## Covariance Models Based on Local Interaction (Spartan) Functionals

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- Need for flexible positive-definite kernel functions [Genton, 2002]
- Faster interpolation and simulation methods for "big data"


## Environmental Applications



SSRF Covariance
Models Models

## Groundwater monitoring

Groundwater level estimation in sparsely monitored basins [Varouchakis and Hristopulos, 2013];
Spatiotemporal variability estimates


Response to environmental threats
Radioactivity monitoring and emergency warning system [Dubois et al., 2011]


## Outline

SSRF
Covarianc Covariance
Models Models
(7) Conclusions

## Applications in Mineral Reserves Estimation

Coal reserves \& quality
Modeling of complex geological structures: Interpolation and simulation


Estimated lower calorific value (kcal/kg) - Amyndeo
Mine (Western Macedonia)


## Fluctuation-Gradient-Curvature (FGC) SSRF

## FGC-SSRF Coefficients

$\eta_{0}:$ scale, $\eta_{1}:$ stiffness, $\xi$ : characteristic length; $k_{c}:$ spectral cutoff

## Covariance Spectral Density



SSRF Covariance Models

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$\qquad$

## FGC-SSRF Covariance \& Spectral Density

- Covariance: $G(\mathbf{r})=\mathbb{E}[\phi(\mathbf{s}) \phi(\mathbf{s}+\mathbf{r})]$. Fourier transform pair:

$$
\tilde{G}(\mathbf{k})=\int d \mathbf{r} e^{-\jmath \mathbf{k} \cdot \mathbf{r}} G(\mathbf{r})
$$

$$
G(\mathbf{r})=\frac{1}{(2 \pi)^{d}} \int d \mathbf{k} e^{\jmath^{\mathbf{k} \cdot \mathbf{r}}} \tilde{G}(\mathbf{k})
$$

- Covariance spectral density:

$$
\tilde{G}(k)=\frac{\mathbb{1}_{k_{\mathrm{c}} \geq \kappa}(\kappa) \eta_{0} \xi^{d}}{1+\eta_{1} \kappa^{2} \xi^{2}+\kappa^{4} \xi^{4}}, \kappa=\|\mathbf{k}\|, \mathbb{1}_{B}(\cdot) \text { : indicator function, }
$$

- Permissibility conditions (Bochner's theorem) Hristopulos [2003]:

$$
\begin{array}{ll}
\text { For any } k_{c} \text { : } & \text { For finite } k_{c} \text { : } \\
\eta_{0}>0, \xi>0, \eta_{1}>-2 & \eta_{1}<-2, \text { if } k_{c} \xi<\sqrt{\frac{\left|\eta_{1}\right|-\Delta}{2}} \\
& \Delta=\sqrt{\eta_{1}^{2}-4}
\end{array}
$$

## Covariance functions

## Covariance ( $d=2$ ): Positive stiffness



Covariance $(d=2)$ : Negative stiffness


## Spectral Representation of Covariance

 Functions
## Spectral Representation (Inverse Hankel transform)

- For isotropic covariance functions the following holds: [Schoenberg, 1938]

$$
G(\mathbf{r})=\frac{\eta_{0} \xi^{d}\|\mathbf{r}\|}{(2 \pi\|\mathbf{r}\|)^{d / 2}} \int_{0}^{k_{\mathrm{c}}} d \kappa \frac{\kappa^{d / 2} J_{d / 2-1}(\kappa\|\mathbf{r}\|)}{1+\eta_{1}(\kappa \xi)^{2}+(\kappa \xi)^{4}}
$$

- $J_{d / 2-1}(\|\mathbf{r}\|)$ : Bessel function of the first kind of order d/2-1
- For $k_{\mathrm{c}} \rightarrow \infty$ (limit of infinite UV cutoff) the spectral integral exists for $d \leq 3$ -

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SSRF Covariance function $d=1$


## SSRF Covariance function $d=1$

## Unlimited band, $k_{\mathrm{c}} \rightarrow \infty$ [Hristopulos and Elogne, 2007]

$$
\begin{aligned}
& G(h)=\frac{\eta_{0}}{4} e^{-h \beta_{2}}\left[\frac{\cos \left(h \beta_{1}\right)}{\beta_{2}}+\frac{\sin \left(h \beta_{1}\right)}{\beta_{1}}\right], \quad\left|\eta_{1}\right|<2 \\
& G(h)=\eta_{0} \frac{(1+h)}{4 e^{h}}, \quad \eta_{1}=2 \\
& G(h)=\frac{\eta_{0}}{2 \Delta}\left(\frac{e^{-h \omega_{1}}}{\omega_{1}}-\frac{e^{-h \omega_{2}}}{\omega_{2}}\right), \quad \eta_{1}>2
\end{aligned}
$$

