ACM40290: Numerical Algorithms

Numerical Differentiation

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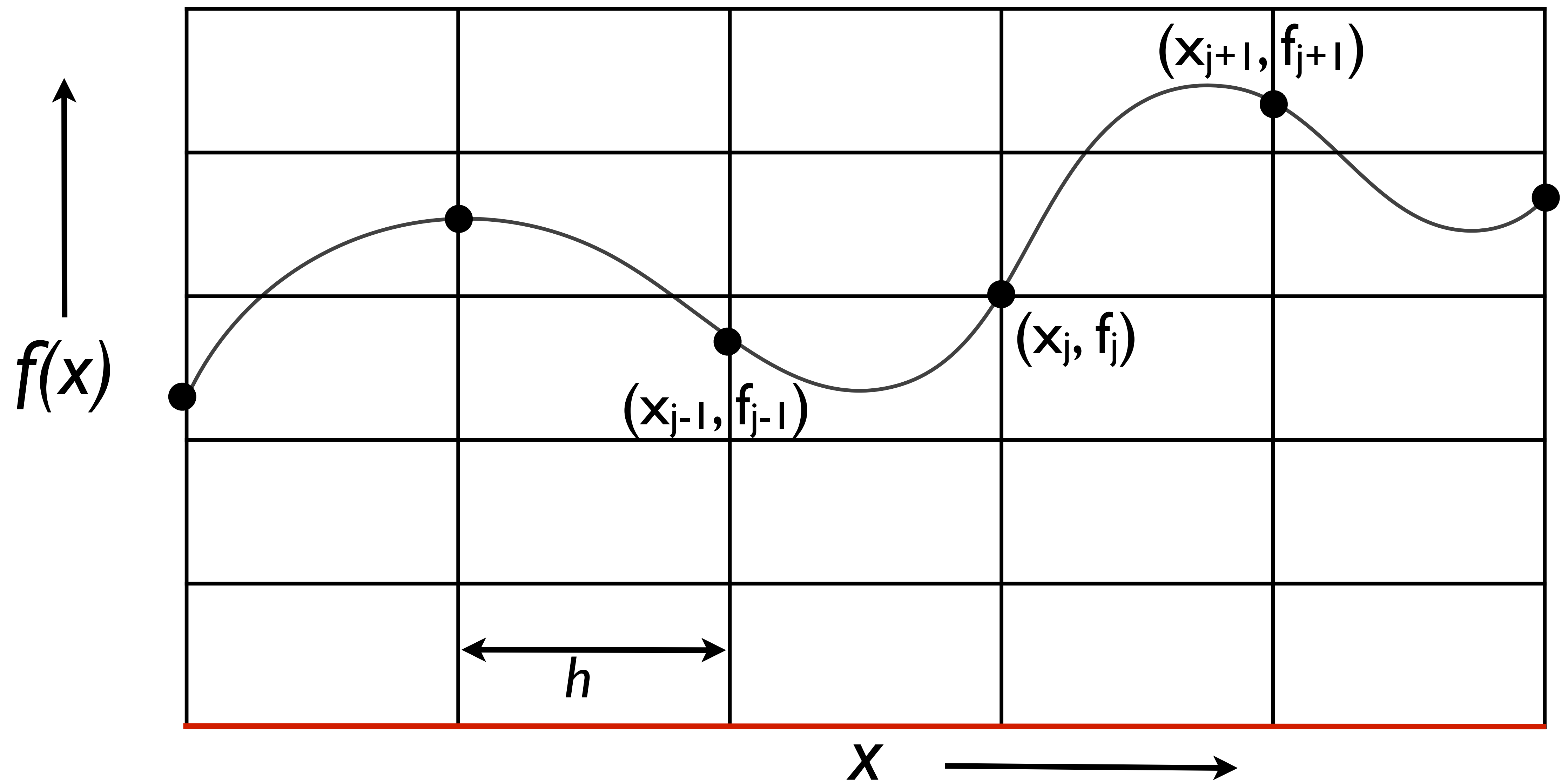
Finite differencing

- We want a method for computing the derivatives of a function.
- Finite differencing is a simple, straightforward approach. In fact, we have already encountered it.
- Start from the definition of a derivative

$$\frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Discretise

Introduce a grid of points on which we have values for a function, define $f_j=f(x_j)$.



