Supplement materials for example derivation in "A multiscale finite element method for coupled heat and water transfer in heterogeneous soils"

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May 2022

1 Correlation Kernel with Manhattan Distance (Example 2.1)

In Example 2.1, we present the solutions of eigenvalues and eigenfunctions when the covariance kernel is constructed with Manhattan distance.

The Manhattan distance of two points in a 2D spatial domain $\vec{x}_1 = (x_1, y_1), \vec{x}_2 = (x_2, y_2) \in \Omega$ is defined as

$$dist(\vec{x}_1, \vec{x}_2) = |x_1 - x_2| + |y_1 - y_2|$$

Using Manhattan distance, the 2D covariance kernel becomes

$$Ker(\vec{x}_1, \vec{x}_2) = \sigma^2 \exp\left[-\frac{|x_1 - x_2| + |y_1 - y_2|}{\eta}\right]$$

The 2D covariance kernel is separable, i.e.,

$$Ker(\vec{x}_1, \vec{x}_2) = \sigma^2 \exp\left[-\frac{|x_1 - x_2|}{\eta}\right] \exp\left[-\frac{|y_1 - y_2|}{\eta}\right]$$

Therefore, it is sufficient to study $\exp\left[-\frac{|x_1-x_2|}{\eta}\right]$ first. And we expect the result can be generalized to the 2D covariance kernel.

Consider $\exp\left[-\frac{|x_1-x_2|}{\eta}\right]$. Since we do not know the form of the eigenfunction, we can take $\cos wx$ or $\sin wx$ as the trials, and plug them into the Fredholm integrals and see what we can get.

First, let us try $\cos wx$

$$\begin{aligned}
&\int_0^L \exp\left[-\frac{|x_1 - x_2|}{\eta}\right] \cos wx_1 dx_1 \\
&= \int_0^{x_2} \exp\left[\frac{x_1 - x_2}{\eta}\right] \cos wx_1 dx_1 + \int_{x_2}^L \exp\left[-\frac{x_1 - x_2}{\eta}\right] \cos wx_1 dx_1 \\
&= \frac{1}{1+\eta^2 w^2}\left[\eta \cos wx_2 - \eta \exp\left(-\frac{x_2}{\eta}\right) + \eta^2 w \sin wx_2\right] \\
&\quad + \frac{1}{1+\eta^2 w^2}\left[\eta \cos wx_2 - \eta \exp\left(-\frac{L - x_2}{\eta}\right) \cos wL + \eta^2 w \exp\left(-\frac{L - x_2}{\eta}\right) \sin wL - \eta^2 w \sin wx_2\right] \\
&= \frac{1}{1+\eta^2 w^2}\left[2\eta \cos wx_2 - \eta \exp\left(-\frac{x_2}{\eta}\right) - \eta \exp\left(-\frac{L - x_2}{\eta}\right) \cos wL + \eta^2 w \exp\left(-\frac{L - x_2}{\eta}\right) \sin wL\right] \\
&= \frac{2\eta \cos wx_2}{1+\eta^2 w^2} + \frac{\eta}{1+\eta^2 w^2}\left[-\exp\left(-\frac{x_2}{\eta}\right) - \exp\left(-\frac{L - x_2}{\eta}\right) \cos wL + \eta w \exp\left(-\frac{L - x_2}{\eta}\right) \sin wL\right]
\end{aligned}$$

