**Task:** Given a table of some quantity $q$

| $i$ | 0 | 1 | 2 | ... | $n$ |
|---|---|---|---|---|---|
| $x_i$ | 0.00 | 0.51 | 1.05 | ... | $x_n$ |
| $q_i$ | 0.00 | 0.22 | 0.25 | ... | $q_n$ |

compute approximations of $q(x)$, $q'(x)$, $\int_a^b q(x)\,dx$ ?

i.e. easy to evaluate, derive, integrate

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

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

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

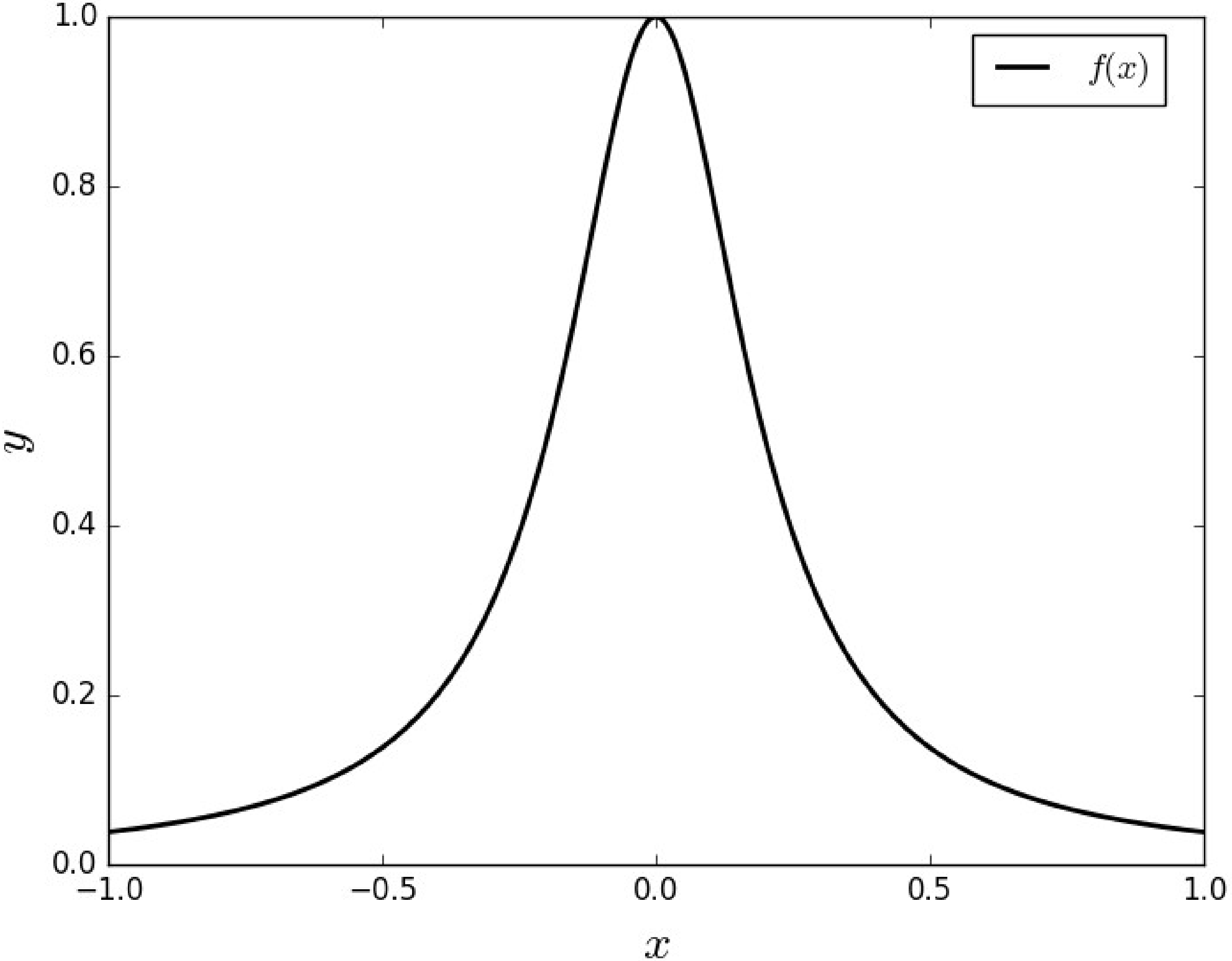
$$p_2(x) = 2 \cdot L_0^2(x) + 5 \cdot L_1^2(x) + 4 \cdot L_2^2(x)$$

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

(like Ex.(1), indeed!)

# Runge's example

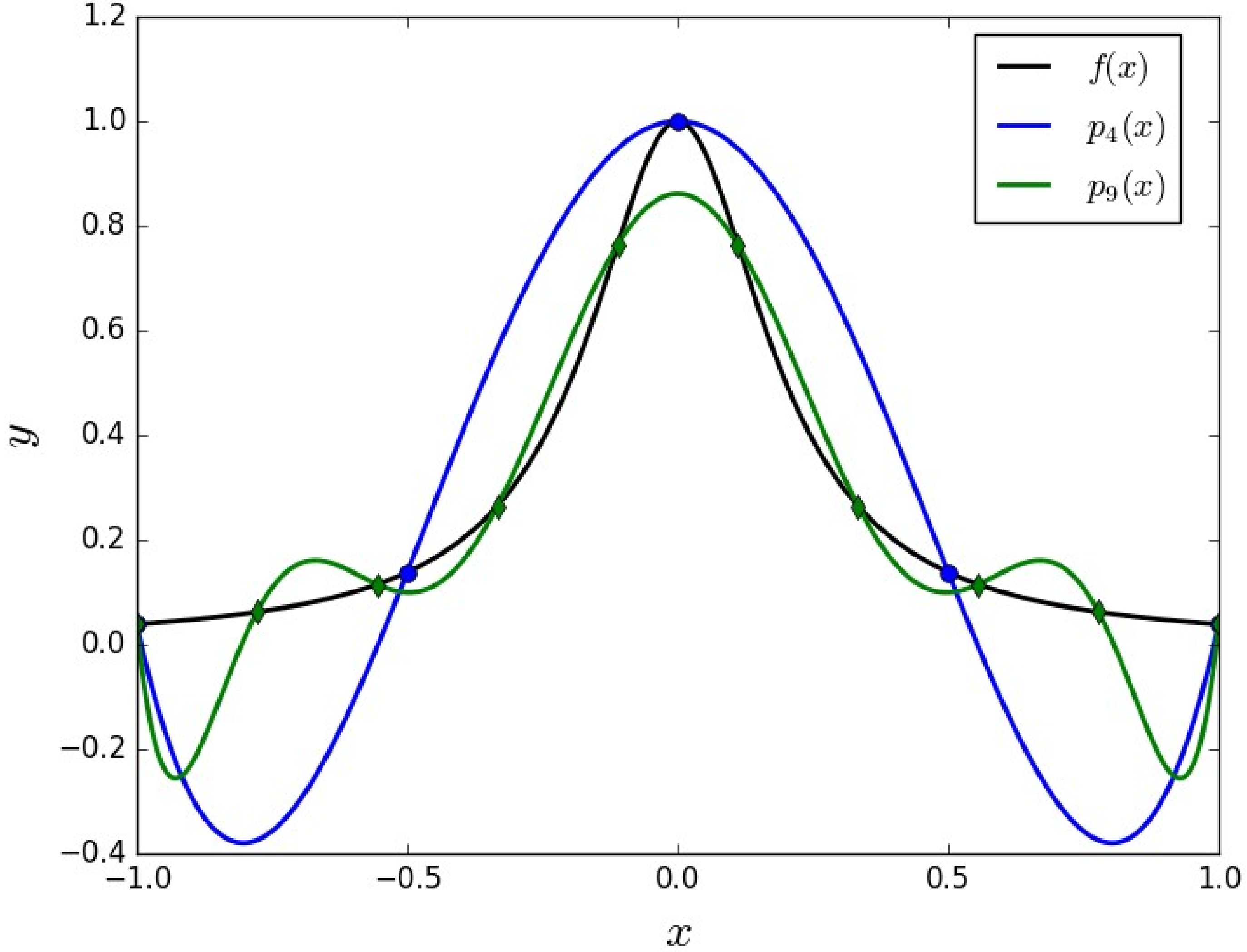
$$f(x) = \frac{1}{1 + 25x^2} \qquad x \in [-1, 1]$$



Ex.: (3)

