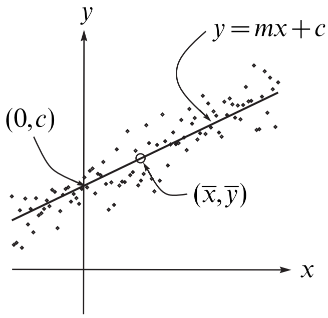
2.14 Numerical methods

Straight-line fitting[a]

Data	$\left(\{x_i\},\{y_i\}\right)$ n points	(2.570)
Weights[b]	$\{w_i\}$	(2.571)
Model	$y = mx + c$	(2.572)
Residuals	$d_i = y_i - mx_i - c$	(2.573)
Weighted centre	$(\overline{x},\overline{y}) = \dfrac{1}{\sum w_i}\left(\sum w_i x_i, \sum w_i y_i\right)$	(2.574)
Weighted moment	$D = \sum w_i (x_i - \overline{x})^2$	(2.575)
Gradient	$m = \dfrac{1}{D}\sum w_i (x_i - \overline{x}) y_i$	(2.576)
	$\mathrm{var}[m] \simeq \dfrac{1}{D}\dfrac{\sum w_i d_i^2}{n-2}$	(2.577)
Intercept	$c = \overline{y} - m\overline{x}$	(2.578)
	$\mathrm{var}[c] \simeq \left(\dfrac{1}{\sum w_i} + \dfrac{\overline{x}^2}{D}\right)\dfrac{\sum w_i d_i^2}{n-2}$	(2.579)



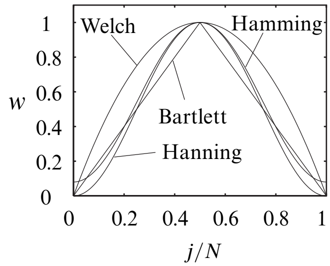
[a]Least-squares fit of data to $y = mx + c$. Errors on y-values only.
[b]If the errors on y_i are uncorrelated, then $w_i = 1/\mathrm{var}[y_i]$.

Time series analysis[a]

Discrete convolution	$(r \star s)_j = \sum_{k=-(M/2)+1}^{M/2} s_{j-k} r_k$	(2.580)
Bartlett (triangular) window	$w_j = 1 - \left\lvert \dfrac{j - N/2}{N/2} \right\rvert$	(2.581)
Welch (quadratic) window	$w_j = 1 - \left[\dfrac{j - N/2}{N/2}\right]^2$	(2.582)
Hanning window	$w_j = \dfrac{1}{2}\left[1 - \cos\left(\dfrac{2\pi j}{N}\right)\right]$	(2.583)
Hamming window	$w_j = 0.54 - 0.46\cos\left(\dfrac{2\pi j}{N}\right)$	(2.584)

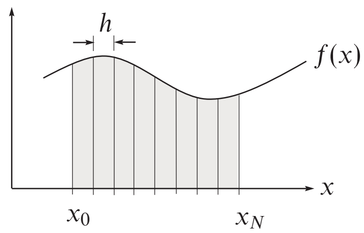
r_i response function
s_i time series
M response function duration

w_j windowing function
N length of time series



[a]The time series runs from $j = 0 \ldots (N-1)$, and the windowing functions peak at $j = N/2$.

Numerical integration



Trapezoidal rule	$\int_{x_0}^{x_N} f(x)\,\mathrm{d}x \simeq \frac{h}{2}(f_0+2f_1+2f_2+\cdots +2f_{N-1}+f_N)$	(2.585)	h $=(x_N-x_0)/N$ (subinterval width) f_i $f_i=f(x_i)$ N number of subintervals
Simpson's rule[a]	$\int_{x_0}^{x_N} f(x)\,\mathrm{d}x \simeq \frac{h}{3}(f_0+4f_1+2f_2+4f_3+\cdots +4f_{N-1}+f_N)$	(2.586)	

[a] N must be even. Simpson's rule is exact for quadratics and cubics.

Numerical differentiation[a]

$$\frac{\mathrm{d}f}{\mathrm{d}x} \simeq \frac{1}{12h}[-f(x+2h)+8f(x+h)-8f(x-h)+f(x-2h)] \quad (2.587)$$

$$\sim \frac{1}{2h}[f(x+h)-f(x-h)] \quad (2.588)$$

$$\frac{\mathrm{d}^2f}{\mathrm{d}x^2} \simeq \frac{1}{12h^2}[-f(x+2h)+16f(x+h)-30f(x)+16f(x-h)-f(x-2h)] \quad (2.589)$$

$$\sim \frac{1}{h^2}[f(x+h)-2f(x)+f(x-h)] \quad (2.590)$$

$$\frac{\mathrm{d}^3f}{\mathrm{d}x^3} \sim \frac{1}{2h^3}[f(x+2h)-2f(x+h)+2f(x-h)-f(x-2h)] \quad (2.591)$$

[a] Derivatives of $f(x)$ at x. h is a small interval in x.
Relations containing "$\simeq$" are $O(h^4)$; those containing "$\sim$" are $O(h^2)$.

Numerical solutions to $f(x)=0$

Secant method	$x_{n+1}=x_n-\frac{x_n-x_{n-1}}{f(x_n)-f(x_{n-1})}f(x_n)$	(2.592)	f function of x x_n $f(x_\infty)=0$
Newton–Raphson method	$x_{n+1}=x_n-\frac{f(x_n)}{f'(x_n)}$	(2.593)	f' $=\mathrm{d}f/\mathrm{d}x$

Numerical solutions to ordinary differential equations[a]

Euler's method	if	$\dfrac{dy}{dx} = f(x,y)$	(2.594)
	and	$h = x_{n+1} - x_n$	(2.595)
	then	$y_{n+1} = y_n + hf(x_n, y_n) + O(h^2)$	(2.596)
Runge–Kutta method (fourth-order)	if	$\dfrac{dy}{dx} = f(x,y)$	(2.597)
	and	$h = x_{n+1} - x_n$	(2.598)
		$k_1 = hf(x_n, y_n)$	(2.599)
		$k_2 = hf(x_n + h/2, y_n + k_1/2)$	(2.600)
		$k_3 = hf(x_n + h/2, y_n + k_2/2)$	(2.601)
		$k_4 = hf(x_n + h, y_n + k_3)$	(2.602)
	then	$y_{n+1} = y_n + \dfrac{k_1}{6} + \dfrac{k_2}{3} + \dfrac{k_3}{3} + \dfrac{k_4}{6} + O(h^5)$	(2.603)

[a]Ordinary differential equations (ODEs) of the form $\frac{dy}{dx} = f(x,y)$. Higher order equations should be reduced to a set of coupled first-order equations and solved in parallel.