Finite differencing

- First-order accurate approximation to the derivative is given by using the limiting definition of a derivative on the grid

$$\frac{df}{dx} \approx \frac{f_{j+1} - f_j}{h}$$

- Could equivalently also use a different pair of points on the grid

$$\frac{df}{dx} \approx \frac{f_j - f_{j-1}}{h}$$

- The two approximations have *first order* errors

Finite differencing

- We can get a *second-order* accurate result using a centred derivative

$$\frac{df}{dx} \approx \frac{f_{j+1} - f_{j-1}}{2h}$$

- Likewise for second derivatives,

$$\frac{d^2 f}{dx^2} \approx \frac{f_{j+1} - 2f_j + f_{j-1}}{h^2}$$

Accuracy

- A finite differencing derivative is only an approximation to the actual derivative.
- It becomes increasingly accurate as the grid spacing decreases.
- Can we say more than this?

Finite differencing

- Taylor's theorem

$$f(x+h) = f(x) + f'(x)h + \tfrac{1}{2}f''(x)h^2 + \cdots$$

- Rearranging this, we recover exactly our finite difference formula

$$\frac{df}{dx} \approx \frac{f_{j+1} - f_j}{h} + \mathcal{O}(h)$$

- We call this is a first-order accurate finite difference since the error is order h^1 (assuming f is sufficiently smooth — in this case that it is twice differentiable).

Finite differencing

- Similarly, can also use Taylor's theorem at *x-h*

$$f(x-h) = f(x) + f'(x)(-h) + \tfrac{1}{2} f''(x)(-h)^2 + \cdots$$

- Rearranging this, we recover exactly our finite difference formula

$$\frac{df}{dx} \approx \frac{f_j - f_{j-1}}{h} + \mathcal{O}(h)$$

- Again, this is a first-order accurate finite difference derivative.

Higher order finite differencing

- Combining the two previous results,

$$f(x+h) - f(x-h) =$$

$$f(x) + f'(x)h + \tfrac{1}{2}f''(x)h^2 + \tfrac{1}{6}f'''(x)h^3$$

$$- f(x) - f'(x)(-h) - \tfrac{1}{2}f''(x)(-h)^2 - \tfrac{1}{6}f'''(x)(-h)^3 + \cdots$$

we find that the order h errors cancel and we have a second-order accurate finite-difference formula