# Runge's example

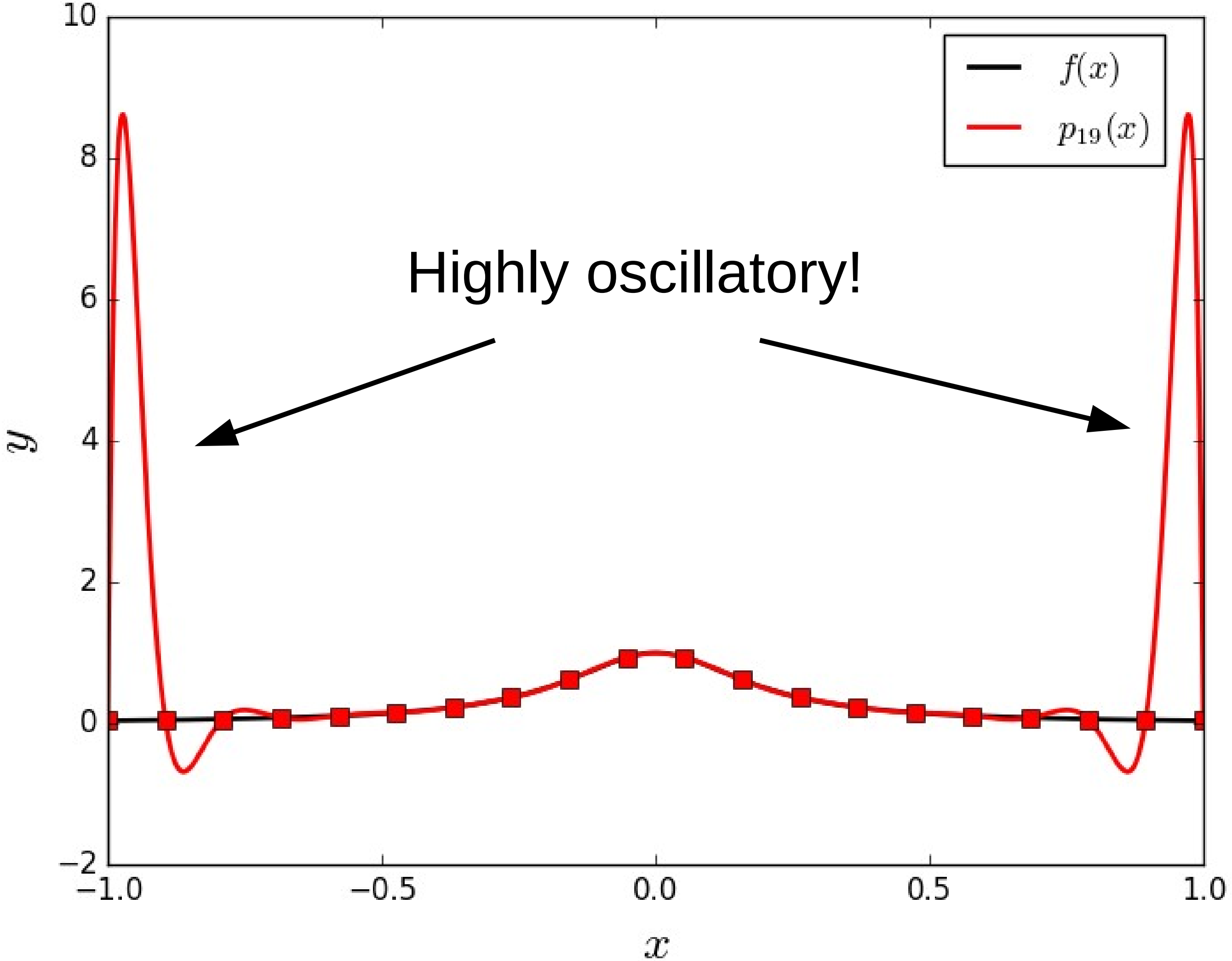
Equidistant: $$x_j = -1 + \frac{2}{n} j \text{ for } j = 0, 1, ..., n$$



Ex.: (3)

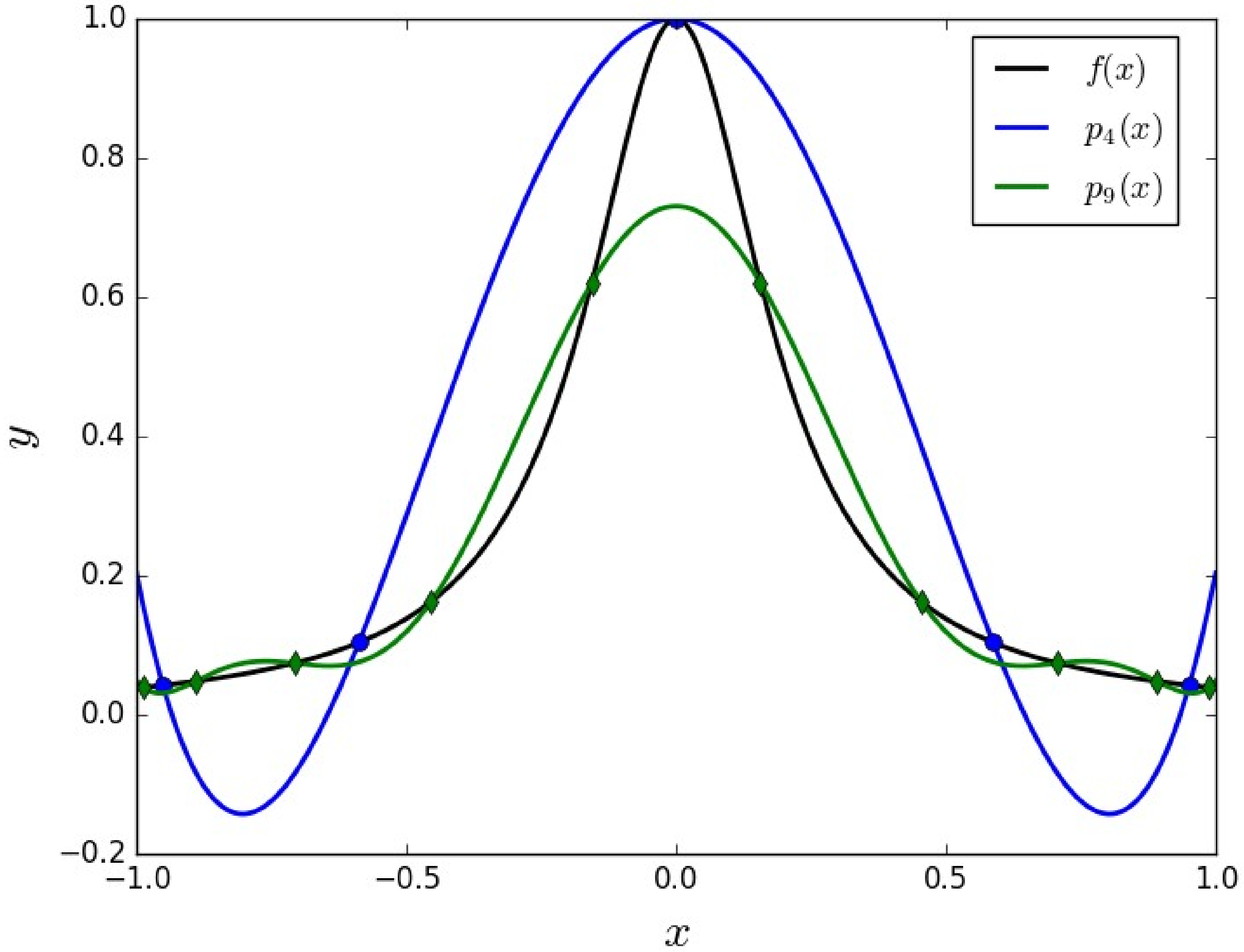
# Runge's example

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



# Runge's example

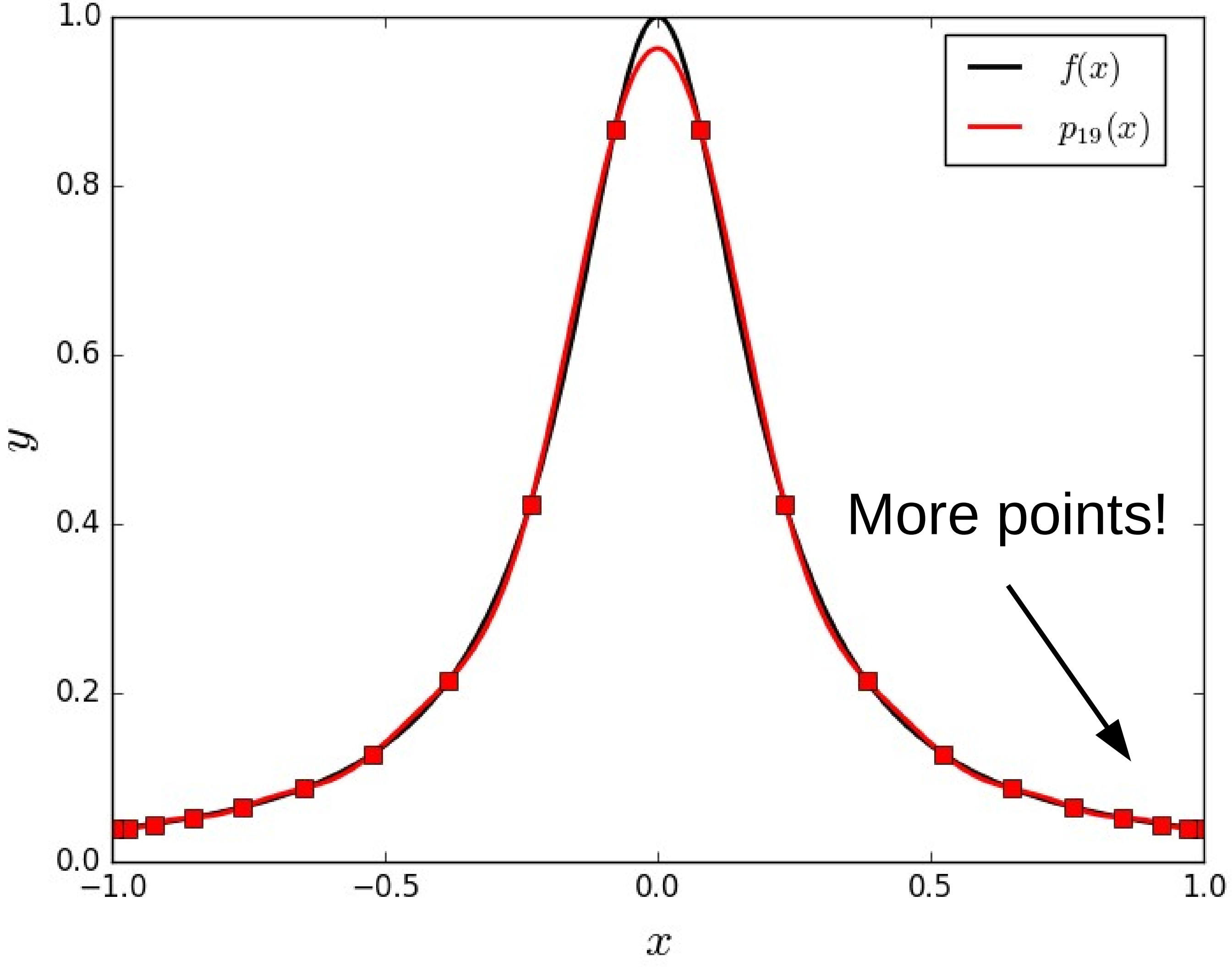
Chebyshev: $x_j = \cos\left(\frac{2j+1}{2(n+1)}\pi\right)$ for $j = 0, 1, ..., n.$



Ex.: (3)

