Task: Given a table of some quantity q

i	0	1	2	$\cdots$	n
x_i	0.00	0.51	1.05	$\cdots$	x_n
q_i	0.00	0.22	0.25	$\cdots$	q_n

compute approximations of $q(x)$

$q'(x)$

$\int_a^b q(x)\, dx$ $\quad \cdot$

?

i.e. easy to evaluate, derive, integrate

$\leadsto$ find a simple (& reasonable) function
$q(x)$ that matches the data

$$q(x_i) = q_i \quad , \quad i = 0, 1, \ldots, n$$

Ex.: (2) find IP through $(x_0, y_0) = (1, 2)$

$(x_1, y_1) = (3, 5)$

$(x_2, y_2) = (4, 4)$

↖ same as Ex.(1)

with LI.

Compute the LPs:

$$L_0^2(x) = \frac{x - x_1}{x_0 - x_1} \cdot \frac{x - x_2}{x_0 - x_1} = \frac{x - 3}{1 - 3} \cdot \frac{x - 4}{1 - 4}$$

$$= \frac{1}{6}(x - 3)(x - 4)$$

$$L_1^2(x) = \frac{x - x_0}{x_1 - x_0} \cdot \frac{x - x_2}{x_1 - x_2} = \frac{x - 1}{3 - 1} \cdot \frac{x - 4}{3 - 4}$$

$$= -\frac{1}{2}(x - 1)(x - 4)$$

$$L_2^2(x) = \frac{x - x_0}{x_2 - x_0} \cdot \frac{x - x_1}{x_2 - x_1} = \frac{x - 1}{4 - 1} \cdot \frac{x - 3}{4 - 3}$$

$$= \frac{1}{3}(x - 1)(x - 3)$$
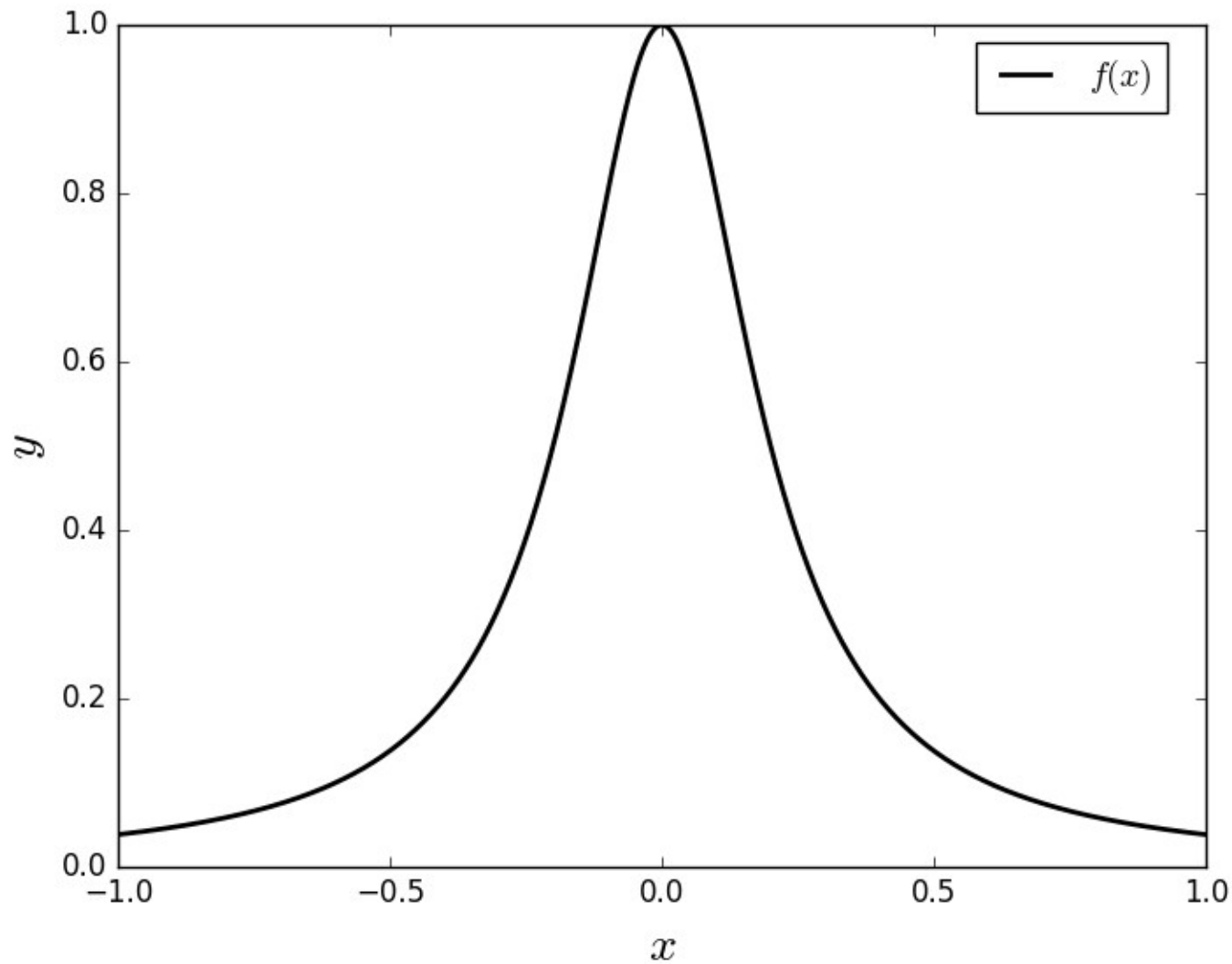
Now inserting into the LI

$$p_2(x) = 2 \cdot L_0^2(x) + 5 \cdot L_1^2(x) + 4 \cdot L_2^2(x)$$

$$= \ldots = 2 + \frac{29}{6}x - \frac{5}{6}x^2$$

(like Ex.(1), indeed!)

Runge's example
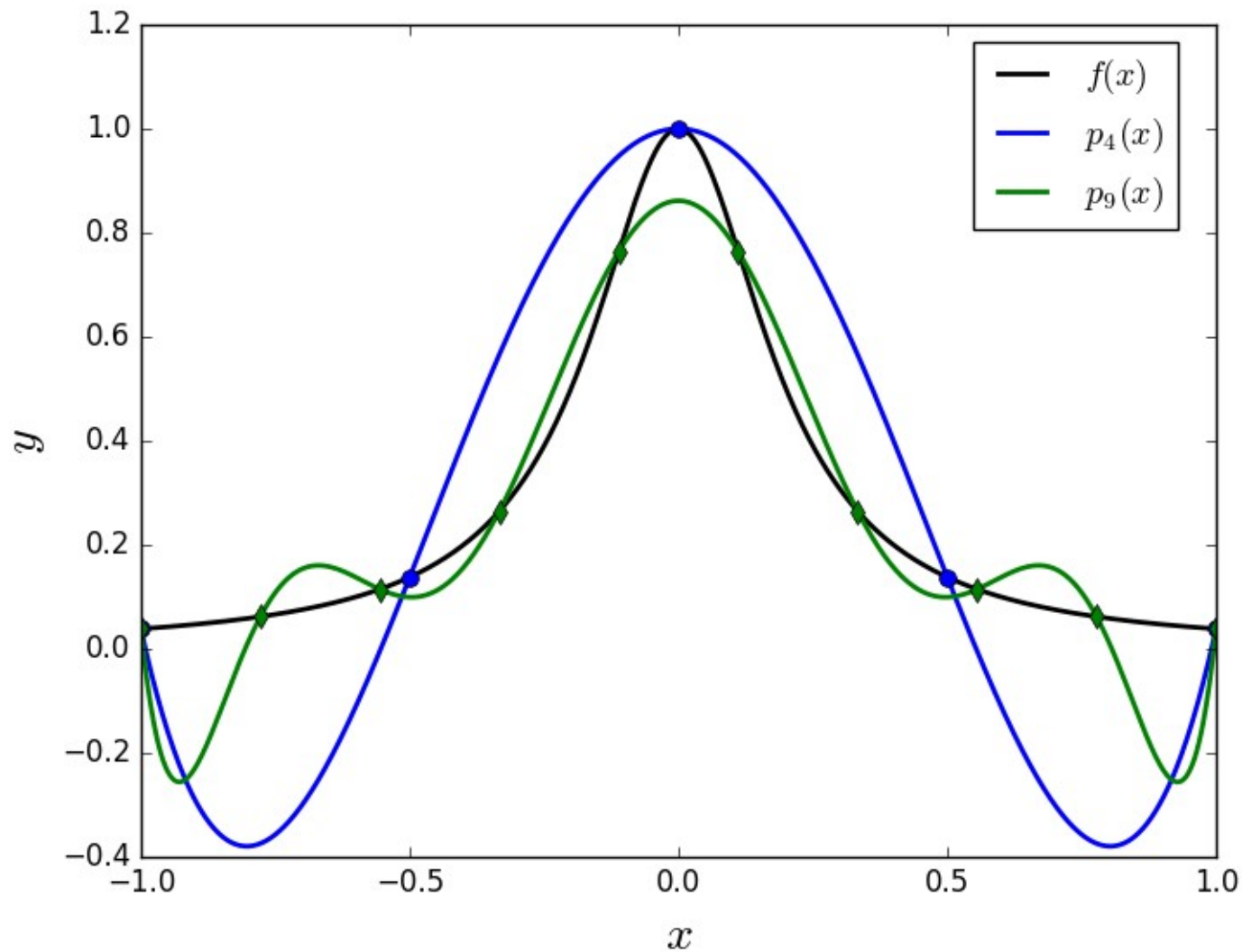
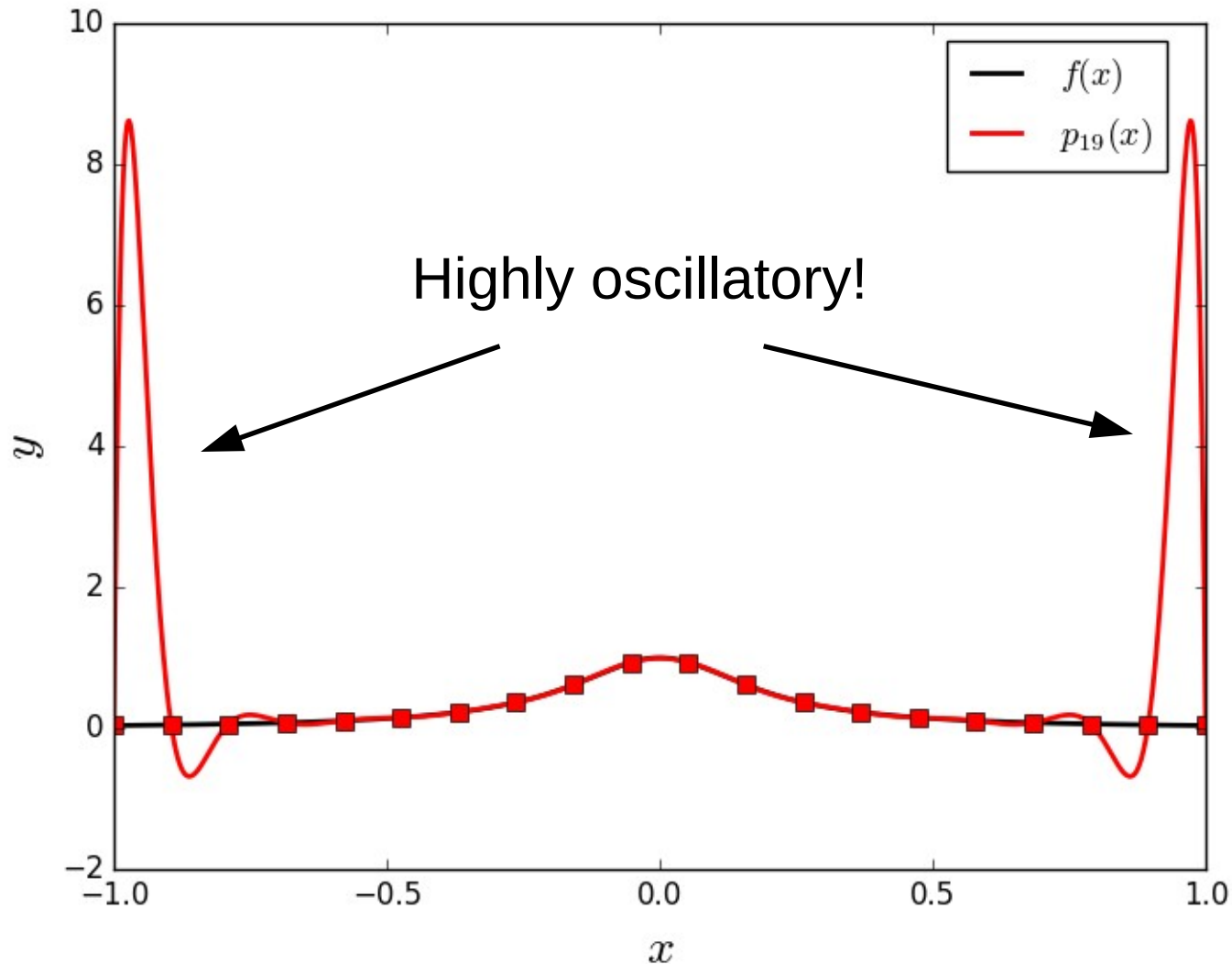$$f(x) = \frac{1}{1 + 25x^2} \qquad x \in [-1, 1]$$

