Spatiotemporal Models Inspired from Statistical Physics

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Overview of the Presentation

- Introduction
- Boltzmann-Gibbs representations of random fields
- Spartan composite-metric covariance functions
- Space-time covariances from linear response theory
- Space-time stochastic local interaction model (SLI)
- Examples of SLI data application (synthetic, reanalysis)
- Conclusions

Introduction

- Statistical physics uses equations of motion (leading to partial differential equations) and Boltzmann-Gibbs (exponential) probability density functions
- There is a long history of interplay between statistical physics and statistical data analysis (Ising model, Metropolis updating, Markov Chain Monte Carlo, variational Gaussian approximations in machine learning, etc.)
- For the purpose of this talk, the main themes are how to use:
  (i) Boltzmann-Gibbs formulations with *local* energies to derive computationally efficient models
  (ii) the framework of *equations of motion* to obtain new forms of spatiotemporal dependence

Local Random Fields: SPDEs & Boltzmann-Gibbs PDFs

Langevin Equation

$LX = \epsilon, \quad \epsilon$: GWN

L: Linear partial differential operator

$$\phi(t) = E[e^{it\cdot(L^{-1}\epsilon)}]$$

$$C(\mathbf{k}) = \frac{1}{L^{\dagger}(\mathbf{k})L(\mathbf{k})}$$

Boltzmann–Gibbs PDF

$f \sim \exp(-H(X))$

$H(X)$: Quadratic function of the field

Rational Spectral Densities

$$C(\mathbf{k}) = \frac{A}{\sum_{i=0}^{n} c_i \, \|\mathbf{k}\|^{2i}}, \quad A > 0, \ \{c_i\}_{i=0}^{n} > 0$$

Local Random Fields

Whittle-Matérn case: L is a pseudo-differential operator. The spectral density is a rational function only if $\nu + \frac{d}{2} = n \in N$

Spartan Spatial Random Fields (SSRFs) are Boltzmann-Gibbs RFs with “local” structure

- Boltzmann-Gibbs probability density function (PDF)

$$f[x(\mathbf{s})] = Z^{-1}\, \mathrm{e}^{-\mathcal{H}[x(\mathbf{s})]}, \quad \mathcal{H}[x(\mathbf{s})]: \text{ energy functional,}$$

- Z: partition function $Z = \int \mathcal{D}x(\mathbf{s})\, \mathrm{e}^{-\mathcal{H}[x(\mathbf{s})]}$
- $\mathcal{H}_{\mathrm{fgc}}[x(\mathbf{s})] = \int \frac{d\mathbf{s}}{2\eta_0 \xi^d} \left\{ [x(\mathbf{s})]^2 + \eta_1\, \xi^2\, [\nabla x(\mathbf{s})]^2 + \xi^4\, \left[\nabla^2 x(\mathbf{s})\right]^2 \right\}$

How to extend the above continuum representation to discrete data?

- Regular grids: Use finite differences ⇒ GMRFs
- Scattered data: Use kernel functions ⇒ SLI model

D. T. Hristopulos, 2003. *SIAM J. Sci. Comput.*, 24(6), 2125–2162

Spartan Spatial Random Fields (SSRFs) are Boltzmann-Gibbs RFs with "local" structure

Langevin Equation

$$\mathcal{L}\, X(\mathbf{s}) = \varepsilon(\mathbf{s}), \text{ where } \varepsilon(\cdot) \text{ is GWN (Gaussian white noise)}$$

$$\mathcal{L} = \frac{1}{\sqrt{\eta_0 \xi^d}} \left[1 - \left(\sqrt{2+\eta_1}\right) \xi \, (-\triangle)^{1/2} + \xi^2 \triangle \right], \quad \triangle : \text{ Laplacian}$$

Spectral density

$$\tilde{C}(\mathbf{k}) = \frac{1}{\left|\tilde{\mathcal{L}}(\mathbf{k})\right|^2} = \frac{\eta_0 \xi^d}{1 + \eta_1 (\|\mathbf{k}\|\xi)^2 + (\|\mathbf{k}\|\xi)^4}.$$