# Runge’s example

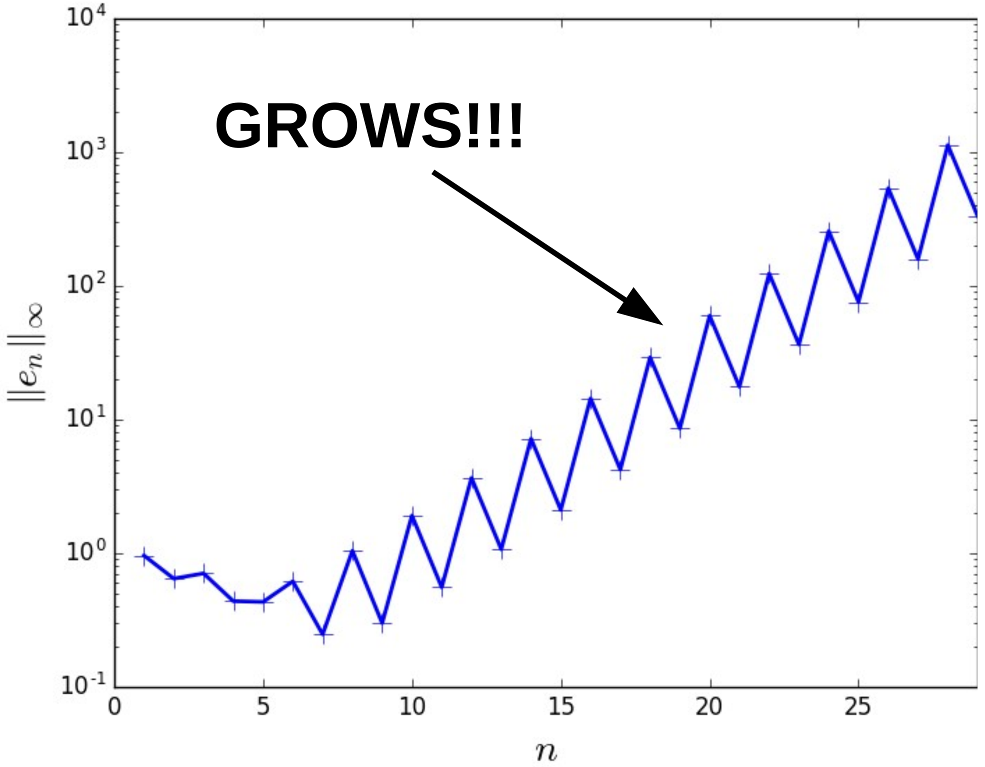
Chebyshev: $$x_j = \cos\left(\frac{2j+1}{2(n+1)}\pi\right) \quad \text{for} \quad j = 0, 1, ..., n.$$



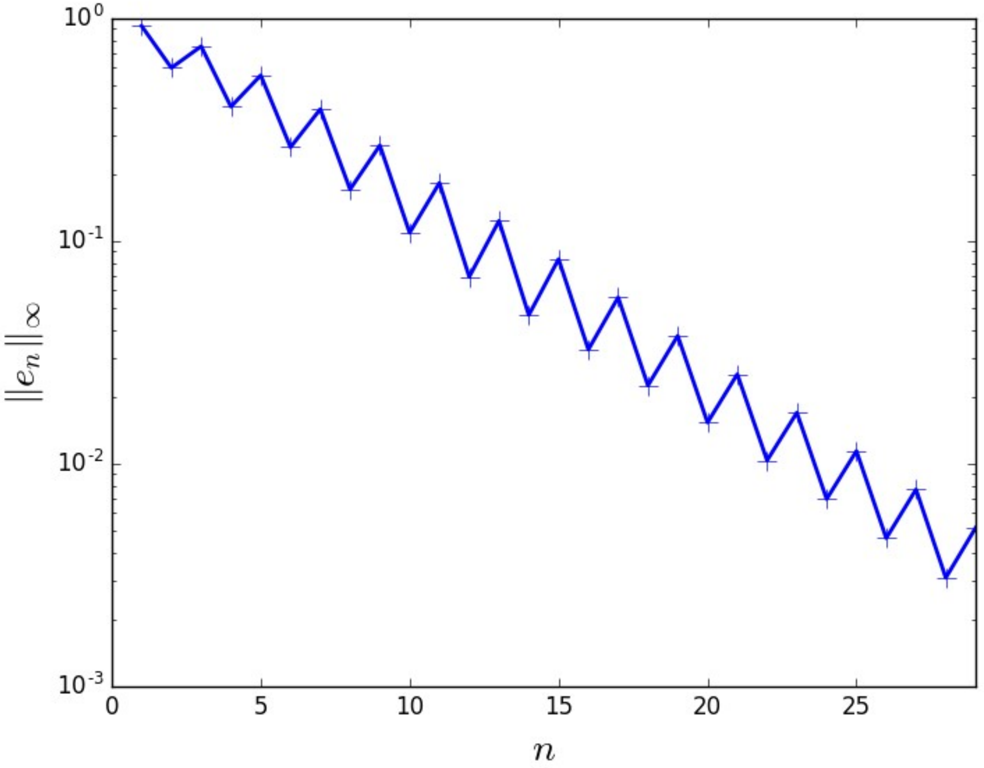
Ex.: (3)

# Runge's example

**Equidistant**




**Chebyshev**

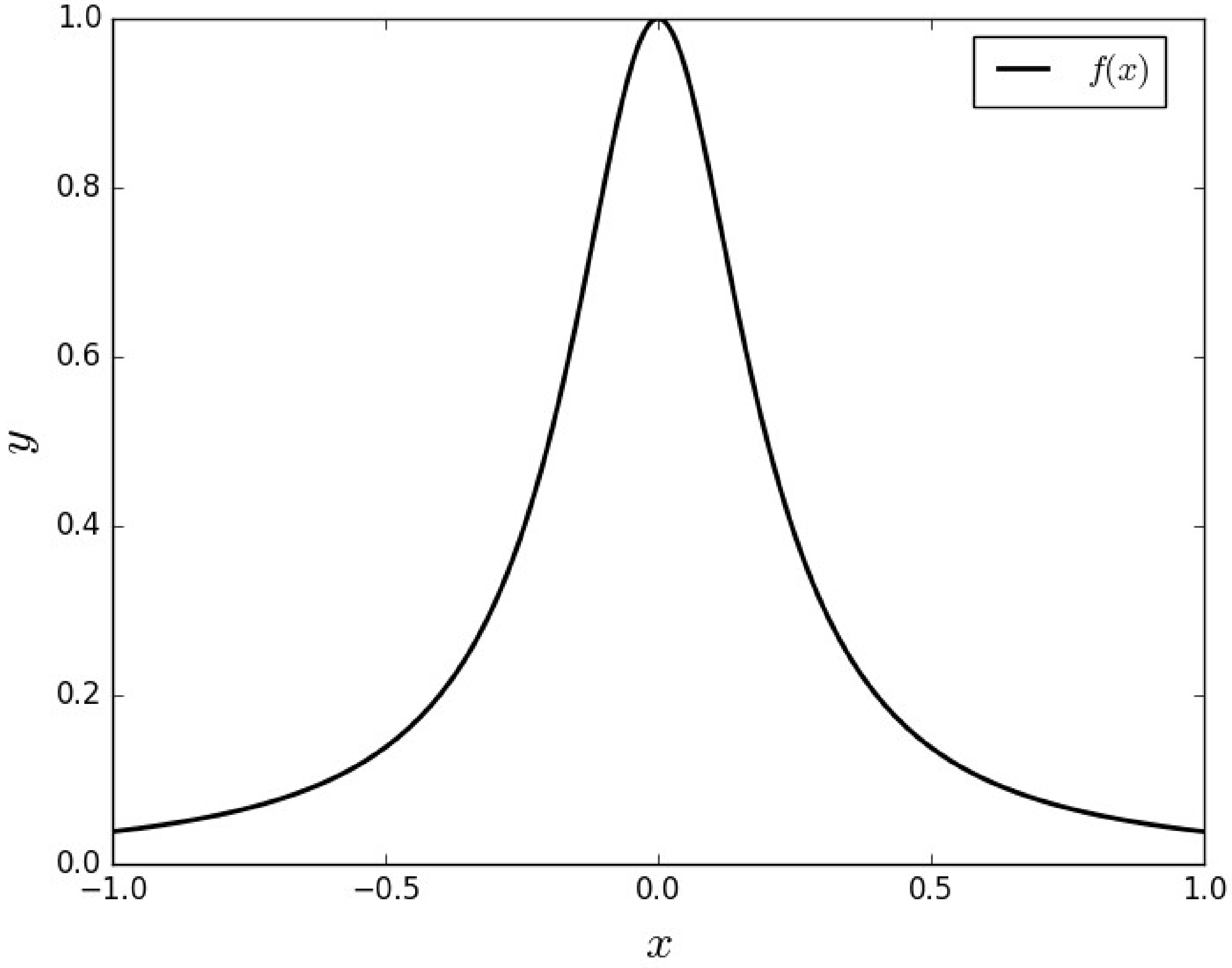



**Interpolation error:** $\|e_n\|_\infty = \|f - p_n\|_\infty$

Ex.: (3)

