

Covariance function from a Poisson PDE

The two-dimensional Poisson equation in a rectangular Cartesian coordinate sytem has the form

$$\frac{\partial^2 v(x, y)}{\partial x^2} + \frac{\partial^2 v(x, y)}{\partial y^2} = - \sum_{\forall i} s_i f_i(x, y) \quad (1)$$

1 Solving the Poisson equation

The exact solution for Eq. (1) is subject to particular boundary conditions. For a first boundary value problem with domain $0 \leq x \leq a$, $0 \leq y \leq b$, and conditions given by

$$\begin{aligned} v(x=0, y) &= f_1(y) \\ v(x=a, y) &= f_2(y) \\ v(x, y=0) &= f_3(x) \\ v(x, y=b) &= f_4(x) \end{aligned}$$

the solution to this equation is given by [1]

$$\begin{aligned} v(x, y) &= \sum_{\forall i} s_i \int_0^a \int_0^b f_i(\xi, \eta) G(x, y, \xi, \eta) d\eta d\xi \\ &+ \int_0^b f_1(\eta) H_1(x, y, \xi, \eta) d\eta - \int_0^b f_2(\eta) H_2(x, y, \xi, \eta) d\eta \\ &+ \int_0^a f_3(\xi) H_3(x, y, \xi, \eta) d\xi - \int_0^a f_4(\eta) H_4(x, y, \xi, \eta) d\xi, \end{aligned} \quad (2)$$

where the Green function $G(x, y, \xi, \eta)$ and the functions $H_1(x, y, \xi, \eta)$, $H_2(x, y, \xi, \eta)$, $H_3(x, y, \xi, \eta)$ and $H_4(x, y, \xi, \eta)$ are given by

$$\begin{aligned} G(x, y, \xi, \eta) &= \frac{4}{ab} \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{\sin(p_n x) \sin(q_m y) \sin(p_n \xi) \sin(q_m \eta)}{p_n^2 + q_m^2}, \\ H_1(x, y, \xi, \eta) &= \left. \frac{\partial}{\partial \xi} G(x, y, \xi, \eta) \right|_{\xi=0}, \quad H_2(x, y, \xi, \eta) = \left. \frac{\partial}{\partial \xi} G(x, y, \xi, \eta) \right|_{\xi=a}, \\ H_3(x, y, \xi, \eta) &= \left. \frac{\partial}{\partial \eta} G(x, y, \xi, \eta) \right|_{\eta=0}, \quad H_4(x, y, \xi, \eta) = \left. \frac{\partial}{\partial \eta} G(x, y, \xi, \eta) \right|_{\eta=b}, \end{aligned} \quad (3)$$

where $p_n = \frac{n\pi}{a}$, and $q_m = \frac{m\pi}{b}$.

Assuming $f_1(y) = f_2(y) = f_3(x) = f_4(x) = 0$, equation (2) is equal to

$$v(x, y) = \sum_{\forall i} s_i \int_0^a \int_0^b f_i(\xi, \eta) G(x, y, \xi, \eta) d\eta d\xi \quad (4)$$

where $G(x, y, \xi, \eta)$ is given by (3).

2 Covariance matrix bewteen the outputs

We assume that $f_i(x, y)$ are independent Gaussian processes with mean value equal to zero and covariance matrix equal to $K_i(x, x', y, y') = K_i(x, x')K_i(y, y')$. Since the PDE equation is linear, the $v_q(x, y)$ are Gaussian processes with covariance matrix given by

$$\text{cov}[v_q(x, y), v_s(x', y')] = \text{E} \left[\sum_{\forall i} s_{qi} \int_0^a \int_0^b f_i(\xi, \eta) G(x, y, \xi, \eta) d\xi d\eta \right. \quad (5)$$

$$\left. \sum_{\forall k} s_{sk} \int_0^a \int_0^b f_k(\xi', \eta') G(x', y', \xi', \eta') d\xi' d\eta' \right] \quad (6)$$

Then, the covariance $\text{cov}[v_q(x, y), v_s(x', y')]$ is given as

$$\sum_{\forall i} s_{qi} \sum_{\forall k} s_{sk} \int_0^a \int_0^a \int_0^b \int_0^b G(x, y, \xi, \eta) G(x', y', \xi', \eta') \mathbb{E}[f_i(\xi, \eta) f_k(\xi', \eta')] d\xi' d\xi d\eta' d\eta$$