Covariance function PDE

$$\left[1 - \eta_1 \, \xi^2 \, \triangle_{\mathbf{s}} + \xi^4 \, \triangle^2_{\mathbf{s}}\right] C(\mathbf{s} - \mathbf{s}') = -\eta_0 \xi^d \, \delta(\mathbf{s} - \mathbf{s}')$$

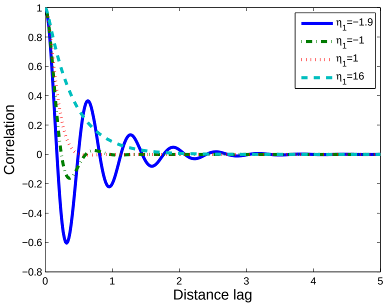
SSRF covariance for time series

$$C(h) = \frac{\eta_0}{4}\, e^{-h\beta_2} \left[\frac{\cos(h\beta_1)}{\beta_2} + \frac{\sin(h\beta_1)}{\beta_1} \right], \quad |\eta_1| < 2$$

$$C(h) = \eta_0 \, \frac{(1+h)}{4\, e^{h}}, \quad \eta_1 = 2$$

$$C(h) = \frac{\eta_0}{2\,\Delta} \left(\frac{e^{-h\,\omega_1}}{\omega_1} - \frac{e^{-h\,\omega_2}}{\omega_2} \right), \quad \eta_1 > 2$$

d=1



Hristopulos & Elogne (2007), *IEEE Trans. Inform. Theory*, 53(12), 4667–4679

Notation

- $h = |r|/\xi$: normalized lag
- $\beta_{1,2} = \left(\frac{|2 \mp \eta_1|}{4} \right)^{1/2}$
- $\omega_{1,2} = \left(\frac{|\eta_1 \mp \Delta|}{2} \right)^{1/2}$
- $\Delta = |\eta_1{}^2 - 4|^{\frac{1}{2}}$

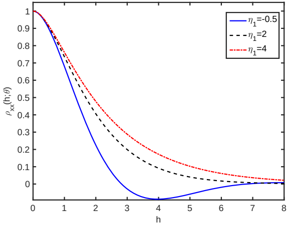
Damped harmonic oscillator in a heat bath is a one-dimensional SSRF

Langevin equation: $\ddot{x}(t) + \Gamma\, \dot{x}(t) + \omega_0^2\, x(t) = \epsilon(t)$

$$C(h) = \frac{\eta_0}{4}\, \mathrm{e}^{-h\beta_2} \left[\frac{\cos(h\beta_1)}{\beta_2} + \frac{\sin(h\beta_1)}{\beta_1} \right], \quad |\eta_1| < 2,$$ Underdamping

$$C(h) = \eta_0\, \frac{(1+h)}{4\, \mathrm{e}^{h}}, \quad \eta_1 = 2,$$ Critical damping

$$C(h) = \frac{\eta_0}{2\,\Delta} \left(\frac{\mathrm{e}^{-h\,\omega_1}}{\omega_1} - \frac{\mathrm{e}^{-h\,\omega_2}}{\omega_2} \right), \quad \eta_1 > 2$$ Overdamping



$$\Gamma^2 = \frac{\eta_1 + 2}{\xi^2}, \; 2k_B T = \frac{\eta_0\, m}{\xi^2 \sqrt{e+2}}$$

$\Leftarrow$ Oscillator displacement correlation function

Nørrelykke, S.F., Flyvbjerg, H. *Phys. Rev. E* **83**, 041103 (2011)

SSRF covariance functions for planar processes

$$C(h) = \frac{\eta_0 \, \Im \left[K_0(h z_+) \right]}{\pi \sqrt{4 - {\eta_1}^2}}, \quad |\eta_1| < 2$$