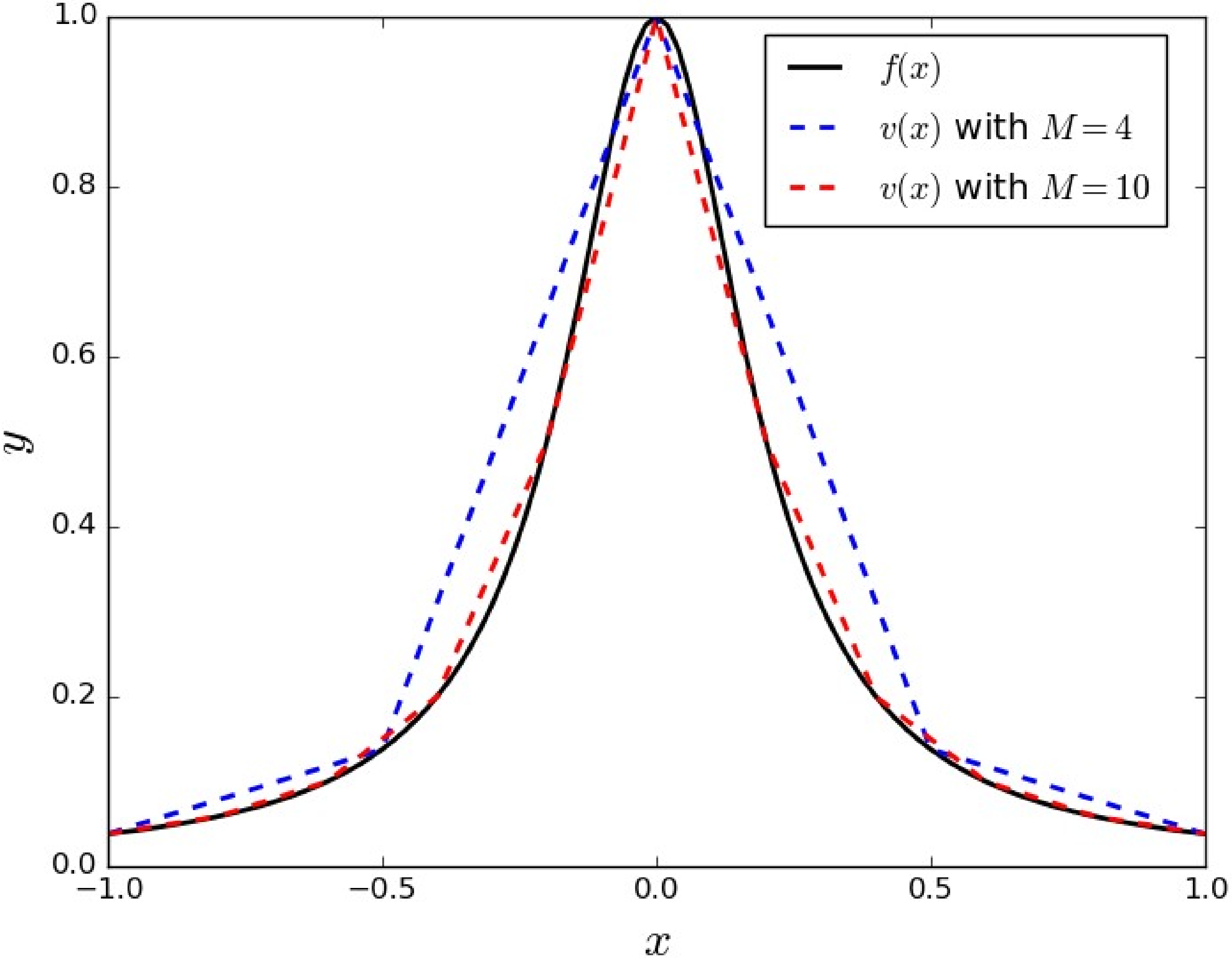
# Runge's example

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



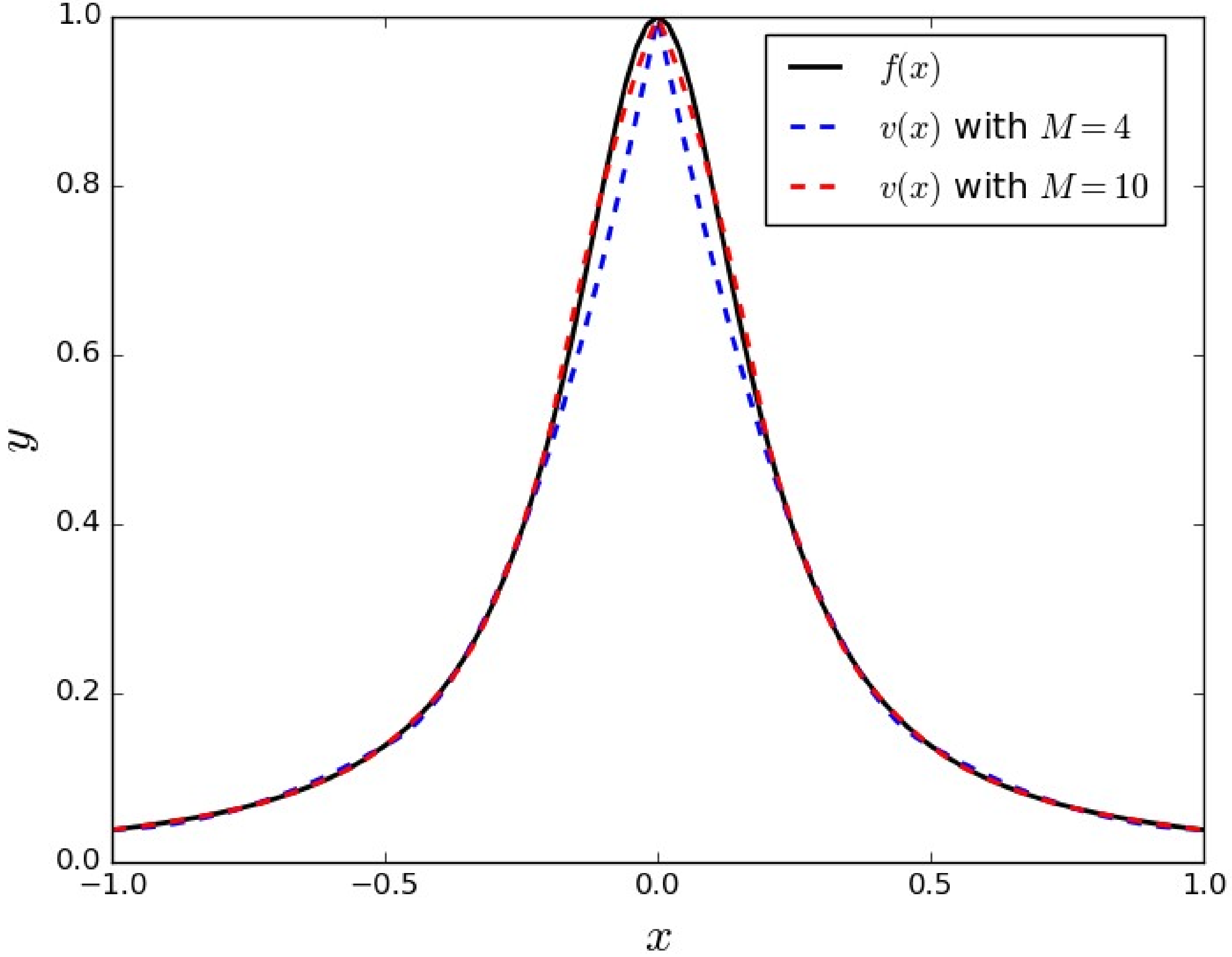
# Runge's example

Piecewise linear



# Runge’s example

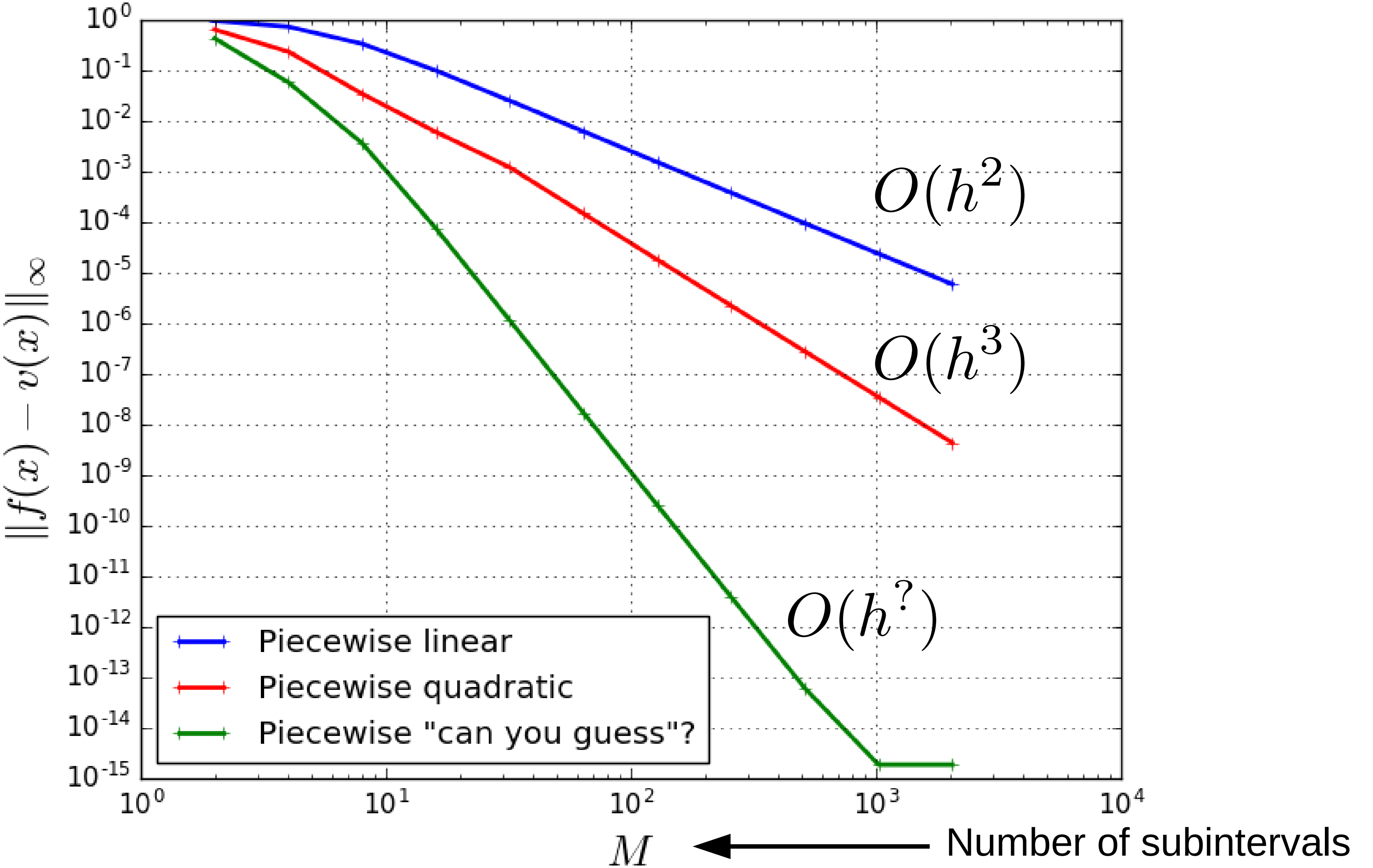
Piecewise quadratic



Ex.: (4)

