Numerical Differentiation

Replace continuous derivative with a finite-difference of sampled data on a grid, for example using Taylor expansion on a uniform grid

$$\frac{\partial f}{\partial x} = \underbrace{\frac{1}{2\Delta x}\left(f_{j+1} - f_{j-1}\right)}_{\text{2nd order approx}} + \underbrace{O(\Delta x^2)}_{\text{truncation error}}$$

or, more accurately with a wider stencil

$$\frac{\partial f}{\partial x} = \underbrace{\frac{1}{12\Delta x}\left(f_{j-2} - 8f_{j-1} + 8f_{j+1} - f_{j+2}\right)}_{\text{fourth order}} + O(\Delta x^4)$$

or

$$\frac{\partial f}{\partial x} = \underbrace{\frac{1}{60\Delta x}\left(-f_{j-3} + 9f_{j-2} - 45f_{j-1} + 45f_{j+1} - 9f_{j+2} + f_{j+3}\right)}_{\text{sixth order}} + O(\Delta x^6)$$

and we can extend the stencil to include more points to obtain higher order approximations.

The above are examples of <u>central-difference</u> schemes, but it turns out that we can do better if we also add extra terms to the 'left-hand-side'; this leads to <u>compact schemes</u>. For example,

$$\alpha\left(\frac{\partial f}{\partial x}\right)_{j+1} + \left(\frac{\partial f}{\partial x}\right)_j + \alpha\left(\frac{\partial f}{\partial x}\right)_{j-1} = \frac{a}{2\Delta x}\left(f_{j+1} - f_{j-1}\right) + \frac{b}{4\Delta x}\left(f_{j+2} - f_{j-2}\right)$$

and choose α, a, and b for best accuracy. Putting $\alpha \to 0$ recovers the standard central scheme, at fourth order, but

$$\alpha = \frac{1}{3}, \quad a = \frac{14}{9}, \quad b = \frac{1}{9}$$

produces a sixth-order compact scheme with both a narrower stencil and smaller truncation error than the 6th-order central diff above. The extra complexity added is that we have to solve a linear system (tri-diagonal matrix) to calculate the derivative rather than just calculate it directly.

Modified Wavenumber

One way to characterise the error in a numerical sheme (e.g. approx. of derivative) is to apply it to a Fourier component e^{ikx} and compare the numerical differentiator $\delta/\delta x$ to the exact one $\partial/\partial x$.

For example: numerical $\dfrac{\delta}{\delta x}\left(e^{ikx}\right) = (ik^*)\,e^{ikx}$

exact $\dfrac{\partial}{\partial x}\left(e^{ikx}\right) = ik\,e^{ikx}$

or for second derivative:

numerical $\dfrac{\delta^2}{\delta x^2}\left(e^{ikx}\right) = -k^{*2}\cdot e^{ikx}$

$\dfrac{\partial^2}{\partial x^2}\left(e^{ikx}\right) = -k^2 e^{ikx}$

Here the numerical operator produces a <u>modified wavenumber</u> k^* which differs from the exact one, as defined above.

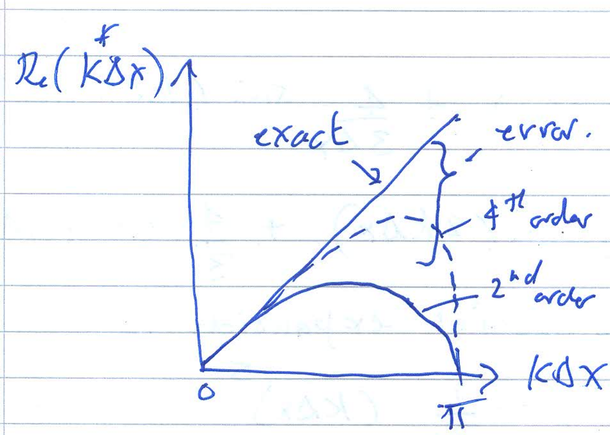
We can define k^* as:

$$k^* = \frac{1}{i} e^{-ikx} \frac{\delta}{\delta x}\left(e^{ikx}\right) \qquad \text{first deriv } \delta/\delta x$$

or

$$k^* = \frac{1}{-1} e^{-ikx} \frac{\delta^2}{\delta x^2}\left(e^{ikx}\right) \qquad \text{second deriv } \delta^2/\delta x^2$$