Second, let us try $\sin wx$

$$
\begin{aligned}
&\int_0^L \exp\left[-\frac{|x_1-x_2|}{\eta}\right]\sin wx_1 dx_1 \\
&= \int_0^{x_2} \exp\left[\frac{x_1-x_2}{\eta}\right]\sin wx_1 dx_1 + \int_{x_2}^L \exp\left[-\frac{x_1-x_2}{\eta}\right]\sin wx_1 dx_1 \\
&= \frac{1}{1+\eta^2 w^2}\left[\eta \sin wx_2 - \eta^2 w\cos wx_2 + \eta^2 w \exp\left(-\frac{x_2}{\eta}\right)\right] \\
&\quad + \frac{1}{1+\eta^2 w^2}\left[\eta\sin wx_2 - \eta\exp\left(-\frac{L-x_2}{\eta}\right)\sin wL - \eta^2 w\exp\left(-\frac{L-x_2}{\eta}\right)\cos wL + \eta^2 w\cos wx_2\right] \\
&= \frac{1}{1+\eta^2 w^2}\left[2\eta\sin wx_2 + \eta^2 w\exp\left(-\frac{x_2}{\eta}\right) - \eta\exp\left(-\frac{L-x_2}{\eta}\right)\sin wL - \eta^2 w\exp\left(-\frac{L-x_2}{\eta}\right)\cos wL\right] \\
&= \frac{2\eta\sin wx_2}{1+\eta^2 w^2} + \frac{\eta}{1+\eta^2 w^2}\left[\eta w\exp\left(-\frac{x_2}{\eta}\right) - \exp\left(-\frac{L-x_2}{\eta}\right)\sin wL - \eta w\exp\left(-\frac{L-x_2}{\eta}\right)\cos wL\right]
\end{aligned}
$$

Therefore, it is natural to combine $\cos wx$ and $\sin wx$ in the way $\eta w\cos wx + \sin wx$, and we can have

$$
\begin{aligned}
&\int_0^L \exp\left[-\frac{|x_1-x_2|}{\eta}\right](\eta w\cos wx_1 + \sin wx_1)dx_1 \\
&= \frac{2\eta}{1+\eta^2 w^2}(\eta w\cos wx_2 + \sin wx_2) \\
&\quad + \frac{\eta}{1+\eta^2 w^2}\exp\left(-\frac{L-x_2}{\eta}\right)\left[(\eta^2 w^2 - 1)\sin wL - 2\eta w\cos wL\right]
\end{aligned}
$$

Comparing this integral with the characteristic equation, we can define the eigenvalue and eigenfunction of the 1D kernel $\exp\left[-\frac{|x_1-x_2|}{\eta}\right]$ as

$$
\widetilde{\omega_n} = \frac{2\eta}{1+\eta^2 w_n^2},\ \widetilde{f_n(x)} = \frac{1}{A_n}(\eta w_n\cos w_n x + \sin w_n x)
$$

But at this time, we have to ensure that the residue term varnishes, i.e.,

$$
\frac{\eta}{1+\eta^2 w^2}\exp\left(-\frac{L-x_2}{\eta}\right)\left[(\eta^2 w^2-1)\sin wL - 2\eta w\cos wL\right] = 0
$$

That is to say, w_n solves

$$
(\eta^2 w_n^2 - 1)\sin w_n L - 2\eta w_n\cos w_n L = 0
$$

A_n is the normalizer of $\widetilde{f_n(x)}$, i.e.,

$$
\begin{aligned}
A_n &= \left[\int_0^L (\eta w_n\cos w_n x + \sin w_n x)^2 dx\right]^{1/2} \\
&= \left[\int_0^L \left(\eta^2 w_n^2\cos^2 w_n x + \sin^2 w_n x + 2\eta w_n\cos w_n x\sin w_n x\right)dx\right]^{1/2} \\
&= \left[\frac{\eta^2 w_n^2+1}{2}L + \frac{\eta^2 w_n^2 - 1}{2w_n}\sin w_n L\cos w_n L - \eta\cos^2 w_n L + \eta\right]^{1/2} \\
&= \left[\frac{\eta^2 w_n^2+1}{2}L + \eta\right]^{1/2}
\end{aligned}
$$

From the second step to the third step, we just need to explicitly calculate all the integrals, while from the third step to the fourth step, we need the fact that w_n satisfies $(\eta^2 w_n^2 - 1)\sin w_n L - 2\eta w_n\cos w_n L = 0$.

Hence, we conclude the analysis of eigenvalues and eigenfunctions for the 1D kernel $\exp\left[-\frac{|x_1-x_2|}{\eta}\right]$.