$$\frac{df}{dx} \approx \frac{f_{j+1} - f_{j-1}}{2h} + \mathcal{O}(h^2)$$

Higher order finite differencing

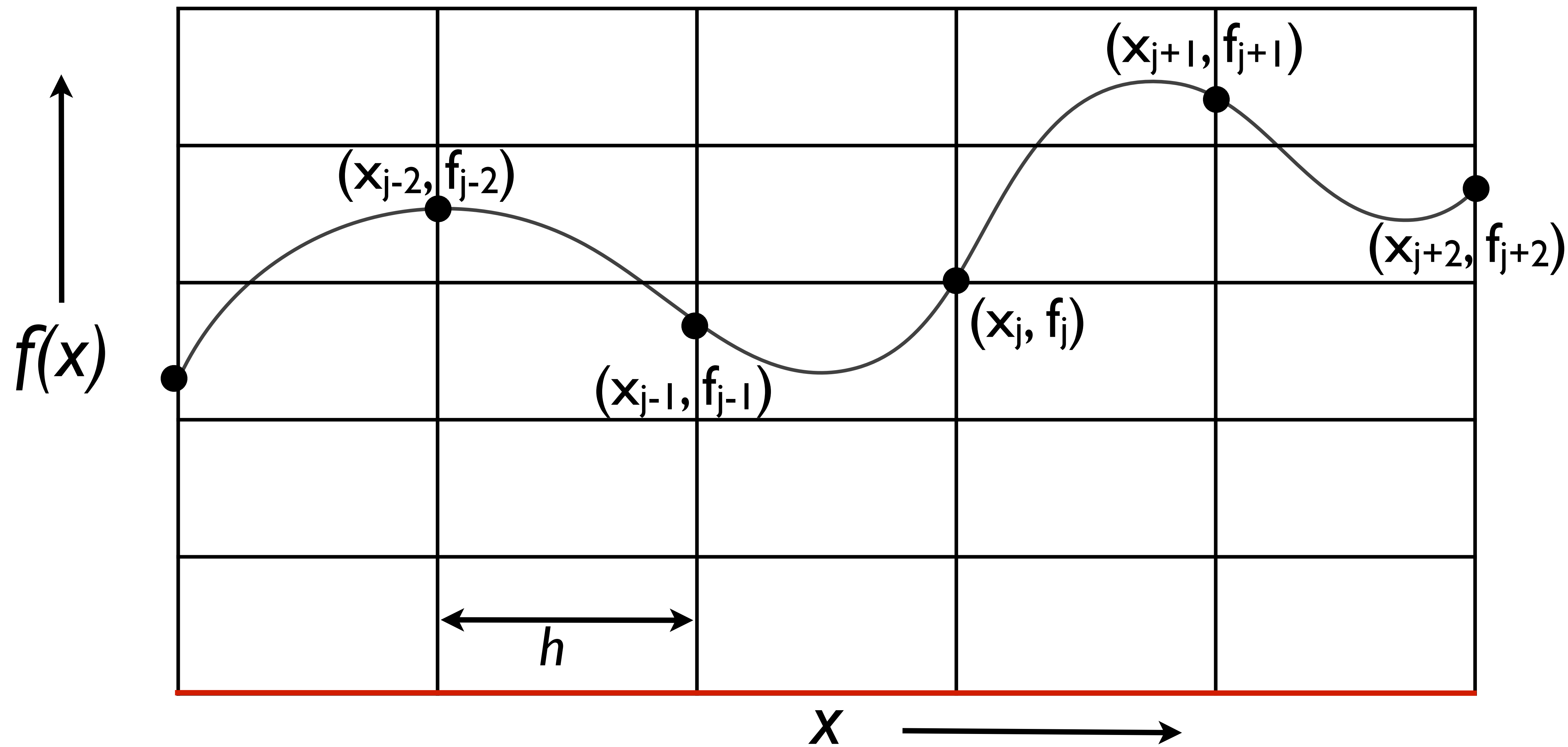
- Even higher order approximations are also possible.
- Fourth order finite difference:

$$\frac{df}{dx} = \frac{f_{j-2} - 8f_{j-1} + 8f_{j+1} - f_{j+2}}{12h} + \mathcal{O}(h^4)$$

- We could have derived this formula by combining the Taylor series for *f(x-2h)*, *f(x-h)*, *f(x+h)* and *f(x+2h)*.
- Higher order is more accurate, but requires more points (more calculation).

Higher order finite differencing

Higher order is more accurate, but requires more points (more calculation).



Higher order finite differencing

- High-order finite difference formulas can be derived by combining the Taylor series for different points, but this is cumbersome.
- A more general approach is to fit a polynomial and differential that.
- Example: determine the unique quadratic passing through the three points (x_{j-1}, f_{j-1}), (x_j, f_j), (x_{j+1}, f_{j+1}), differentiate it and this gives the second-order finite difference formula.
- In general, a finite difference formula using n points will be exact for functions that are polynomials of degree $n-1$ and have asymptotic order at least $n-m$. Sometimes higher asymptotic order because of cancellation.