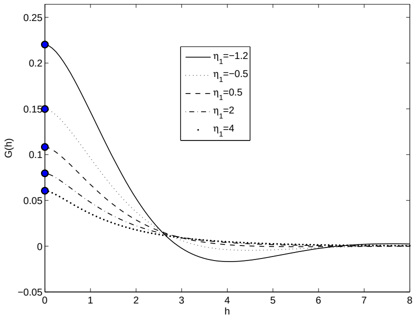
$$C(h) = \left(\frac{\eta_0 \, h}{4\pi} \right) K_{-1}(h), \quad \eta_1 = 2$$

$$C(h) = \frac{\eta_0 \left[K_0(h z_+) - K_0(h z_-) \right]}{2\pi \sqrt{{\eta_1}^2 - 4}}, \quad \eta_1 > 2$$

Notation

- $\Im$: Imaginary part
- $z_{\pm} = \sqrt{-t^*_{\pm}}$
- $t^*_{\pm} = \left(-\eta_1 \pm \sqrt{{\eta_1}^2 - 4} \right) / 2$
- $K_\nu(z)$: modified Bessel function of the second kind and order ν

d=2



Hristopulos (2015), *Stoch. Environ. Res. Risk Assesss.*, 29(3), 739–754.

SSRF Covariance functions in $\mathbb{R}^3$ or in $\mathbb{R}^2 \times T$

$$C(h) = \eta_0 \frac{e^{-h\beta_2}}{2\pi\Delta}\left[\frac{\sin(h\beta_1)}{h}\right], \quad |\eta_1| < 2$$

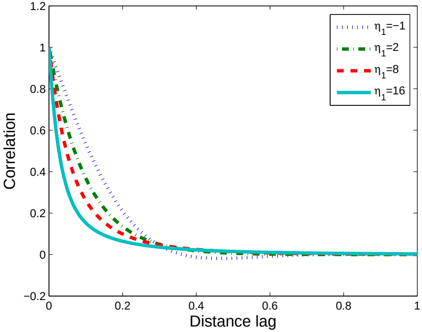
$$C(h) = \frac{\eta_0}{8\pi} e^{-h}, \quad \eta_1 = 2$$

$$C(h) = \frac{1}{4\pi\Delta}\left[\frac{e^{-h\omega_1} - e^{-h\omega_2}}{h(\omega_2 - \omega_1)}\right], \quad \eta_1 > 2$$

Notation

- $h = \|\mathbf{r}\|/\xi$,
- $\beta_{1,2} = \left(\frac{|2 \mp \eta_1|}{4}\right)^{1/2}$
- $\omega_{1,2} = \left(\frac{|\eta_1 \mp \Delta|}{2}\right)^{1/2}$
- $\Delta = |\eta_1{}^2 - 4|^{\frac{1}{2}}$

d=3



Hristopulos and Elogne, 2007, *IEEE Trans. Inform. Theory*, 53(12), 4667–4679

SSRF composite space-time covariance in $\mathbb{R}^2 \times T$

$$C(h) = \eta_0 \, \frac{e^{-h\beta_2}}{2\,\pi\,\Delta} \left[\frac{\sin(h\beta_1)}{h} \right], \quad |\eta_1| < 2$$

$$C(h) = \frac{\eta_0}{8\,\pi} \, e^{-h}, \quad \eta_1 = 2$$

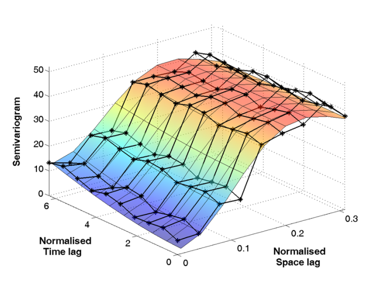
$$C(h) = \frac{1}{4\,\pi\,\Delta} \left[\frac{e^{-h\omega_1} - e^{-h\omega_2}}{h\,(\omega_2 - \omega_1)} \right], \quad \eta_1 > 2$$

Notation

- $h = \|\mathbf{r}\|/\xi$,
- $\beta_{1,2} = \left(\frac{|2 \mp \eta_1|}{4} \right)^{1/2}$
- $\omega_{1,2} = \left(\frac{|\eta_1 \mp \Delta|}{2} \right)^{1/2}$
- $\Delta = |\eta_1{}^2 - 4|^{\frac{1}{2}}$

Composite space-time metric

$$h = \sqrt{\|\mathbf{r}\|^2/\xi^2 + \alpha\tau^2/\tau_c^2}$$



Varouchakis & Hristopulos, 2017. *Spatial Statistics*, https://doi.org/10.1016/j.spasta.2017.07.003.

