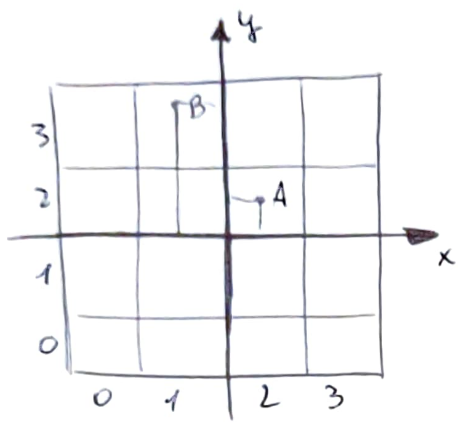
Matteo Zortea, Anja Heim

24/11/2021

Fundamentals of Simulation Methods
Sheet 05

(1)



$x, y \in [-H, H] \Rightarrow$ side $2H$

N number of squares per each side

$h = \frac{2H}{N}$ square side length

$\tilde{x}, \tilde{y}$ are coordinates in units of h, i.e.

$$\tilde{x} = x/h \qquad \tilde{y} = y/h$$

Cells are labelled by indices (k, ℓ)

Given coordinates of a point (x_p, y_p), the indices corresponding to the closest cell are

$$k = \lfloor x_p + \tfrac{N}{2} \rfloor \qquad \ell = \lfloor y_p + \tfrac{N}{2} \rfloor$$

For example, for the figure above, if $A = (\frac{1}{2}, \frac{1}{2})$ and $B = (-\frac{1}{2}, \frac{5}{3})$

$$\left.\begin{aligned} k_A &= \lfloor \tfrac{1}{2} + 2 \rfloor = \lfloor \tfrac{5}{2} \rfloor = 2 \\ \ell_A &= \lfloor \tfrac{1}{2} + 2 \rfloor = \lfloor \tfrac{5}{2} \rfloor = 2 \end{aligned}\right\} (k, \ell) = (2, 2)$$

$$\left.\begin{aligned} k_B &= \lfloor -\tfrac{1}{2} + 2 \rfloor = \lfloor \tfrac{3}{2} \rfloor = 1 \\ \ell_B &= \lfloor \tfrac{5}{3} + 2 \rfloor = \lfloor \tfrac{11}{3} \rfloor = 3 \end{aligned}\right\} (k, \ell) = (1, 3)$$

In units of h

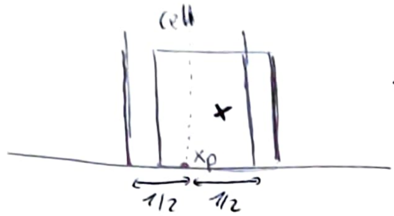
(2) $W_{k,\ell}(\bar{x}_i) = \int \Pi(\bar{x}_i - \bar{x}_p)\, \delta(\bar{x}_i - \bar{x}_\ell)\, d\bar{x} =$

$$= \int \Pi(\bar{x}_0 - \bar{x}_p)\, \delta(\bar{x} - \bar{x}_i)\, d\bar{x} =$$

$$= \left(\int \Pi(x_i - x_p)\, \delta(x - x_i)\, dx \right) \left(\int \Pi(y_i - y_p)\, \delta(y - y_\ell)\, dy \right) =$$

$$= \Pi(x_i - x_p)\, \Pi(y_i - y_p)$$

=> Calculate distances from the centers of the cells and position of the point. If distance (both along x and y) is less than 1/2 $W_{kl} = 1$.
Else $W_{kl} = 0$



$$\Pi(x - x_p) = \begin{cases} 1 & \text{if } |x_p - x| < 1/2 \\ 0 & \text{otherwise} \end{cases}$$

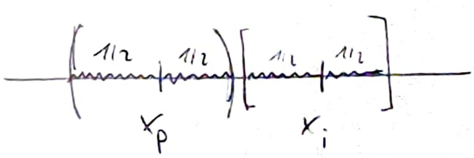
Practically speaking only the cell closest to $\bar{x}_i$ contributes to W, hence once we found the indices of the closest cell, we can sum up 1 to the weight of that cell.