Runge's example

Equidistant: $x_j = -1 + \dfrac{2}{n}j$ for $j = 0, 1, ..., n$

Runge's example
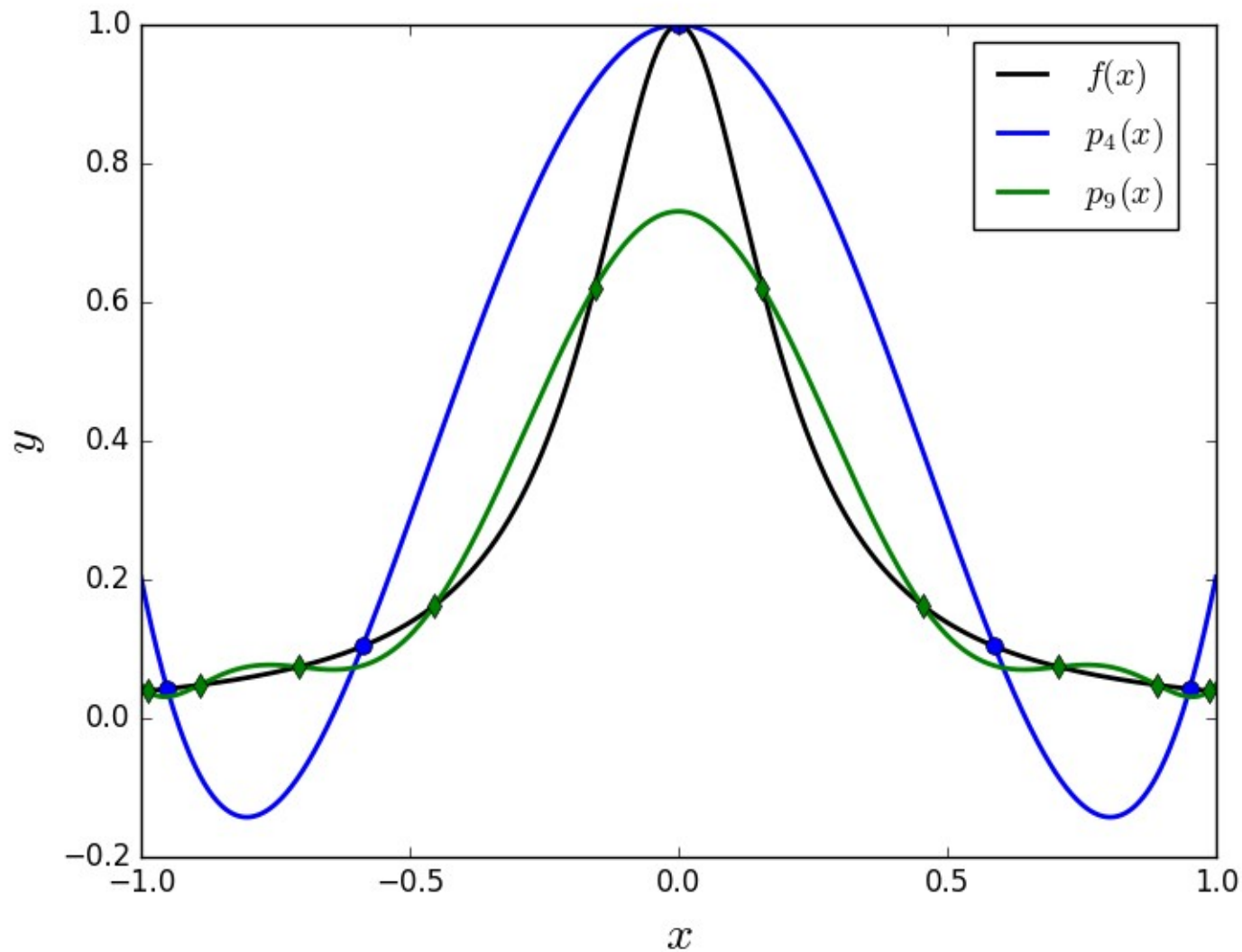
Equidistant: $x_j = -1 + \dfrac{2}{n}j$ for $j = 0, 1, ..., n$

Runge's example
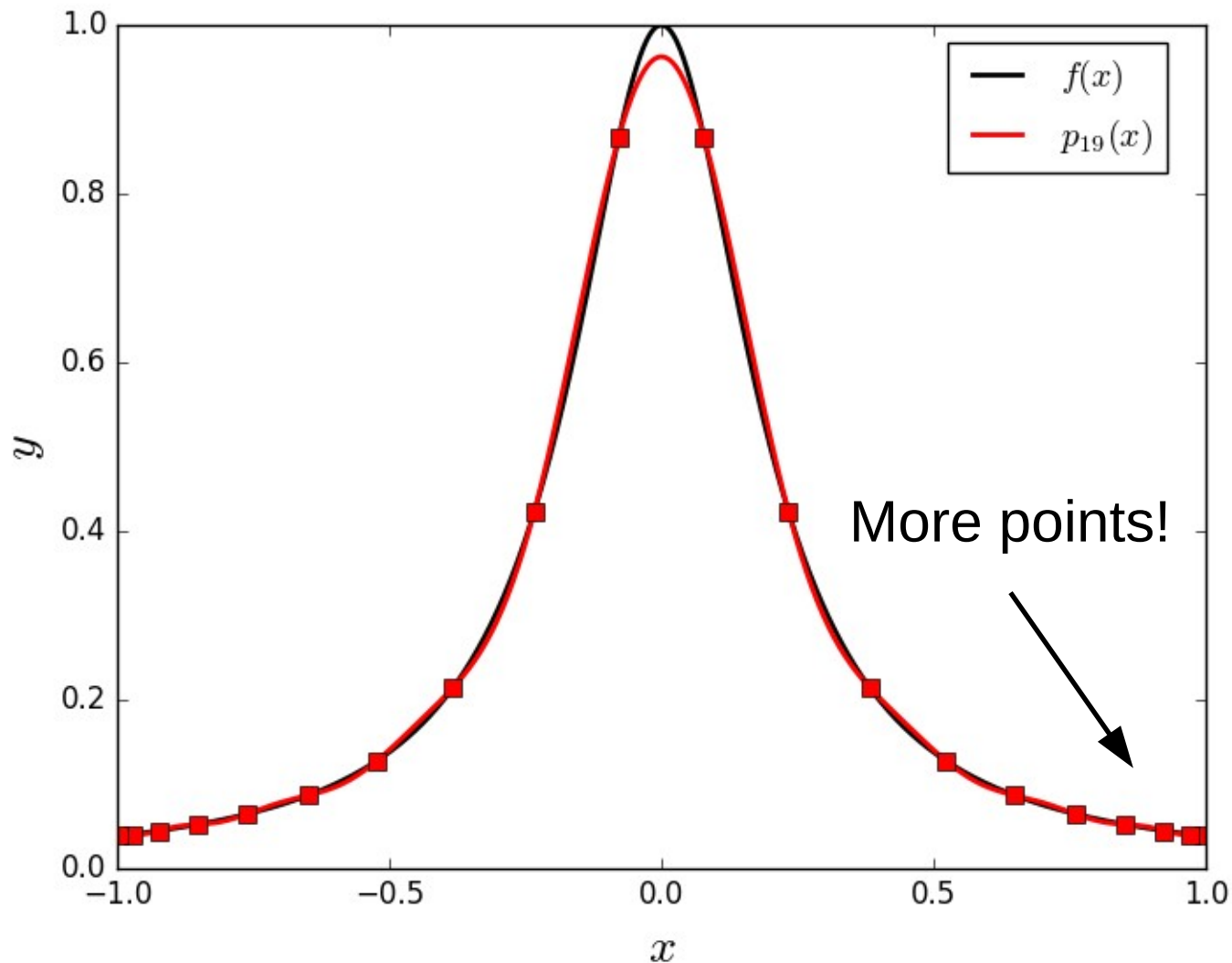
Chebyshev: $x_j = \cos\left(\dfrac{2j+1}{2(n+1)}\pi\right)$ for $j = 0, 1, ..., n.$
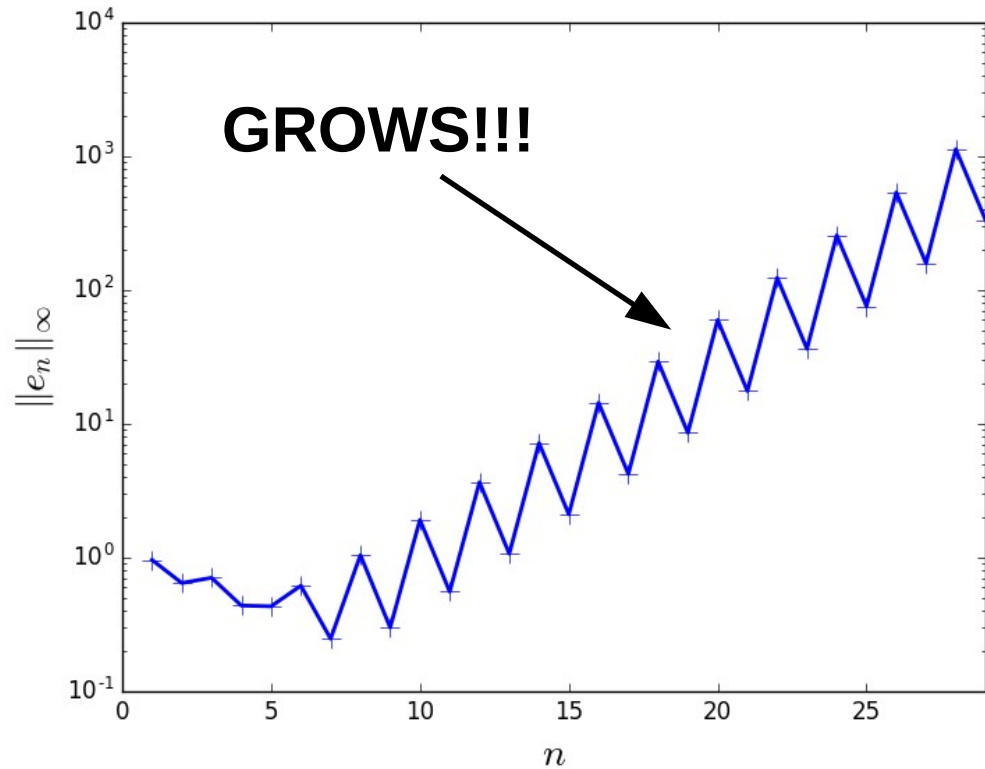
Runge's example

