Stochastic Partial Differential Equations and Geostatistics

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Section 1

Introduction

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SPDE and Geostatistics

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What are the connection between these approches?

Consider a SPDE of the form

$$\mathcal{L}U = X$$

with $\mathcal{L}$ some differential operator X a Gaussian random *function*. We look at for a Gaussian random *function* U solution to this equation. Imagine there exists an unique random function solution to this equation.

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→ We could describe **completely** this solution through its covariance and mean!

→ There **must** be some connections!

SPDE and Geostatistics: Example

Following *Lindgren and Rue* (2011), consider the SPDE over the space $\mathbb{R}^d$:

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with $\kappa > 0$, $\alpha > d/2$ and W the White Noise.

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Its solution has a Matérn stationary covariance function:

$$\rho(x-y) = \frac{1}{(2\pi)^{d/2} 2^{\alpha-1} \kappa^{2\alpha-d} \Gamma(\alpha)} (\kappa|x-y|)^{\alpha-d/2} K_{\alpha-d/2}(\kappa|x-y|)$$

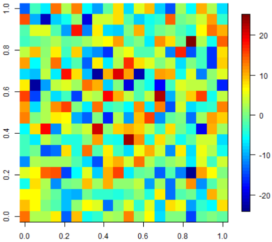
with $K_{\alpha-d/2}$ the modified Bessel function of second kind of order $\alpha - d/2 > 0$.

SPDE and Geostatistics: Example

Consider the spatio-temporal covariance model

$$C_Z((x,t),(y,s)) = \frac{\sigma^2}{(4\alpha\pi(t+s))^{d/2}} e^{-\frac{|x-y|^2}{4\alpha(t+s)}}$$

with $\alpha > 0$.



Simulation by Cholesky decomposition with $\alpha = 0.01$ and $\sigma^2 = 20$.

SPDE and Geostatistics: Example

This covariance describes the **Diffusion of a White Noise**

$$\begin{cases} \dfrac{\partial Z}{\partial t} - \alpha \Delta Z = 0 \\ \\ Z_{t=0} = \sigma W \end{cases} \tag{1}$$

with $\alpha, \sigma > 0$.

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We have both theoretical and practical motivations:

- Connection between geostatistical models and physical phenomena.
- Source of new geostatistical models, based on solutions of SPDE, eventually with special properties. Specially adapted for the spatio-temporal case.
- Utilisation of PDE solvers to obtain fast and precise simulations of complicated geostatistical models.

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- Some mathematical basis for our results.
- Results on existence and uniqueness of stationary models solutions of some SPDE's, and application to some notable cases.
- Analysis of some evolution models, which involve physical phenomena like diffusion, convection, reaction, etc.

Section 2

Mathematical Basis

Classical Geostatistic model

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- **Mean function:** $m_Z(x) = \mathbb{E}(Z(x))$ is any real function.
- **Covariance function:** $C_Z(x, y) = \mathbb{C}ov(Z(x), Z(y))$ is a positive-definite real function.

Stationary Gaussian random function: $(Z(x))_{x \in \mathbb{R}^d}$ Gaussian random field such that,

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Bochner's Theorem

ρ_Z is a stationary positive-definite continuous function if and only if it is the Fourier transform of an even, positive and *finite* measure μ_Z:

$$\rho_Z(h) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-ih^T\xi} d\mu_Z(\xi) \qquad \forall h \in \mathbb{R}^d$$

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The measure μ_Z is called the **Spectral Measure** of Z, and can be used to describe the covariance structure.

Linear SPDE's

Let $\mathcal{L}$ be a real linear operator defined for functions (or something more *general*...). Let X be a Gaussian random *function*. We look at for a Gaussian random *function* U such that

$$\mathcal{L}U = X \tag{2}$$

We call this type of equation a linear SPDE (abuse of language). We interpret this equation in two senses:

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  In this Gaussian framework, this is equivalent to ask:

$$m_X = m_{\mathcal{L}U} \;\; (= \mathcal{L}m_U) \qquad C_X = C_{\mathcal{L}U} \;\; (= (\mathcal{L} \otimes \mathcal{L})C_U)$$

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All of this equation have a rigorous meaning in a distributional sense.

Consequence of the distributional approach

We have a meaning for not necessarily finite spectral measures in the stationary case.

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Bochner-Schwartz Theorem:

If ρ is a real stationary positive-definite distribution, then it is tempered and it is the Fourier transform of an even, positive and tempered measure,

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- We call **Spectral Measure** to any positive, even and tempered measure μ.