# Runge's example

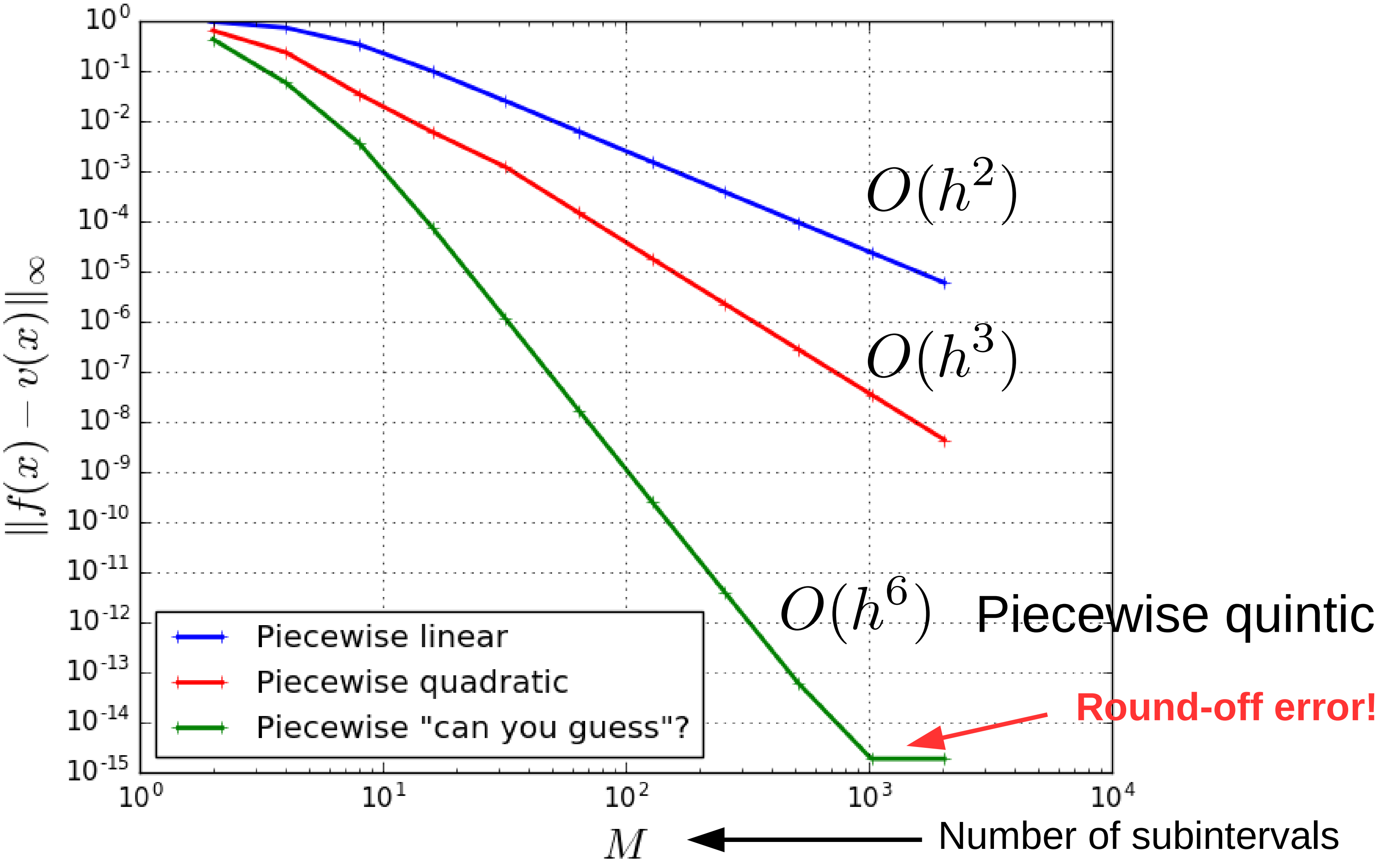
Piecewise interpolation error



Ex.: (4)

# 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 ⇝ Chap. 2
- function not known analytically
  ... e.g. numerical solution of differential equations ⇝ Chap. 3 & 4

<u>Idea:</u> Find IP $p[f|x_0,\dots,x_n]$ approx. the function $f(x)$ and compute

$$f(x) \approx p[f|x_0,\dots,x_n](x)$$

$$f'(x) \approx p'[f|x_0,\dots,x_n](x)$$

$$f''(x) \approx p''[f|x_0,\dots,x_n](x)$$

$$\vdots$$

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

$$f: I = [a,b] \to \mathbb{R}$$

Let $p[f|x_1,\dots,x_n]$ be the IP, then

k-th derivative

$$\frac{d^k f}{dx^k}(x) \approx \frac{d^k}{dx^k} p[f|x_0,\dots,x_n](x) = \frac{d^k}{dx^k} \sum_{j=0}^{n} L_j^n(x) \cdot f(x_j)$$

approx.

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

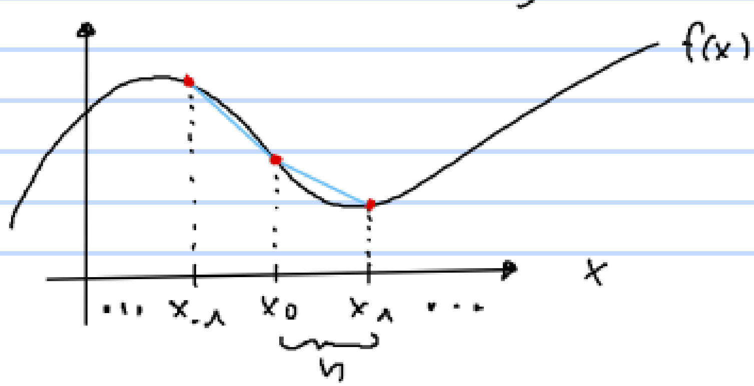
This general procedure leads to so-called finite difference (FD) approximations of derivatives.

Usually one uses equidistantly spaced nodes

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

integers

where $h$ is a constant spacing between nodes.



The resulting formulas are usually evaluated at $x_0$.

Using a linear IP:

$$f'(x_0) \approx p'[f|x_0, x_1](x_0) = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

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

(so-called forward FD)

$$f'(x_0) \approx p'[f|x_{-1}, x_0](x_0) = \frac{f(x_0) - f(x_{-1})}{x_0 - x_{-1}}$$

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

(so-called backward FD)

What about approx. to $f''$ ?

Using a quadratic IP:

$$f'(x_0) \approx p'[f|x_{-1},x_0,x_1] = \frac{f(x_1)-f(x_{-1})}{x_1-x_{-1}}$$

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

$$f''(x_0) \approx p''[f|x_{-1},x_0,x_1] = \frac{f(x_1)-2f(x_0)+f(x_{-1})}{h^2}$$

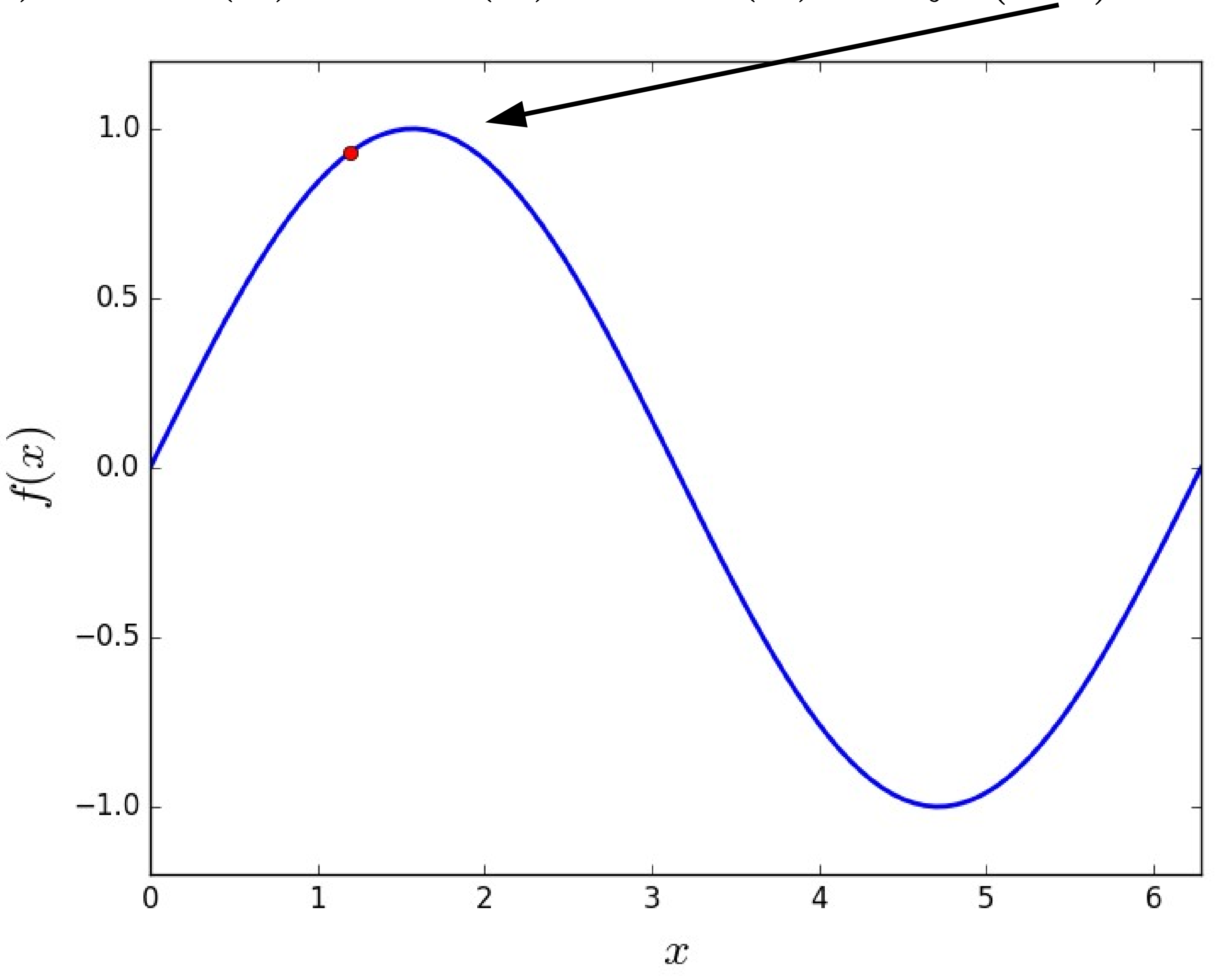
$$= \frac{f(x_0+h)-2f(x_0)+f(x_0-h)}{h^2}$$

