Particle Approximations

1 Approximation of a Continuous function f using Particles

A function $f(x)$ can be written in terms of a convolution with the Dirac delta function as follows

$$f(x) = \int_{-\infty}^{\infty} f(y)\delta(y-x)\,\mathrm{d}y. \tag{1}$$

The integral in the above equation can be approximated at discrete points x_i by the summation

$$f_\varepsilon^h(x) = \sum_i f(x_i)V_i\eta_\varepsilon(x_i - x), \tag{2}$$

where η_ε is an approximation of the Dirac delta

$$\delta(x) = \lim_{\varepsilon\to 0}\frac{1}{\varepsilon^d}\eta\left(\frac{x}{\varepsilon}\right) = \lim_{\varepsilon\to 0}\eta_\varepsilon(x), \tag{3}$$

with ε the kernel radius and V_i is the volume or weight associated to point x_i. The function η defines the shape while ε defines the scale. The parameter d corresponds to the number of *dimensions* for the problem. The Dirac delta satisfies the following properties:

$$\int_{-\infty}^{\infty} f(x-y)\delta(x)\,\mathrm{d}x = f(y) \tag{4}$$

$$\int_{-\infty}^{\infty} \delta(x)\,\mathrm{d}x = 1 \tag{5}$$

$$\int_{-\infty}^{\infty} x^m\delta(x)\,\mathrm{d}x = 0 \quad \forall m > 0 \tag{6}$$

Naturally, the mollification kernel η_ε must satisfy similar properties which are discussed below.

2 Smooth Particles

Given the scaled kernel

$$\eta_\varepsilon(x) = \frac{1}{\varepsilon^d}\eta\left(\frac{x}{\varepsilon}\right) \tag{7}$$

we can distinguish two cases:

Point Particles approximate a function $f(x)$ using the Dirac function:

$$f(x) = \int_{-\infty}^{\infty} f(y)\delta(x-y)\,\mathrm{d}y \to f^h(x) = \sum_{p=1}^{N} f(x_p)V_p\delta(x-x_p). \tag{8}$$

The values of this function are only defined at the points x_p, everywhere else the function values are zero. V_p is the volume of particle p which is associated to a characteristic particle spacing h. N is the number of particles in the system.

Smooth Particles approximate a function $f(x)$ using a mollifier kernel given in Equation (7) instead of the Dirac delta $\delta(x)$:

$$f_\varepsilon(x) = \int_{-\infty}^{\infty} f(y)\eta_\varepsilon(x-y)\,\mathrm{d}y \rightarrow f_\varepsilon^h(x) = \sum_{p=1}^{N} f(x_p)V_p\eta_\varepsilon(x-x_p). \quad (9)$$

Here the function values are defined within the radius of the kernel $\eta_\varepsilon(x)$. The notation f_ε^h is used for the approximation, where ε denotes the width or radius of the kernel and h denotes a characteristic separation of neighboring particles which is associated to the particle volume V_p for particle p. N is the number of particles in the system.

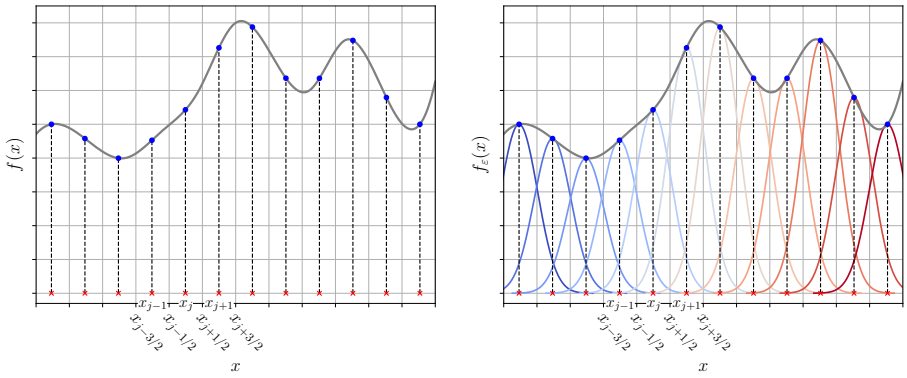

Figure 1: Point particles (left) and smooth particle (right) approximations

Figure 1 compares two approximations, where the left figure approximates the function $f(x)$ using samples obtained by the Dirac delta function (point particles), while the approximation on the right uses a smooth Gaussian kernel (smooth particles)

$$\eta_\varepsilon(x) = \frac{1}{\sqrt{2\pi}\varepsilon} e^{-\frac{x^2}{2\varepsilon^2}}. \quad (10)$$

The approximation of $f(x)$ is obtained from the superposition of a series of such kernels at each particle position x_j. Note that the volume V_j for these uniformly spaced particles (in the figure the particles are arranged on a regular lattice) corresponds to $V_j = x_{j+1/2} - x_{j-1/2}$.