Space-Time models using Linear Response Theory

- Linear response theory describes the non-equilibrium response due to small deviation from equilibrium, leading to S-T Langevin equations

$$\frac{\partial x(\mathbf{s},t)}{\partial t} = -D\,\frac{\delta \mathcal{H}[x(\mathbf{s})]}{\delta x(\mathbf{s})}\bigg|_{x(\mathbf{s})=x(\mathbf{s},t)} + \zeta(\mathbf{s},t) = V[x(\mathbf{s},t)] + \zeta(\mathbf{s},t)$$

- Equilibrium-restoring rate for the *ST-SRRF* random field

$$V[x(\mathbf{s},t)] = -\frac{1}{2\xi^d\,\eta_0}\left(1-\eta_1\xi^2\nabla^2+\mu\,\xi^4\nabla^4\right)x(\mathbf{s})\bigg|_{x(\mathbf{s})=x(\mathbf{s},t)}$$

- D is a diffusion coefficient
- $\zeta(\mathbf{s},t)$ is the random perturbation (e.g., Gaussian white noise)

Hohenberg and Halperin (1977), *Reviews of Modern Physics*, **49**(3), 435–479

Equations of motion for ST-SSRF covariance can be derived using Linear Response Theory

EOM: $$\frac{\partial C(\mathbf{r},\tau)}{\partial \tau} = -\frac{\mathrm{sign}(\tau)}{\tau_c}\left(1-\eta_1 \xi^2 \nabla^2 + \mu\, \xi^4 \nabla^4\right) C(\mathbf{r},\tau),$$

where $\tau_c^{-1} = D/(2\xi^d\, \eta_0)$, and the *initial condition* is the SSRF spectral density

$$\tilde{C}(k,\tau=0) = \frac{\eta_0\, \xi^d}{1+\eta_1 (k\xi)^2 + \mu (k\xi)^4}.$$

Zero-μ solution in $d=1$ dimension

$$C_1(h,u) = \frac{\eta_0\, \lambda}{4}\left[\mathrm{e}^{-\lambda\, h}\, \mathrm{erfc}\left(\sqrt{u} - \frac{\lambda\, h}{2\sqrt{u}}\right) + \mathrm{e}^{\lambda\, h}\, \mathrm{erfc}\left(\sqrt{u} + \frac{\lambda\, h}{2\sqrt{u}}\right)\right],$$

$\lambda = 1/\sqrt{\eta_1}$, $h = r/\xi$, $u = |\tau|/\tau_c$, and $\mathrm{erfc}(\cdot)$ is the complementary error function.

$C_1(h,u)$ is equivalent (except for different parametrization) to the covariance derived from a parabolic SPDE in 1+1 dimensions (Heine (1955); Biometrika, 42(1-2), 170–178.)

Taming the variance divergence with space transforms

- In 3D the variance of the zero-μ solution diverges
- Space transforms are mathematical operations that can generate covariance functions based on lower-dimensional projections
  [Mantoglou and Wilson (1982). *Water Resources Research*, **18**(5), 1379–1394]

$$C_3(r,\tau) = \frac{1}{r}\int_0^r \mathrm{d}x\, C_1(x,\tau) = \frac{1}{h}\int_0^h \mathrm{d}y\, C_1(y,u)$$