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

SSRF Covariance function $d=2$

Unlimited band, $k_{\mathrm{c}} \rightarrow \infty$ [Hristopulos, 2013]

$$
\begin{array}{rr}
G(h)=\frac{\eta_{0} \Im\left[K_{0}\left(h z_{+}\right)\right]}{\pi \sqrt{4-\eta_{1}^{2}}}, & \left|\eta_{1}\right|<2 \\
G(h)=\left(\frac{\eta_{0} h}{4 \pi}\right) K_{-1}(h), & \eta_{1}=2 \\
G(h)=\frac{\eta_{0}\left[K_{0}\left(h z_{+}\right)-K_{0}\left(h z_{-}\right)\right]}{2 \pi \sqrt{\eta_{1}^{2}-4}}, & \eta_{1}>2
\end{array}
$$

- $h=\|\mathbf{r}\| / \xi, \quad$ §: Imaginary part
- $z_{ \pm}=\sqrt{-t_{ \pm}^{*}}, \quad t_{ \pm}^{*}=\left(-\eta_{1} \pm \sqrt{\eta_{1}^{2}-4}\right) / 2$
- $K_{\nu}(z)$ : modified Bessel function of the second kind and order $\nu$

SSRF Covariance function $d=2$


SSRF Covariance function $d=3$


SSRF Covariance function $d=3$

## Unlimited band, $k_{\mathrm{c}} \rightarrow \infty$ [Hristopulos and Elogne, 2007]

$$
\begin{aligned}
G(h)=\eta_{0} \frac{e^{-h \beta_{2}}}{\Delta}\left[\frac{\sin \left(h \beta_{1}\right)}{h}\right], & \left|\eta_{1}\right|<2 \\
G(h)=\frac{\eta_{0}}{4} e^{-h}, & \eta_{1}=2 \\
G(h)=\frac{1}{2 \Delta}\left(\frac{e^{-h \omega_{1}}-e^{-h \omega_{2}}}{h}\right), & \eta_{1}>2
\end{aligned}
$$

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

FGC-SSRF Realizations $d=1$



## FGC-SSRF Length Scales

FGC-SSRF covariance functions have non-linear dependence of correlation scales on model parameters [Hristopulos and Žukovič, 2011]

## Definitions

$$
\ell_{c} \doteq\left[\frac{\int d \mathbf{r} G(r)}{G(0)}\right]^{1 / d}=A_{d} \xi
$$

(2) Correlation length:

$$
\begin{aligned}
& r_{c} \doteq\left[\frac{\int d \mathbf{r} r^{2} G(r)}{\int d \mathbf{r} G(r)}\right]^{1 / 2} \\
& =\sqrt{\left[\left|\frac{d^{2} \tilde{G}(k) / d k^{2}}{2 \tilde{G}(k)}\right|_{k=0}\right]}=\sqrt{\left|\eta_{1}\right| \xi}
\end{aligned}
$$

## Integral range:

$$
\begin{aligned}
& \text { Definitions } \\
& \text { (1) Integral range: } \\
& \qquad \ell_{c} \doteq\left[\frac{\int d \mathbf{r} G(r)}{G(0)}\right]^{1 / d}=A_{d} \xi \\
& \text { (2) Correlation length: } \\
& \quad r_{c} \doteq\left[\frac{\int d \mathbf{r} r^{2} G(r)}{\int d \mathbf{r} G(r)}\right]^{1 / 2} \\
& =\sqrt{\left[\left|\frac{d^{2} \tilde{G}(k) / d k^{2}}{2 \tilde{G}(k)}\right|_{k=0}\right]}=\sqrt{\left|\eta_{1}\right|} \xi
\end{aligned}
$$

FGC-SSRF covariance functions have non-linear dependence of correlation scales on model parameters [Hristopulos and Žukovič, 2011]

