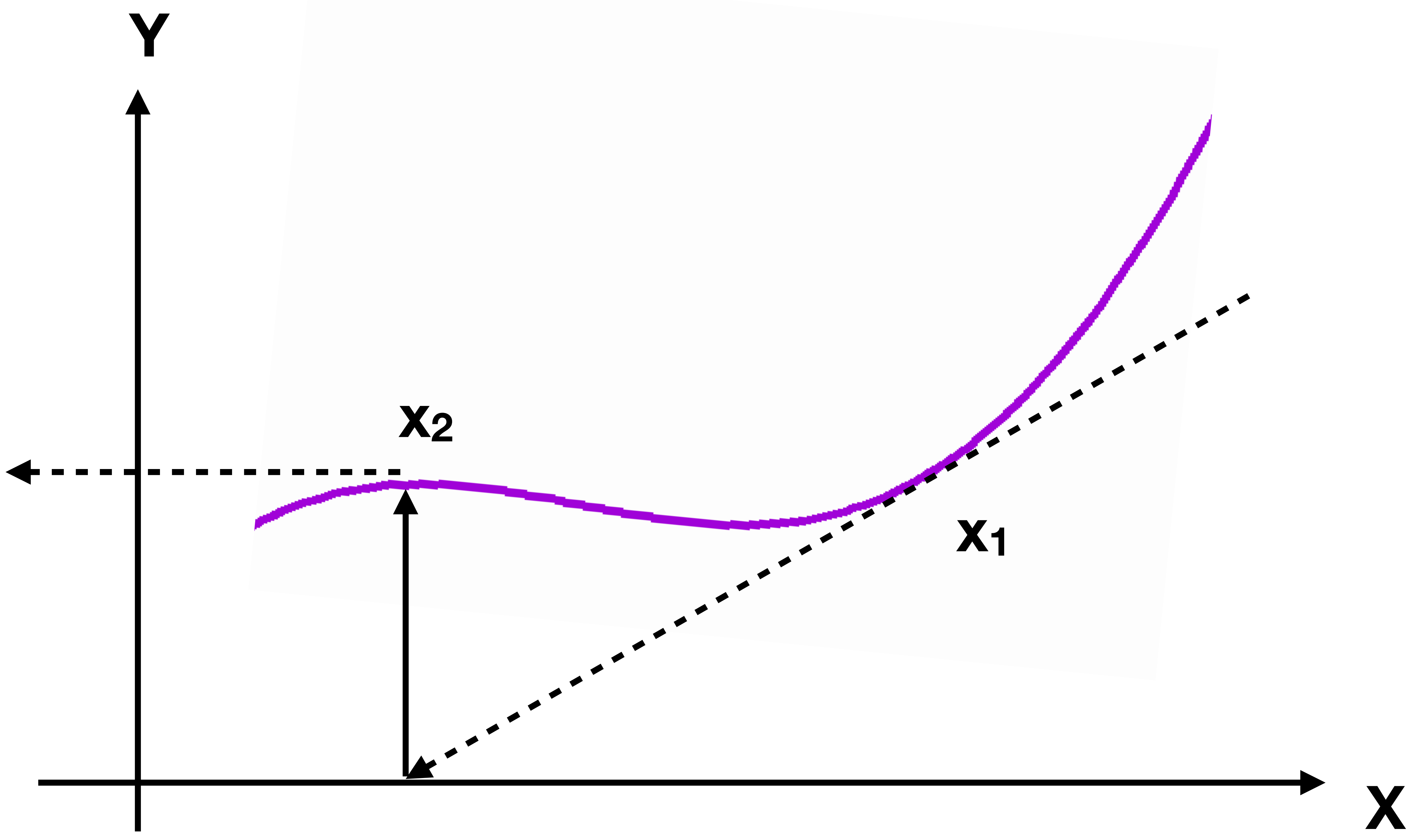
$$f(x) + f'(x)h = 0$$

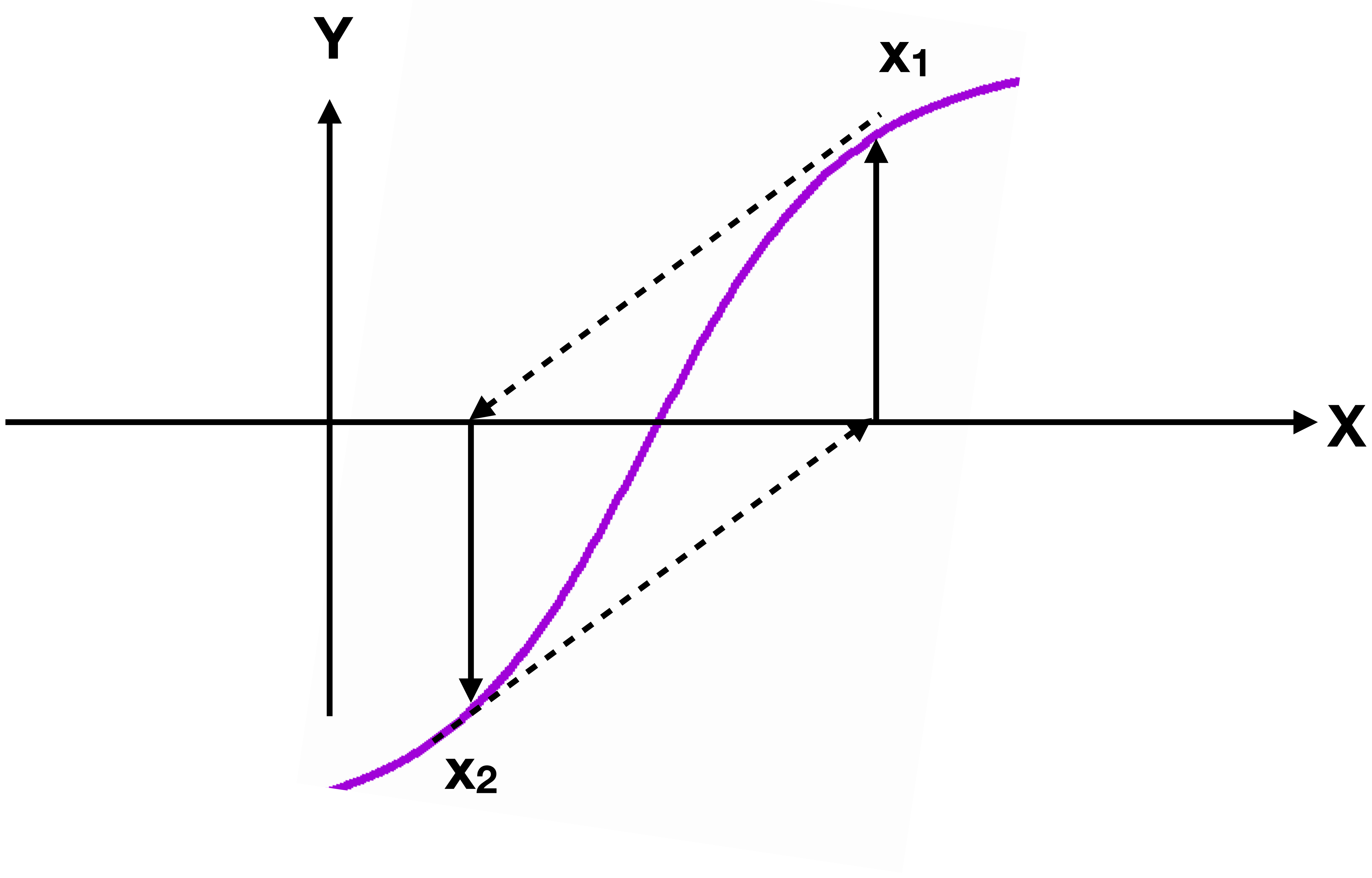
$$h = x_{k+1} - x_k$$

$$x_{k+1} = x_k - f(x_k)/f'(x_k)$$

Newton-Raphson Method

However





Newton-Raphson Method

Problems:

(1) both f(x) and f'(x) must be evaluated at each iteration

(2) when f'(x) -> 0, we go for a "wide ride"

(3) cannot compute f'(x) easily

Secant Method

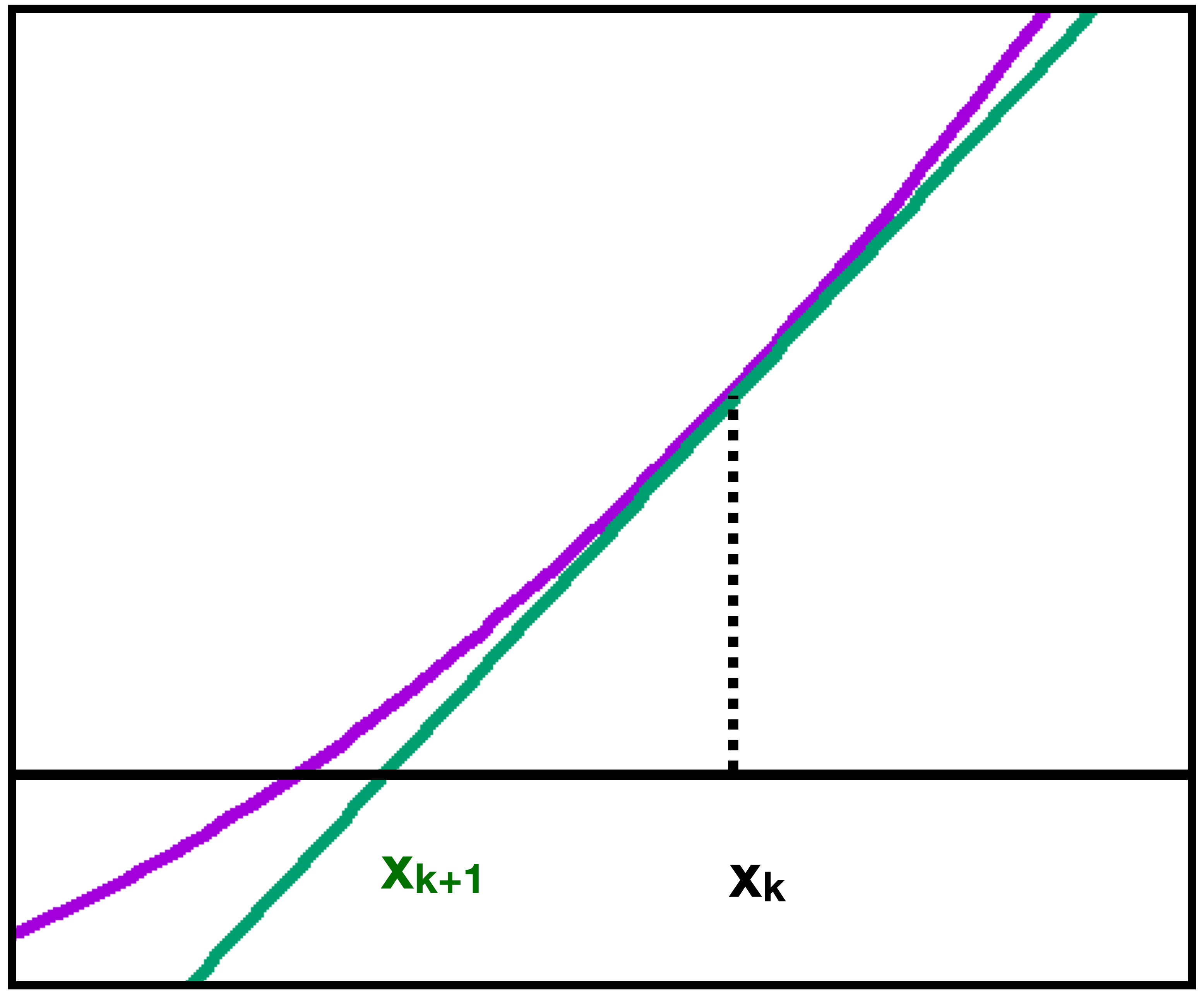
We can approximate f'(x) by finite difference

$$f'(x_k) \sim \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}$$

Will require two initial guess, x_0 and x_1

Exercise: Secant Method

$$f(x) = x^2 - 4\sin(x) = 0$$



$$x_{k+1} = x_k - f(x_k)/f'(x_k)$$

$$f'(x_k) \sim \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}$$

Halley's method

Consider the next term in Taylor series,

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)\left(1 - \frac{f(x_i)f''(x_i)}{2f'(x_i)^2}\right)}$$

If f"(x) is almost free,

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} / \max\left[0.8, \min\left(1.2, 1 - \frac{f(x_i)f''(x_i)}{2f'(x_i)^2}\right)\right]$$

Convergence rates

$$\lim_{k\to\infty} \frac{||e_{k+1}||}{||e_k||^r} = C$$

If r = 1 and C <1, the convergence rate is linear
If r > 1, the convergence rate is superlunar
If r = 2, the convergence rate is quadratic
If r = 3, the convergence rate is cubic, and so on