- Applying the above to $C_1(h,u)$ we obtain

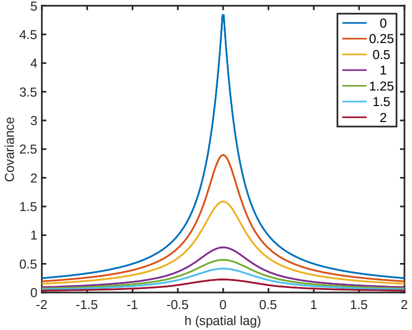
Space-transformed ST-SSRF covariance

$$C_3(h,u) = \frac{\eta_0}{4h}\left[2\,\mathrm{e}^{-u}\,\mathrm{erf}\left(\frac{\lambda h}{2\sqrt{u}}\right) + \mathrm{e}^{\lambda\,h}\,\mathrm{erfc}\left(\sqrt{u}+\frac{\lambda h}{2\sqrt{u}}\right) - \mathrm{e}^{-\lambda\,h}\,\mathrm{erfc}\left(\sqrt{u}-\frac{\lambda h}{2\sqrt{u}}\right)\right]$$

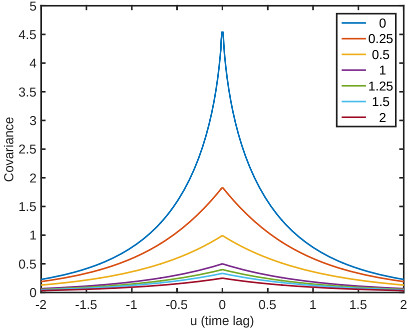
[Hristopulos & Tsantili, 2017. *Spatial Statistics*, 22(2):321–337]

Visualization of the ST-SSRF covariance

The ST-SSRF covariance is fully symmetric, continuous, non-differentiable at $u = 0$, and *is not* in the Gneiting class (smoothness at origin does not determine smoothness along both the space and time axes)



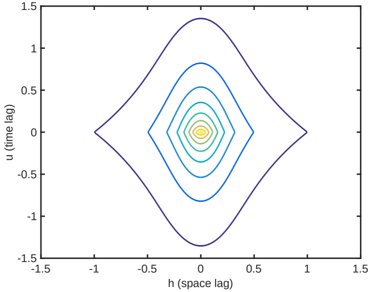
Dependence of covariance function on space lag for different temporal lags.

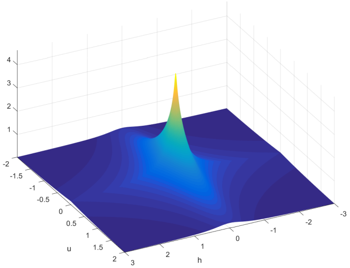


Dependence of covariance function on time lag for different spatial lags.

Visualization of the ST-SSRF covariance

The ST-SSRF covariance is fully symmetric, continuous, non-differentiable at $u = 0$, and *is not* in the Gneiting class (smoothness at origin does not determine smoothness along both the space and time axes)





Stochastic Local Interaction (SLI) model for space-time data

- The vector $\mathbf{x}_{\mathrm{S}} \equiv (x_1, x_2, \ldots, x_N)^\top$ comprises the field values at the space-time point set $\{(\mathbf{s}_1, t_1), (\mathbf{s}_2, t_2), \ldots (\mathbf{s}_N, t_N)\}$
- Space-time energy function

$$\mathcal{H}(\mathbf{x}_{\mathrm{S}}; \boldsymbol{\theta}) = \frac{1}{2\,\lambda} \left[\frac{(\mathbf{x}_{\mathrm{S}} - m_{\mathrm{x}} \mathbf{I})^2}{N} + c_1\, \mathcal{S}_1(\mathbf{x}_{\mathrm{S}}; \mathbf{h}_s, \mathbf{h}_t) \right],$$