FGC-SSRF Integral Range


## Karhunen-Loève Expansions of SSRFs

## Karhunen-Loève Theorem

(1) A second-order $\phi(\mathbf{s})$ with continuous covariance covariance $G\left(\mathbf{s}, \mathbf{s}^{\prime}\right)$ can be expanded on a closed and bounded domain $\mathcal{D}$ as:

$$
\phi(\mathbf{s})=m_{\mathrm{x}}(\mathbf{s})+\sum_{m=1}^{\infty} \sqrt{\lambda_{m}} c_{m} \psi_{m}(\mathbf{s})
$$

The convergence is uniform on $\mathcal{D}$.
(2) The $\lambda_{m}$ and $\psi_{m}(\mathbf{s})$ are respectively, eigenvalues and eigenfunctions of the covariance operator, that satisfy the Fredholm integral equation

$$
\int_{\mathcal{D}} d \mathbf{s}^{\prime} G\left(\mathbf{s}, \mathbf{s}^{\prime}\right) \psi_{m}\left(\mathbf{s}^{\prime}\right)=\lambda_{m} \psi_{m}\left(\mathbf{s}^{\prime}\right)
$$The $c_{m}$ are zero-mean, uncorrelated random variables, i.e,

$\mathbb{E}\left[c_{m}\right]=0$ and $\mathbb{E}\left[c_{m} c_{n}\right]=\delta_{n, m}, \forall n, m \in \mathbb{N}$.

## Karhunen-Loève Expansions of SSRFs

Simulations on Square Domain

- Square lattice $100 \times 100$, Modes used: $100 \times 100$ wave-vectors
- Pinned boundaries (no fluctuations)
- SSRF eigenvalues

$$
\lambda_{m}=\frac{\eta_{0} \xi^{2}}{1+\eta_{1} \xi^{2}\left\|\mathbf{k}_{m}\right\|^{2}+\xi^{4}\left\|\mathbf{k}_{m}\right\|^{4}}, \mathbf{k}_{m}=\left(\frac{2 \pi n_{m, 1}}{L}, \frac{2 \pi n_{m, 2}}{L}\right)^{T}
$$

- SSRF K-L eigenfunctions

$$
\psi_{m}\left(s_{1}, s_{2}\right)=\frac{1}{L} \sin \left(k_{m, 1} s_{1}\right) \sin \left(k_{m, 2} s_{2}\right)
$$

| $\eta_{0}=2, \eta_{1}=-1.5, \xi=5$ | $\eta_{0}=2, \eta_{1}=1.5, \xi=5$ |
| :---: | :---: |
|  |  |
| $\eta_{0}=2, \eta_{1}=0, \xi=5$ | $\eta_{0}=2, \eta_{1}=15, \xi=5$ |
|  |  |

## SSRF Inverse Covariance Kernel with Ultraviolet Cutoff

- Spectral integral of $\tilde{\mathbb{J}}_{S}(\|\mathbf{k}\|)=\left(\eta_{0} \xi^{d}\right)^{-1}\left[1+\eta_{1}(\xi\|\mathbf{k}\|)^{2}+c_{2}(\xi\|\mathbf{k}\|)^{4}\right]$,

$$
\mathbb{J}_{S}(\mathbf{r} ; \boldsymbol{\theta})=\frac{\|\mathbf{r}\|}{(2 \pi\|\mathbf{r}\|)^{d / 2}} \int_{0}^{k_{\mathrm{c}}} d\|\mathbf{k}\|\|\mathbf{k}\|^{d / 2} J_{d / 2-1}(\|\mathbf{k}\|\|\mathbf{r}\|) \tilde{\mathbb{J}}_{S}(\|\mathbf{k}\| ; \boldsymbol{\theta}),
$$

- Lommel functions

$$
z^{2} \frac{d^{2} w(z)}{d z^{2}}+z \frac{d w(z)}{d z}+\left(z^{2}-\nu^{2}\right) w(z)=z^{\mu+1} .
$$

- If $\mu-\nu=2 I+1$ the following Lommel series terminates after $I+1$ terms $S_{\mu, \nu}(z)=z^{\mu-1}\left[1-\frac{(\mu-1)^{2}-\nu^{2}}{z^{2}}+\frac{\left[(\mu-1)^{2}-\nu^{2}\right]\left[(\mu-3)^{2}-\nu^{2}\right]}{z^{4}}-\ldots\right]$