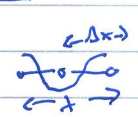
and so on. Ideally $k^* \to k$ for well resolved wave components, i.e. for $k\Delta x \ll 1$, but in general k^* will contain errors which are largest as $k\Delta x$ increases, up to $k\Delta x = \pi$, grid limit (Nyquist).

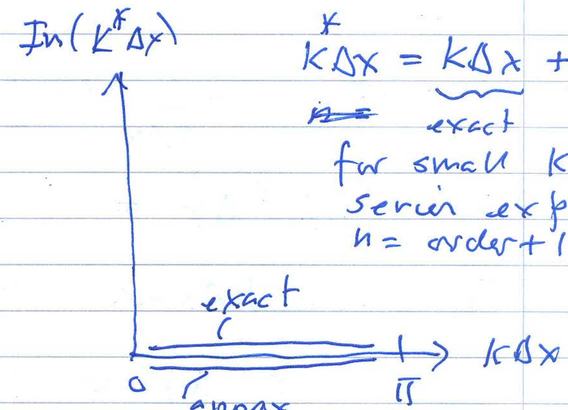


upper limit

$\lambda = \dfrac{2\pi}{k} = 2\Delta x$

$\Rightarrow k\Delta x = \pi$



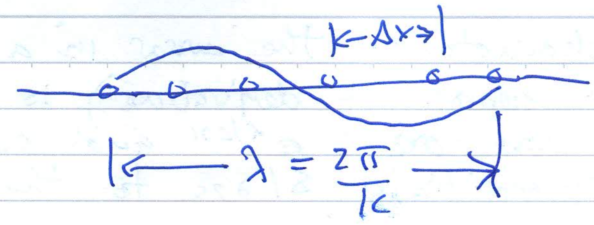


$$k^*\Delta x = \underbrace{k\Delta x}_{\text{exact}} + \underbrace{c\cdot(k\Delta x)^n}_{\text{error}}$$

for small $k\Delta x \ll 1$ series expansion. n = order + 1.

for central schemes, by symmetry.

Resolution of waves: suppose we have m grid points

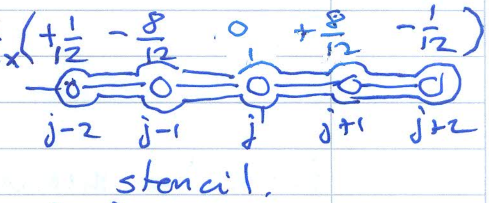


to resolve a fourier component, (per cycle) then

$$\lambda = \frac{2\pi}{k} = m\,\Delta x, \qquad K\Delta x \simeq \frac{2\pi}{m}$$

and the upper limit (smallest wave on grid) is $m=2$ or $K\Delta x = \pi$. For well resolved waves m is large and $K\Delta x$ is small, $\Rightarrow$ approximations are good here.

<u>Example</u> – 4^{th} order central scheme.



$$\frac{\delta f}{\delta x} = \frac{-1}{12\Delta x}\left(f_{j+2} - f_{j-2}\right) + \frac{8}{12\Delta x}\left(f_{j+1} - f_{j-1}\right)$$

Put $f = e^{ikx}$

$$\frac{\delta f}{\delta x} = -\frac{1}{12\Delta x}\, e^{ikx}\left(e^{i2k\Delta x} - e^{-i2k\Delta x}\right) + \frac{8e^{ikx}}{12\Delta x}\left(e^{ik\Delta x} - e^{-ik\Delta x}\right)$$

convert to trig (cos, sin) form

$$\frac{\delta f}{\delta x} = \frac{-(i)e^{ikx}}{6\Delta x}\sin(2k\Delta x) + \frac{(i)4}{3\Delta x}e^{ikx}\sin(k\Delta x)$$

and compare with, hence find k^*.