Example: Convergence rates

$$\lim_{k \to \infty} \frac{||e_{k+1}||}{||e_k||^r} = C$$

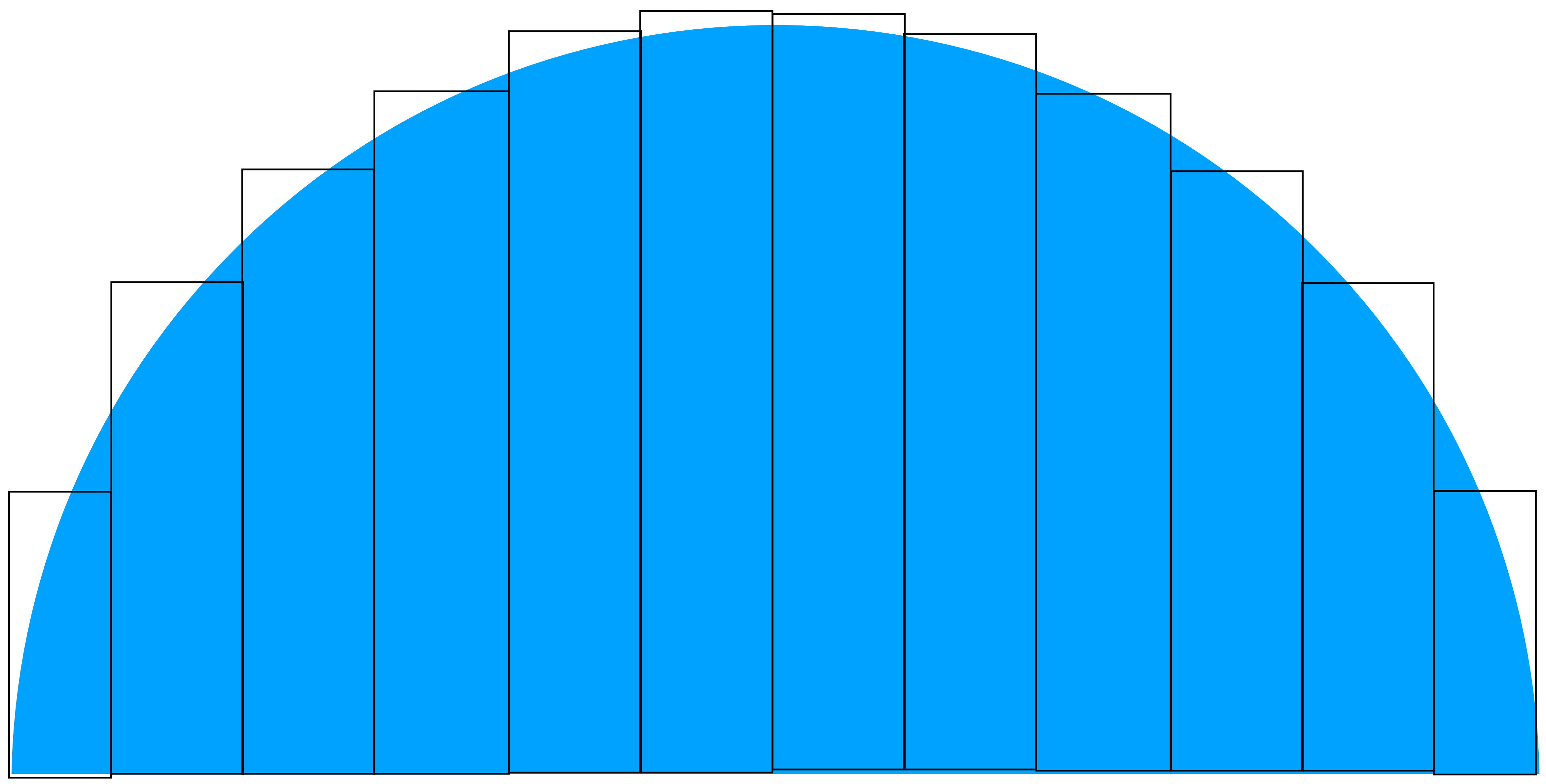
$$f(x) = x^2 - 4\sin(x) = 0$$

(See convergence.ipynb)

Numerical Integration

Recall the PI calculation in lecture 2

The area of the circle can be approximated by the area of sum of these small rectangles x 2