(so-called centered FD)

Ex.: (5)

# Numerical Differentiation

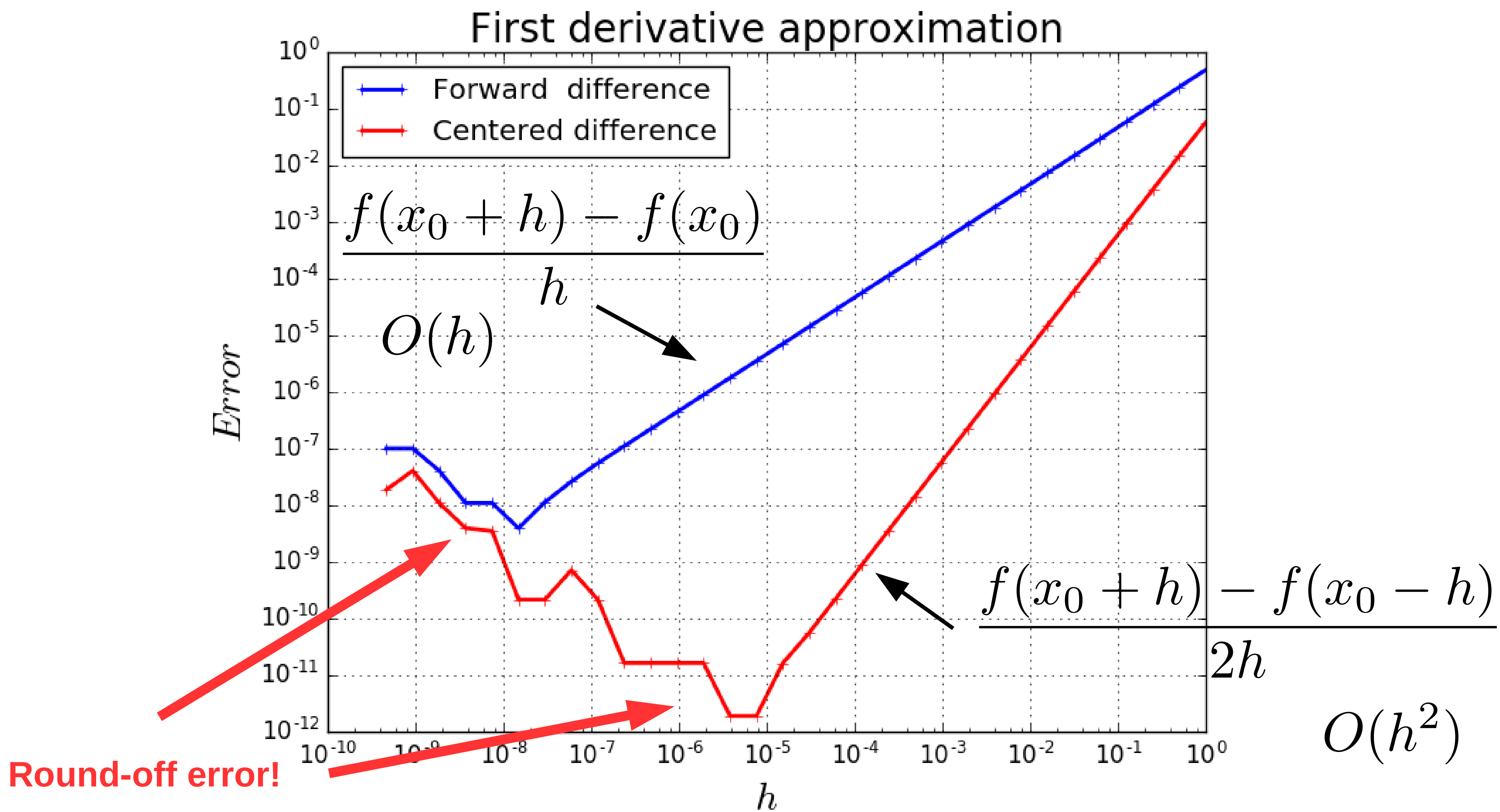
$$f(x) = \sin(x) \qquad f'(x) = \cos(x) \qquad f'(1.2) = \cos(1.2)$$



Ex.: (5)

# Numerical Differentiation

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



# Numerical Differentiation

$$f(x+h) = f(x) + f'(x)\cdot h + \frac{f''(x)}{2}h^2 + \dots + \frac{f^{(k)}(x)}{k!}h^k + \frac{f^{(k+1)}(\xi)}{(k+1)!}h^{k+1}$$

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

remainder term (sometimes error term)

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

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

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

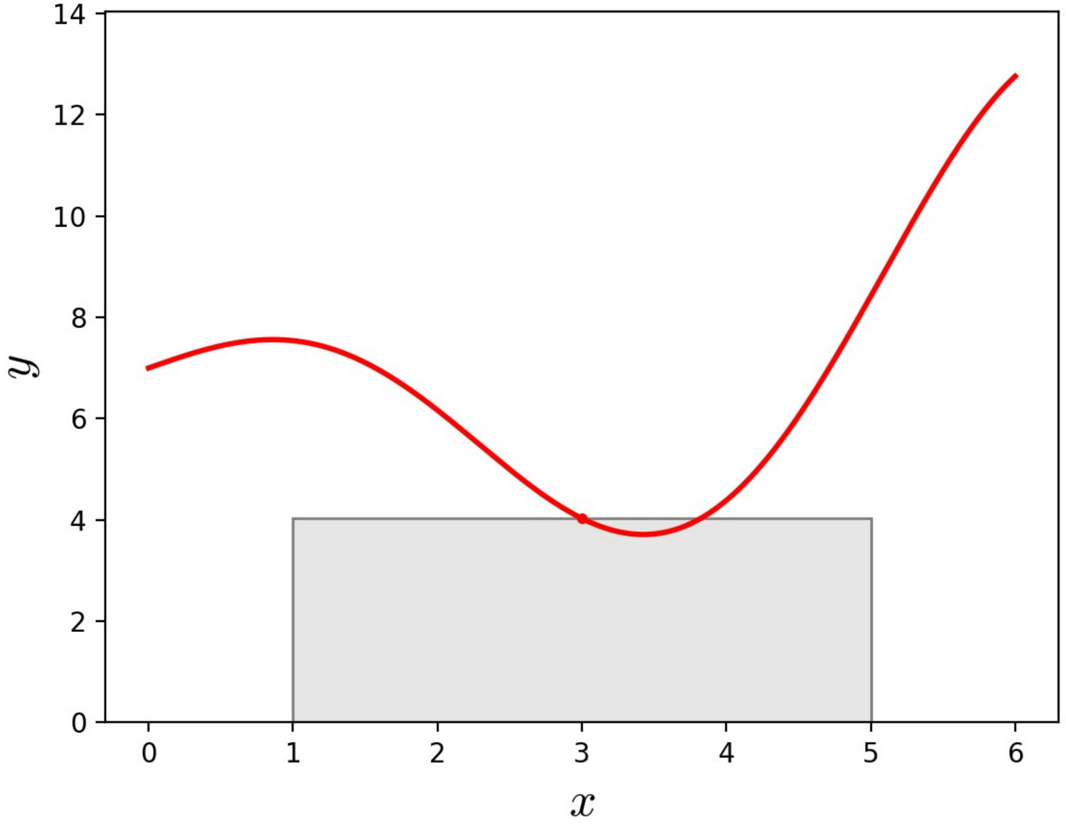
$$= f'(x_0) + \mathcal{O}(h) \quad ✓.$$

So, for forward FD we have an order of accuracy of $r = 1$

Ex.: (7)

# Midpoint rule

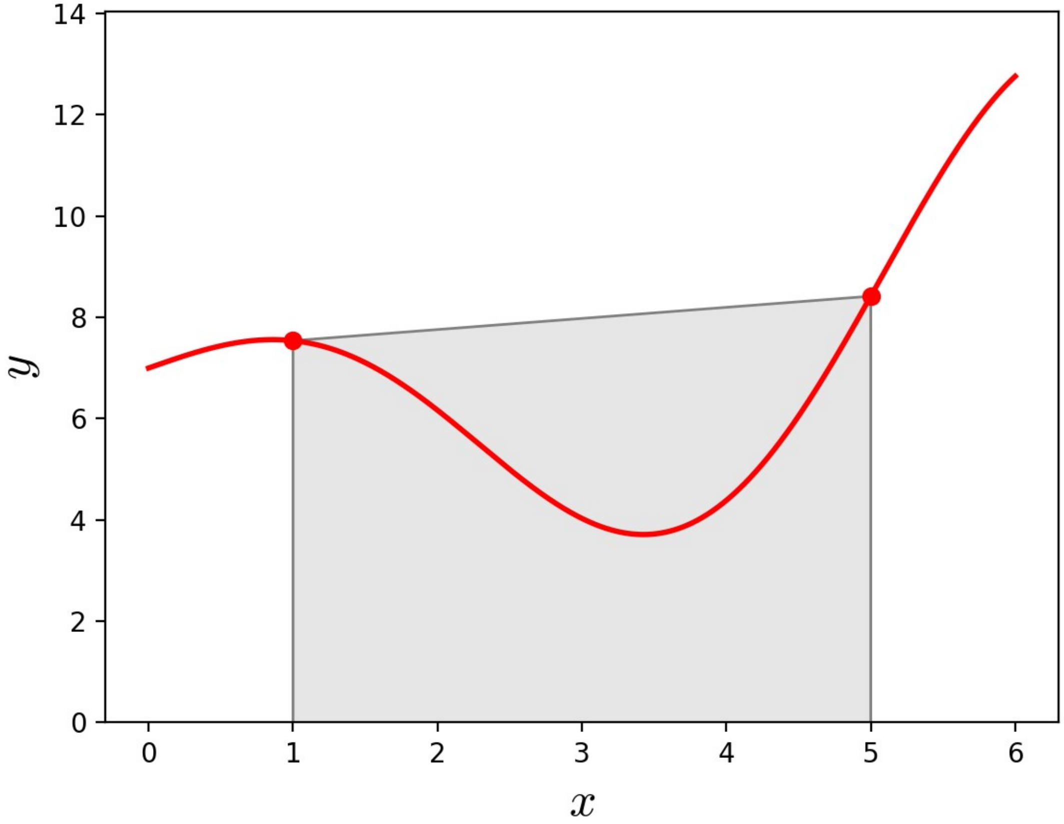
$$Q_0[f] = (b-a)f\left(\frac{a+b}{2}\right)$$