$$\frac{\delta f}{\delta x} = i k^* e^{ikx}$$

$$\Rightarrow \quad k^* = -\frac{1}{6\Delta x}\sin(2k\Delta x) + \frac{4}{3\Delta x}\sin(k\Delta x)$$

$$\Rightarrow \quad k^*\Delta x = -\frac{1}{6}\sin(2k\Delta x) + \frac{4}{3}\sin(k\Delta x)$$

For small $k\Delta x \ll 1$ the series expansion is

$$k^*\Delta x = k\Delta x - \frac{1}{30}(k\Delta x)^5 + \cdots$$

This is fourth-order accurate.

Example - second derivative. $\partial^2/\partial x^2$

Find modified wavenumber for 2^{nd} order second derivative - central differences,

$$\frac{\delta^2 f}{\delta x^2} = \frac{1}{\Delta x^2}\left(f_{j+1} - 2f_j + f_{j-1}\right)$$

We put $f = e^{ikx}$ and apply the numerical operator and compare with the exact one,

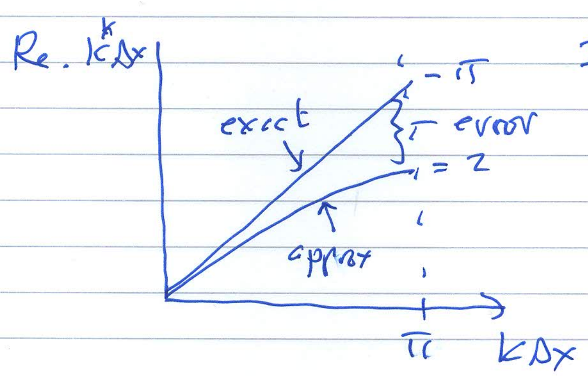
$$\underbrace{\frac{\partial^2}{\partial x^2}\left(e^{ik^* x}\right)}_{\text{equivalent modified.}} \qquad \underbrace{\frac{\delta^2}{\delta x^2}\left(e^{ikx}\right)}_{\text{approx}}$$

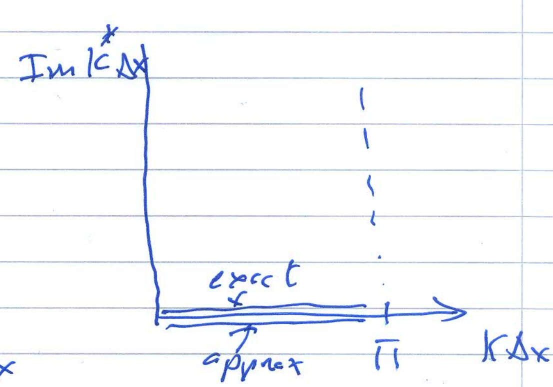
$$-k^{*2} e^{ikx} = \frac{1}{\Delta x^2} \cdot e^{ikx} \cdot \left(e^{ik\Delta x} - 2 + e^{-ik\Delta x}\right)$$

cancelling common factors, rearrange,

$$(k^*\Delta x)^2 = 2 - 2\cos(k\Delta x)$$

$$k^*\Delta x = \sqrt{2}\sqrt{(1 - \cos(k\Delta x))}$$





Series expansion for small $k\Delta x << 1$

$$k^*\Delta x = k\Delta x - \frac{1}{24} k^3\Delta x^3 + \frac{1}{1920} k^5\Delta x^5 + \cdots$$

and is accurate to 2^{nd} order in $k\Delta x$.

Why is k^* useful?

Any numerical difference operator will have (small) errors, and hence modify k when used to differentiate a Fourier component, the modified wavenumber characterises these errors, and these errors can lead to modified behaviour of our solutions.