First order method

$$W_{k,l}(\bar{x}_i) = \int d\bar{x} \; \Pi(\bar{x} - \bar{x}_p)\, \Pi(\bar{x} - \bar{x}_i) =$$

$$= \underbrace{\left(\int dx \; \Pi(x - x_p)\, \Pi(x - x_i) \right)}_{} \left(\int dy \; \Pi(y - y_p)\, \Pi(y - y_i) \right) =$$

$\neq 0$ only if $|x - x_p| < 1/2$ and $|x - x_i| < 1/2$



=> The result is the overlap area between $[x_p - 1/2, x_p + 1/2]$ and $[x_i - 1/2, x_i + 1/2]$

=> ① Calculate ε_x (ε_y), that is the overlap with the closest cell along x (y) direction

② W_{kl} is updated by those weights, i.e. $W_{kl} \mathrel{+}= \varepsilon_x \varepsilon_y$

③ If ε_x (ε_y) is less than 1/2, there is some overlap also in the previous cell. The overlap is $1 - \varepsilon_x$ ($1 - \varepsilon_y$)

④ Otherwise there is overlap with the successive cell and it amounts to $1 - \varepsilon_x$ ($1 - \varepsilon_y$).

Second order method

The height of the triangle must be 1 in order to be 1 the total "volume".

$\Rightarrow$ the height must be 1

$\Rightarrow$ the angle θ is such that $tg\,\theta = \frac{\text{height}}{\text{length}} = \frac{1}{2}$

$\Rightarrow$ if ε_x is the distance from the leftmost cell edge, the portion of triangle in the previous cell is $(1-\varepsilon)\,\frac{(1-\varepsilon)}{2} = \frac{(1-\varepsilon)^2}{2}$

In the one after it is $[1-(1-\varepsilon)] \cdot \frac{[1-(1-\varepsilon)]}{2} = \frac{\varepsilon^2}{2}$

In the closest cell we can just take the total area and subtract the overlap area of the cells before and after

$$1 - \frac{\varepsilon^2}{2} - \frac{(1-\varepsilon)^2}{2} = \frac{1}{2} - \varepsilon^2 + \varepsilon$$

Thus, we can also follow another approach. We may make use of the fact that

Order	Assignement function
Zeroth order	Π
first order	$\Pi * \Pi$
second order	$\Pi * \Pi * \Pi$

We might want to obtain the function $W(x)$ analitically. In order to do this, instead of solving the convolution analitically, we could take the Fourier transform, using the fact that $\mathcal{F}[f * g] = \mathcal{F}[f] \cdot \mathcal{F}[g]$

$$\mathcal{F}[\Pi] = \int_{-\infty}^{+\infty} dx\; \Pi(x)\, e^{-ikx} = \int_{-1/2}^{1/2} e^{-ikx}\, dx = \frac{e^{-ik/2} - e^{+ik/2}}{2-ik/2} = \frac{\sin(k/2)}{k/2} = \mathrm{sinc}(k/2)$$

In the Fourier domain:

$$\text{zeroth order} \longrightarrow \operatorname{sinc}(k) = \frac{\sin k}{k}$$

$$\text{first order} \longrightarrow \left(\operatorname{sinc}(k)\right)^2 = \frac{\sin^2 k}{k^2}$$

$$\text{second order} \longrightarrow \left(\operatorname{sinc}(k)\right)^3 = \frac{\sin^3 k}{k^3}$$

$\Rightarrow$ To antitransform we need to evaluate integrals of the type

$$f_\alpha(x) = \int_{-\infty}^{+\infty} dk \; \operatorname{sinc}^\alpha(k)\, e^{ikx} = \int_{-\infty}^{+\infty} dk \; \frac{\sin^\alpha(k)}{k^\alpha}\, e^{ikx}$$

One can note that

$$\frac{d^\alpha f_\alpha(x)}{dx^\alpha} = \int_{-\infty}^{+\infty} dk \; \frac{\sin^\alpha(k)}{k^\alpha} \frac{\partial^\alpha}{\partial x^\alpha}\left(e^{ikx}\right) = \int_{-\infty}^{+\infty} dk \; \sin^\alpha(k)\, i^\alpha\, e^{ikx}$$

This last integral can be evaluated for some α:

zeroth order ($\alpha=1$)

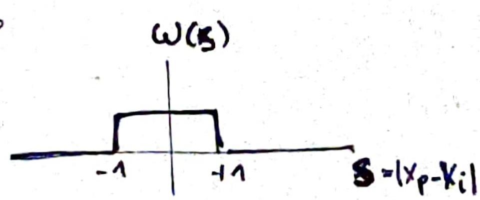
$$\int_{-\infty}^{+\infty} dk \; \sin(k)\, e^{ikx} = \frac{1}{2i}\left(\delta(x+1) - \delta(x-1)\right)$$