Example: the White Noise

We can define the Gaussian **White Noise** as a zero mean Gaussian process indexed on the measurable sets $\mathcal{B}(\mathbb{R}^d)$, $(W(A))_{A\in\mathcal{B}(\mathbb{R}^d)}$ such that

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The White Noise is *stationary in distributional sense*, and has a not finite spectral measure

$$\mu_W = (2\pi)^{-d/2}\mathbf{1}$$

Section 3

Stationary Solutions for some SPDE's

Let us consider the next kind of linear real operators $\mathcal{L}_h$ defined as:

$$\mathcal{L}_h(\cdot) = \mathscr{F}^{-1}(h\mathscr{F}(\cdot))$$

where h is a smooth function with slow growing behaviour and such that $h = \check{\bar{h}}$, and $\mathscr{F}$ is the Fourier Transform. This function h is called the **symbol** of $\mathcal{L}_h$.
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- $h(\xi) = (\kappa^2 + \xi^T \xi)^{\alpha/2} \quad \Rightarrow \quad \mathcal{L}_h = (\kappa^2 - \Delta)^{\alpha/2}$
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- $h(\omega, \xi) = i(\omega + v^T\xi) + \alpha\xi^T\xi + \kappa^2 \quad \Rightarrow \quad \mathcal{L}_h = \frac{\partial}{\partial t} - \alpha\Delta + v^T\nabla + \kappa^2 I$
  with $v \in \mathbb{R}^d, \kappa^2 > 0, \alpha > 0$ (spatio-temporal framework).

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  with $v \in \mathbb{R}^d, \kappa^2 > 0, \alpha > 0$ (spatio-temporal framework).
- $h(\omega, \xi) = -\omega^2 + c^2\xi^T\xi \quad \Rightarrow \quad \frac{\partial^2}{\partial t^2} - c^2\Delta$
  with $c > 0$ (spatio-temporal framework).

Stationary Solutions for some SPDE's

The operators of this type **maintain stationarity**:

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$\rightarrow$ If U is a centred stationary random field with spectral measure μ_U, then $\mathcal{L}_h U$ is also stationary and its spectral measure is

$$\mu_{\mathcal{L}_h U} = |h|^2 \mu_U$$

Stationary Solutions for some SPDE's

Objective

To find stationary solutions to the equation

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$\rightarrow$ **a division problem**.

Result: Existence and Uniqueness

Proposition

There exists a stationary solution to $\mathcal{L}_h U \overset{law}{=} X$ *if and only if*

$$\int_{\mathbb{R}^d} \frac{d\mu_X(\xi)}{|h(\xi)|^2(1+\xi^T\xi)^N} < \infty$$

for some $N \in \mathbb{N}$*. In this case, we have that*

$$\mu_U := \frac{\mu_X}{|h|^2}$$

is a well-defined spectral measure solution to $|h|^2\mu_U = \mu_X$*. In addition, the solution is unique if and only if* $|h| > 0$*.*

Examples of uniqueness

Matérn Model: consider de equation over $\mathbb{R}^d$:

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with W the White Noise, $\kappa^2 > 0$, $\alpha \in \mathbb{R}$, and Δ the Laplace operator.

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$\rightarrow$ **there exists an unique stationary solution, and its spectral measure is**

$$d\mu_U(\xi) = \frac{d\mu_X(\xi)}{|h(\xi)|^2} = \frac{1}{(2\pi)^{d/2}} \frac{d\xi}{(\kappa^2 + \xi^T \xi)^{\alpha}}$$

If $\alpha > d/2$, this measure is finite $\rightarrow$ **Matérn!**

Examples of uniqueness

Stein Model: (*Stein* (2005)) it is known as a stationary spatio-temporal model with spectral measure

$$d\mu_U(\omega,\xi) = \frac{1}{(2\pi)^{(d+1)/2}} \frac{d\omega d\xi}{\left(a(s^2+\omega^2)^{\beta} + b(k^2+\xi^T\xi)^{\alpha}\right)^{\nu}}$$

with $\kappa^2, s, a, b > 0$, $\alpha, \beta, \nu \in \mathbb{R}$.

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$$h(\omega,\xi) = \left(a(s^2+\omega^2)^\beta + b(k^2+\xi^T\xi)^\alpha\right)^{\nu/2}$$

And we propose an SPDE for this model:

$$\left(a(s^2 - \frac{\partial^2}{\partial t^2})^\beta + b(\kappa^2 - \Delta)^\alpha\right)^{\nu/2} S = W$$

where W is a (spatio-temporal) White Noise.