Recall the PI calculation in lecture 2

The area of each rectangle is dA =

Midpoint rule

$$\int_a^b f(x)dx \sim (b-a)f(\frac{a+b}{2})$$

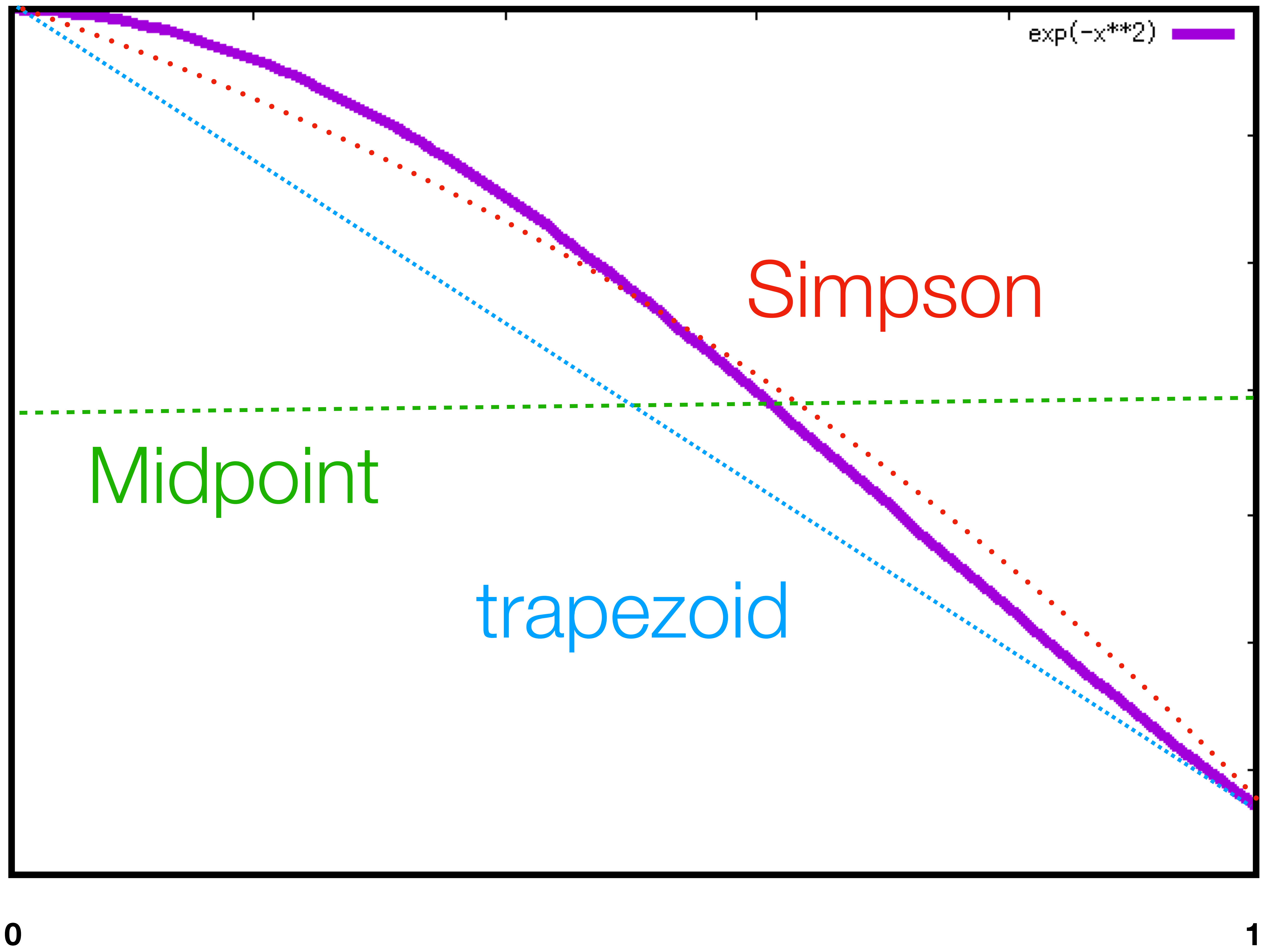
Trapezoidal rule

$$\int_a^b f(x)dx \sim (b-a)(\frac{f(a)+f(b)}{2})$$

Simpson's rule

$$\int_a^b f(x)dx \sim \frac{(b-a)}{6}(f(a)+4f(\frac{a+b}{2})+f(b))$$

Midpoint / Trapezoid / Simpson

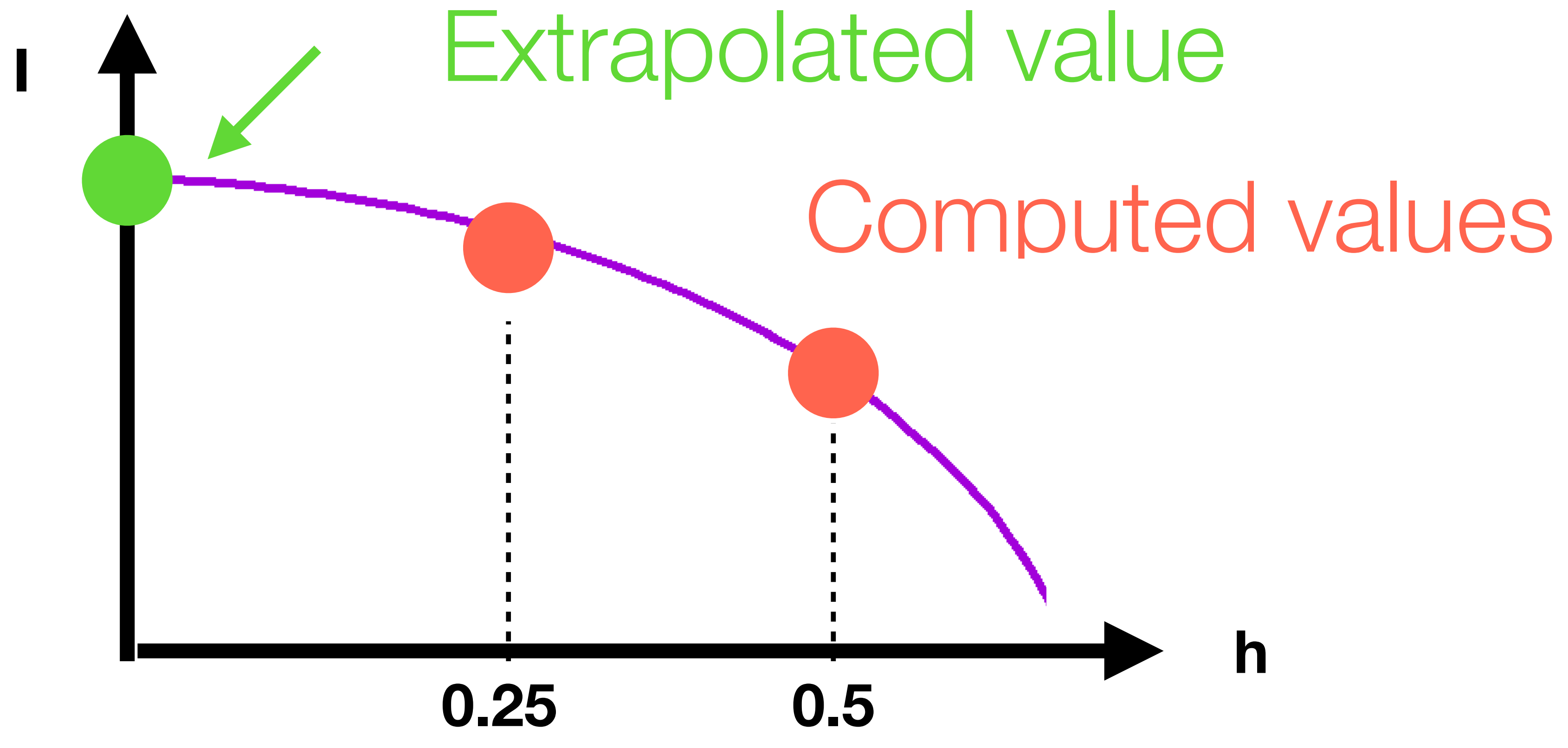


Romberg Integration

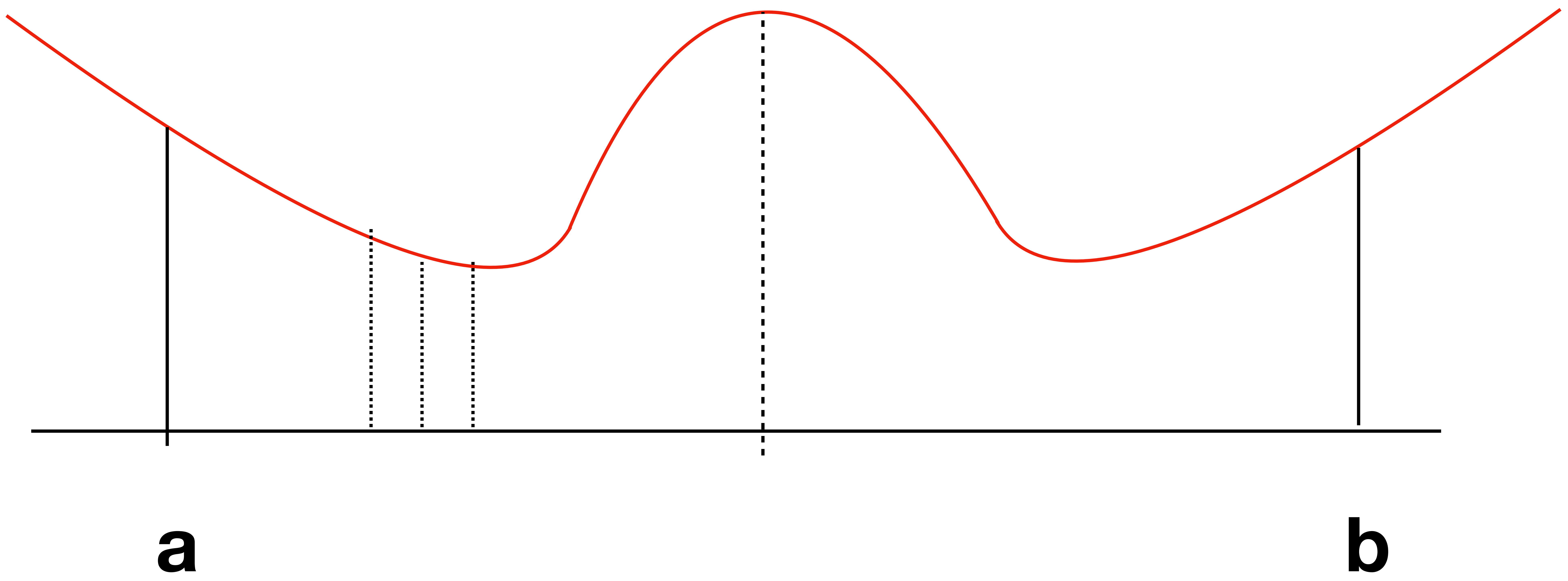
$$I(h) = a_0 + a_1 h^p + O(h^r)$$

I is the obtained value with step h (with p < r).
e.x. When using trapezoid rule, we have p=2, r=4

$$I(h) = a_0 + a_1 h^2 + O(h^4)$$



Adaptive quadrature method



Adaptive quadrature method

- Start with pair of quadrature rules whose difference gives error estimate
- Apply both rules on initial interval [a,b]
- If difference between rules exceeds error tolerance, subdivide interval and apply rules in each subinterval
- Continue subdividing, as necessary, until tolerance is met on all subintervals

Adaptive quadrature method

Implementation issues:

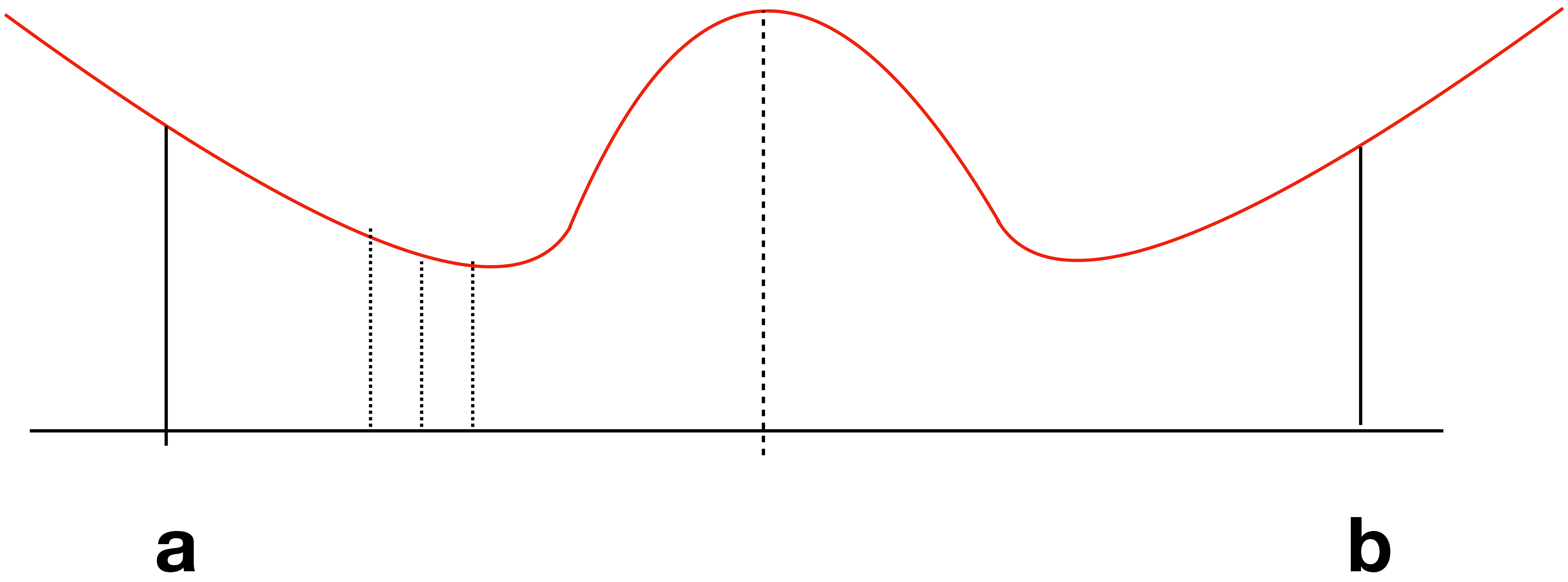
(1) what’s the stopping criterion?

(2) Can the error tolerance always met?

(3) how to avoid wasting time subdividing unconverted subintervals

Exercise: Adaptive quadrature method

Use the adaptive quadrature method to do the Pi calculation again



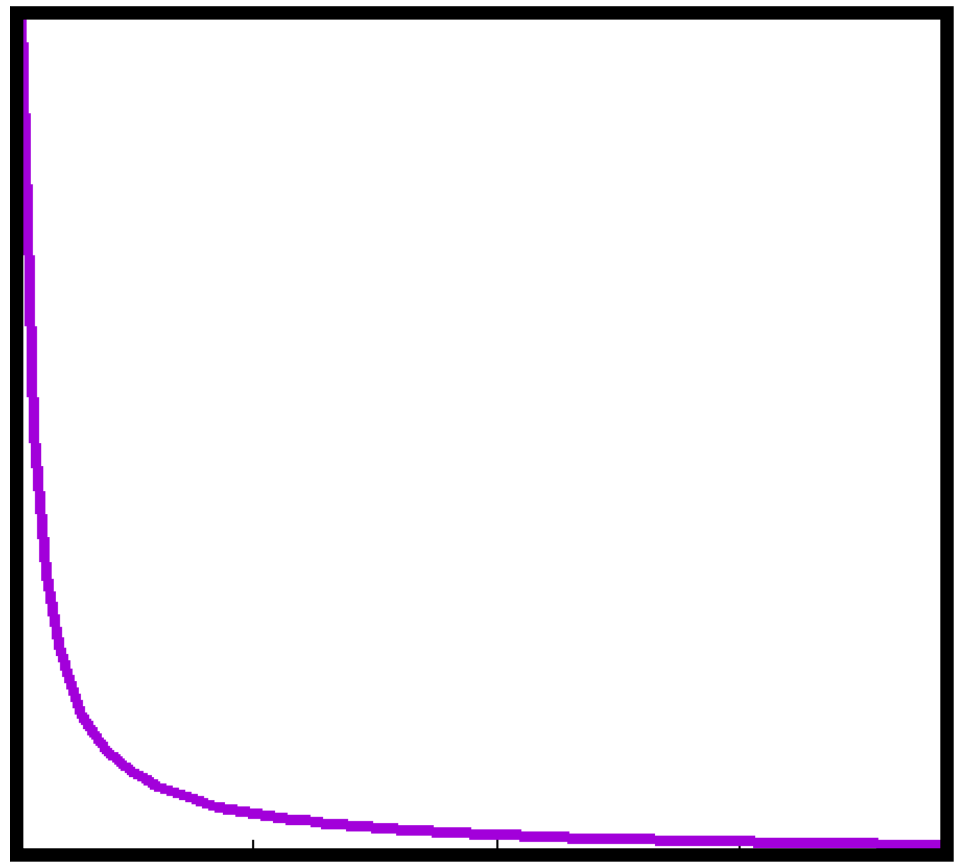
Integral of Tabular data

- A reasonable approach to integrate tabular data is by piecewise interpolation.
- Piecewise linear interpolation gives a composite trapezoid rule.
- An excellent method for integrating tabular data is provided by Hermit cubic or cubic spline interpolation
- This facility is provided by many spline interpolation packages

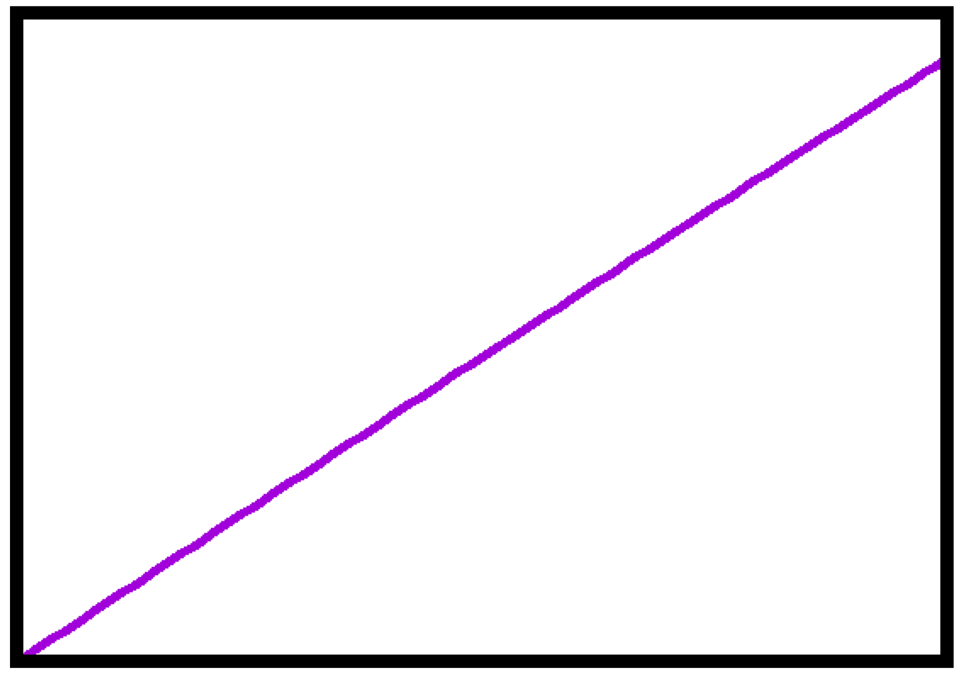
Singularities in the integration

Philosophy: subtract them away …

$$\int_{0.01}^{1} \frac{dx}{e^x - 1}$$



As $x \to 0$ $\qquad \dfrac{1}{e^x - 1} \to \dfrac{1}{x}$



$$I = \int_{0.01}^{1} \left(\frac{1}{e^x - 1} - \frac{1}{x} \right) dx + \boxed{\int_{0.01}^{1} \frac{dx}{x}}$$