2.1 Taylor Series Expansion

We use a Taylor series expansion of the function evaluation $f(y)$ around x and write

$$f(y) = \sum_{k=0}^{\infty} \frac{f^{(k)}(x)}{k!}(y-x)^k, \quad (11)$$

where $f^{(k)} = \mathrm{d}^k f/\mathrm{d}x^k$ denotes the k-th derivative of the function f. Next, we subtract $f(x)$ and convolve both sides of the equation with the yet unknown function η_ε:

$$\begin{aligned}\int_{-\infty}^{\infty}[f(y)-f(x)]\eta_\varepsilon(x-y)\,\mathrm{d}y &= \int_{-\infty}^{\infty}\sum_{k=1}^{\infty}\frac{f^{(k)}(x)}{k!}(y-x)^k\eta_\varepsilon(x-y)\,\mathrm{d}y \\ &= \sum_{k=1}^{\infty}\frac{f^{(k)}(x)}{k!}\frac{\varepsilon^k}{\varepsilon^k}\int_{-\infty}^{\infty}(y-x)^k\frac{1}{\varepsilon}\eta\left(\frac{x-y}{\varepsilon}\right)\mathrm{d}y,\end{aligned} \tag{12}$$

where we have used Equation (7) with $d = 1$. Next we introduce the variable

$$z = \frac{x-y}{\varepsilon} \tag{13}$$

$$\frac{\mathrm{d}z}{\mathrm{d}y} = -\frac{1}{\varepsilon}. \tag{14}$$

Substituting variable z into Equation (12) yields

$$\int_{-\infty}^{\infty}[f(y)-f(x)]\eta_\varepsilon(x-y)\,\mathrm{d}y = \sum_{k=1}^{\infty}\frac{f^{(k)}(x)}{k!}(-1)^k\varepsilon^k M_k, \tag{15}$$

where the k-th moment M_k is defined by

$$M_k = \int_{-\infty}^{\infty} z^k\eta(z)\,\mathrm{d}z. \tag{16}$$

Note that the negative sign of the differential $\mathrm{d}z$ in Equation (14) cancels after substituting variable z for the integration bounds and inverting them such that integration is from $-\infty$ to $+\infty$.

2.2 Smooth Particle Approximations

Equation (15) can be used to derive derivatives expressed by an integral operator by choosing a particular kernel $\eta(x)$ which we determine by satisfying certain moment conditions M_k given in Equation (16). For ease of notation, we multiply Equation (15) by $\varepsilon^{-\beta}$ and rewrite it as

$$\frac{1}{\varepsilon^\beta}\int_{-\infty}^{\infty}[f(y)-f(x)]\eta_\varepsilon(x-y)\,\mathrm{d}y = \sum_{k=1}^{\infty}\frac{\mathrm{d}^k f}{\mathrm{d}x^k}\frac{(-1)^k}{k!}\varepsilon^{k-\beta}M_k, \tag{17}$$

where $\beta > 0$ denotes the order of the derivative we would like to retain. For example, the β-th derivative is obtained if all terms on the right hand side of Equation (17) vanish for $k \neq \beta$. We then obtain an expression for the derivative in terms of an integral operator

$$\frac{\mathrm{d}^\beta f}{\mathrm{d}x^\beta} = \frac{1}{\varepsilon^\beta}\int_{-\infty}^{\infty}[f(y)-f(x)]\eta_\varepsilon(x-y)\,\mathrm{d}y, \tag{18}$$

which is exact only if the kernel $\eta_\varepsilon(x)$ satisfies the following conditions:

$$\begin{aligned}M_\beta &= (-1)^\beta\beta!, \\ M_k &= 0 \quad k \neq \beta.\end{aligned}$$

In practice it is not feasible to impose infinite moment conditions on the kernel $\eta_\varepsilon(x)$. There are two approximations that arise:

1. Truncation of the Taylor series
2. Use of a quadrature rule to approximate the integral operator

For an accuracy r, we truncate the summation in Equation (17) after a certain term. The leading order error term in Equation (17) depends on the number of satisfied conditions on the moments M_k for $k \in \mathcal{S}$, where $\mathcal{S} = \{1, \ldots, \beta + r - 1\} - \{\beta\}$. For example, Equation (18) is approximated with a leading error norm of $\|f - f_\varepsilon\|_\infty \leq C_1 \varepsilon^r \|f^{(r)}\|_\infty$, where $C_1 > 0$ is a constant, by the following moment conditions:

$$\begin{aligned} M_k &= 0 \quad k \in \mathcal{S}, \\ M_\beta &= (-1)^\beta \beta!, \\ M_k &< \infty \quad k \notin \mathcal{S}. \end{aligned}$$

The approximation of the integral operator in Equation (18) is achieved with an appropriate quadrature rule that introduces an error norm $\|f_\varepsilon - f_\varepsilon^h\|_\infty \leq C_2 (h/\varepsilon)^m \|f^{(m)}\|_\infty$, where $C_2 > 0$ is a constant and m depends on the smoothness properties of $\eta(x)$. From this error norm, it is clear that $h/\varepsilon < 1$ must hold for convergence (the kernels η_ε must *overlap* for neighboring particles).

Given that the moment conditions M_k are satisfied, we can construct a kernel $\eta_\varepsilon(x)$ to approximate the β-th derivative with associated error norm $\|f - f_\varepsilon^h\|_\infty \leq C_1 \varepsilon^r \|f^{(r)}\|_\infty + C_2 (h/\varepsilon)^m \|f^{(m)}\|_\infty$. The complexity of constructing such kernels is greatly reduced by taking into account symmetry in the form of

$$\eta(x) = (-1)^\beta \eta(-x), \tag{19}$$

where the shape of the kernel depends on the derivative order β and is *symmetric* for even derivatives and *anti-symmetric* for odd derivatives.

2.3 Example: Approximation for Second Derivative

We want to approximate the second derivative up to second order accuracy. Therefore, $\beta = 2$ and $r = 2$. The task is to find a kernel $\eta(x)$ with the symmetry property

$$\eta(x) = \eta(-x)$$

and it must satisfy the following moment conditions:

$$\begin{aligned} M_1 &= 0, \\ M_2 &= 2, \\ M_3 &= 0, \\ M_k &< \infty \quad \forall k > 3. \end{aligned}$$

It is easy to show that the Gaussian kernel

$$\eta(x) = \frac{4}{\sqrt{\pi}} e^{-x^2} \tag{20}$$

satisfies these properties. To retain a second order accurate approximation, we use the mid-point rule to approximate the integral operator and arrive at the following expression for the second derivative

$$\left.\frac{\mathrm{d}^2 f_\varepsilon^h}{\mathrm{d}x^2}\right|_{x_i} = \frac{1}{\varepsilon^2}\sum_{p=1}^{N}[f(x_p) - f(x_i)]V_p\eta_\varepsilon(x_i - x_p), \tag{21}$$

where N is the number of quadrature points and η_ε corresponds to Equation (7) ($d = 1$) with $\eta(x)$ the Gaussian kernel from Equation (20).

3 Particle Strength Exchange

Particle strength exchange (PSE) is a method that aims at high order approximations for the diffusion operator in particle systems. Assume $q = q(\mathbf{x}, t)$ is the density of some quantity q (e.g. concentration density) with spatial coordinates $\mathbf{x}$ and t time. We express the integral of the density q over the domain Ω as

$$Q(t) = \int_\Omega q(\mathbf{x}, t)\,\mathrm{d}V. \tag{22}$$

Assume we discretize the domain Ω using N particles. Equation (22) is then rewritten in the form

$$Q(t) = \sum_{p=1}^{N}\int_{\Omega_p} q(\mathbf{x}, t)\,\mathrm{d}V = \sum_{p=1}^{N} Q_p(t), \tag{23}$$

where $\Omega_p \subseteq \Omega$ is the domain occupied by particle p and $Q_p(t)$ the "strength" of the quantity of interest carried by particle p. Note that $V_p = \int_{\Omega_p}\mathrm{d}V$ is the volume of particle p.

