University of Cape Town - Department of Physics
Honours Computational Physics

TOPIC 2 - ROOT-FINDING, INTERPOLATION & EXTRAPOLATION : SMOOTH PARTICLE INTERPOLATION

This worksheet accompanies the EJS simulation `Interpolation_No1_SPI.jar`

Smooth Particle Interpolation (SPI) is an interpolation scheme based on the Smooth Particle Hydrodynamics (SPH) technique of solving PDE's.

Consider a function $f(x)$. From the definition of the δ-function,

$$f(\bar{x}) = \int_{-\infty}^{+\infty} f(x')\,\delta(\bar{x} - x')\,dx'.$$

The smoothed approximation of SPH involves replacing the δ-function by a kernel function $W(\bar{x} - x'; h)$, with h a parameter known as the smoothing length. The kernel function satisfies the following criteria:

- $W(\bar{x} - x'; h) \geq 0$;
- $\int_{-\infty}^{+\infty} W(\bar{x} - x'; h)\,dx' = 1$ (normalisation);
- $W(\bar{x} - x'; h)$ has compact support (i.e. $\exists$ a δ such that $W(\bar{x} - x'; h) = 0$ when $|\bar{x} - x'| > \delta$);
- $W(\bar{x} - x'; h)$ approaches $\delta(\bar{x} - x')$ as $h \to 0$;
- $W(\bar{x} - x'; h)$ should be an even function of $\bar{x} - x'$ to ensure reasonable accuracy.

This results in:

$$f(\bar{x}) \approx \int_{-\infty}^{+\infty} f(x')\,W(\bar{x} - x'; h)\,dx' \equiv \langle f(\bar{x}) \rangle.$$

The second approximation involves evaluating the integral in the smoothed approximation $\langle f(\bar{x}) \rangle$ using only the function values at the N points $x_1, x_2, \ldots x_N$:

$$f(\bar{x}) \approx \sum_{i=1}^{N} \Delta x_i\, f(x_i)\,W(\bar{x} - x_i; h) \equiv [f(\bar{x})]\,.$$

In SPI terminology, particles are said to be positioned at $x_1, x_2, \ldots x_N$ and the Δx_i are then particle spacings. Given $f(x)$ evaluated at the N points $x_1, x_2, \ldots x_N$, the particle approximation allows the estimation of the function at some point $\bar{x}$ (i.e. interpolation).

A number of SPI kernel functions exist, although the most common is the Gaussian kernel:

$$W(\bar{x} - x'; h) = \frac{1}{h\sqrt{\pi}} \exp\left(-\left(\frac{\bar{x} - x'}{h}\right)^2\right).$$

Strictly speaking, the Gaussian kernel does not have compact support. However, it does tend to zero quickly enough for most applications.

A very useful feature of SPI is that it can be used to approximate derivatives as well as functions. Consider the smoothed approximation of the first derivative $f'(x)$:

$$\langle f'(\bar{x}) \rangle \equiv \int_{-\infty}^{+\infty} f'(x') \, W(\bar{x} - x'; h) \, dx'.$$

We can use integration by parts to shift the derivative to the kernel function:

$$\langle f'(\bar{x}) \rangle = \cancelto{0}{f(x') \, W(\bar{x} - x'; h) \Big|_{-\infty}^{+\infty}} - \int_{-\infty}^{+\infty} f(x') \, \frac{dW(\bar{x} - x'; h)}{dx'} dx',$$

where the compact support of the kernel function has been used to cancel the boundary term. Finally, using the particle approximation, we obtain an estimate for the first derivative:

$$f'(\bar{x}) \approx -\sum_{i=1}^{N} \Delta x_i \, f(x_i) \, W'(\bar{x} - x_i; h) \equiv [f'(\bar{x})] \, .$$

A similar procedure can be applied to higher derivatives.

Questions:

1. Show that SPI is not strictly speaking an interpolation scheme by considering the particle approximation $[f(x_i)]$.
2. Show that normalisation of the kernel function is required in order to ensure agreement between the smoothed approximation $\langle f(\bar{x}) \rangle$ and $f(\bar{x})$ for a constant function $f(x) = C$.
3. Show that $\langle f(\bar{x}) \rangle = f(\bar{x}) + \frac{h^2}{4} f''(\bar{x}) + O(h^4)$, for the Gaussian kernel. (Hint: Taylor expand $f(x')$ about $\bar{x}$, multiply by $W(\bar{x} - x'; h)$ and integrate.)
4. Derive the particle approximation to the second derivative $[f''(\bar{x})]$.
5. Use the associated EJS simulation to investigate the use of SPI in approximating the function

$$f(x) = 3x^4 - x^3 + 2x + 3,$$

   defined over the interval $[-10, +10]$.

   (a) Confirm that SPI is not truly an interpolation scheme.

   (b) Account for the behaviour of the SPI approximation to $f(x)$ with a parameter choice $h = 0.1$ and $N = 10$.

   (c) **Focus on the central region $x \in [-2, 2]$.**
   Investigate the effect that variation of h and N has on the SPI approximation to $f(x)$ over this interval. Obviously there is considerable interplay between the parameters h and N. Can you suggest a combination of the two that serves as a more sensible single parameter to keep track of?

   (d) **Consider the entire interval $[-10, 10]$.**
   What do you notice near the interval boundaries? Does adjusting the number of SPI particles and/or the smoothing length h remedy the situation?

i. Can you suggest a reason for this failure? (Hint: consider the criteria that the kernel function is assumed to meet.)

ii. Propose a correction to alleviate the problem near the boundaries.

(e) Consider the SPI approximations to the first and second derivative of $f(x)$.

i. Do the derivative approximations suffer from similar weaknesses at the boundaries?

ii. Investigate the effect that variation of h and N has on the SPI approximations to the derivatives.

(f) Is the h-dependence of the error derived in Question 3 confirmed by the simulation? Discuss.