Chebyshev: $x_j = \cos\left(\dfrac{2j+1}{2(n+1)}\pi\right)$ for $j = 0, 1, ..., n.$

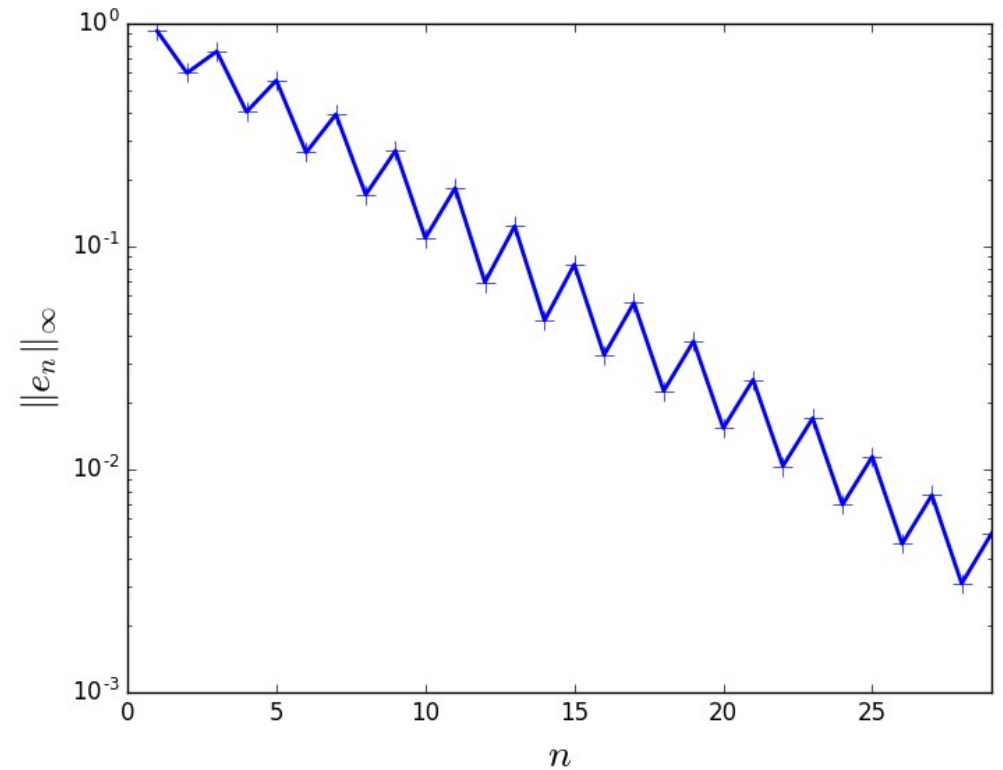More points!

Runge's example

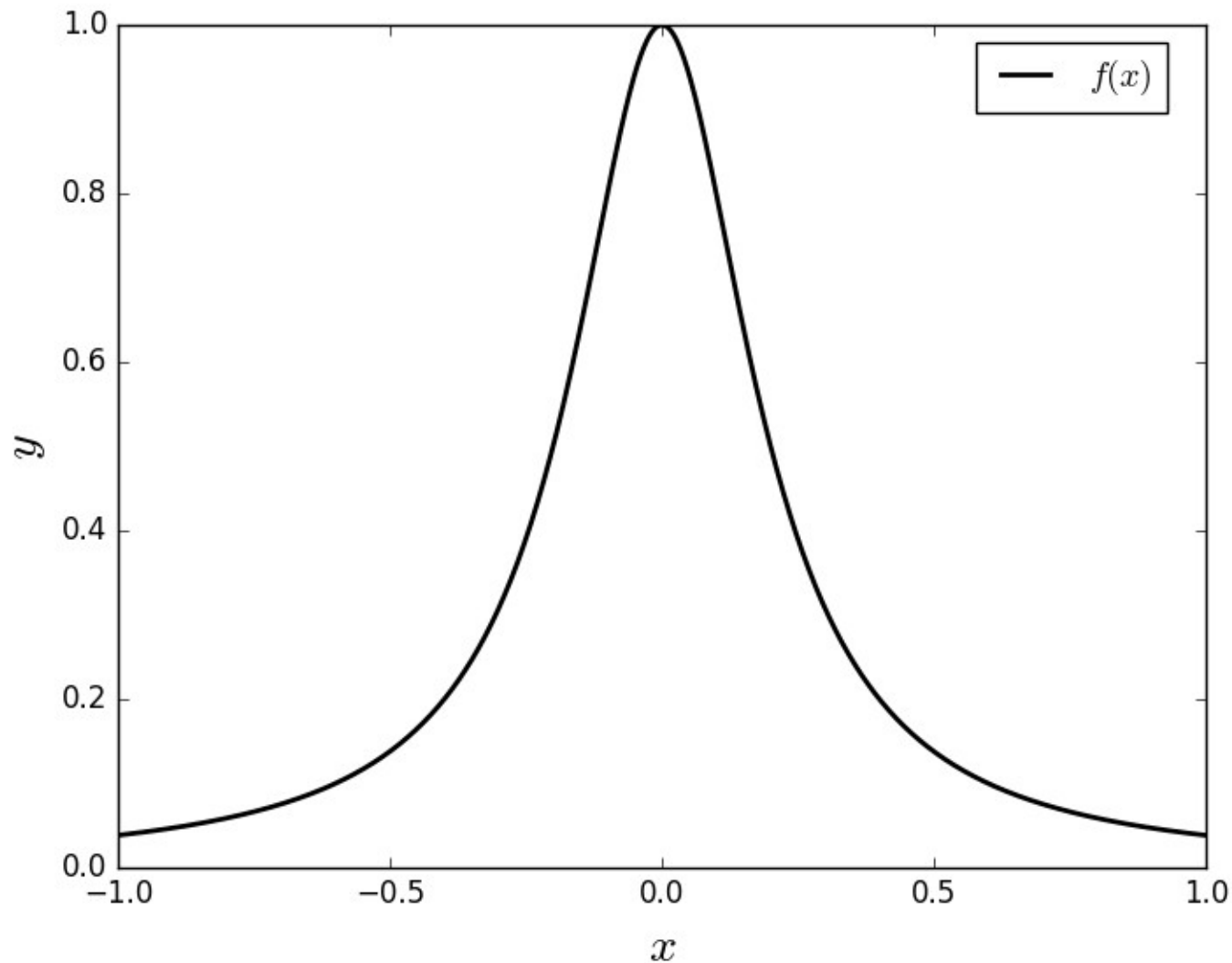**Equidistant**

Chebyshev

GROWS!!!