Ex.: (8)

# Trapezoidal rule

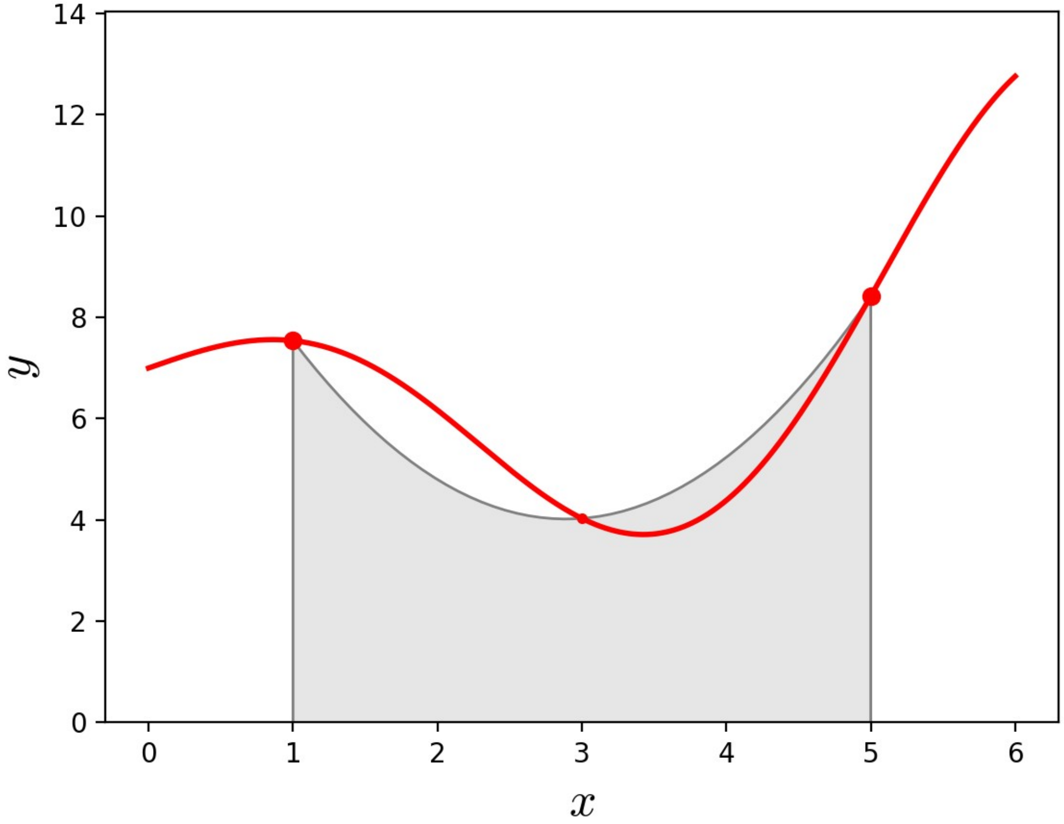
$$Q_1[f] = \frac{b-a}{2}\left(f(a) + f(b)\right)$$



Ex.: (9)

# Simpson rule

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



Measure of quality

# Degree of exactness

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

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

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

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

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

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

→ $q = 3$

# Composite quadrature rules

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

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

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

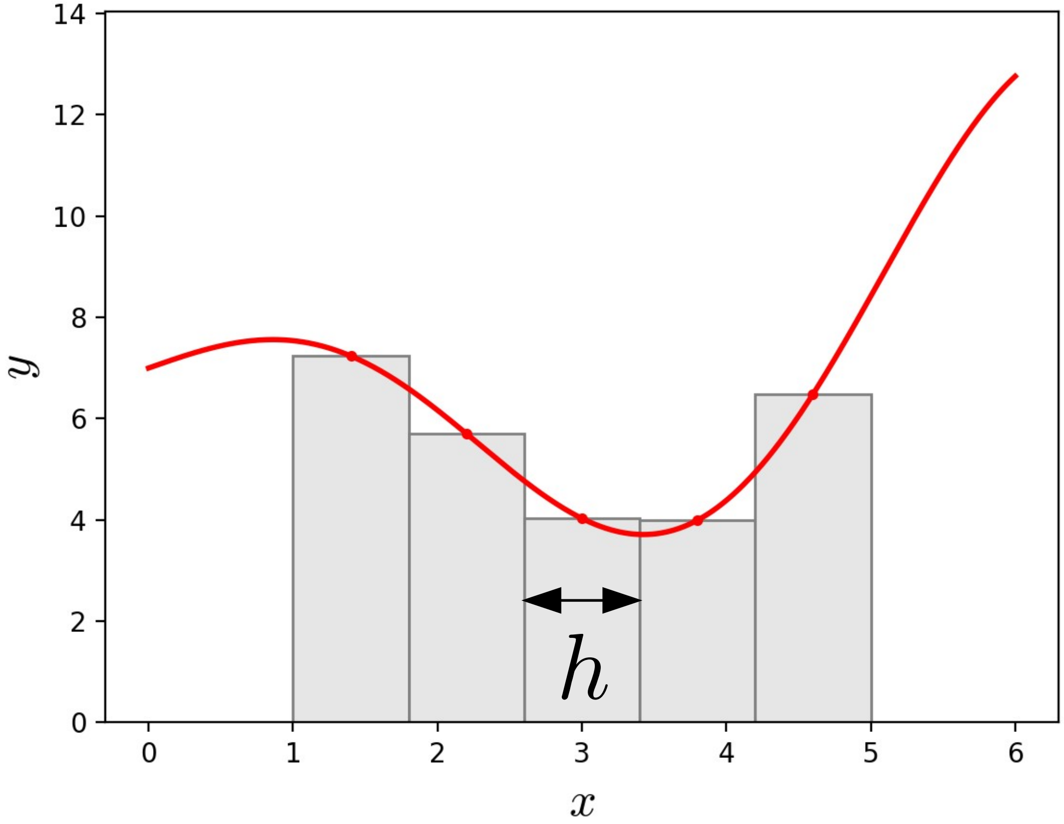
and apply a QR over each $I_j$.

This leads to so-called <u>composite QRs</u>

Ex.: (10)

# Composite midpoint rule

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

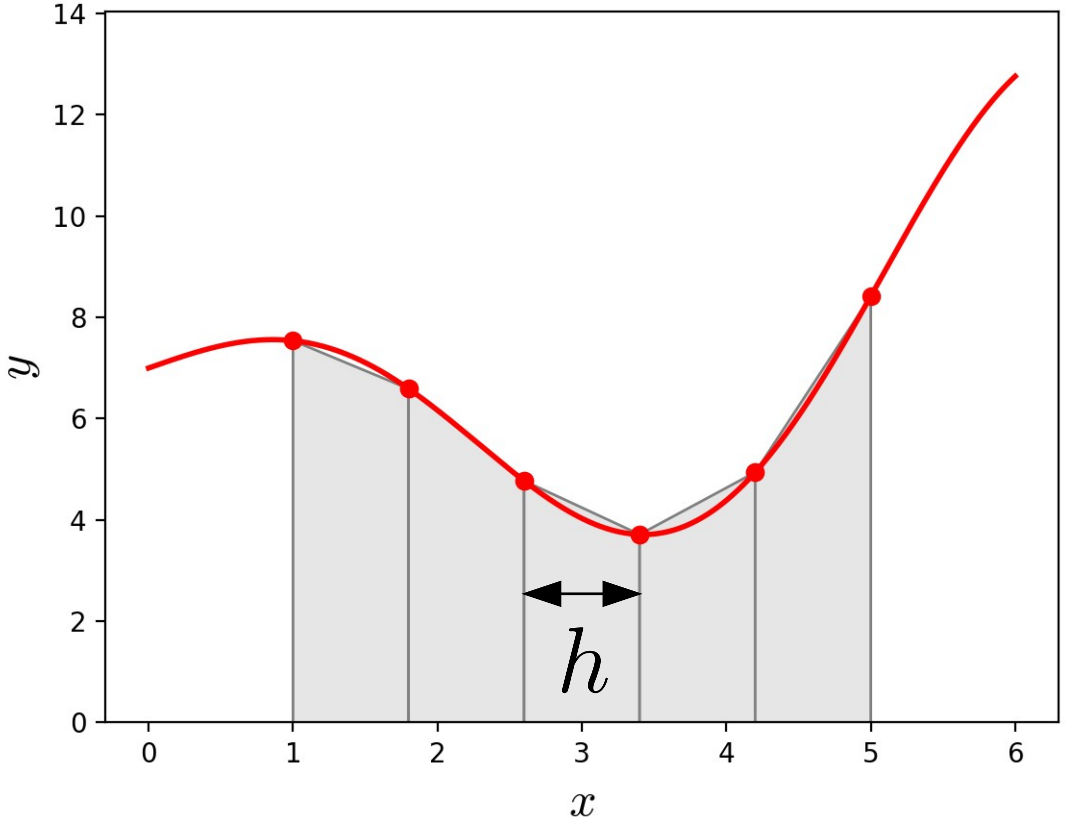



$$N = 5$$

Ex.: (11)