I used that $\sin(k) = \frac{e^{ik} - e^{-ik}}{2i}$ and that $\int e^{ikx}\, dx = \delta(k)$

hence

$$\frac{d f(x)}{dx} = \frac{\cancel{i}}{2\cancel{i}}\left(\delta(x+1) - \delta(x-1)\right)$$

$$f(x) = \frac{1}{2\cancel{i}}\int_{-\infty}^{x} dx' \left(\delta(x'+1) - \delta(x'-1)\right) = \frac{1}{2}\left(\theta(x+1) - \theta(x-1)\right)$$



$$f(x) = \begin{cases} 0 & \text{if } |x| > 1 \\ \frac{1}{2} & \text{if } |x| < 1 \end{cases}$$

First order ($\alpha=2$)

$$\int_{-\infty}^{+\infty} dk \; \sin^2(k)\, e^{ikx} = \int_{-\infty}^{+\infty} dk \left(\frac{e^{ik} - e^{-ik}}{2i}\right)^2 e^{ikx} = \int_{-\infty}^{+\infty} \frac{e^{ik(x+2)} + e^{ik(x-2)} - 2e^{ikx}}{-4} =$$

$$= \frac{\delta(x)}{2} - \frac{\delta(x+2)}{4} - \frac{\delta(x-2)}{4}$$

hence

$$\frac{d^2 f(x)}{dx^2} = i^2\left(\frac{\delta(x)}{2} - \frac{\delta(x+2)}{4} - \frac{\delta(x-2)}{4}\right) = \frac{\delta(x+2)}{4} + \frac{\delta(x-2)}{4} - \frac{\delta(x)}{2}$$

$$\Rightarrow \frac{df}{dx} = \int_{-\infty}^{x} dx' \, \frac{\delta(x'+2)}{4} + \frac{\delta(x'-2)}{4} - \frac{\delta(x')}{2} = \frac{\Theta(x+2)}{4} + \frac{\Theta(x-2)}{4} - \frac{\Theta(x)}{2}$$

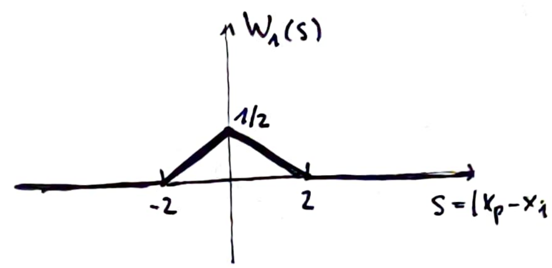
$$f(x) = \int_{-\infty}^{x} dx' \, \frac{\Theta(x+2)}{4} + \frac{\Theta(x-2)}{4} - \frac{\Theta(x)}{2} = \frac{x+2}{4}\Theta(x+2) + \frac{x-2}{4}\Theta(x-2) - \frac{x}{2}\Theta(x)$$

$x > 2 \longrightarrow f(x) = 0$

$x < -2 \longrightarrow f(x) = 0$

$-2 \leq x < 0 \longrightarrow f(x) = \frac{1}{4}x + \frac{1}{2}$

$0 < x \leq 2 \longrightarrow f(x) = -\frac{1}{4}x + \frac{1}{2}$



$$\Rightarrow f(x) = \left(\frac{1}{2} - \frac{|x|}{4}\right)\Theta(2 - |x|) = \frac{1}{4}(2 - |x|)\,\Theta(2 - |x|)$$

Second order ($\alpha = 3$)

$$\int_{-\infty}^{+\infty} dk \, \sin^3(k) \, e^{ikx} = \int_{-\infty}^{+\infty} \left(\frac{e^{2ik} + e^{-2ik} - 2}{-4}\right)\left(\frac{e^{ik} - e^{-ik}}{2i}\right) e^{ikx} \, dk =$$

$$= \int_{-\infty}^{+\infty} \frac{e^{ik(x+3)} - e^{ik(x+1)} + e^{-ik(x-1)} - e^{ik(x-3)} - 2e^{ik(x+1)} + 2e^{ik(x-1)}}{-8i} \, dk =$$

$$= \int_{-\infty}^{+\infty} \frac{e^{ik(x+3)}}{-8i} + \frac{3e^{ik(x+1)}}{8i} - \frac{3e^{ik(x-1)}}{8i} + \frac{e^{ik(x-3)}}{8i} \, dk \Longrightarrow$$

$$\Longrightarrow \frac{d^3 f(x)}{dx^3} = i^3\left(\frac{\delta(x+3)}{-8i} + \frac{3\delta(x+1)}{8i} - \frac{3\delta(x-1)}{8i} + \frac{\delta(x+3)}{8i}\right) =$$