Interpolation error: $\|e_n\|_\infty = \|f - p_n\|_\infty$
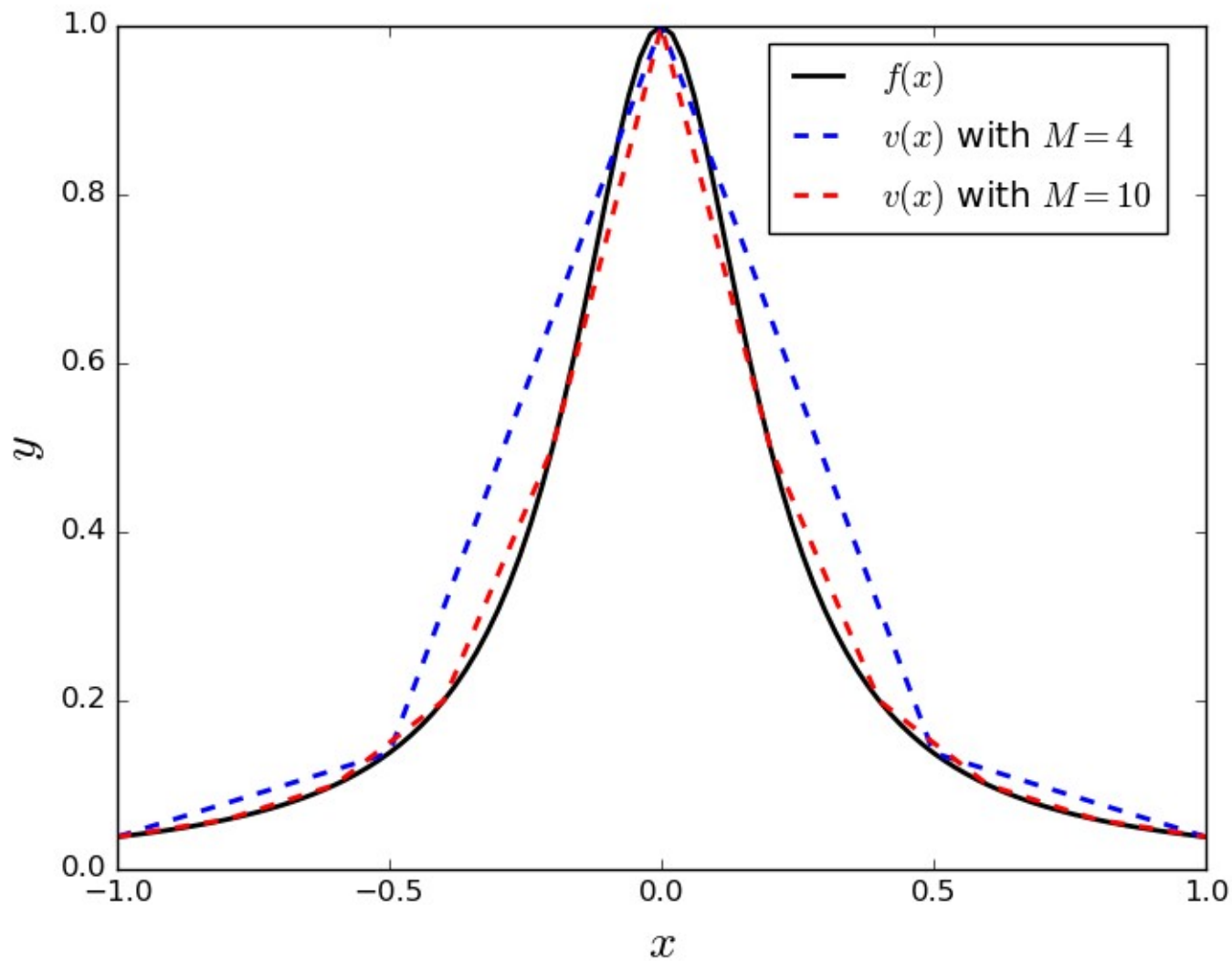
Ex.: (3)

Runge's example

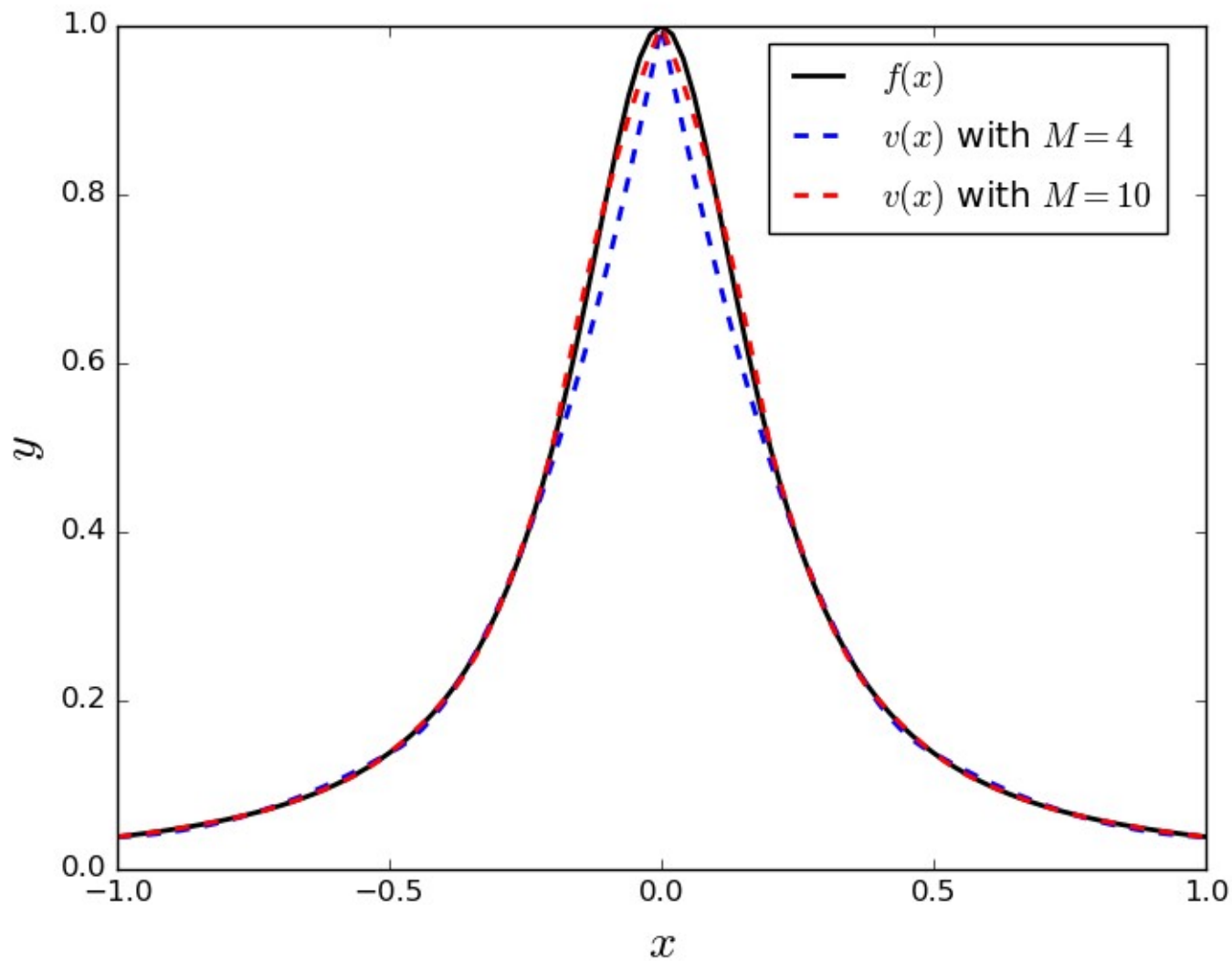$$f(x) = \frac{1}{1 + 25x^2} \qquad x \in [-1, 1]$$
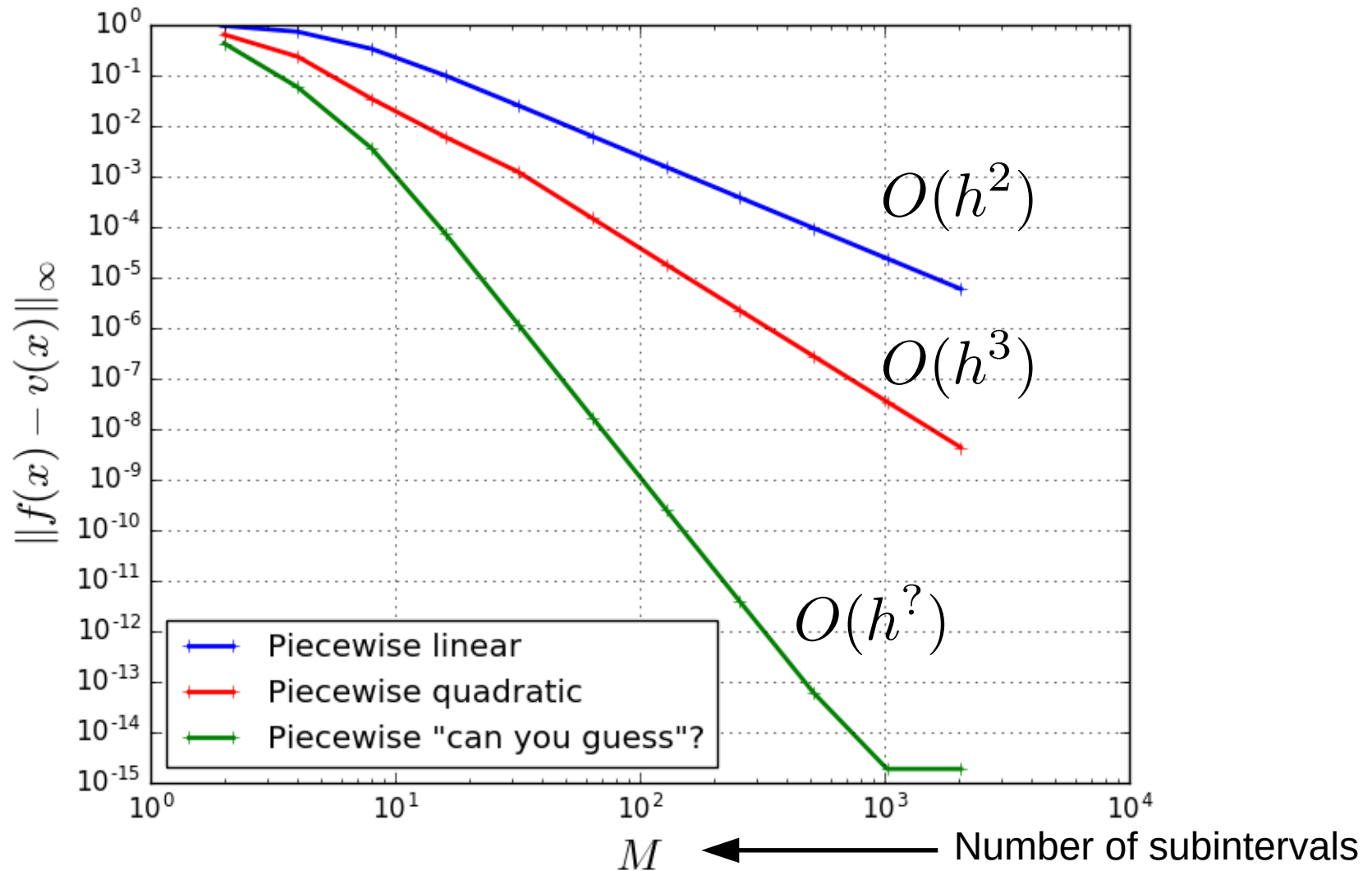
Runge's example