Can do it analytically

Example: Singularities in the integration

This kind of integral are very common in stellar interior.

$$I = \int_r^R \frac{dr}{(r^2 - 2m(r)r)^{1/2}}, \qquad m(r) \propto r^3$$

$$= \int_r^R \left[\frac{1}{(r^2 - 2m(r)r)^{1/2}} - \frac{1}{r} \right] dr + \int_r^R \frac{dr}{r}$$

Example: Singularities in the integration

Or, you could change of variables

$$I = \int_0^1 \frac{dt}{t^{1/2}}$$

$$x \equiv 1/t$$

$$= \int_1^\infty \frac{dx}{x^{3/2}} \qquad dx = -\frac{1}{t^2}dt = -x^2 dt$$

Open integral!

Double Integral

$$\int_a^b \int_c^d f(x,y)dxdy$$

Use a pair of adaptive 1D quadrature routines.

Use a Cartesian product rule

Multiple Integral

To compute integral in higher dimensions (n>3), the *Monte Carlo* method is preferred.

Sample N points randomly in the domain of integration, and then mean of these function values is multiplied by the area (or volume, etc.)

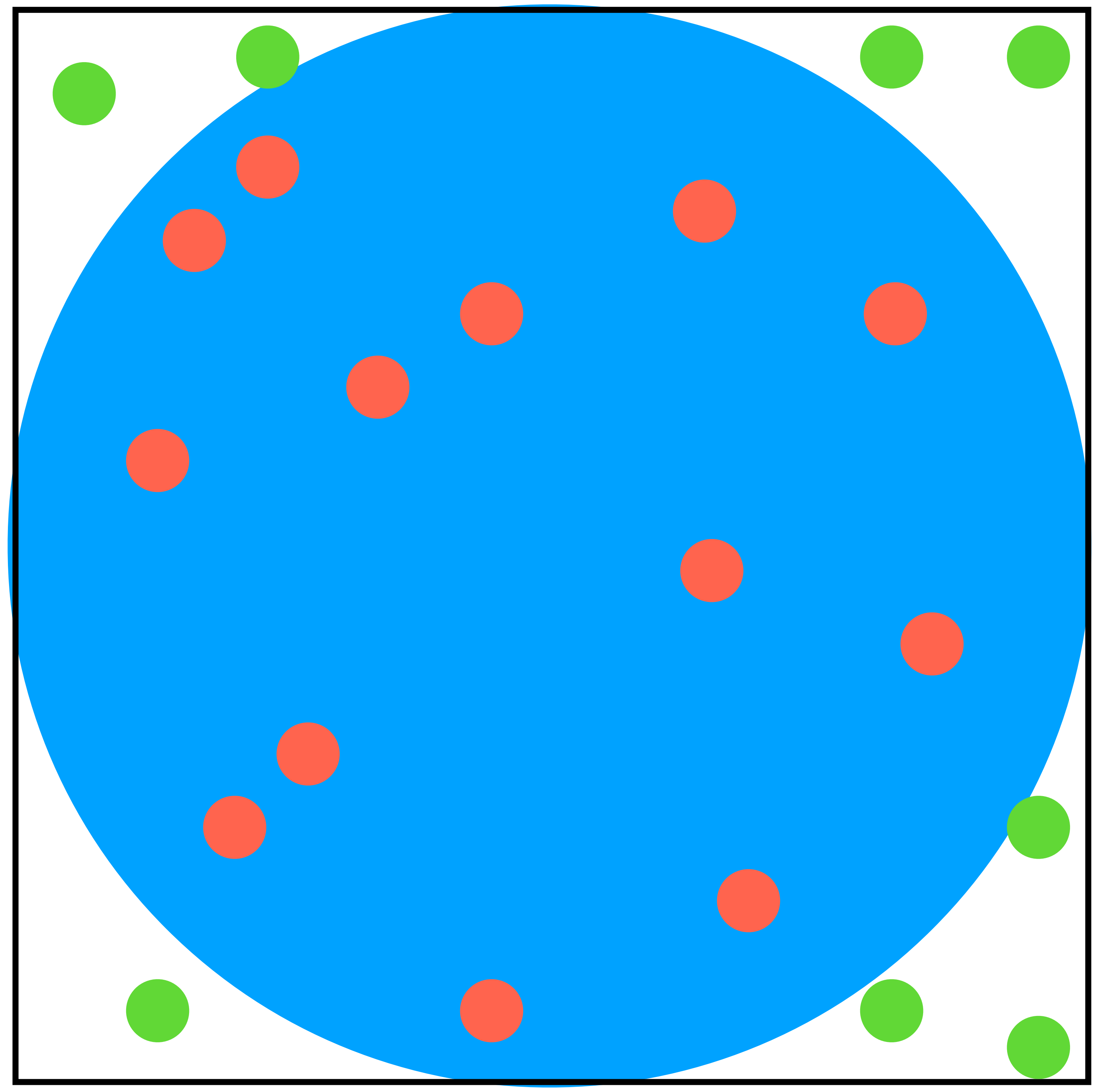
The error in this estimate goes to zero as 1/sqrt(N)

-> 1digit accuracy requires 100x samples

But the converge rate is independent of dimensions

Exercise: Monte Carlo method

The Pi calculation (again)



Random numbers

Random number generator

An algorithm for generating random number is a short description of the sequence it yields, which therefore by definition is not truly random.
-> “pseudo random”

A good random number generator:
(1) random pattern
(2) long period
(3) efficiency
(4) Repeatability
(5) Portability

Congruential generator

$$x_k = (a x_{k-1} + b) \pmod M,$$

x_0: seed

a, b : given integers (chosen very carefully)

M : (often) the largest integer

e.g.