SSRF Inverse Covariance Kernel with Ultraviolet Cutoff

## Theorem

In $d \geq 2$, the SSRF inverse covariance kernel $\mathbb{J}_{S}(z ; \theta)$ is given by means of the following tripartite sum, where $u_{c}=k_{c} \xi, z=k_{c}\|\mathbf{r}\|$, and $\nu=d / 2-1$

$$
\begin{gathered}
\mathbb{J}_{S}(z ; \theta)=\sum_{I=0,1,2} \frac{g_{I}(\theta)}{z^{2 \nu+2 l+1}}\left[(2 \nu+2 I) J_{\nu}(z) S_{\nu+2 I, \nu-1}(z)-J_{\nu-1}(z) S_{\nu+2 I+1, \nu}(z)\right] \\
g_{0}(\theta)=\frac{k_{c}^{d}}{(2 \pi)^{d / 2} \eta_{0} \xi^{d}}, g_{1}(\theta)=\eta_{1} u_{c}^{2} g_{0}(\theta), g_{2}(\theta)=u_{c}^{4} g_{0}(\theta),
\end{gathered}
$$

The above equations define a positive semidefinite kernel function for $\eta_{1}>-2$. In particular, the value at the origin is

$$
\mathbb{J}_{S}(0 ; \theta)=\frac{g_{0}(\theta)}{2^{\nu+1} \Gamma(\nu+2)}\left[1+\eta_{1} u_{c}^{2}\left(\frac{\nu+1}{\nu+2}\right)+u_{c}^{4}\left(\frac{\nu+1}{\nu+3}\right)\right]
$$

## SSRF Inverse Covariance Kernel with

 Ultraviolet Cutoff

## SSRF Inverse Covariance Kernel with Ultraviolet Cutoff

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Normalized inverse SSRF covariance function vs $d$
SSRF parameters are $\eta_{0}=1, \xi=1, \eta_{1}=2$, and $k_{c}=2$.


## Fast optimal interpolation

## Theorem

Let $\mathbf{X}_{s}=\left(X_{1}, \ldots, X_{N}\right)^{T}$ a vector of measurements at $\mathbf{s}_{n}, n=1, \ldots, N$, and $X_{p}=X_{N+1}$ the SSRF value at unmeasured location $\mathbf{s}_{N+1}$. Assume that the data are samples of the SSRF with the energy functional

$$
H_{\mathrm{fgc}}\left[\mathbf{X}_{s ; p} ; \boldsymbol{\theta}\right]=\frac{1}{2} \mathbf{X}_{s ; p}^{T} \mathbf{J}(\boldsymbol{\theta}) \mathbf{X}_{s ; p},
$$

where $\mathbf{X}_{s ; p}=\left(X_{1}, \ldots, X_{N}, X_{p}\right)^{T}$, and $\mathbf{J}(\theta)$ is the inverse covariance (precision) matrix. The mode estimate $\hat{X}_{p}$ which maximizes the joint pdf is given by

$$
\begin{equation*}
\hat{X}_{p}=-\frac{\mathbf{J}_{p ; s}^{T}(\boldsymbol{\theta}) \mathbf{X}_{s}}{J_{p ; p}(\boldsymbol{\theta})}=-\sum_{i=1}^{N} \frac{J_{p, i}(\boldsymbol{\theta}) X_{i}}{J_{p ; p}(\boldsymbol{\theta})} . \tag{1}
\end{equation*}
$$

Grid Approximation of Continuum SSRF

$$
\mathbb{J}_{S}\left(\mathbf{r}_{\mathbf{n}} ; \boldsymbol{\theta}\right)=c_{0}\left[1-\eta_{1}\left(\sum_{i=1}^{d} \frac{\xi^{2}}{a_{i}^{2}} \mathrm{D}_{\mathbf{n}, i}^{2}\right)+\left(\sum_{i=1}^{d} \sum_{j=1}^{d} \frac{\xi^{4}}{a_{i}^{2} a_{j}^{2}} \mathrm{D}_{\mathbf{n}, i}^{2} D_{\mathbf{n}, j}^{2}\right)\right] \delta\left(\mathbf{r}_{\mathbf{n}}\right) .
$$

On a grid with lattice step $a \rightarrow 0: \delta\left(\mathbf{s}_{i}-\mathbf{s}_{j}\right) \rightarrow \delta_{i, j} / v_{c}, v_{c}=a^{d}$.