Piecewise linear

Runge's example
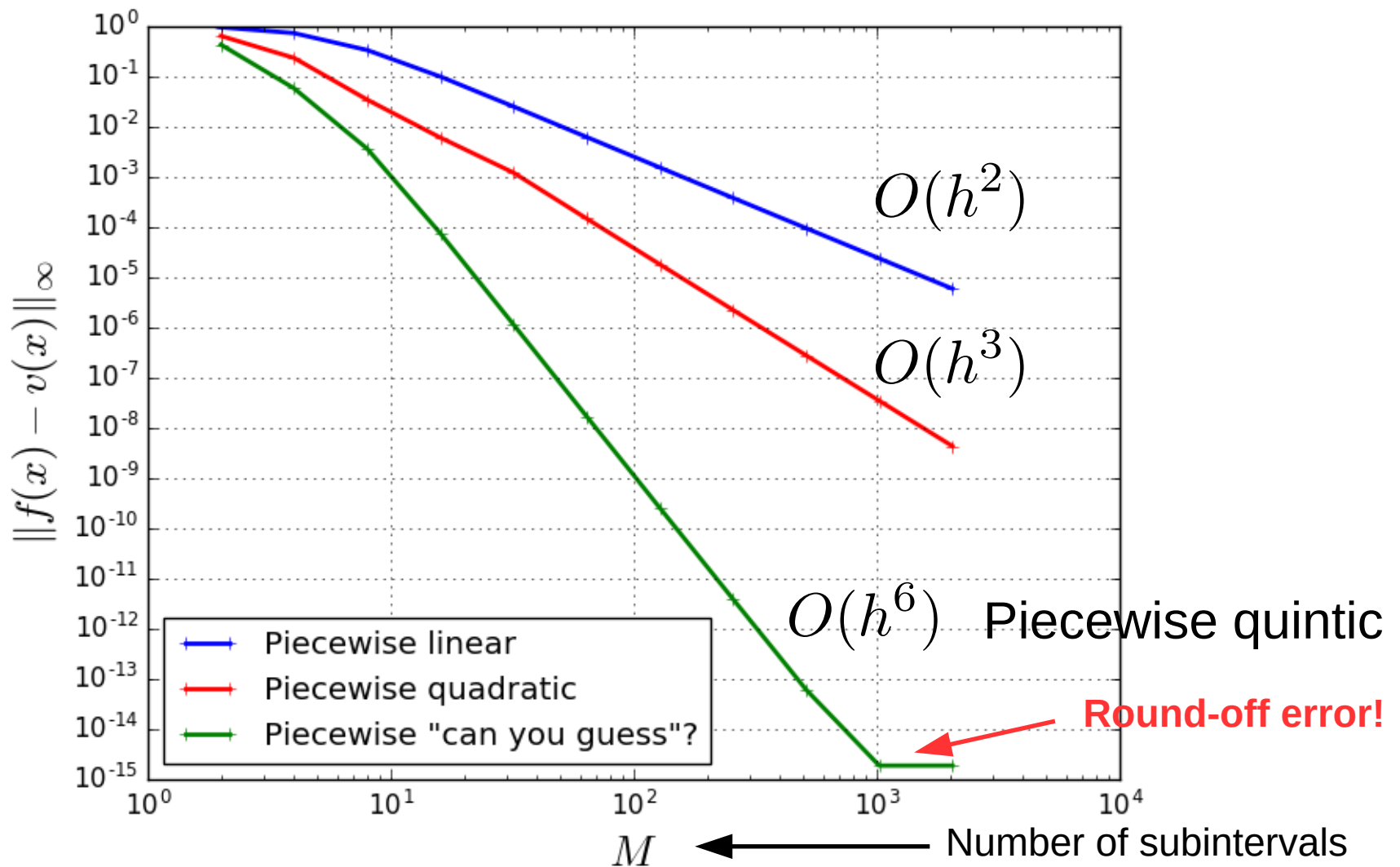
Piecewise quadratic

Runge's example

Piecewise interpolation error

Runge's example

Piecewise interpolation error

I.3 Numerical differentiation

We all know how to differentiate a function analytically...

However, sometimes there are reasons to do this numerically:

- very complicated function (error prone)
  ... e.g. quasi-Newton methods $\leadsto$ Chap. 2

- function not known analytically
  ... e.g. numerical solution of differential equations $\leadsto$ Chap. 3 & 4

Idea: Find IP $p[f \mid x_0, \ldots, x_n]$ approx. the function $f(x)$ and compute

$$f(x) \approx p[f \mid x_0, \ldots, x_n](x)$$

$$f'(x) \approx p'[f \mid x_0, \ldots, x_n](x)$$

$$f''(x) \approx p''[f \mid x_0, \ldots, x_n](x)$$

$$\vdots$$

So suppose we want to approx. the derivatives
of a (sufficiently) smooth function

$$f : I = [a, b] \to \mathbb{R}$$
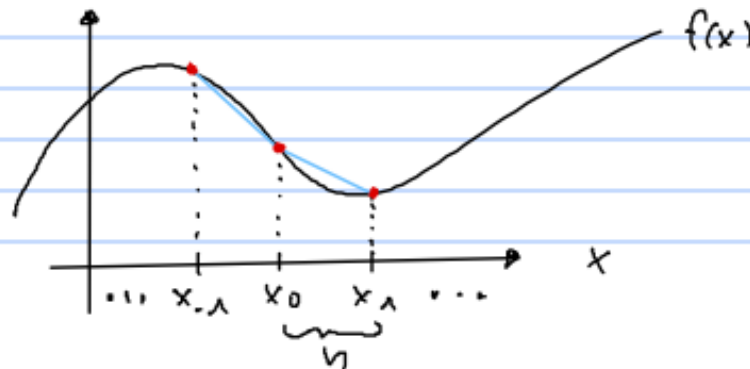
Let $p[f \mid x_1, \dots, x_c]$ be the IP, then

k-th derivative

$$\frac{d^k f}{dx^k}(x) \underset{\approx}{\underset{\text{approx.}}{\approx}} \frac{d^k}{dx^k} p[f \mid x_0, \dots, v_n](x) = \frac{d^k}{dx^k} \sum_{j=0}^{\hat{n}} \hat{L}_j(x) \cdot f(x_j)$$

$$= \sum_{j=0}^{\hat{n}} \frac{d^k \hat{L}_j}{dx^k}(x) \cdot f(x_j)$$

This general procedure leads to so-called
<u>finite difference</u> (FD) approximations of
derivatives.
Usually one uses equidistantly spaced nodes

integers

$$x_j = x_0 + j \cdot h, \quad j \in \mathbb{Z}$$

where h is a constant spacing between nodes.

The resulting formulas are usually evaluated at x_0.

Using a linear IP:

$$f'(x_0) \approx p'[f|x_0, x_\wedge](x_0) = \frac{f(x_\wedge) - f(x_0)}{x_\wedge - x_0}$$

$$= \frac{f(x_0 + h) - f(x_0)}{h}$$

(so-called forward FD)

$$f'(x_0) \approx p'[f|x_{-\wedge}, x_0](x_0) = \frac{f(x_0) - f(x_{-\wedge})}{x_0 - x_{-\wedge}}$$

$$= \frac{f(x_0) - f(x_0 - h)}{h}$$

(so-called backward FD)

What about approx. to f''?

Using a quadratic IP:

$$f'(x_0) \approx p'[f \mid x_{-\wedge}, x_0, x_\wedge] = \frac{f(x_\wedge) - f(x_{-\wedge})}{x_\wedge - x_{-\wedge}}$$

$$= \frac{f(x_0+h) - f(x_0-h)}{2h}$$

$$f''(x_0) \approx p''[f \mid x_{-\wedge}, x_0, x_\wedge] = \frac{f(x_\wedge) - 2f(x_0) + f(x_{-\wedge})}{h^2}$$

$$= \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2}$$

$$\left(\text{so-called} \ \underline{\text{centered}} \ \text{FD} \right)$$
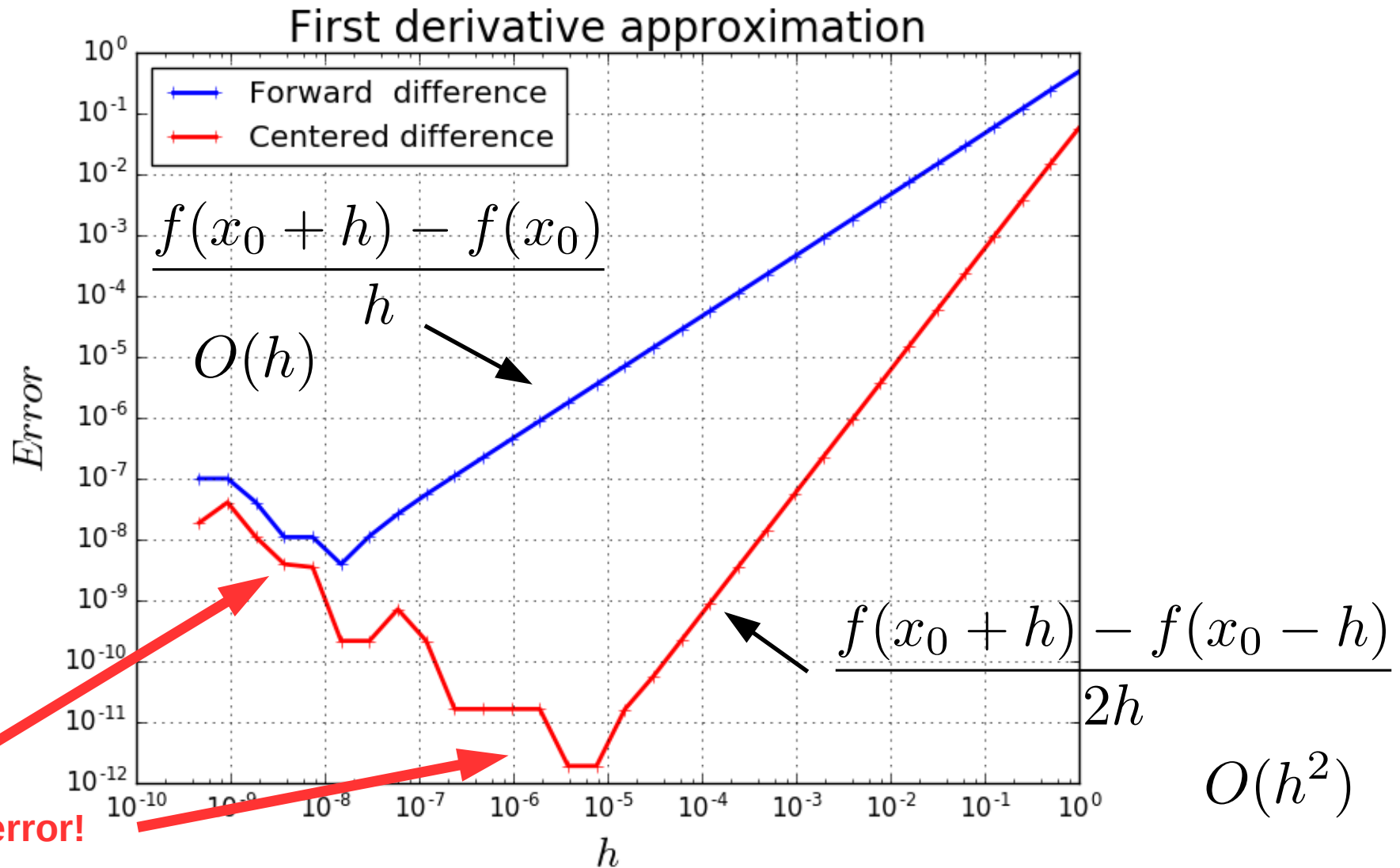
Numerical Differentiation

$$f(x) = \sin(x) \qquad f'(x) = \cos(x) \qquad f'(1.2) = \cos(1.2)$$

Numerical Differentiation

$$f(x) = \sin(x) \qquad f'(x) = \cos(x) \qquad f'(1.2) = \cos(1.2)$$

First derivative approximation

Forward difference

Centered difference

$$\frac{f(x_0 + h) - f(x_0)}{h}$$

$$O(h)$$

$$\frac{f(x_0 + h) - f(x_0 - h)}{2h}$$

$$O(h^2)$$

Round-off error!