For the 2D covariance kernel, using the fact that the 2D covariance kernel is separable,

$$Ker(\vec{x}_1, \vec{x}_2) = \sigma^2 \exp\left[-\frac{|x_1 - x_2|}{\eta}\right] \exp\left[-\frac{|y_1 - y_2|}{\eta}\right]$$

we can apply our previous results to $\exp\left[-\frac{|x_1-x_2|}{\eta}\right]$ and $\exp\left[-\frac{|y_1-y_2|}{\eta}\right]$ one-by-one. Then the conclusion shown in the paper follows.

2 Correlation Kernel with Euclidean Distance (Example 2.2)

In Example 2.2, we claim the analytical solution to the eigenvalues and eigenfunctions can be challenging. Hence, we follows the semi-analytic method via 2D Fourier expansion, proposed in Li et al. (2006).

The Euclidean distance of two points in a 2D spatial domain $\vec{x}_1 = (x_1, y_1), \vec{x}_2 = (x_2, y_2) \in \Omega$ is defined as

$$dist(\vec{x}_1, \vec{x}_2) = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$$

Using Euclidean distance, the 2D covariance kernel becomes

$$Ker(\vec{x}_1, \vec{x}_2) = \sigma^2 \exp\left[-\frac{\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}}{\eta}\right]$$

With the Euclidean distance, the 2D covariance kernel is not separable any more.

To make the derivations clear, we explicitly write down the basis functions of 2D Fourier expansion, i.e.,

$$\left\{\sin\frac{2\pi kx}{L}\sin\frac{2\pi ly}{L}, \cos\frac{2\pi kx}{L}\sin\frac{2\pi ly}{L}, \sin\frac{2\pi kx}{L}\cos\frac{2\pi ly}{L}, \cos\frac{2\pi kx}{L}\cos\frac{2\pi ly}{L}\right\}_{k,l=0,1,2,\ldots,M}$$

If there exists an eigenfunction $f(x, y)$, we can namely write it as

$$f(x,y) = \sum_{k,l=0}^{M} a_{kl}\sin\frac{2\pi kx}{L}\sin\frac{2\pi ly}{L} + b_{kl}\cos\frac{2\pi kx}{L}\sin\frac{2\pi ly}{L} + c_{kl}\sin\frac{2\pi kx}{L}\cos\frac{2\pi ly}{L} + d_{kl}\cos\frac{2\pi kx}{L}\cos\frac{2\pi ly}{L}$$

The way we wrote the 2D Fourier expansion is not 100% correct, because there will be some redundant terms, such as when $k, l = 0$,

$$\sin\frac{2\pi kx}{L}\sin\frac{2\pi ly}{L} = \cos\frac{2\pi kx}{L}\sin\frac{2\pi ly}{L} = \sin\frac{2\pi kx}{L}\cos\frac{2\pi ly}{L} = 0$$

However, in this way, we can observe that there exists some symmetrical characteristics in this 2D Fourier expansion.

Because of the orthogonality of the base functions, we can now simply write all the base functions as

$$\{\varphi_i\}_{i=0,1,2,\ldots,N}$$

where φ_i stands for $\sin\frac{2\pi kx}{L}\sin\frac{2\pi ly}{L}$, $\cos\frac{2\pi kx}{L}\sin\frac{2\pi ly}{L}$, $\sin\frac{2\pi kx}{L}\cos\frac{2\pi ly}{L}$, or $\cos\frac{2\pi kx}{L}\cos\frac{2\pi ly}{L}$. Without loss of generality, we assume $\{\varphi_i\}_{i=0,1,2,\ldots,N}$ are normalized. Then, the 2D Fourier expansion of $f(x, y)$ can be written in a concise form,

$$f(x, y) = \sum_{n=1}^{N} c_n\varphi_n(x, y)$$

Hence, we obtain the 2D Fourier expansion of the assumed eigenfunction $f(x, y)$.