With $\mathbb{E}[f_i(\xi, \eta) f_k(\xi', \eta')] = K_{ik}(\xi, \xi', \eta, \eta') \delta_{ik} = K_{ik}(\xi, \xi') K_{ik}(\eta, \eta') \delta_{ik}$, the last expression can be written as

$$\sum_{\forall i} s_{qi} s_{si} \int_0^a \int_0^a \int_0^b \int_0^b G(x, y, \xi, \eta) G(x', y', \xi', \eta') K_i(\xi, \xi') K_i(\eta, \eta') d\xi' d\xi d\eta' d\eta$$

Using the expression (3) for $G(x, y, \xi, \eta)$ and SE kernels for the covariances of the latent processes, we have

$$\begin{aligned} \sum_{\forall i} s_{qi} s_{si} \int_0^a \int_0^a \int_0^b \int_0^b \left\{ \left[\frac{4}{ab} \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{\sin(p_n x) \sin(q_m y) \sin(p_n \xi) \sin(q_m \eta)}{p_n^2 + q_m^2} \right] \times \right. \\ \left. \left[\frac{4}{ab} \sum_{n'=1}^{\infty} \sum_{m'=1}^{\infty} \frac{\sin(p_{n'} x') \sin(q_{m'} y') \sin(p_{n'} \xi') \sin(q_{m'} \eta')}{p_{n'}^2 + q_{m'}^2} \right] \right\} \times \\ \exp \left[-\frac{(\xi - \xi')^2}{\sigma_x^2} \right] \exp \left[-\frac{(\eta - \eta')^2}{\sigma_y^2} \right] d\xi' d\xi d\eta' d\eta \end{aligned}$$

The above expression can be separated in two different sets of integrals

$$\begin{aligned} \sum_{\forall i} s_{qi} s_{si} \left\{ \frac{16}{(ab)^2} \sum_{\forall n} \sum_{\forall n'} \sum_{\forall m} \sum_{\forall m'} \frac{1}{(p_n^2 + q_m^2)(p_{n'}^2 + q_{m'}^2)} \sin(p_n x) \sin(p_{n'} x') \sin(q_m y) \sin(q_{m'} y') \times \right. \\ \left. \left\{ \int_0^a \int_0^a \sin(p_n \xi) \sin(p_{n'} \xi') \exp \left[-\frac{(\xi - \xi')^2}{\sigma_x^2} \right] d\xi' d\xi \right\} \left\{ \int_0^b \int_0^b \sin(q_m \eta) \sin(q_{m'} \eta') \exp \left[-\frac{(\eta - \eta')^2}{\sigma_y^2} \right] d\eta' d\eta \right\} \right\}. \end{aligned}$$

In this sense, we have

$$\text{cov}[v_q(x, y), v_s(x', y')] = \sum_{\forall i} s_{qi} s_{si} \left\{ \frac{16}{(ab)^2} \sum_{\forall n} \sum_{\forall n'} \sum_{\forall m} \sum_{\forall m'} \frac{C_{v_q, v_s}^x(n, n') \sin(p_n x) \sin(p_{n'} x') C_{v_q, v_s}^y(m, m') \sin(q_m y) \sin(q_{m'} y')}{(p_n^2 + q_m^2)(p_{n'}^2 + q_{m'}^2)} \right\}$$

for which

$$C_{v_q, v_s}^x(n, n') = \int_0^a \int_0^a \sin(p_n \xi) \sin(p_{n'} \xi') \exp \left[-\frac{(\xi - \xi')^2}{\sigma_x^2} \right] d\xi' d\xi \quad (7)$$

$$C_{v_q, v_s}^y(m, m') = \int_0^b \int_0^b \sin(q_m \eta) \sin(q_{m'} \eta') \exp \left[-\frac{(\eta - \eta')^2}{\sigma_y^2} \right] d\eta' d\eta. \quad (8)$$