Numerical Differentiation

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

$$+ \cdots$$

$$+ \frac{f^{(k)}(x)}{k!} h^k$$

for some
$\xi \in [x, x+h]$

remainder term $\leadsto$ $+ \dfrac{f^{(k+1)}(\xi)}{(k+1)!} h^{k+1}$

(sometimes error term)

Ex.: (6) forward FD approx of f':

$$\frac{f(x_0 + h) - f(x_0)}{h} = \frac{f(x_0) + f'(x_0) \cdot h + \frac{f''(x_0)}{2} h^2 + \ldots - f(x_0)}{h}$$

$$= f'(x_0) + \frac{h}{2} f''(x_0) + \ldots \quad ?$$

$$= f'(x_0) + \mathcal{O}(h) \quad \checkmark$$
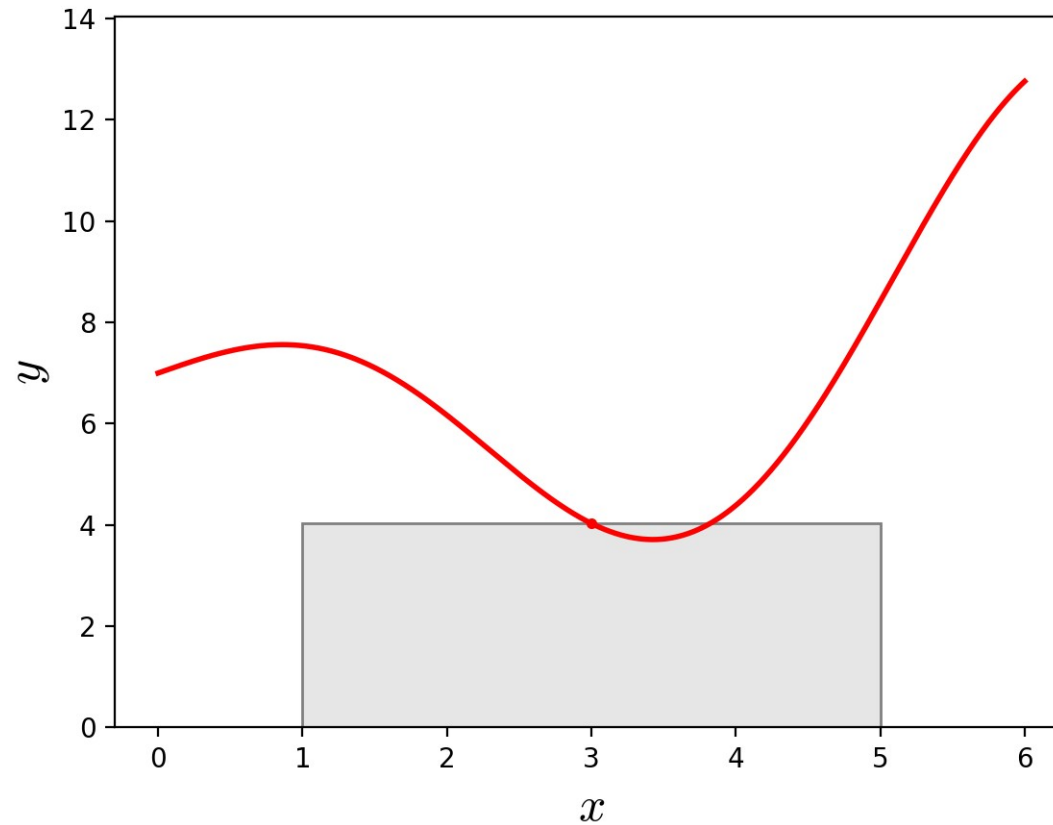
So, for forward FD we have an order of accuracy of $r = 1$
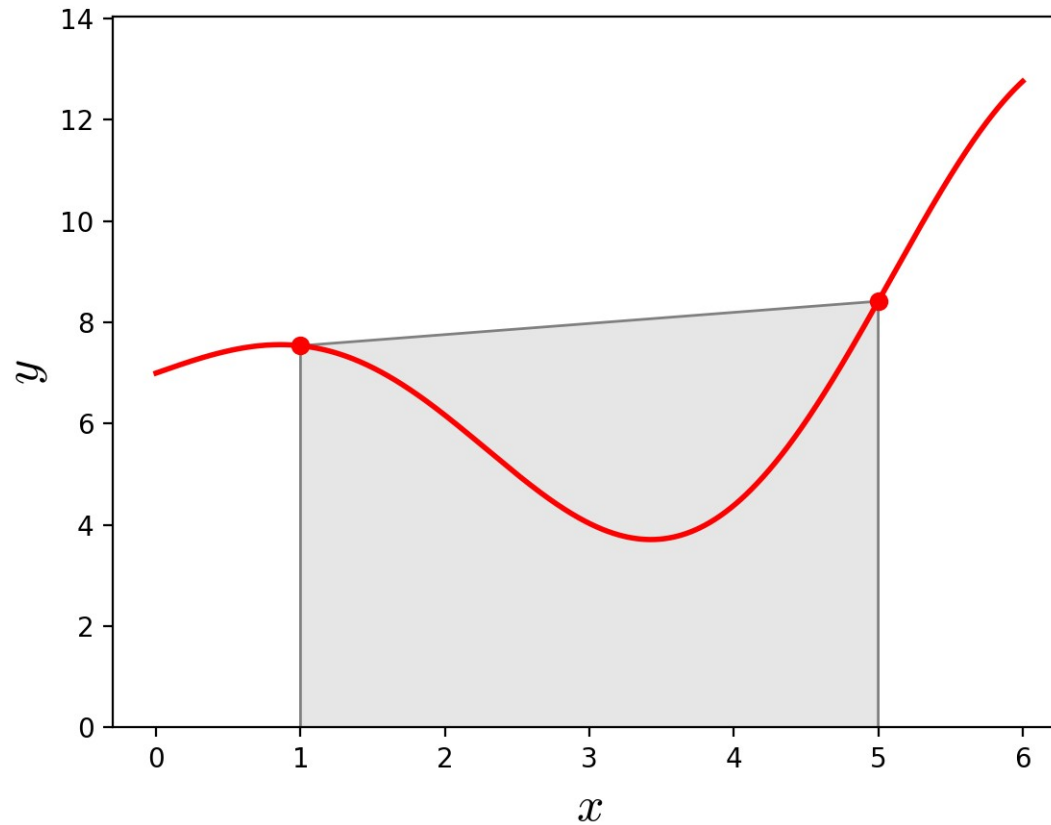
Midpoint rule

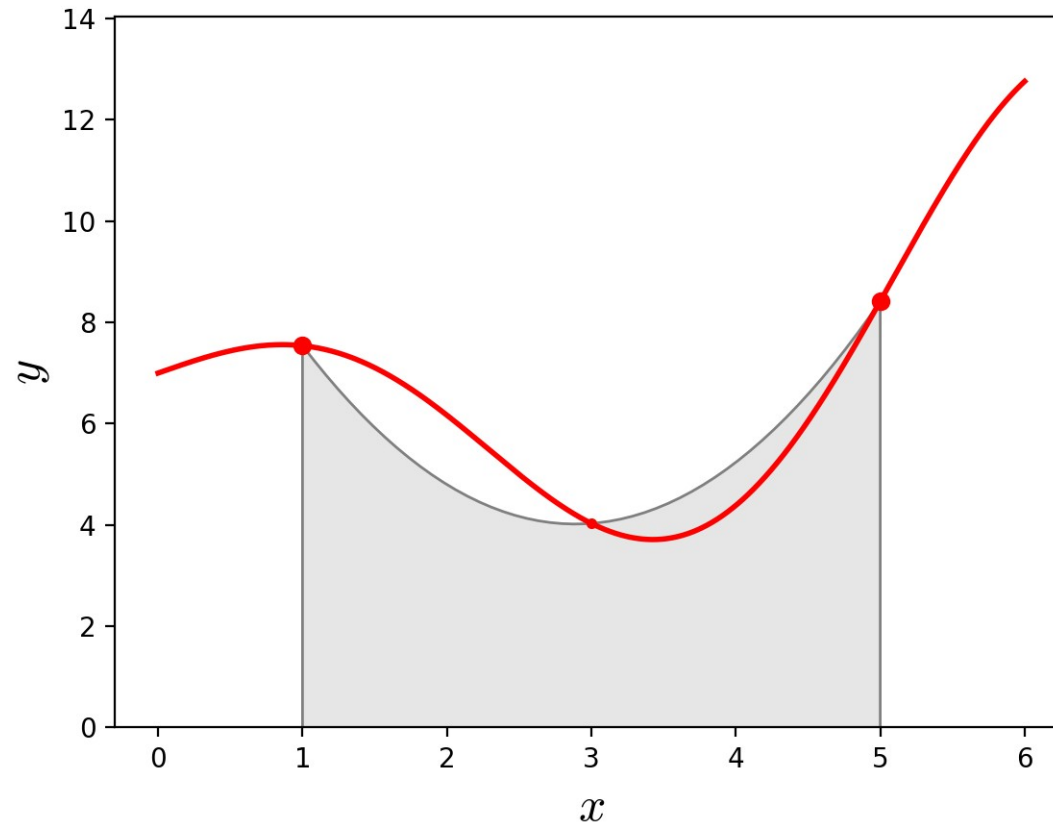$$Q_0[f] = (b-a) f\left(\frac{a+b}{2}\right)$$

