Diffusion and Matern functions

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1 Goal

The aim is to find a practical way to compute the Matern function:

$$c_\nu(\tilde{r}) = \alpha_\nu \tilde{r}^\nu K_\nu(\tilde{r}) \tag{1}$$

where K_ν is the modified Bessel function of second kind and the factor α_ν ensures that c_ν is normalized ($c_\nu(0) = 1$).

2 Explicit formula

For the particular case where $\nu - 1/2 \in \mathbb{Z}$, there is a special formula for the modified Bessel function of second kind (http://functions.wolfram.com/Bessel-TypeFunctions/BesselK/introductions/Bessels/05/):

$$K_\nu(\tilde{r}) = \sqrt{\pi} e^{-\tilde{r}} \sum_{j=0}^{\lfloor |\nu|-1/2 \rfloor} \frac{(|\nu| - 1/2 + j)!}{j!\,(|\nu| - 1/2 - j)!} (2\tilde{r})^{-j-1/2} \tag{2}$$

Thus for $\nu > 0$:

$$\begin{aligned} c_\nu(\tilde{r}) &= \alpha_\nu \tilde{r}^\nu K_\nu(\tilde{r}) && (3)\\ &= \alpha_\nu \frac{\sqrt{\pi}}{2^\nu} e^{-\tilde{r}} \sum_{j=0}^{\nu-1/2} \frac{(\nu - 1/2 + j)!}{j!\,(\nu - 1/2 - j)!} (2\tilde{r})^{\nu-1/2-j} && (4)\\ & && (5) \end{aligned}$$

3 Practical computation

For the implicit diffusion, $\nu = M - d/2$ where $M \in \mathbb{N}$ is the number of implicit steps, and d the dimension. So only the cases $d = 1$ and $d = 3$ are valid here:

$$c_\nu(\tilde{r}) = \alpha_\nu \frac{\sqrt{\pi}}{2^{M-d/2}} e^{-\tilde{r}} \sum_{j=0}^{M-(d+1)/2} \beta_{j,M-(d+1)/2} (2\tilde{r})^{M-(d+1)/2-j} \tag{6}$$

where

$$\beta_{j,M} = \frac{(M+j)!}{j!\,(M-j)!} \tag{7}$$

can be computed recursively:

$$\beta_{0,M} = 1 \tag{8}$$

and

$$\begin{aligned} \beta_{j+1,M} &= \frac{(M+j+1)!}{(j+1)!\,(M-(j+1))!} && (9) \\ &= \frac{(M+j+1)(M-j)}{j+1} \beta_{j,M} && (10) \end{aligned}$$

Thus, the normalization becomes:

$$c_\nu(0) = \alpha_\nu \frac{\sqrt{\pi}}{2^{M-d/2}} \beta_{M-(d+1)/2,M-(d+1)/2} = 1 \tag{11}$$

leading to

$$\alpha_\nu = \frac{2^{M-d/2}}{\sqrt{\pi}} \frac{1}{\beta_{M-(d+1)/2,M-(d+1)/2}} \tag{12}$$

And finally:

$$c_\nu(\tilde{r}) = \frac{1}{\beta_{M-(d+1)/2,M-(d+1)/2}} e^{-\tilde{r}} \sum_{j=0}^{M-(d+1)/2} \beta_{j,M-(d+1)/2} (2\tilde{r})^{M-(d+1)/2-j} \tag{13}$$

The case $d = 2$ would require another method.