- Kernel function based approximation of the square gradient

$$\mathcal{S}_1(\mathbf{x}_{\mathrm{S}}; \mathbf{h}_s, \mathbf{h}_t) = \left\langle\, (x_n - x_k)^2 \,\right\rangle,$$

$$\langle (x_n - x_k)^2 \rangle = \frac{\sum_{n=1}^{N} \sum_{k=1}^{N} w_{n,k}(\mathbf{r}_{n,k}, \tau_{n,k}; h_{s,n}, h_{t,n})\,(x_n - x_k)^2}{\sum_{n=1}^{N} \sum_{k=1}^{N} w_{n,k}(\mathbf{r}_{n,k}, \tau_{n,k}; h_{s,n}, h_{t,n})}.$$

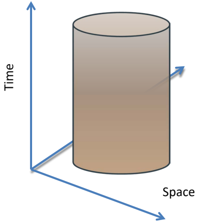
- Parameters: λ, c_1, m_{x}, μ_s , μ_t
- Kernel based weights: $w_{n,k}(\mathbf{r}_{n,k}, \tau_{n,k}; h_{s,n}, h_{t,n})$

Different approaches for kernel weight selection

Separable space-time structure

$$w_{n,k} = K\left(\frac{\|\mathbf{r}_{n,k}\|}{h_{s,n}}\right) K\left(\frac{|\tau_{n,k}|}{h_{t,n}}\right)$$

This does not imply *separable covariance*

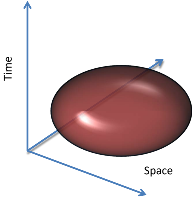


Composite space-time metric

$$w_{n,k} = K\left(\frac{\sqrt{\mathbf{r}^2_{n,k} + \tau^2_{n,k}/\alpha^2}}{h_{s,n}}\right)$$

Relation of S-T bandwidths: $h_{t,n} = \alpha h_{s,n}$

Currently we use this approach



Different approaches for kernel weight selection

Weight matrix for separable space-time kernel structure

Sampling pattern: N_s locations and N_t times

$$\mathbf{K}_s = \begin{bmatrix} K\left(\frac{\|\mathbf{r}_{1,1}\|}{h_{s,1}}\right) & \dots & K\left(\frac{\|\mathbf{r}_{1,N_s}\|}{h_{s,1}}\right) \\ \vdots & \vdots & \vdots \\ K\left(\frac{\|\mathbf{r}_{N_s,1}\|}{h_{s,N_s}}\right) & \dots & K\left(\frac{\|\mathbf{r}_{N_s,N_s}\|}{h_{s,N_s}}\right) \end{bmatrix}, \mathbf{K}_t = \begin{bmatrix} K\left(\frac{\|\tau_{1,1}\|}{h_{t,1}}\right) & \dots & K\left(\frac{\|\tau_{1,N_t}\|}{h_{t,1}}\right) \\ \vdots & \vdots & \vdots \\ K\left(\frac{\|\tau_{N_t,1}\|}{h_{t,N_t}}\right) & \dots & K\left(\frac{\|\tau_{N_t,N_t}\|}{h_{t,N_t}}\right) \end{bmatrix}$$

Kernel weight matrix: $\mathbf{W} = \mathbf{K}_s \otimes \mathbf{K}_t$

For positive-valued kernel functions the *normalized-weight matrix* is

$$\mathbf{U} = \frac{\mathbf{W}}{\|\mathbf{W}\|_1}, \text{ where } \|\mathbf{W}\|_1 = \sum_{k=1}^{N}\sum_{l=1}^{N} |W_{k,l}|, \text{ is the entry-wise } L_1 \text{ norm}$$

SLI precision matrix formulation

Quadratic Form of SLI Energy Functional

$$\mathcal{H}(\mathbf{x}_{\mathrm{S}};\boldsymbol{\theta}) = \frac{1}{2}(\mathbf{x}_{\mathrm{S}} - m_{\mathrm{x}}\mathbf{I})^{\top}\,\mathbf{J}(\boldsymbol{\theta})\,(\mathbf{x}_{\mathrm{S}} - m_{\mathrm{x}}\mathbf{I})$$