Higher order finite differencing

- There is a general prescription for a finite difference approximation to an order *m* derivative with *n*+*1* points, evaluated at a point *s* (relative to the left-most point)

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CALCULATION OF WEIGHTS IN FINITE DIFFERENCE FORMULAS*

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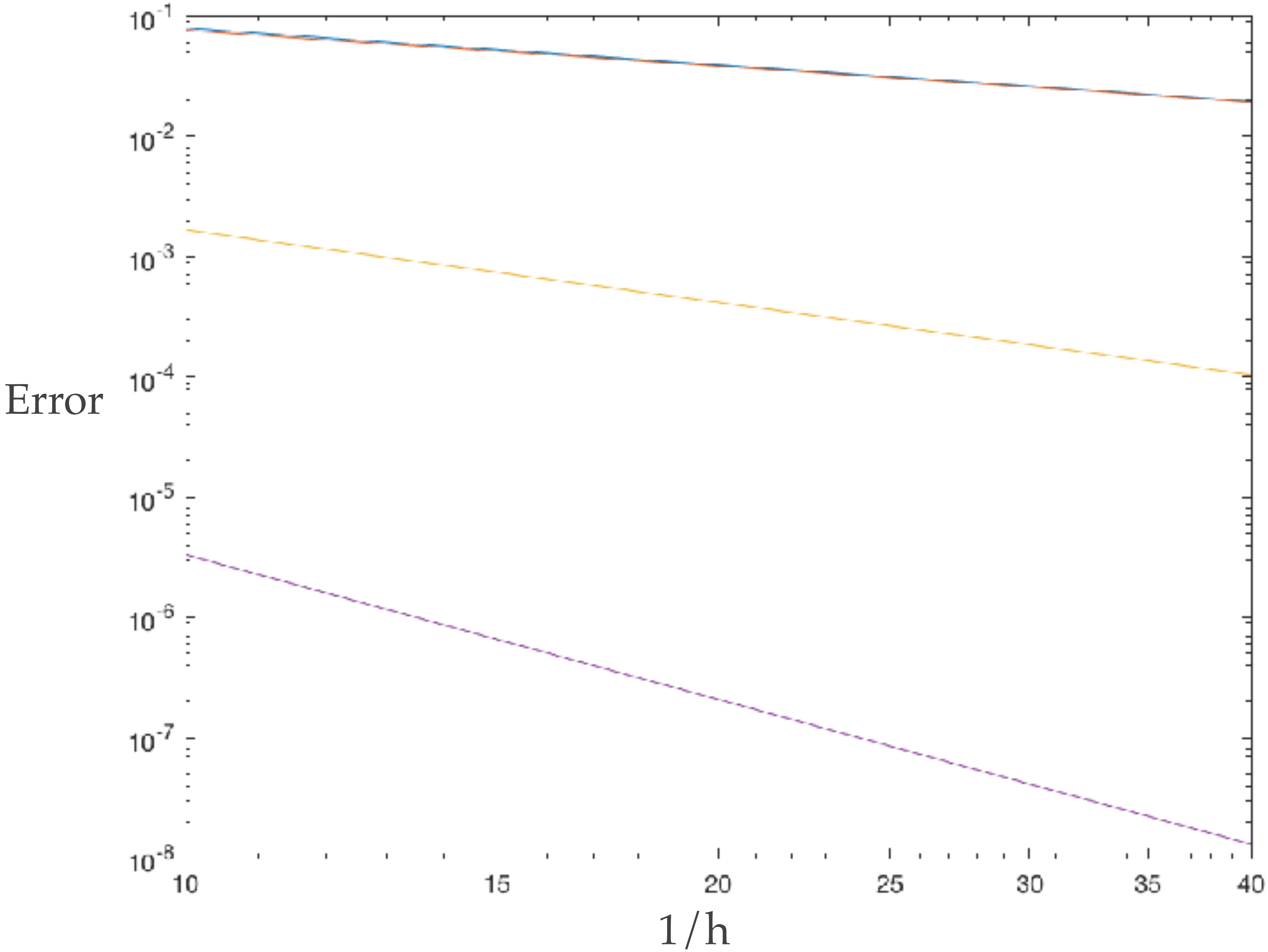
Abstract. The classical techniques for determining weights in finite difference formulas were either computationally slow or very limited in their scope (e.g., specialized recursions for centered and staggered approximations, for Adams–Bashforth-, Adams–Moulton-, and BDF-formulas for ODEs, etc.). Two recent algorithms overcome these problems. For equispaced grids, such weights can be found very conveniently with a two-line algorithm when using a symbolic language such as Mathematica (reducing to one line in the case of explicit approximations). For arbitrarily spaced grids, we describe a computationally very inexpensive numerical algorithm.