Trapezoidal rule

$$Q_1[f] = \frac{b-a}{2}\left(f(a) + f(b)\right)$$

Ex.: (9)

Simpson rule

$$Q_2[f] = \frac{b-a}{6}\left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right)$$

Degree of exactness

<u>Def.:</u> the degree of exactness (DoE) q is defined as the maximum polynomial degree a QR can integrate exactly

The property is easily check by comparing the exact value of the integral over a reference interval

$$I[x^k] = \int_0^1 x^k \ \mathrm{d}x = \left.\frac{x^{k+1}}{k+1}\right|_0^1 = \frac{1}{k+1}$$

with the result of the QR $Q[x^k]$

Example: DoE of Simpson rule $Q_2[f] = \frac{b-a}{6}\left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right)$

$$I[1] = 1 = Q_2[1] = \frac{1}{6}(1+1+1) = 1$$

$$I[x] = \frac{1}{2} = Q_2[x] = \frac{1}{6}(0+2+1) = \frac{1}{2}$$

$$I[x^2] = \frac{1}{3} = Q_2[x^2] = \frac{1}{6}(0+1+1) = \frac{1}{3}$$

$$I[x^3] = \frac{1}{4} = Q_2[x^3] = \frac{1}{6}\left(0+\frac{1}{2}+1\right) = \frac{1}{4}$$

$$I[x^4] = \frac{1}{5} \neq Q_2[x^4] = \frac{1}{6}\left(0+\frac{1}{4}+1\right) = \frac{5}{24}$$

$\implies$ $q = 3$

Composite quadrature rules

Divide the integration interval $I = [a, b]$ in N subintervals

$$I_j = [x_{j-1}, x_j] \quad , \quad j = 1, 2, \ldots, N$$

$$x_j = a + \frac{b-a}{N} \cdot j \quad , \quad j = 0, 1, \ldots, N$$
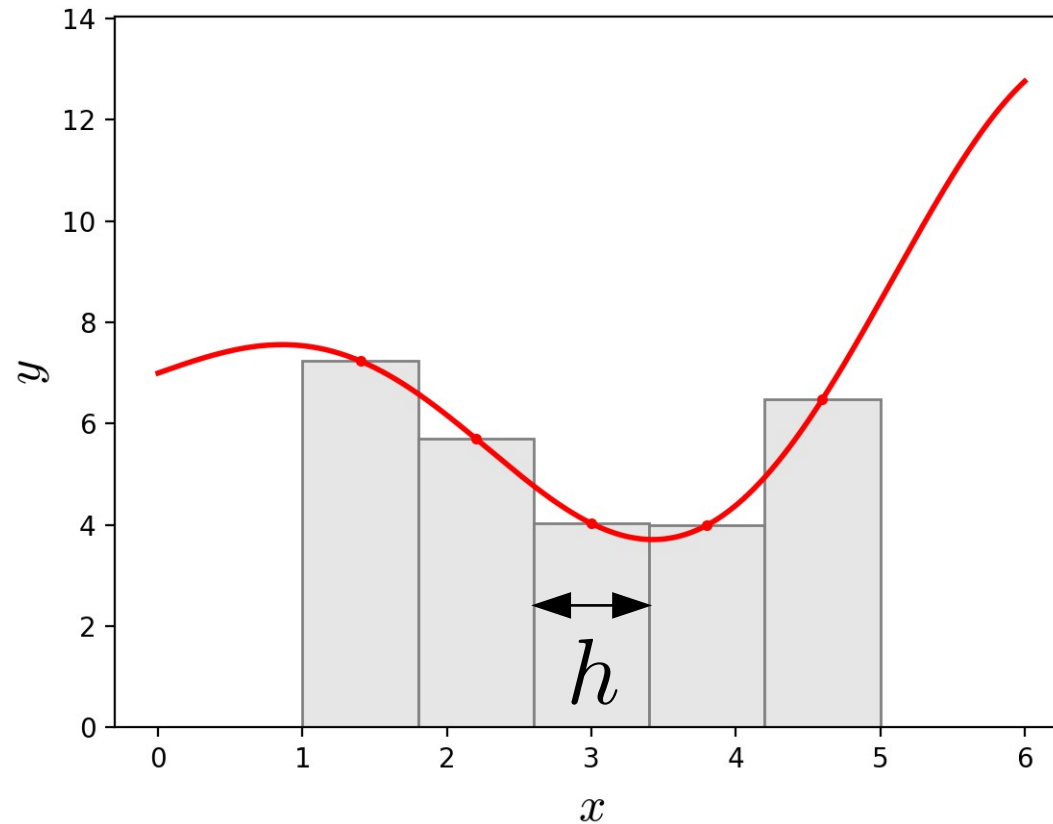
$$\underbrace{\qquad}_{h}$$

and apply a QR over each I_j.

This leads to so-called composite QRs

Composite midpoint rule

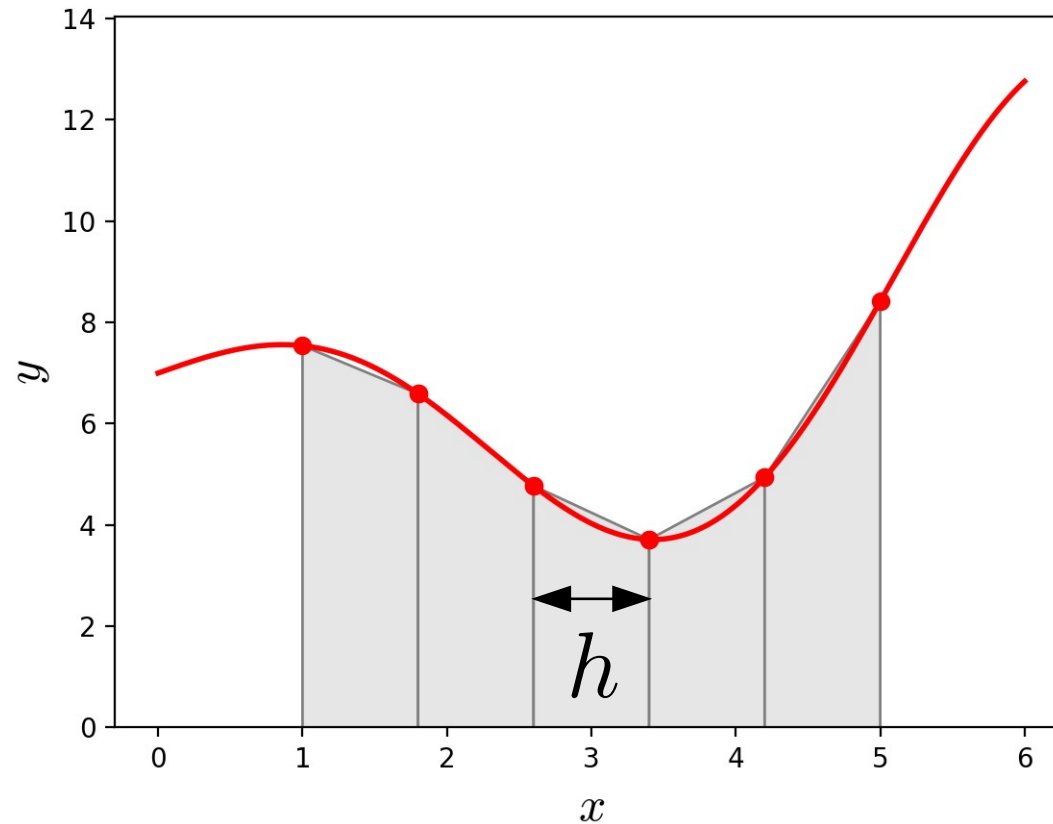$$Q_0^N[f] = h \sum_{k=1}^{N} f\left(\frac{x_{k-1} + x_k}{2}\right)$$

$$N = 5$$

Composite trapezoidal rule

$$Q_1^N[f] = \frac{h}{2}\left(f(a) + 2\sum_{k=1}^{N-1} f(x_k) + f(b)\right)$$

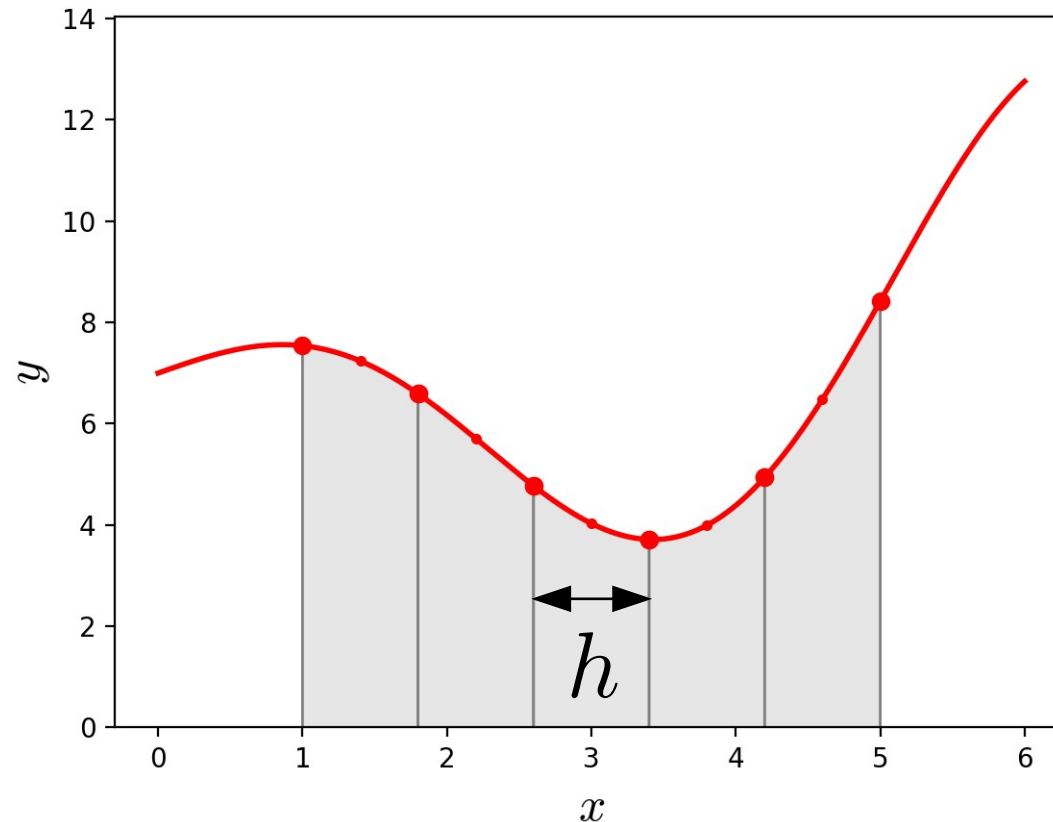$$N = 5$$

Composite Simpson rule

$$Q_1^N[f] = \frac{h}{6}\left(f(a) + 2\sum_{k=1}^{N-1} f(x_k) + 4\sum_{k=1}^{N} f\left(\frac{x_{k-1} + x_k}{2}\right) + f(b)\right)$$