Precision matrix (sparse, explicit) using only the first two terms

$$\mathbf{J}(\boldsymbol{\theta}) = \frac{1}{\lambda}\left\{\frac{\mathbf{I}}{N} + c_1\,\mathbf{J}_1(\mathbf{h}_s, \mathbf{h}_t)\right\},\ \boldsymbol{\theta} = \left(\lambda, c_1, \mathbf{h}_s^{\top}, \mathbf{h}_t^{\top}\right)^{\top}$$

Gradient Precision sub-matrix based on the normalized-weight matrix

$$[\mathbf{J}_1(\mathbf{h}_s, \mathbf{h}_t)]_{i,j} = -u_{i,j}(\mathbf{h}_s, \mathbf{h}_t) - u_{j,i}(\mathbf{h}_s, \mathbf{h}_t) + \delta_{i,j}\sum_{k=1}^{N}[u_{i,k}(\mathbf{h}_s, \mathbf{h}_t) + u_{k,i}(\mathbf{h}_s, \mathbf{h}_t)]$$

Normalized kernel weights: $u_{i,j}(\mathbf{h}_s, \mathbf{h}_t) = [\mathbf{U}]_{i,j}$

SLI Mode Predictor for Interpolation of Missing Data

- The prime ($'$) indicates a fluctuation around m_{x}
- Modified energy functional in the presence of an unknown value

$$\mathcal{H}(\mathbf{x}_{\mathrm{S}};\boldsymbol{\theta}) = \frac{1}{2}\begin{bmatrix} \mathbf{x}'^{\top}_{\mathrm{S}} & x'_p \end{bmatrix} \begin{bmatrix} \mathbf{J}_{S,S} & \mathbf{J}_{S,P} \\ \mathbf{J}_{P,S} & J_{p,p} \end{bmatrix} \begin{bmatrix} \mathbf{x}'_{\mathrm{S}} \\ x'_p \end{bmatrix}$$

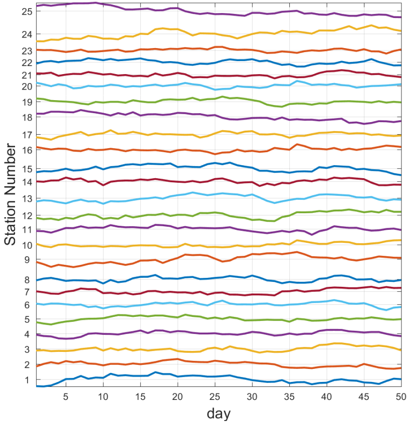
- $\hat{x}_p = \arg\min_{x_p} \hat{\mathcal{H}}(\mathbf{x}_{\mathrm{S}}, x_p; \boldsymbol{\theta}^*)$
- x_p is value at the *prediction point*
- The predictor is a linear equation that can be evaluated in $\mathcal{O}(N)$:

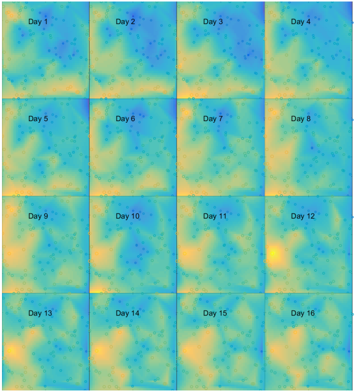
$$\hat{x}_p = m_{\mathrm{x}} - \frac{1}{J_{p,p}(\boldsymbol{\theta}^*)} \sum_{i=1}^{N} J_{p,i}(\boldsymbol{\theta}^*)\,(x_i - m_{\mathrm{x}})$$

Hristopulos, Stochastic Local Interaction (SLI) model, *Comput. & Geosci.*, 2015

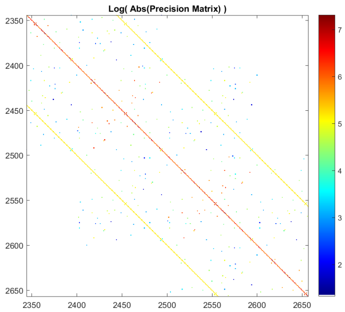
Simulated S-T data from stationary random field