$$
\delta_{\mathbf{n}, i}\left[f\left(\mathbf{r}_{n}\right)\right]=f\left(\mathbf{r}_{n}+\frac{a_{i}}{2} \hat{\mathbf{e}}_{i}\right)-f\left(\mathbf{r}_{n}-\frac{a_{i}}{2} \hat{\mathbf{e}}_{i}\right), i=1, \ldots, d
$$

$$
\delta_{\mathbf{n}, i}^{2}\left[f\left(\mathbf{r}_{n}\right)\right]=f\left(\mathbf{r}_{n}+a_{i} \hat{\mathbf{e}}_{i}\right)+f\left(\mathbf{r}_{n}-a_{i} \hat{\mathbf{e}}_{i}\right)-2 f\left(\mathbf{r}_{n}\right)
$$

$\mathrm{D}_{\mathbf{n}, i}$ is related to the centered difference operator by [Hildebrand, 1974]

$$
a_{i} \mathrm{D}_{\mathbf{n}, i}=2 \sinh ^{-1}\left(\frac{\delta_{\mathbf{n}, i}}{2}\right)
$$

Taylor series expansions of $D_{\mathbf{n}, i}^{2}$ and $D_{\mathbf{n}, i}^{4}$ in terms of $\delta_{\mathbf{n}, i}$

$$
\begin{aligned}
& a_{i}^{2} \mathrm{D}_{\mathbf{n}, i}^{2}=\delta_{\mathbf{n}, i}^{2}-\frac{\delta_{\mathbf{n}, i}^{4}}{12}+\frac{\delta_{\mathbf{n}, i}^{6}}{90}-\frac{\delta_{\mathbf{n}, i}^{8}}{560}+\frac{\delta_{\mathbf{n}, i}^{10}}{3150}-\frac{\delta_{\mathbf{n}, i}^{12}}{16632}+O\left(\delta_{\mathbf{n}, i}^{14}\right) \\
& a_{i}^{4} \mathrm{D}_{\mathbf{n}, i}^{4}=\delta_{\mathbf{n}, i}^{4}-\frac{\delta_{\mathbf{n}, i}^{6}}{6}+\frac{7 \delta_{\mathbf{n}, i}^{8}}{240}-\frac{41 \delta_{\mathbf{n}, i}^{10}}{7560}+\frac{479 \delta_{\mathbf{n}, i}^{12}}{453600}+O\left(\delta_{\mathbf{n}, i}^{14}\right)
\end{aligned}
$$

## Inverse SSRF Covariance Kernel on Hypercubic Grid

Table: Central finite differences of orders $2 k, k=1, \ldots, 6$ on hypercubic grid with uniform step $a=1$ in each orthogonal direction $i=1, \ldots, d$. FD stands for finite difference. The $f_{\mathrm{n}}$ denotes any lattice function.