Our goal is to solve the diffusion equation

$$\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial x^2} \tag{24}$$

in a particle system for a function $f(x, t)$ and diffusion coefficient D. For simplicity, we assume a one dimensional system and set $d = 1$. We are interested in the integral quantity $Q(t)$ for which we define a function $f_p(t)$ as follows

$$f_p(t) = \frac{\int_{\Omega_p} q(x, t)\,\mathrm{d}x}{\int_{\Omega_p}\mathrm{d}x} = \frac{Q_p(t)}{V_p}, \tag{25}$$

which is defined at each particle location x_p. In Equation (21) we have found a second order accurate approximation for the second derivative, which we now use together with the function $f_p(t)$ to reduce the partial differential equation of Equation (24) into a system of ordinary differential equations for N particles, that is

$$\frac{\mathrm{d}Q_i}{\mathrm{d}t} = \frac{D}{\varepsilon^2}\sum_{p=1}^{N}[Q_pV_i - Q_iV_p]\eta_\varepsilon(x_i - x_p). \tag{26}$$

Integration of the system can be carried out using a suitable numerical scheme. The scheme in Equation (26) is called particle strength exchange. Note that the PSE scheme is *conservative* for a symmetric kernel η_ε.

3.1 PSE for Particles Arranged on a Regular Lattice

The PSE scheme shown in Equation (26) is general and can be applied for arbitrary particle positions x_p for a kernel η_ε that satisfies the necessary moment conditions. The Gaussian kernel shown in Equation (20) would be a possible choice for a second order accurate approximation. It is important to note that this kernel does not have local support, even though it decays fast. Nevertheless, the computational complexity associated with evaluating this kernel is high. We can derive a kernel which is much cheaper to evaluate if we are allowed to restrict the particle locations to a regular lattice. Assume particle locations are constrained to a uniform grid with grid spacing h. We define the kernel

$$\eta(x) = \begin{cases} 2\left(1 - \frac{1}{2}|x|\right) & \text{for} |x| \leq 2 \\ 0 & \text{otherwise} \end{cases} \tag{27}$$

Figure 2 illustrates the shape of this kernel. Note that this special kernel does

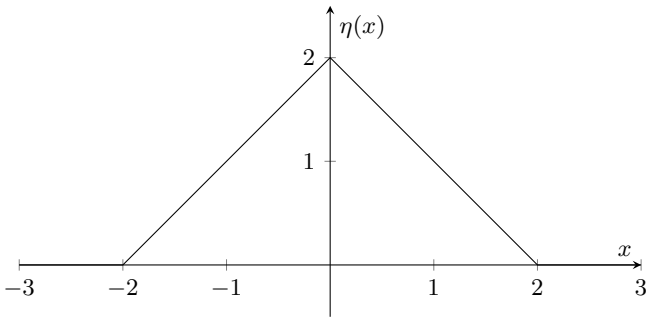

Figure 2: Shape of kernel defined in Equation (27)

not satisfy the condition for the second moment $M_2 = 8/3 \neq 2$ and can not be used in general. Such a "small" kernel exhibits discrete behavior as it only takes into account a small neighborhood of points. Because particles are arranged on a lattice, the kernel will only be evaluated at known locations x_i. Therefore, we enforce the discrete moment conditions at grid points i

$$\hat{M}_k = \sum_i i^k \eta(i) \tag{28}$$

which will result in the correct normalization $\hat{M}_2 = 2$ for this special discrete kernel. Note that because of the regular lattice restriction and the requirement of discrete moment conditions, the kernel in Equation (27) can only be used if particles are arranged on a regular lattice.

The distance between particle i and p on a uniform grid simply is $(i - p)h$ and the associated particle volume is $V_i = V_p = V = h$. Furthermore, we set the kernel radius equal to the grid spacing $\varepsilon = h$. Using Equations (26) and (7)

we can plugin our kernel in Equation (27) to arrive at the expression

$$\frac{\mathrm{d}Q_i}{\mathrm{d}t} = \frac{D}{h^2}\sum_{p=1}^{N}[Q_p h - Q_i h]\frac{1}{h}\eta\left(\frac{(i-p)h}{h}\right) \tag{29}$$

$$= \frac{D}{h^2}\sum_{p=1}^{N}[Q_p - Q_i]\eta(i-p) \tag{30}$$

$$= \frac{D}{h^2}(Q_{i-1} - 2Q_i + Q_{i+1}). \tag{31}$$

The spatial discretization on the right hand side results in second order accurate centered finite differences given the kernel in Equation (27). This shows that if particles are arranged on a regular lattice, provided we make a clever choice for η_ε, any finite difference scheme can be obtained. Kernel choices that recover finite differences are special kernels in the sense that their kernel radius is the smallest possible to achieve a certain accuracy. This results in much higher efficiency regarding the evaluation of the kernel η_ε which is a direct consequence of enforcing the particle locations to a regular lattice.