$$N = 5$$

The QE of a CQR is (obviously) the sum of QEs over each subinterval.
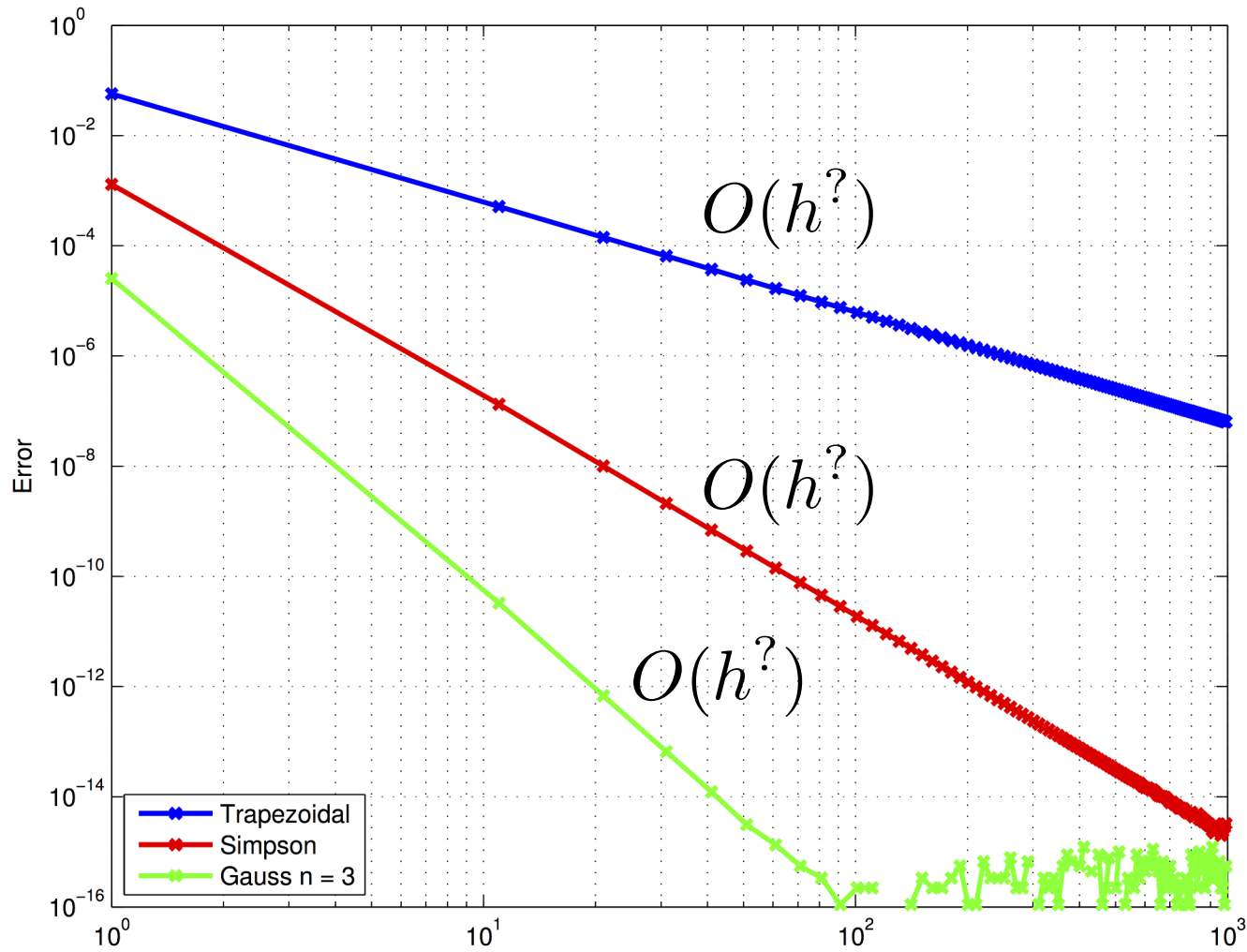
One can show that

$$E^N(f) = |Q_n^N(f) - I[f]|$$

$$\leq \frac{\|f^{(q+1)}\|_\infty}{(q+1)!}(b-a)h^{q+1} = \frac{\|f^{(s)}\|_\infty}{s!}(b-a)h^s$$
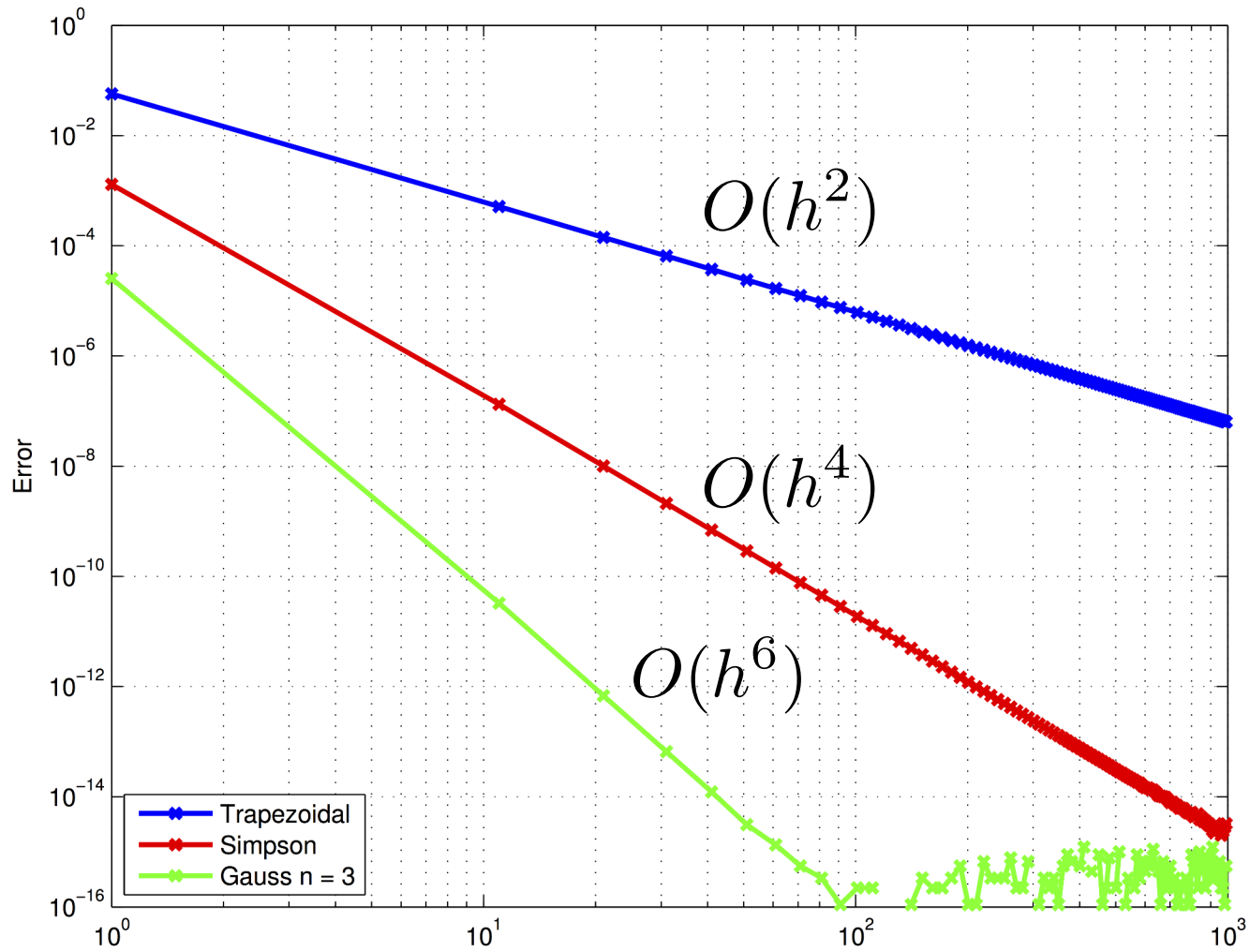
DoE

order of accuracy

Quadrature

$$E^N[f] = \left| I[f] - Q^N[f] \right|$$

$$\int_0^1 \frac{1}{1+x} \mathrm{d}x = \log(2)$$

Quadrature

$$\int_0^1 \frac{1}{1+x}\mathrm{d}x = \log(2)$$

Adaptive Quadrature

Idea: Compute an approximation of the integral with two methods

$Q_1[f]$ method 1

$Q_2[f]$ method 2 (more precise than method 1)

and compare the results to get an estimate of the quadrature error.

Adaptive Quadrature

Adaptive quadrature (~ Pseudo-MATLAB-Code)

Function $Q = adapt\_quad (f, a, b, tol)$

$\quad Q1 = quad1 (f, a, b)$ method 1

$\quad Q2 = quad2 (f, a, b)$ method 2

$\quad E = abs (Q1 - Q2)$

$\quad$ if $E < tol$

$\quad\quad Q = Q2$ (keep the more precise
$\quad\quad\quad\quad\quad\quad$ result)

$\quad$ else

$\quad\quad Ql = adapt\_quad (f, a, \frac{a+b}{2}, \frac{tol}{2})$

$\quad\quad Qr = adapt\_quad (f, \frac{a+b}{2}, b, \frac{tol}{2})$

$\quad\quad Q = Qr + Ql$

$\quad$ end

end

Adaptive Quadrature

$$I[f] = \int_{3/2}^{4} \left(\frac{200}{2x^3 - x^2} \right) \left(5 \sin(20/x) \right)^2 \, \mathrm{d}x$$

Adaptive Quadrature

$$I[f] = \int_{3/2}^{4} \left(\frac{200}{2x^3 - x^2} \right) \left(5 \sin(20/x) \right)^2 \, \mathrm{d}x$$

Adaptive Quadrature

$$I[f] = \int_0^1 e^{-x^2}\,\mathrm{d}x$$

Adaptive Quadrature

$$I[f] = \int_0^1 e^{-x^2}\,\mathrm{d}x$$

Adaptive Quadrature

$$I[f] = \int_0^1 e^{-x} \sin(4\pi x) \mathrm{d}x$$

Adaptive Quadrature

$$I[f] = \int_0^1 e^{-x}\sin(4\pi x)\mathrm{d}x$$