Numerical Methods for Astrophysics:

NUMERICAL DERIVATIVES

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Numerical derivatives. Concept

Textbooks of computational physics usually skip numerical derivs. because:

– too easy to implement

– in many cases we do not need to calculate derivative numerically because we can do it analytically (but see Newton-Raphson)

– significant problems of accuracy when noisy data

Numerical derivatives. Forward, backward and central differences

Definition of derivative:

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

Numerical definitions of derivative:

1. forward difference

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

where *h* is small interval
"forward" refers to the fact that we consider the interval after *x*

2. backward difference

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

"backward" refers to the fact that we consider the interval before *x*

3. central difference:

$$\frac{\mathrm{d}f}{\mathrm{d}x} \sim \frac{f(x+h/2) - f(x-h/2)}{h}$$

calculated with respect to the midpoint *x* of the interval
more accurate than 1. and 2.

Numerical derivatives. Second derivatives

Calculate central differences in the following points

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

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

Apply again the central difference for the second derivative

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

$$= \frac{[f(x+h)-f(x)]/h - [f(x)-f(x-h)]/h}{h}$$

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

Numerical derivatives. Partial derivatives

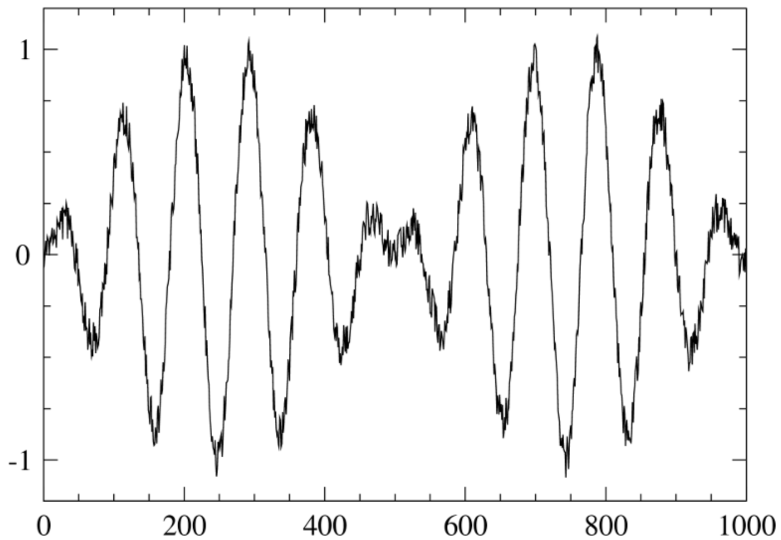
Partial derivatives with central differences:

$$\frac{\partial f}{\partial x} = \frac{f(x+h/2,y)-f(x-h/2,y)}{h}$$
$$\frac{\partial f}{\partial y} = \frac{f(x,y+h/2)-f(x,y-h/2)}{h}$$

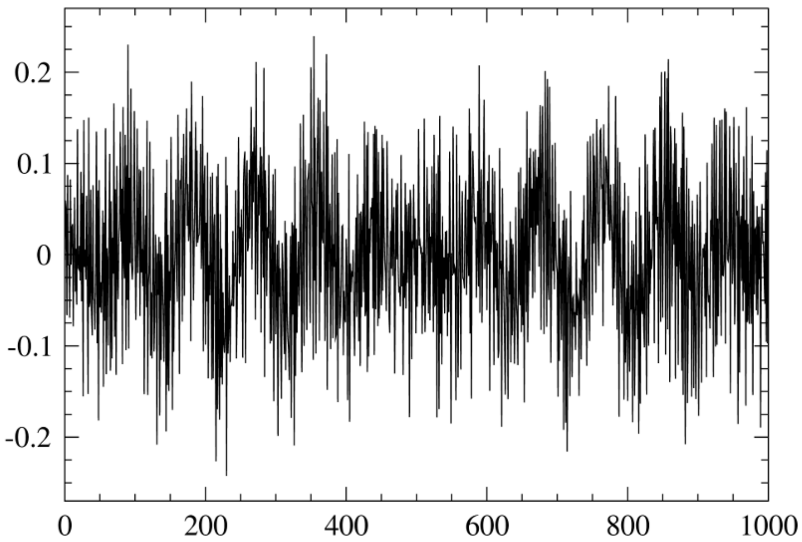
I apply the central difference to each variable at a time

Numerical derivatives. Derivatives of noisy data

Real-life data have noise:



Num. derivative enhances that noise:



because locally the slope of the function might be dominated by noise

Ways to improve this:
i) *h* larger smooths the features

ii) fit a smooth curve to the data and then take the derivative of the fit

iii) calculate the Fourier transform of the data,
which makes them smoother

Numerical derivatives. Exercise

EXERCISE:

You have already written a script to perform root finding with the Newton-Raphson method. Now modify that script to include a numerical derivative (for the case of eccentric anomaly) with the central difference method.