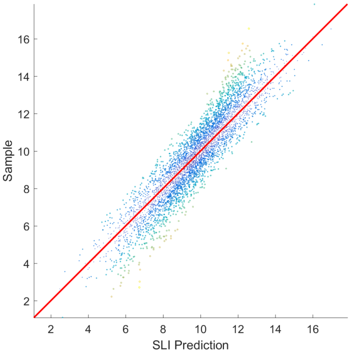
100 random locations and 50 time slices





Simulated S-T data from stationary random field



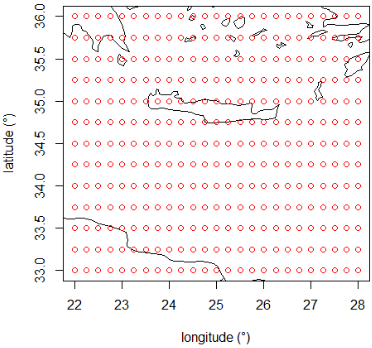


Reanalysis temperature data around Crete

Study design

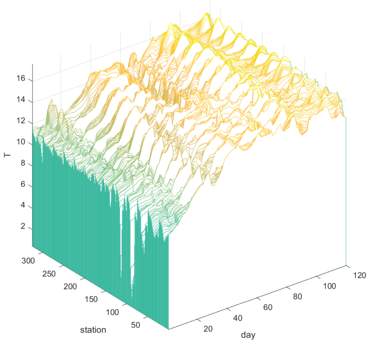
- Hourly temperature data (degrees) for five days from 01-01-2017 00:00:00 to 05-01-2017 23:00:00
- Total of 39 000 data points
- SLI parameter estimation with LOO-CV based on MAE
- Remove one time slice each time and predict using SLI

Spatial grid 13×25

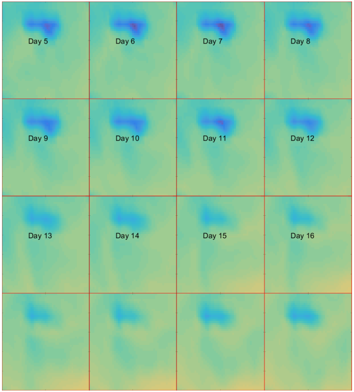


Reanalysis temperature data around Crete

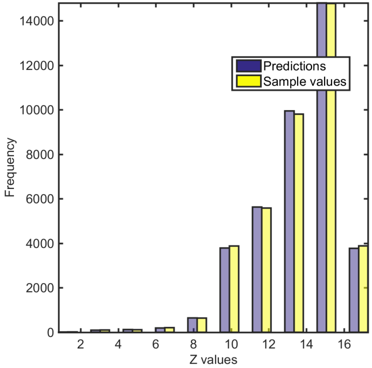
Time series - all sites

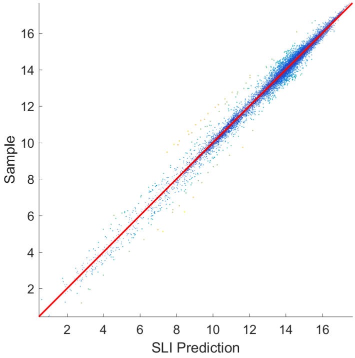


First few time slices



Reanalysis temperature data around Crete





SLI precision matrix *sparsity index* $\approx 0.08\%$, i.e., $\approx 123\,000$ non-zero entries out of 1.521×10^9

Conclusions

- Statistical mechanics is a useful framework for developing local S-T methods
- Linear Langevin equations ⇒ Rational spectral densities & Boltzmann-Gibbs probability density functions
- Linear Langevin equations ⇒ Linear covariance PDE
- The stochastic local interaction model (SLI) extends GMRF ideas to scattered data without solving an SPDE
- SLI employs compactly supported kernel functions with adaptive kernel bandwidths to build an explicit precision matrix. This structure leads to semi-explicit prediction equations

Thank you for your attention!

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For more information ...

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