Since $f(x, y)$ is the eigenfunction, we can insert it into the characteristic equation, i.e.,

$$\iint_\Omega \exp\left[-\frac{\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}}{\eta}\right] f(x_1, y_1)dx_1dy_1 = \widetilde{\omega} f(x_2, y_2)$$

Exchange $f(x, y)$ by its Fourier expansion, $f(x, y)$

$$\iint_\Omega \exp\left[-\frac{\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}}{\eta}\right] \sum_{n=1}^{N} c_n\varphi_n(x_1, y_1)dx_1dy_1 = \widetilde{\omega}\sum_{p=1}^{N} c_p\varphi_p(x_2, y_2)$$

Now, multiply both side by $\varphi_q(x,y)$, and integrate over Ω, we can obtain

$$\begin{aligned}\iint_\Omega \varphi_q(x_2,y_2)\left[\iint_\Omega \exp\left[-\frac{\sqrt{(x_1-x_2)^2+(y_1-y_2)^2}}{\eta}\right]\sum_{n=1}^{N} c_n\varphi_n(x_1,y_1)dx_1dy_1\right]dx_2dy_2 \\ = \iint_\Omega \varphi_q(x_2,y_2)\left[\widetilde{\omega}\sum_{p=1}^{N} c_p\varphi_p(x_2,y_2)\right]dx_2dy_2\end{aligned}$$

The left-hand side (LHS) can be converted by changing the order to integrals, and we can further define the quadra-integral as Φ, i.e.

$$LHS = \sum_{n=1}^{N} c_n\left[\iint_\Omega \varphi_q(x_2,y_2)\left[\iint_\Omega \exp\left[-\frac{\sqrt{(x_1-x_2)^2+(y_1-y_2)^2}}{\eta}\right]\varphi_n(x_1,y_1)dx_1dy_1\right]dx_2dy_2\right] \equiv \sum_{n=1}^{N}\Phi_{qn}c_n$$

The right-hand side (RHS) can be simplified due to the orthonormality of $\{\varphi_i\}$, i.e.,

$$RHS = \widetilde{\omega}c_q$$

Therefore, the simplified characteristic equation can be written as

$$\sum_{n=1}^{N}\Phi_{qn}c_n = \widetilde{\omega}c_q$$

We notice that for $q, n = 1, 2, 3, ..., N$, the equation above can be written into a matrix form, i.e.,

$$\begin{pmatrix}\Phi_{11} & \Phi_{12} & \cdots & \Phi_{1N}\\ \Phi_{21} & \Phi_{22} & \cdots & \Phi_{2N}\\ \vdots & \vdots & & \vdots\\ \Phi_{N1} & \Phi_{N2} & \cdots & \Phi_{NN}\end{pmatrix}\begin{pmatrix}c_1\\ c_2\\ \vdots\\ c_N\end{pmatrix} = \widetilde{\omega}\begin{pmatrix}c_1\\ c_2\\ \vdots\\ c_N\end{pmatrix}$$

This is the eigenvalue problem of matrix $\begin{pmatrix}\Phi_{11} & \Phi_{12} & \cdots & \Phi_{1N}\\ \Phi_{21} & \Phi_{22} & \cdots & \Phi_{2N}\\ \vdots & \vdots & & \vdots\\ \Phi_{N1} & \Phi_{N2} & \cdots & \Phi_{NN}\end{pmatrix}$, and if it can be solved, $\widetilde{\omega}$ will be the eigenvalue of the 2D covariance kernel, and the associated eigenfunction will be the 2D Fourier expansion with the coefficients $\begin{pmatrix}c_1 & c_2 & \cdots & c_N\end{pmatrix}^T$, i.e.,

$$\widetilde{f_n(x,y)} = \sum_{n=1}^{N} c_n\phi_n(x,y)$$

Therefore, the intuition of the semi-analytic method is to convert the eigenvalue problem of the characteristic equation into the eigenvalue problem of a matrix Φ_{qn}, $q, n = 1, 2, ..., n$.