| FD | Expressions |
| :---: | :---: |
| $\delta_{\mathbf{n}, i}^{2} \mathrm{f}_{\mathbf{n}}=$ | $f_{\mathrm{n}+\hat{\mathrm{e}}_{i}}+f_{\mathrm{n}-\hat{\mathbf{e}}_{i}}-2 f_{\mathrm{n}}$ |
| $\delta_{\mathrm{n}, i}^{4} \mathrm{f}_{\mathbf{n}}=$ | $f_{\mathbf{n}+2 \hat{e}_{i}}+f_{\mathbf{n}-2 \hat{e}_{i}}-4 f_{\mathbf{n}+\hat{\mathbf{e}}_{i}}-4 f_{\mathbf{n}-\hat{\mathbf{e}}_{i}}+6 f_{\mathrm{n}}$ |
| $\delta_{\mathbf{n}, i}^{6} f_{\mathbf{n}}=$ | $f_{\mathbf{n}+3 \hat{\mathbf{e}}_{i}}+f_{\mathbf{n}-3 \hat{\mathbf{e}}_{i}}-6 f_{\mathbf{n}+2 \hat{e}_{i}}-6 f_{\mathbf{n}-2 \hat{\mathbf{e}}_{i}}+15 f_{\mathbf{n}+\hat{\mathbf{e}}_{i}}+15 f_{\mathrm{n}-\hat{\mathbf{e}}_{i}}-20 f_{\mathrm{n}}$ |
| $\delta_{\mathbf{n}, i}^{8} f_{\mathbf{n}}=$ | $\begin{aligned} & f_{\mathbf{n}+4 \hat{e}_{i}}+f_{\mathbf{n}-4 \hat{\mathbf{e}}_{i}}-8 f_{\mathbf{n}+3 \hat{e}_{i}}-8 f_{\mathbf{n}-3 \hat{e}_{i}}+28 f_{\mathbf{n}+2 \hat{e}_{i}}+28 f_{\mathbf{n}-2 \hat{e}_{i}}-56 f_{\mathbf{n}+\hat{\mathbf{e}}_{i}} \\ & -56 f_{\mathbf{n}}-\hat{\mathbf{e}}_{i}+70 f_{\mathbf{n}} \end{aligned}$ |
| $\delta_{\mathbf{n}, i}^{10} f_{\mathbf{n}}=$ | $\begin{aligned} & f_{n_{i}+5, n_{j}}+f_{n_{i}}-5, n_{j}-10 f_{\mathbf{n}+4 \hat{e}_{i}}-10 f_{\mathbf{n}}-4 \hat{\mathbf{e}}_{i}+45 f_{\mathbf{n}+3 \hat{\mathbf{e}}_{i}}+45 f_{\mathbf{n}-3 \hat{\mathbf{e}}_{i}}-120 f_{\mathbf{n}+2 \hat{\mathbf{e}}_{i}} \\ & -120 f_{\mathbf{n}-2 \hat{e}_{i}}+210 f_{\mathbf{n}+\hat{\mathbf{e}}_{i}}+210 f_{\mathbf{n}-\hat{\mathbf{e}}_{i}}-252 f_{\mathbf{n}} \end{aligned}$ |
| $\delta_{\mathbf{n}, i}^{12} \mathrm{f}_{\mathbf{n}}=$ | $\begin{aligned} & f_{n_{i}+6, n_{j}}+f_{n_{i}}-6, n_{j}-12 f_{n_{i}+5, n_{j}}-12 f_{n_{i}}-5, n_{j}+66 f_{\mathbf{n}+4 \hat{e}_{j}}+66 f_{\mathbf{n}-4 \hat{\mathbf{e}}_{i}}-220 f_{\mathbf{n}+3 \hat{\mathbf{e}}_{i}} \\ & -220 f_{\mathbf{n}-3 \hat{e}_{j}}+495 f_{\mathbf{n}+2 \hat{\mathbf{e}}_{j}}+495 f_{\mathbf{n}-2 \hat{e}_{j}}-792 f_{\mathbf{n}+\hat{\mathbf{e}}_{j}}-792 f_{\mathbf{n}-\hat{\mathbf{e}}_{j}}+924 f_{\mathbf{n}} \\ & \hline \end{aligned}$ |

## Inverse SSRF Covariance Kernel on

## Hypercubic Grid

$$
\mathbb{J}\left(\mathbf{r}_{\mathbf{n}} ; \boldsymbol{\theta}\right)=c_{0}\left[\delta_{\mathbf{n}, \mathbf{0}}-\eta_{1} \xi^{2} S\left(\mathbf{r}_{\mathbf{n}}\right)+\xi^{4} C\left(\mathbf{r}_{\mathbf{n}}\right)\right]
$$

where the square gradient, $S\left(\mathbf{r}_{\mathbf{n}}\right)$, and square curvature, $C\left(\mathbf{r}_{\mathbf{n}}\right)$, are given by

$$
S\left(\mathbf{r}_{\mathbf{n}}\right)=\sum_{i=1}^{d} \mathrm{D}_{\mathbf{n}, i}^{2}, \quad C\left(\mathbf{r}_{\mathbf{n}}\right)=\sum_{i=1}^{d} \mathrm{D}_{\mathbf{n}, i}^{4}+\sum_{i=1}^{d} \sum_{j=1}^{d} \mathrm{D}_{\mathbf{n}, i}^{2} \mathrm{D}_{\mathbf{n}, j}^{2} .
$$

Truncating $S\left(\mathbf{r}_{\mathbf{n}}\right)$ and $C\left(\mathbf{r}_{\mathbf{n}}\right)$ at order $2 p=12$, it follows that