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h and μ_W satisfy the conditions $\rightarrow$ **The Stein model is the unique stationary solution.**

Some Spatio-temporal Markov Models: If we take the spatio-temporal SPDE:

$$\kappa^2 U + \sum_{k=1}^{M} a_k \frac{\partial^k U}{\partial t^k} + \sum_{j=1}^{N} (-1)^j b_j \Delta^{(j)} U = W$$

with W a (spatio-temporal) White Noise, $\kappa^2 > 0$ and some suitable conditions for the coefficients $(a_k)_k$ and $(b_j)_j$.

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The symbol is positive and equals to

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The function h and μ_W satisfy the conditions $\rightarrow$ There exists an unique stationary solution with spectral measure,

$$d\mu_U(\omega, \xi) = \frac{1}{(2\pi)^{(d+1)/2}} \frac{d\omega d\xi}{(\kappa^2 + \sum_{\substack{k \leq M \\ k \text{ even}}} a_k (-1)^{k/2} \omega^k + \sum_j b_j |\xi|^{2j})^2 + (\sum_{\substack{k \leq M \\ k \text{ odd}}} a_k (-1)^{(k-1)/2} \omega^k)^2}$$

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$$h(\omega, \xi) = \kappa^2 + \sum_{k=1}^{M} a_k i^k \omega^k + \sum_{j=1}^{N} b_j |\xi|^{2j}$$

The function h and μ_W satisfy the conditions $\rightarrow$ There exists an unique stationary solution with spectral measure,

$$d\mu_U(\omega,\xi) = \frac{1}{(2\pi)^{(d+1)/2}} \frac{d\omega d\xi}{(\kappa^2 + \sum_{\substack{k\leq M \\ k \text{ even}}} a_k (-1)^{k/2} \omega^k + \sum_j b_j |\xi|^{2j})^2 + (\sum_{\substack{k\leq M \\ k \text{ odd}}} a_k (-1)^{(k-1)/2} \omega^k)^2}$$

By Rozanov's Theorem, this is the spectral measure of a **spatio-temporal Markov Model** (*Rozanov* (1982)).

Notable example: Heat Equation

Let us consider the next version of a **Stochastic Heat Equation**:

$$\frac{\partial U}{\partial t} - \alpha \Delta U = X$$

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If there is a stationary solution, it is not unique $\rightarrow$ random constants can be added.

Example: Heat Equation

Case with a White Noise source term:

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There are stationary solutions to this equation **only for dimension** $d \geq 3$.

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Result

There are stationary solutions to this equation **only for dimension** $d \geq 3$.

In dimension $d = 3$, the fundamental stationary covariance solution is:

$$\rho_U(u, h) = \frac{\pi}{2\alpha|h|} - \frac{\pi}{4\alpha\sqrt{|u|}} \operatorname{erfc}\left(\sqrt{\frac{2|u|}{\alpha|h|^2}}\right)$$

Section 4

First order evolution models

First Order Evolution Model

Let us consider the next evolution equation in $\mathbb{R}^+ \times \mathbb{R}^d$:

$$\begin{cases} \dfrac{\partial U}{\partial t} + \mathcal{L}_g U = X \\ U_{t=0} = U_0 \end{cases}$$

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The spatio-temporal symbol of the operator is

$$h(\omega, \xi) = i\omega + g(\xi)$$

First Order Evolution Model: Duhamel's Formula

$$\begin{cases} \dfrac{\partial U}{\partial t} + \mathcal{L}_g U = X \\ U_{t=0} = U_0 \end{cases}$$

Duhamel's formula allows us to solve **strictly** this equation:

$$U(t,x) = \mathscr{F}_S^{-1}\left(e^{-g(\xi)t}\mathscr{F}_S(U_0)(\xi) + \int_0^t e^{-g(\xi)(t-u)}\mathscr{F}_S(X)(u,\xi)du\right)(x)$$

$$\mathscr{F}_S(U)(t,\xi) = e^{-g(\xi)t}\mathscr{F}_S(U_0)(\xi) + \int_0^t e^{-g(\xi)(t-u)}\mathscr{F}_S(X)(u,\xi)du$$

When $X = W$ and U_0 has a spectral measure μ_{U_0}, the covariance of the solution U is spatially stationary, and we can note:

$$C_U((x,t),(y,s)) =$$

$$\mathscr{F}_S^{-1}\left(e^{-ig_I(\xi)(t-s)-g_R(\xi)(t+s)}\mu_{U_0} + \frac{e^{-ig_I(\xi)(t-s)}\left(e^{-g_R(\xi)|t-s|} - e^{-g_R(\xi)(t+s)}\right)}{(2\pi)^{d/2}2g_R(\xi)}\right)(x-y)$$

where g_R and g_I are the real and imaginary parts of g respectively.