Mathematica code: CoefficientList[Normal[Series[x^s Log[x]^m, {x, 1, n}]/h^m], x]

Example: derivative of sin(x)

```
hL=0.1; hM=0.05; hH=0.025; h = [hL, hM, hH];

x0 = 1.0;

fp_exact = cos(x0);

fp_fd1u = (sin(x0+h)-sin(x0))./h;
fp_fd1d = (sin(x0)-sin(x0-h))./h;
fp_fd2 = (sin(x0+h)-sin(x0-h))./(2*h);
fp_fd4 = (sin(x0-2*h)-8*sin(x0-h)+8*sin(x0+h)-sin(x0+2*h))./(12*h);

err_fd1u = abs(1-fp_fd1u/fp_exact);
err_fd1d = abs(1-fp_fd1d/fp_exact);
err_fd2 = abs(1-fp_fd2/fp_exact);
err_fd4 = abs(1-fp_fd4/fp_exact);

loglog(1./h, err_fd1u, 1./h, err_fd1d, 1./h, err_fd2, 1./h, err_fd4)
```

Example: derivative of sin(x)



Convergence

- Numerical approximation approaches exact solution as *h* goes to 0.
- Convergence *rate* depends on the numerical scheme.
- Numerical solution differs from exact solution by an amount which depends on the resolution (i.e. *h*)

$$f'(x_0) = f'_{\text{exact}}(x_0) + Ch^p$$

- *p* is called the *convergence rate*.

Convergence Rate

- If we know the exact solution, we can determine the convergence rate by running at two resolutions

$$f'_L(x_0) = f'_{\text{exact}}(x_0) + Ch_L^p$$
$$f'_H(x_0) = f'_{\text{exact}}(x_0) + Ch_H^p$$

- We know $f'_{exact}(x_0), f'_L(x_0) f'_H(x_0), h_L, h_H$
- Solve 2 equations for 2 unknowns: C, p
- Useful to test a algorithm against a known analytic solution — p is determined by the algorithm.

Convergence Rate

- If we don't have an exact solution, we can still determine the convergence rate by using three resolutions