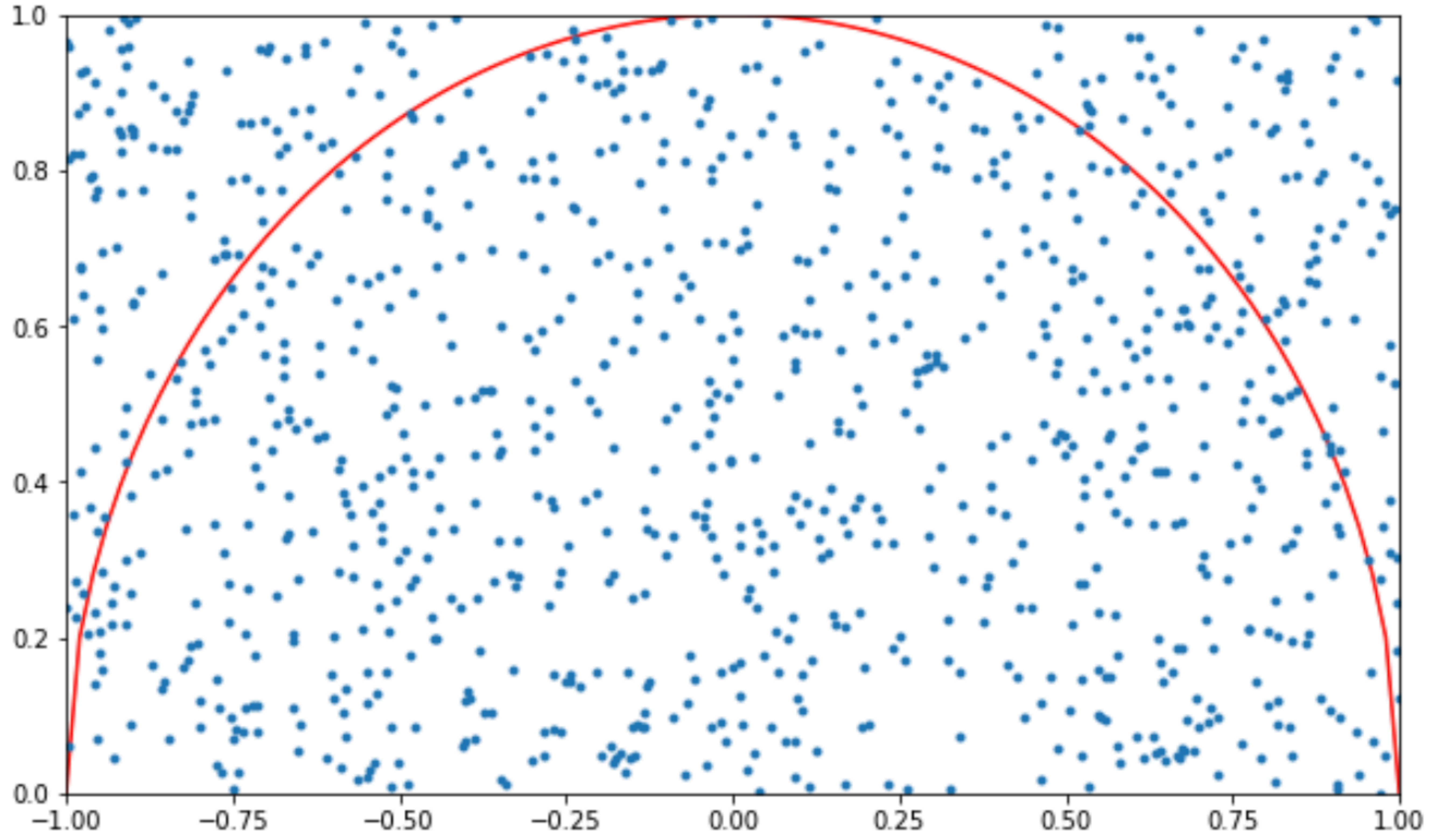
Never use this generator in your research!

a = 1664525

b = 1013904223

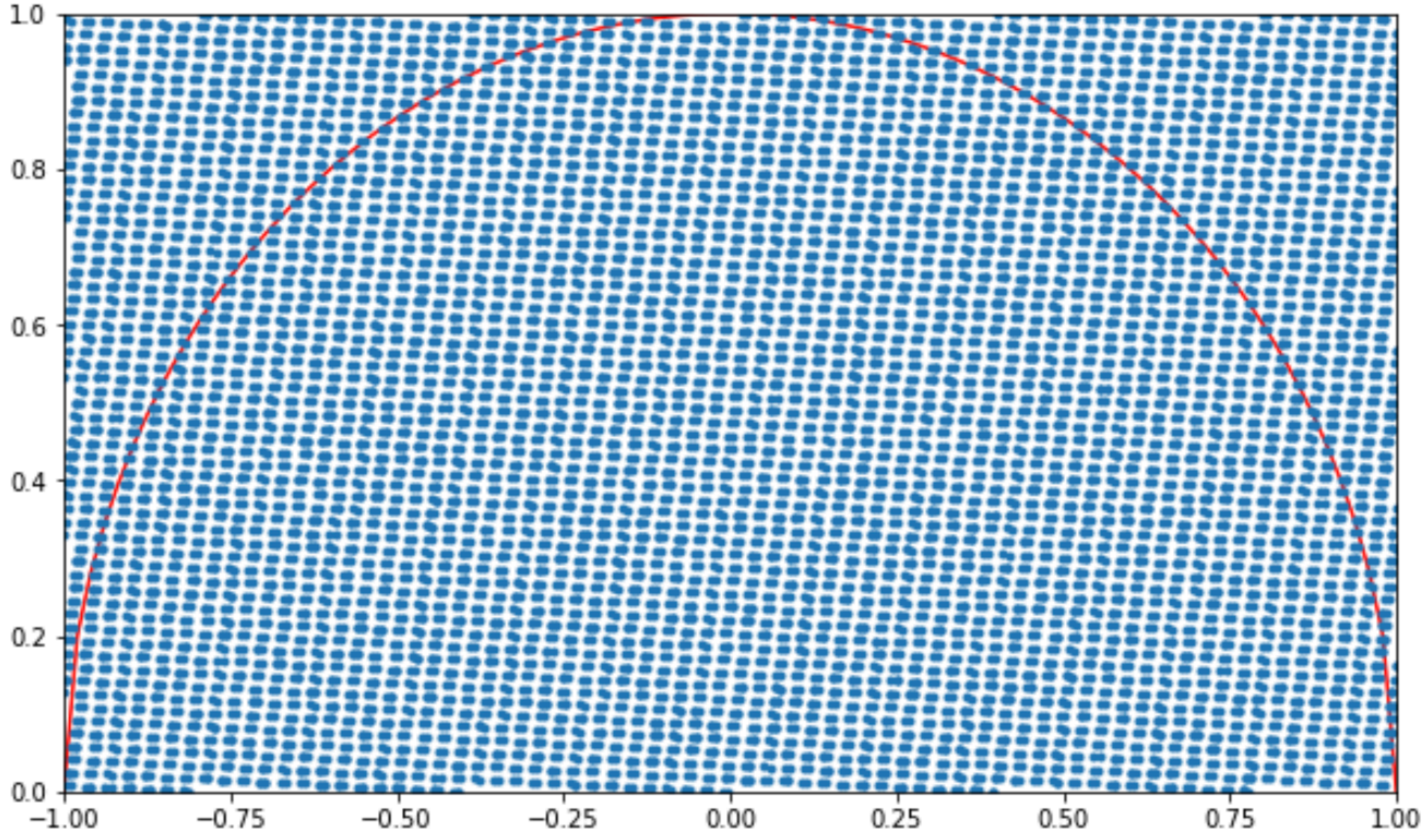
M = 2^32

Example: A bad Random number generator



(See random.ipynb)