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Two possible analysis:

- Choice of μ_{U_0} such that the covariance is stationary.
- Convergence to a stationary model as $t \to \infty$.

First Order Evolution Model: choice of initial condition

If we take μ_{U_0} to be:

$$d\mu_{U_0}(\xi) = \frac{d\xi}{(2\pi)^{d/2} 2 g_R(\xi)} \tag{3}$$

The formula turns to

$$C_U((x,t),(y,s)) = \mathscr{F}_S^{-1}\left(\frac{e^{-ig_I(\xi)(t-s) - g_R(\xi)|t-s|}}{(2\pi)^{d/2} 2 g_R(\xi)}\right)(x-y)$$

and the solution is stationary in space-time.

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$\rightarrow$ use criteria of existence of a stationary solution! With $\mu_X = \mu_W$ and symbol

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In particular if $g_R > 0$ and it inverse doesn't grow very fast, the division is possible.

First Order Evolution Model: convergence

Let us analyse the asymptotic behaviour:

$$C_U((x,t),(y,s)) =$$

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If $g_R > 0$, we can take $t, s \to \infty$ and we re-obtain the expression

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$\rightarrow$ **convergence to a spatially stationary fixed point**, given by the optimal choice of μ_{U_0}.

First Order Evolution Model: Example

Consider the equation

$$\begin{cases} \dfrac{\partial U}{\partial t} + (\kappa^2 - \Delta)^\alpha U = W \\ U_{t=0} = U_0 \end{cases}$$

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We have $g(\xi) = (\kappa^2 + \xi^T \xi)^\alpha$ which is positive and satisfies the division condition.
$\rightarrow$ convergence to the stationary solution:

$$\rho_U(u,h) = \mathscr{F}_S^{-1} \left(\frac{e^{-(\kappa^2+\xi^T\xi)^\alpha |u|}}{(2\pi)^{d/2} 2(\kappa^2 + \xi^T \xi)^\alpha} \right) (|h|)$$

$$\rho_U(u,h) = \frac{1}{|h|^{d/2-1}} \int_0^\infty J_{d/2-1}(|h|r) \frac{e^{-(\kappa^2+r^2)^\alpha |u|} r^{d/2}}{2(\kappa^2 + r^2)^\alpha (2\pi)^{d/2}} dr$$

where $J_{d/2-1}$ is the Bessel function of the first kind. ρ_U is a well defined **function** for $\alpha > d/2$.

First Order Evolution Model: Example

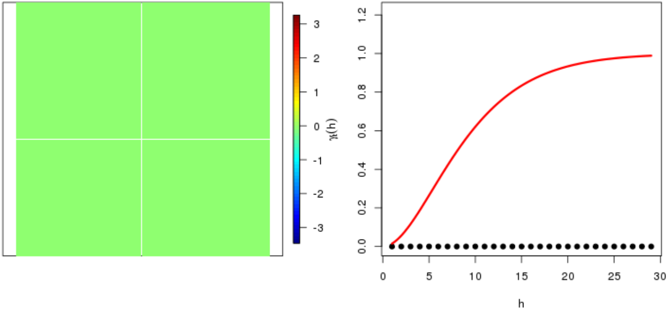
The spatial trace of this solution is a Matérn Model:

$$\rho_U(0,h) = \mathscr{F}_S^{-1}\left(\frac{1}{(2\pi)^{d/2}2(\kappa^2+\xi^T\xi)^\alpha}\right)(|h|)$$

So the spatial trace of the stationary solution, U_S, satisfies the equation

$$\sqrt{2}(\kappa^2-\Delta)^{\alpha/2}U_S = W_S$$

where W_S is a spatial White Noise. $\rightarrow$ Take a Matérn Model as a initial condition.



$\kappa = 1/6$, $\alpha = 4$. Finite Elements method in space, Finites Differences method in time.

Section 5

MUCHAS GRACIAS

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