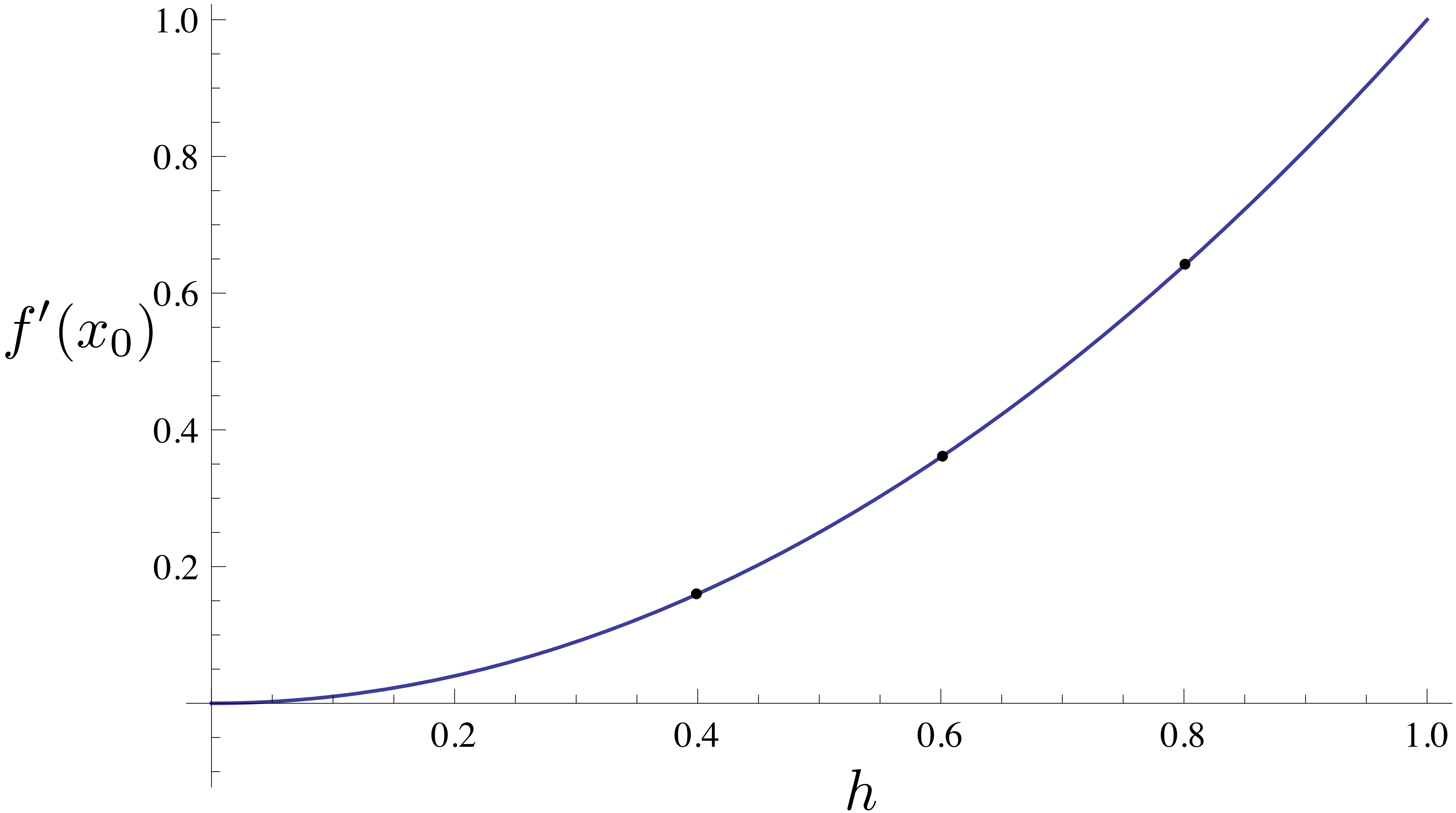
$$f'_L(x_0) = f'_{\mathrm{exact}}(x_0) + Ch_L^p$$
$$f'_M(x_0) = f'_{\mathrm{exact}}(x_0) + Ch_M^p$$
$$f'_H(x_0) = f'_{\mathrm{exact}}(x_0) + Ch_H^p$$

- We know $f'_L(x_0), f'_M(x_0), f'_H(x_0), h_L, h_M, h_H$
- Solve 3 equations for 3 unknowns: $C, p, f'_{\mathrm{exact}}(x_0)$
- Useful when you don't have any known solutions to test against

Richardson Extrapolation

- Having convergence is very powerful
- It allows extrapolation from numerical solutions at specific h to determine what the value would be for infinite resolution.
- The extrapolation procedure is called *Richardson extrapolation* and can dramatically improve the accuracy of numerical results

Richardson Extrapolation



Richardson Extrapolation

- Given numerical solutions at two resolutions

$$f'_L(x) = f'_{\text{exact}}(x) + Ch_L^p$$
$$f'_H(x) = f'_{\text{exact}}(x) + Ch_H^p$$

- If we have already established convergence, then we know p
- We also know $f'_L(x), f'_H(x), h_L, h_H$
- Solve 2 equations for 2 unknowns: $f'_{exact}(x_0), C$
- We now know the exact solution, $f'_{exact}(x_0)$