$$= \frac{\delta(x+3)}{8} - \frac{3\delta(x+1)}{8} + \frac{3\delta(x-1)}{8} - \frac{\delta(x+3)}{8}$$

$$\frac{d^2 f(x)}{dx^2} = \int_{-\infty}^{x} dx' \, \frac{d^3 f(x')}{dx'^3} = \frac{\Theta(x+3)}{8} - 3\frac{\Theta(x+1)}{8} + 3\frac{\Theta(x-1)}{8} - \frac{\Theta(x+3)}{8}$$

$$\frac{df(x)}{dx} = \int_{-\infty}^{x} dx' \, \frac{d^2 f(x')}{dx'^2} = \frac{(x+3)}{8}\Theta(x+3) - \frac{3(x+1)}{8}\Theta(x+1) + \frac{3}{8}(x-1)\,\Theta(x-1) - \frac{1}{8}(x+3)\Theta(x+3)$$

$$f(x) = \int_{-\infty}^{x} \frac{x'+3}{8}\theta(x'+3) - \frac{3(x'+1)}{8}\theta(x'+1) + \frac{3}{8}(x'-1)\,\theta(x'-1) - \frac{1}{8}(x'-3)\,\theta(x'-3)\,dx' =$$

$$= \frac{\theta(x+3)}{8}\int_{-3}^{x} dx'\, x'+3 \; - \frac{3\theta(x+1)}{8}\int_{-1}^{x} x'+1\, dx' \; + \frac{3\theta(x-1)}{8}\int_{1}^{x} x'-1\, dx' - \frac{\theta(x-3)}{8}\int_{3}^{x} x'-3\,dx'$$

$$= \frac{\theta(x+3)}{8}\left(\frac{x^2}{2}+3x-\frac{9}{2}+9\right) - \frac{3\theta(x+1)}{8}\left(\frac{x^2}{2}+x-\frac{1}{2}+1\right) + \frac{3}{8}\theta(x-1)\left(\frac{x^2}{2}-x+\frac{1}{2}-1\right) +$$

$$-\frac{1}{8}\theta(x-3)\left(\frac{x^2}{2}-3x-\frac{9}{2}+9\right)$$

$$= \frac{1}{8}\Bigg[\theta(x+3)\left(\frac{x^2}{2}+3x+\frac{9}{2}\right) - 3\,\theta(x+1)\left(\frac{x^2}{2}+x+\frac{1}{2}\right) + 3\,\theta(x-1)\left(\frac{x^2}{2}-x+\frac{1}{2}\right) +$$

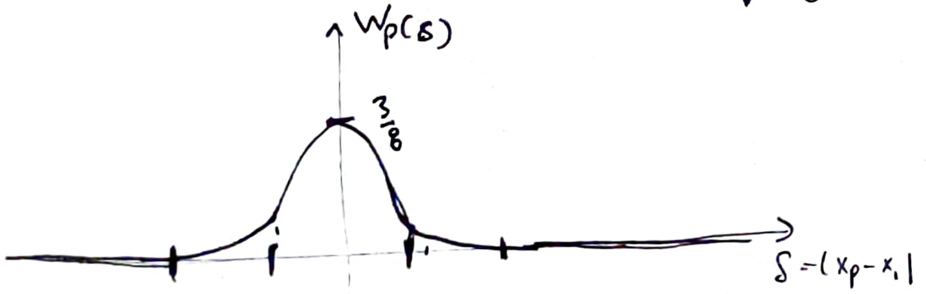
$$- \theta(x-3)\left(\frac{x^2}{2}-3x+\frac{9}{2}\right)\Bigg]$$

$|x| > 3 \rightarrow f(x) = 0$

$-3 < x < -1 \rightarrow f(x) = \frac{1}{16}(x^2+6x+9) = \frac{1}{16}(x+3)^2$

$-1 < x < 1 \rightarrow f(x) = -\frac{1}{8}(x^2-3)$

$1 < x < 3 \rightarrow f(x) = \frac{1}{16}(-x+3)^2 \Rightarrow f(x) = \begin{cases} \frac{1}{16}(3-|x|)^2 & 1<|x|<3 \\ \frac{1}{8}(3-|x|^2) & |x|<1 \\ 0 & \text{otherwise} \end{cases}$