# Composite trapezoidal rule

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

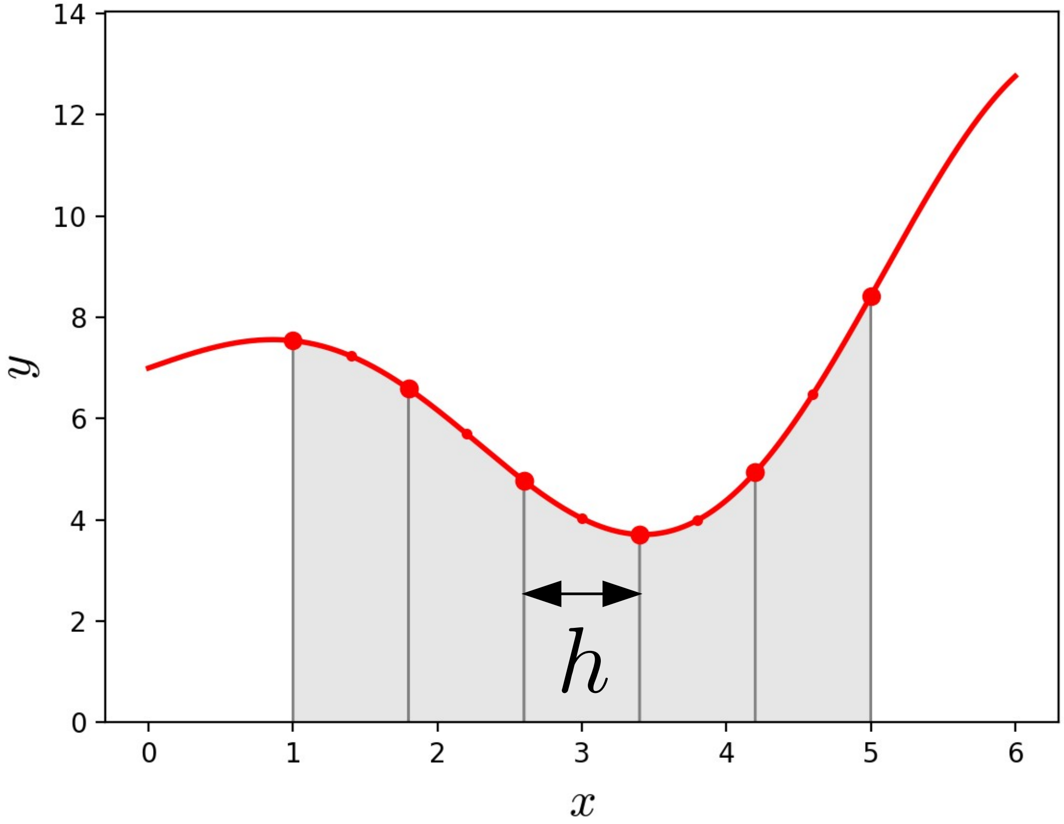



$$N = 5$$

Ex.: (12)

# 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

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

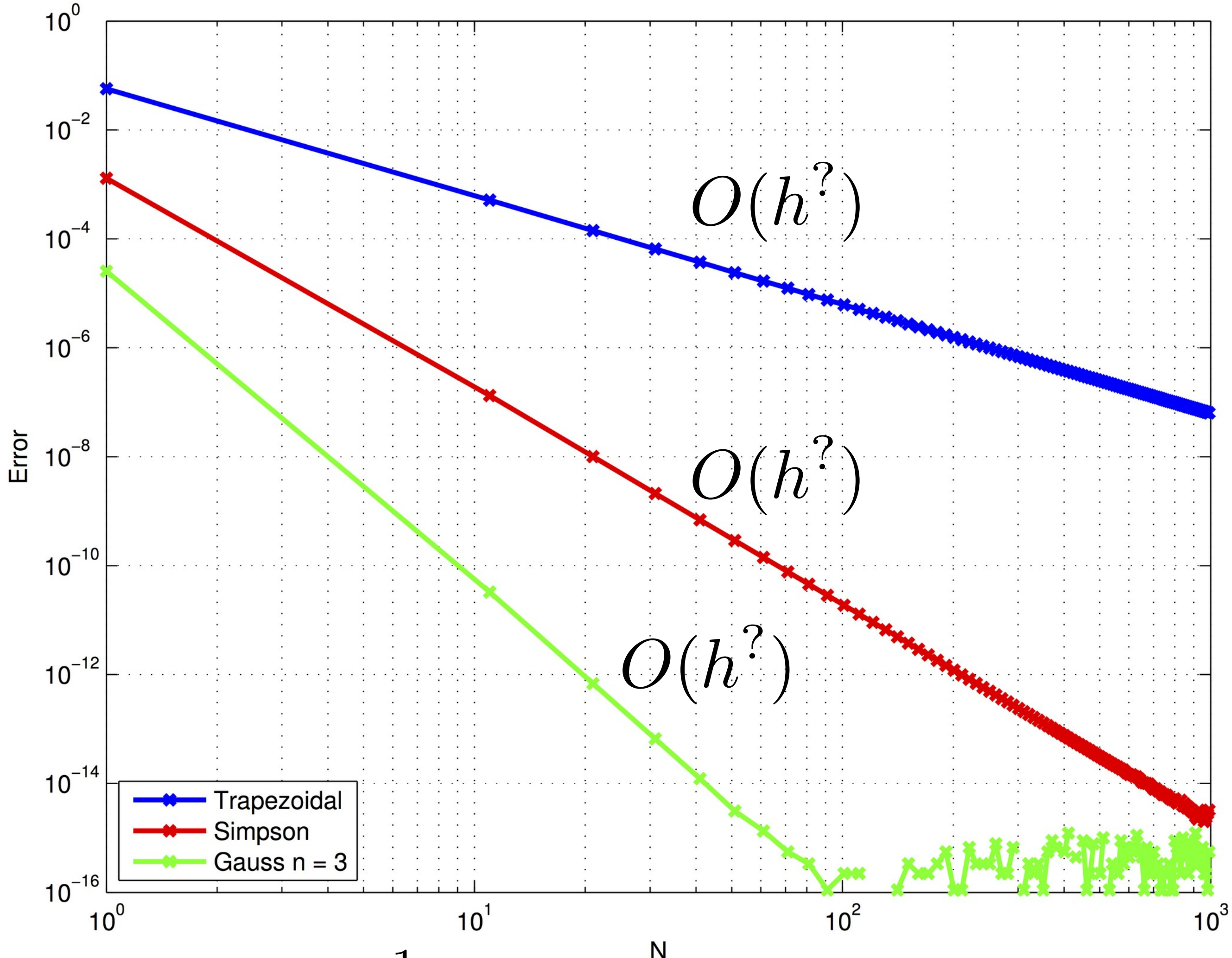
$$\leq \frac{\|f^{(q+1)}\|_\infty}{(q+1)!}(b-a)\,h^{q+1} = \frac{\|f^{(5)}\|_\infty}{5!}(b-a)\,h^5$$

DoE — order of accuracy

Ex.: (13)

# Quadrature

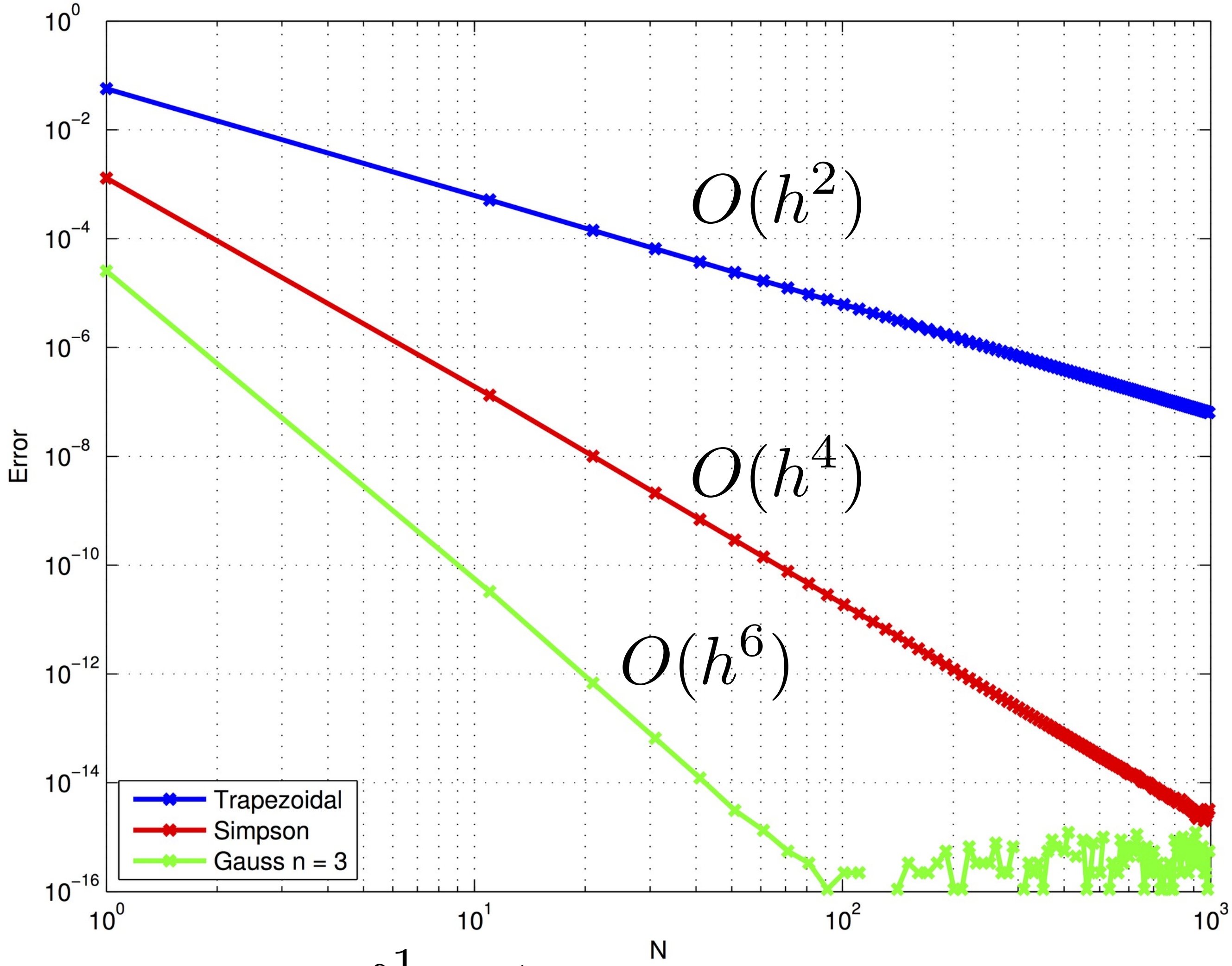
$$E^N[f] = |I[f] - Q^N[f]|$$




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

Ex.: (13)

# Quadrature




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