The expressions above follow an expression that has already been obtained for the solution of the Heat equation in one space variable. See [2] for details. In that case, the one space Heat equation involves the solution of the following double integral

$$C_{y_q, y_s}(n, m) = \int_0^l \int_0^l \sin(w_n \xi) \sin(w_m \xi') \exp \left[-\frac{(\xi - \xi')^2}{\sigma_x^2} \right] d\xi' d\xi,$$

where l is the spatial length, $w_n = \frac{n\pi}{l}$, $w_m = \frac{m\pi}{l}$, and σ_x is the length-scale for the SE kernel assumed for the latent function. It can be shown [2] that the solution for $C_{y_q, y_s}(n, m)$ follows as

$$C_{y_q, y_s}(n, m) = \begin{cases} \left(\frac{\sigma_x l}{\sqrt{\pi}(m^2 - n^2)} \right) \left\{ n e^{(\frac{\gamma_n \sigma_x}{2})^2} \mathcal{I}[\mathcal{H}(\gamma_n, l)] - m e^{(\frac{\gamma_m \sigma_x}{2})^2} \mathcal{I}[\mathcal{H}(\gamma_m, l)] \right\} & \text{if } n \text{ and } m \text{ are both even or both odd} \\ 0 & \text{otherwise} \end{cases} \quad (9)$$

for $n \neq m$, where $\gamma_n = j w_n$, $\gamma_m = j w_m$, and

$$\mathcal{H}(\zeta, v) = \text{erf} \left(\frac{v}{\sigma} + \frac{\sigma \zeta}{2} \right) - \text{erf} \left(\frac{\sigma \zeta}{2} \right).$$

If $n = m$, the following expression must be used instead

$$C_{y_q, y_s}(n) = \frac{\sigma_x \sqrt{\pi} l}{2} e^{(\frac{\gamma_n \sigma_x}{2})^2} \left\{ \mathcal{R}[\mathcal{H}(\gamma_n, l)] - \mathcal{I}[\mathcal{H}(\gamma_n, l)] \left[\frac{\sigma_x^2 n \pi}{2l^2} + \frac{1}{n\pi} \right] \right\} + \frac{\sigma_x^2}{2} \left[e^{-(\frac{l}{\sigma_x})^2} \cos(n\pi) - 1 \right]$$

In the expression for $C_{y_q, y_s}(n, n')$, the term $e^{\left(\frac{\gamma_n \sigma_x}{2}\right)^2} \mathcal{I}[\mathcal{H}(\gamma_n, l)]$ can be replaced for a more numerical stable expression given in terms of the complex error function $w(z)$,

$$e^{\left(\frac{\gamma_n \sigma_x}{2}\right)^2} \mathcal{I}[\mathcal{H}(\gamma_n, l)] = \mathcal{I} \left[w(jz_1^{\gamma_n}) - e^{-\left(\frac{l}{\sigma_x}\right)^2} e^{-\gamma_n l} w(jz_2^{\gamma_n}) \right],$$

with $z_1^{\gamma_n} = \frac{\sigma_x \gamma_n}{2}$ and $z_2^{\gamma_n} = \frac{l}{\sigma_x} + \frac{\sigma_x \gamma_n}{2}$. A similar expression for $e^{\left(\frac{\gamma_n \sigma_x}{2}\right)^2} \mathcal{R}[\mathcal{H}(\gamma_n, l)]$ can be obtained when $n = m$. Derivative for $C_{y_q, y_s}(n, m)$ in terms of σ_x can be found in [2].

3 Covariance matrix bewteen the outputs and the latent functions

The covariance matrix between the outputs $v_q(x, y)$ and the latent functions $f_i(x, y)$ is given by

$$\text{cov}[v_q(x, y), f_i(x', y')] = \mathbb{E} \left[\sum_{\forall k} s_{qk} \int_0^a \int_0^b f_k(\xi, \tau) G(x, y, \xi, \eta) d\xi d\eta f_i(x', y') \right] \quad (10)$$

Then, the covariance $\text{cov}[v_q(x, y), f_i(x', y')]$ is given as

$$\sum_{\forall k} s_{qk} \int_0^a \int_0^b G(x, y, \xi, \eta) \mathbb{E}[f_k(\xi, \eta) f_i(x', y')] d\xi d\eta$$

Using the factorized form for the covariance of the latent functions, the last expression can be written as

$$s_{qi} \int_0^a \int_0^b G(x, y, \xi, \eta) K_i(\xi, x') K_i(\eta, y') d\xi d\eta$$

With the expression (3) for $G(x, y, \xi, \eta)$ and SE kernels for the covariances of the latent processes, we have

$$s_{qi} \int_0^a \int_0^b \left\{ \left[\frac{4}{ab} \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{\sin(p_n x) \sin(q_m y) \sin(p_n \xi) \sin(q_m \eta)}{p_n^2 + q_m^2} \right] \exp \left[-\frac{(\xi - x')^2}{\sigma_x^2} \right] \exp \left[-\frac{(\eta - y')^2}{\sigma_y^2} \right] \right\} d\xi d\eta$$