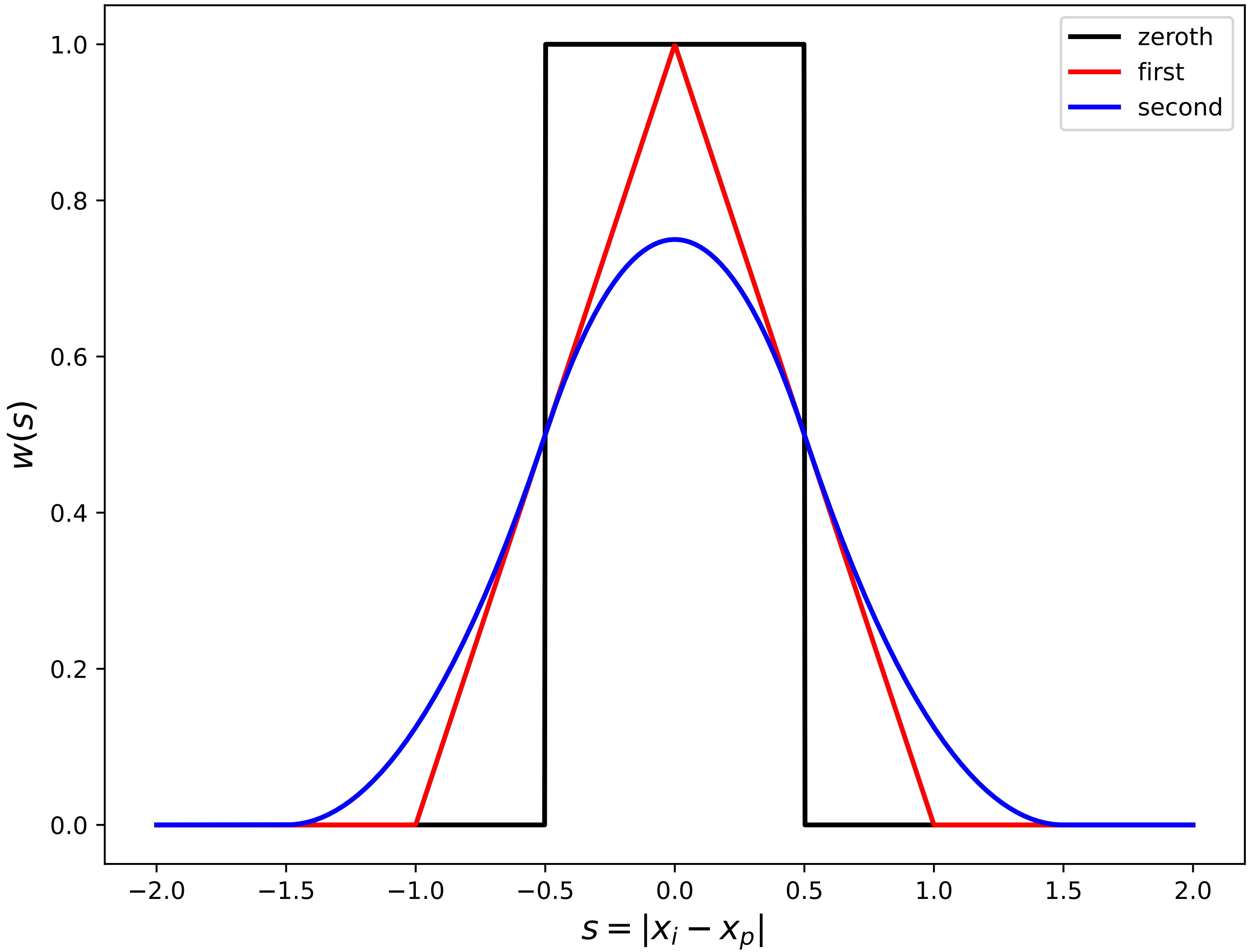
In the real problem our function was $\operatorname{sinc}(x/2)$. Hence our correct weight functions are:

$$W_0(x) = \begin{cases} 1 & \text{if } |x| < 1/2 \\ 0 & \text{otherwise} \end{cases}$$

$$W_1(x) = \begin{cases} \frac{1}{2}(1 - |x|) & \text{if } |x| < 1 \\ 0 & \text{otherwise} \end{cases}$$

$$W_2(x) = \begin{cases} 1(3/4 - x^2) & |x| < 1/2 \\ \frac{1}{2}(3/2 - |x|)^2 & \frac{1}{2} < |x| < \frac{3}{2} \\ 0 & \text{otherwise} \end{cases}$$

The next page reports the plots of the three functions.


zeroth
first
second
$w(s)$
$s = |x_i - x_p|$
1.0
0.8
0.6
0.4
0.2
0.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0