Consider the wave equation (1D - first order)

$$\frac{\partial f}{\partial t} + c\frac{\partial f}{\partial x} = 0$$

and put $f = e^{i(kx-ct)}$ which represents a wave travelling to the right ($+x$) at speed c.

If we integrate $\partial f/\partial t$ exactly but use a numerical operator for $\partial f/\partial x$ then our solutions are

$$(-i\sigma)e^{-i\sigma t}\cdot e^{ikx} + c\frac{\delta}{\delta x}\left(e^{ikx}\right)e^{-i\sigma t} = 0$$

or cancelling common factors + operator

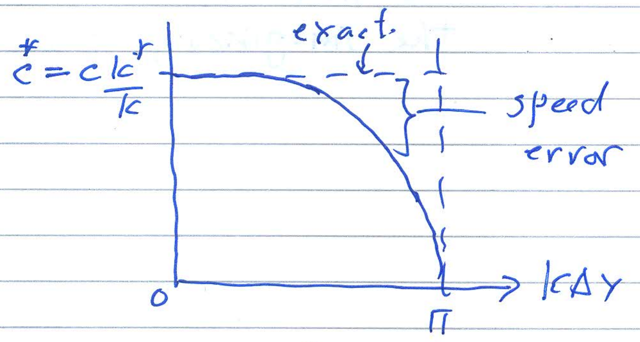
$$-i\sigma + c\,(ik^*) = 0$$

and the dispersive relation gives the frequency $\sigma(k)$ as

$$\sigma(k) = ck^*.$$

and phase speed $c(k) = \dfrac{\sigma(k)}{k} = c\left(\dfrac{k^*}{k}\right)$.

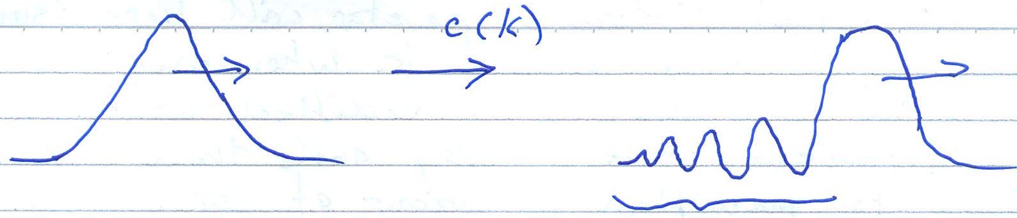
Here the exact speed $c = \text{const}$ is modified to ck^*/k — $\Rightarrow$ dispersive, because speed now depends on the wavenumber $k\Delta x$, and in our examples $k^* < k$ so that (modified) c is slower for shorter waves, and (in example) for $k\Delta x = \pi$ actually stop.



speed vs $k\Delta x$.

Exact system is non-dispersive, but numerical system <u>is</u> dispersive.

Numerical dispersion



initial pulse, wide spectrum of fourier components

short waves travel slower ⇒ left behind ⇒ trailing oscillation $\qquad \frac{k^*}{k} < 1$

What if k^* is complex?

This can happen if the stencil is not balanced in $\pm x$ (e.g. upwind schemes)

In this case $\qquad k^* = k^*_{Re} + i k^*_{Im}$

and the dispersion relation implies complex frequency

$$\sigma = c k^*$$

so that waves that ~~grow~~ propagate as $e^{-i(kx-\sigma t)}$ now behave as:

$$e^{i(kx-\sigma t)} = e^{-i(kx - ck^*_{re}t - c i k^*_{im} t)}$$

$$= \underbrace{e^{-ik(x - c\frac{k^*}{k_{re}}\cdot t)}}_{\text{wave with phase speed } c^* = c\frac{k^*}{k_{re}}} \cdot \underbrace{\boxed{e^{-ck^*_{im}\cdot t}}}_{\text{amplitude growth/decay}}$$

The real part of k^* modifies the phase speed (of 1D - first order) waves, and the imaginary part alters the amplitude.