Again the above expression can be separated in two different sets of integrals

$$\frac{4s_{qi}}{ab} \sum_{\forall n} \sum_{\forall m} \frac{\sin(p_n x) \sin(q_m y)}{p_n^2 + q_m^2} \left\{ \int_0^a \sin(p_n \xi) \exp \left[-\frac{(\xi - x')^2}{\sigma_x^2} \right] d\xi \right\} \left\{ \int_0^b \sin(q_m \eta) \exp \left[-\frac{(\eta - y')^2}{\sigma_y^2} \right] d\eta \right\}$$

We have

$$\text{cov}[v_q(x, y), f_i(x', y')] = \frac{4s_{qi}}{ab} \sum_{\forall n} \sum_{\forall m} \frac{\sin(p_n x) C_{v_q, f_i}^x(x', n) \sin(q_m y) C_{v_q, f_i}^y(y', m)}{p_n^2 + q_m^2}$$

in which

$$C_{v_q, f_i}^x(x', n) = \int_0^a \sin(p_n \xi) \exp \left[-\frac{(\xi - x')^2}{\sigma_x^2} \right] d\xi$$

$$C_{v_q, f_i}^y(y', m) = \int_0^b \sin(q_m \eta) \exp \left[-\frac{(\eta - y')^2}{\sigma_y^2} \right] d\eta.$$

A similar expression to the ones above was obtained when solving the covariance between the output of the Heat equation and the input function. See [2]. That expression is given as

$$C_{y_q, f_i}(x', n) = \int_0^l \sin(w_n \xi) \exp \left[-\frac{(\xi - x')^2}{\sigma_x^2} \right] d\xi.$$

Its solution follows as

$$C_{y_q, f_i}(x', n) = \frac{\sigma_x \sqrt{\pi}}{2} \exp \left(\frac{\gamma_n \sigma_x}{2} \right)^2 \mathcal{I}[\exp(\gamma_n x') \mathcal{H}(\gamma_n, x', l)],$$

where

$$\mathcal{H}(\zeta, v, \varphi) = \text{erf} \left(\frac{v}{\sigma} + \frac{\sigma \zeta}{2} \right) - \text{erf} \left(\frac{v - \varphi}{\sigma} + \frac{\sigma \zeta}{2} \right).$$

In the expression for $C_{y_q, f_i}(x', n)$, the term $\exp \left(\frac{\gamma_n \sigma_x}{2} \right)^2 \mathcal{I}[\exp(\gamma_n x') \mathcal{H}(\gamma_n, x', l)]$ can be replaced for a more numerical stable expression given in terms of the complex error function $w(z)$,

$$e^{\left(\frac{\gamma_n \sigma_x}{2}\right)^2} \mathcal{I} \left[e^{\gamma_n x'} \mathcal{H}(\gamma_n, x', l) \right] = \mathcal{I} \left[e^{-\left(\frac{x' - l}{\sigma_x}\right)^2} e^{\gamma_n l} w(jz_2^{\gamma_n, x'}) - e^{-\left(\frac{x'}{\sigma_x}\right)^2} w(jz_1^{\gamma_n, x'}) \right],$$

with $z_1^{\gamma_n, x'} = \frac{x'}{\sigma_x} + \frac{\sigma_x \gamma_n}{2}$ and $z_2^{\gamma_n, x'} = \frac{x' - l}{\sigma_x} + \frac{\sigma_x \gamma_n}{2}$.

The derivative for $C_{y_q, f_i}(x', n)$ in terms of σ_x can also be found in [2].

References

- [1] Andrei D. Polyanin. *Handbook of Linear Partial Differential Equations for Engineers and Scientists*. Chapman & Hall/CRC, 2002.
- [2] Mauricio A. Álvarez. About the partial differential equation for the drosophila segmentation problem. Technical report, Faculty of Engineering, Universidad Tecnológica de Pereira, 2013.
- [3] M. Abramowitz and I. A. Stegun, editors. *Handbook of Mathematical Functions: With Formulas, Graphs and Mathematical Tables*. Dover Publications Inc., New York, NY, (USA), new edition edition, 1965.
- [4] N. D. Lawrence, G. Sanguinetti, and M. Rattray. Modelling transcriptional regulation using Gaussian processes. In J. C. Platt B. Schölkopf and T. Hofmann, editors, *Advances in Neural Information Processing Systems 19*. MIT Press, Cambridge, MA, 2007.