Example: A bad Random number generator

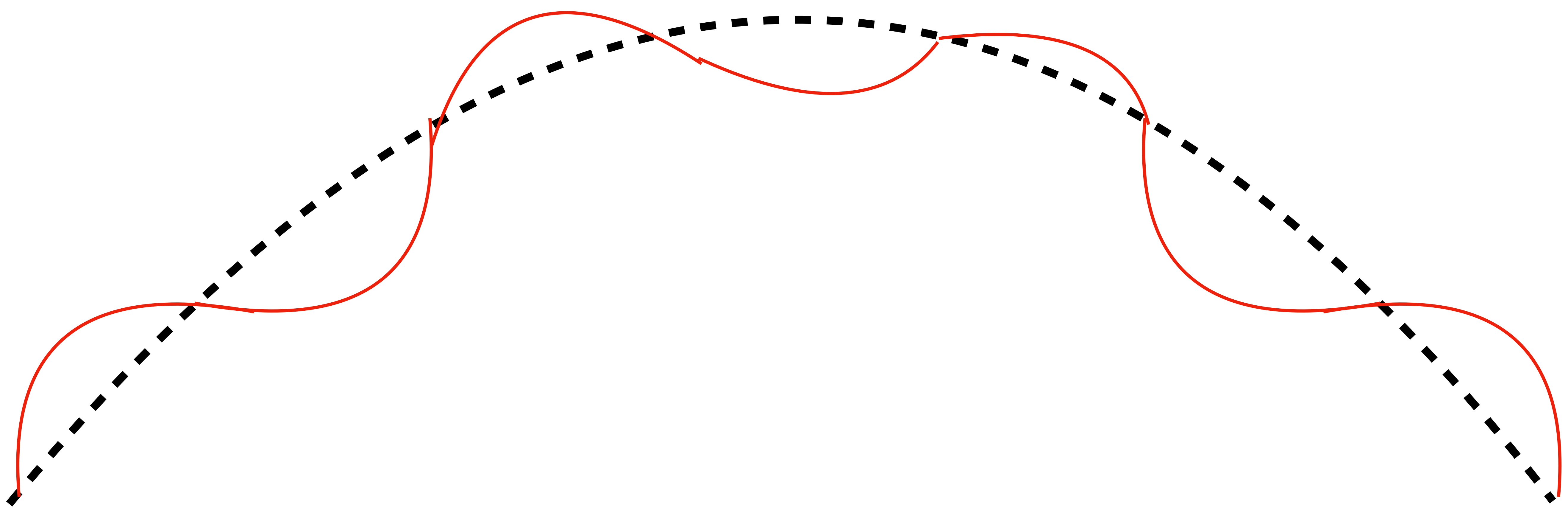


(See random.ipynb)

Numerical Differentiation

Numerical differentiation

Two functions having similar integrals but very different derivatives



For discrete data, it is better to fit with some smooth function before calculating derivatives

Finite difference approximation

From the Taylor expansion, ….

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \frac{f'''(x)}{6}h^3 + \ldots$$

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)}{2}h^2 - \frac{f'''(x)}{6}h^3 + \ldots$$

Finite difference approximation

Forward difference (first order)

$$f'(x) \sim \frac{f(x+h) - f(x)}{h}$$

Backward difference (first order)

$$f'(x) \sim \frac{f(x) - f(x-h)}{h}$$

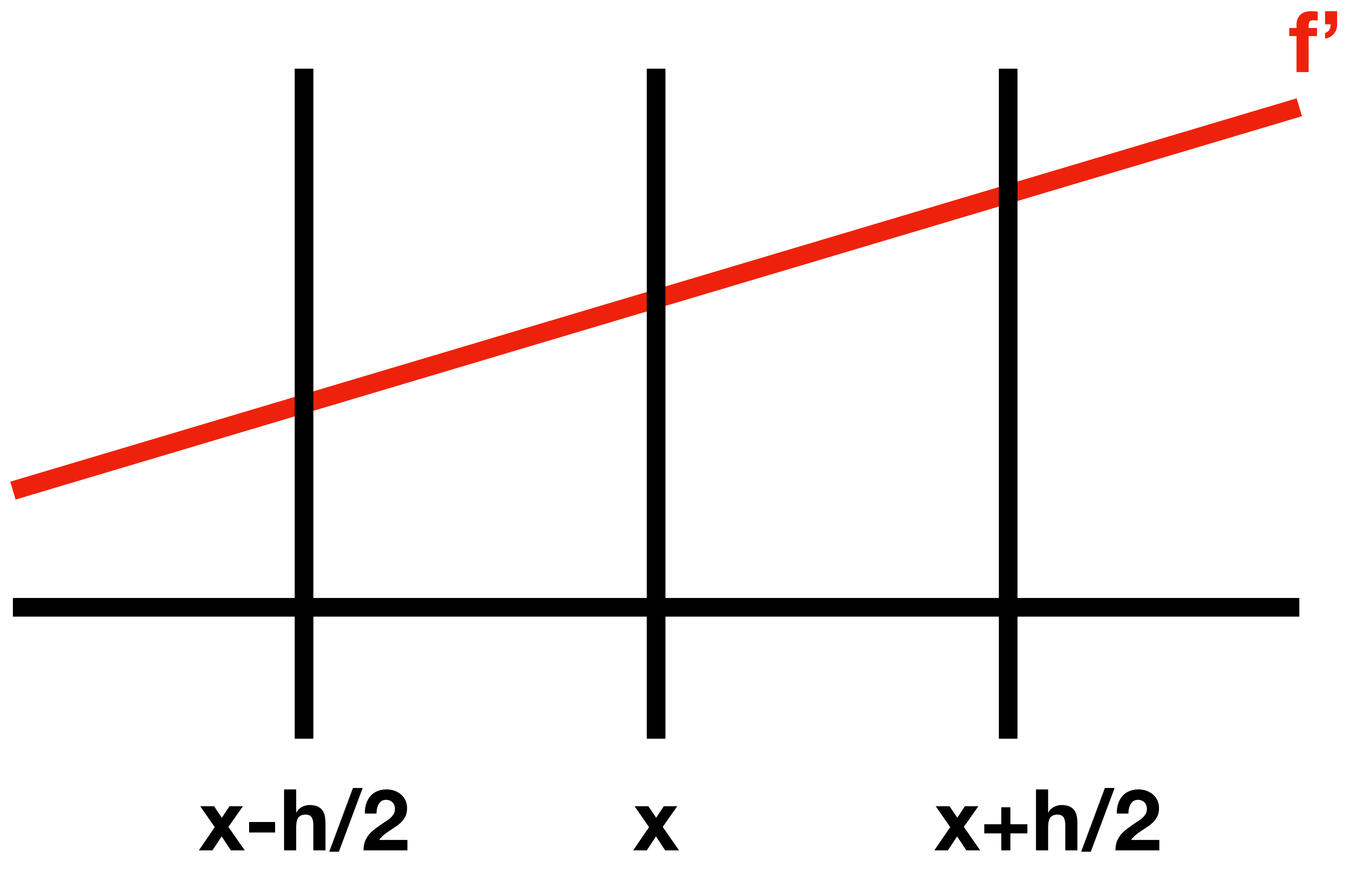
Centered difference (second order)

$$f'(x) \sim \frac{f(x+h) - f(x-h)}{2h}$$

Finite difference approximation

Second derivative (second order)

$$f''(x) \sim \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$



$$f''(x) = \frac{f'(x+\frac{h}{2}) - f'(x-\frac{h}{2})}{h}$$

$$f'(x+\frac{h}{2}) = \frac{f(x+h) - f(x)}{h}$$

$$f'(x-\frac{h}{2}) = \frac{f(x) - f(x-h)}{h}$$

Problem Set 5

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Next lecture

- Ordinary differential equations (ODEs)
- Initial Value Problems (IVPs)
- N-body methods
- Lab: Triple star simulation
- Lab: Solar system simulation