$$
\begin{gathered}
S^{(12)}\left(\mathbf{r}_{\mathbf{n}}\right)=\sum_{i=1}^{d} \delta_{\mathbf{n}, i}^{2}-\frac{\delta_{\mathbf{n}, i}^{4}}{12}+\frac{\delta_{\mathbf{n}, i}^{6}}{90}-\frac{\delta_{\mathbf{n}, i}^{8}}{560}+\frac{\delta_{\mathbf{n}, i}^{10}}{3150}-\frac{\delta_{\mathbf{n}, i}^{12}}{16632}, \\
C^{(12)}\left(\mathbf{r}_{\mathbf{n}}\right)=\sum_{i=1}^{d}\left(\delta_{\mathbf{n}, i}^{4}-\frac{\delta_{\mathbf{n}, i}^{6}}{6}+\frac{7 \delta_{\mathbf{n}, i}^{8}}{240}-\frac{41 \delta_{\mathbf{n}, i}^{10}}{7560}+\frac{479 \delta_{\mathbf{n}, i}^{12}}{453600}\right)+\sum_{i=1}^{d} \sum_{j=1}^{d}\left(\delta_{\mathbf{n}, i}^{2} \delta_{\mathbf{n}, j}^{2}-\frac{\delta_{\mathbf{n}, i}^{2} \delta_{\mathbf{n}, j}^{4}}{6}\right. \\
\left.+\frac{\delta_{\mathbf{n}, i}^{2} \delta_{\mathbf{n}, j}^{6}}{45}-\frac{\delta_{\mathbf{n}, i}^{2} \delta_{\mathbf{n}, j}^{8}}{280}+\frac{\delta_{\mathbf{n}, i}^{2} \delta_{\mathbf{n}, j}^{10}}{1575}+\frac{\delta_{\mathbf{n}, i}^{4} \delta_{\mathbf{n}, j}^{4}}{144}-\frac{\delta_{\mathbf{n}, i}^{4} \delta_{\mathbf{n}, j}^{6}}{540}+\frac{\delta_{\mathbf{n}, i}^{4} \delta_{\mathbf{n}, j}^{8}}{3360}+\frac{\delta_{\mathbf{n}, i}^{6} \delta_{\mathbf{n}, j}^{6}}{8100}\right)
\end{gathered}
$$

## Inverse SSRF Covariance Kernel on Hypercubic Grid



## Conclusions and Future Directions

- We presented three-parameter, positive-definite, isotropic covariance models based on local interaction "energy" (Spartan) functionals
- SSRF models lead to fast (linear complexity) interpolation on regular grids and on unstructured grids as well [Hristopulos and Elogne, 2009]
- A new family of four-parameter, positive-definite kernels valid in $d \geq 2$ based on Lommel functions is proposed
- Continuing research involves extensions to: spatial non-homogeneity, space-time correlations, and non-Gaussian dependence


## References

M. Abramowitz and I. A. Stegun. Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables. National Bureau of Standards, Washington, DC, 1972.
G. Dubois, D. Cornford, D. Hristopulos, E. Pebesma, and J. Pilz. Introduction to this special issue on geoinformatics for environmental surveillance. Computers and Geosciences, 37(3):277-279, 2011.
M. G. Genton. Classes of kernels for machine learning: a statistics perspective. Journal of Machine Learning Research, 2:299-312, March 2002. URL http://dl.acm.org/citation.cfm?id=944790.944815.
F. B. Hildebrand. Introduction to numerical analysis. International Series in Pure and Applied Mathematics. McGraw-Hill, New York, 2nd. edition, 1974.
D. Hristopulos. Spartan Gibbs random field models for geostatistical applications. SIAM Journal of Scientific Computing, 24(6):2125-2162, 2003.
D. Hristopulos and S. Elogne. Analytic properties and covariance functions of a new class of generalized Gibbs random fields. IEEE Transactions on Information Theory, 53(12):4667-4679, 2007.
D. T. Hristopulos. Positive Semidefinite Functions and Karhunen-Loève Expansions Related to Spartan Random Fields. SIAM Journal on Uncertainty Quantification, in review, 2013.
D. T. Hristopulos and S. N. Elogne. Computationally efficient spatial interpolators based on Spartan spatial random fields. 57(9):3475-3487, 2009.
D. T. Hristopulos and M. Žukovič. Relationships between correlation lengths and integral scales for covariance models with more than two parameters. Stochastic Environmental Research and Risk Assessment, 25 (1):11-19, 2011.
I. J. Schoenberg. Metric spaces and completely monotone functions. Annals of Mathematics, 39(4):811-841, 1938.
E. A. Varouchakis and D. T. Hristopulos. Improvement of groundwater level prediction in sparsely gauged basins using physical laws and local geographic features as auxiliary variables. Advances in Water Resources, 52:34-49, 2013. URL DOI:10.1016/j.advwatres.2012.08.002.

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ЕЕПА


