# Continuum limits of Gaussian Markov random fields : resolving the conflict with geostatistics

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## Agenda

- Hidden Markov random fields (MRF's).
- Geostatistical versus MRF approach to spatial data.
- Describe simplest Gaussian intrinsic autoregression on 2–d rectangular array.
- Provide its **exact** and **asymptotic variograms**.
- Reconcile geostatistics and Gaussian MRF's via regional averages.
- Generalizations and wrap-up.

For general theory and some applications of Gaussian MRF's, see

H. Rue & L. Held (2005), Gaussian Markov Random Fields, Chapman & Hall.

For intrinsic autoregressions and the limiting de Wijs process, see

J. Besag & C. Kooperberg (1995), *Biometrika*, **82**, 733–746.

J. Besag & D. Mondal (2005), *Biometrika*, **92**, 909–920.

## Hidden Markov random fields for spatial data

- Markov random fields arise naturally in spatial context.
- Spatial variables observed indirectly, via treatments, covariates, blur, noise, ...
- Data y = response to linear predictor  $\eta$ 
  - $\eta = \mathbf{T} \boldsymbol{ au} + \mathbf{F} \mathbf{x} + \mathbf{z}$
  - $\boldsymbol{\tau}$  = treatment / variety / covariate effects
  - $\mathbf{T}$  = design matrix (covariate information)
  - $\mathbf{x}$  = (secondary) spatial effects
  - $\mathbf{F}$  = linear filter (identity/incidence matrix, averaging operator, ...)
  - $\mathbf{z}$  = residual effects
- Usually, goal is to make **probabilistic inferences** about  $\tau$  (MCMC or ...). Unknown/unmeasured **covariates** might be identified via **x** and **z** (Rumsfeld).
- Stochastic representation of x via MRF : often "prior ignorance". E.g. Ising/Potts model or Gaussian/non–Gaussian smoother.

## EGRET (energetic gamma-ray experiment telescope) astronomy

Raw photon counts L2 deblurring

L1 deblurring





# Markov chain Monte Carlo every 2500 image updates



# Geostatistical approach to spatial component

- Specify continuum spatial process, often chosen via family of Matérn variograms.
- Extract **covariance matrix** for observations.
- Fit surface and make predictions.
- Rescaling OK.
- Substantial computational burden.

# Gaussian Markov random field (MRF) approach

- Assume **discrete space**(?!) **Markov** property.
- If Gaussian  $\Rightarrow$  locations of nonzero elements in precision matrix.
- Estimate parameters in overall scheme.
- Sparse matrix computation OK (e.g. cotton field with 500,000 pixels).
- Scale and prediction problematic at least aesthetically.

## Variety trial for wheat at Plant Breeding Institute, UK



Besag and Higdon (JRSS B, 1999)



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# Markov random fields on pixel arrays

•	•	•	•	•	•	•	•
•	•	•					
•	•	•					
•	•	•	•	•	•		
•	•	•					

Gaussian Markov random fields on rectangular pixel arrays

- Pixel centres  $i = (u, v) \in \mathbb{Z}^2$ .
- Choose **neighbours**  $\partial i$  for each site i

$$\Rightarrow \qquad \pi(x_i \,|\, \mathbf{x}_{-i}) \;\equiv\; \pi(x_i \,|\, \mathbf{x}_{\partial i}).$$

- $\Rightarrow$  Undirected conditional dependence graph  $\mathcal{G}$ .
- Associated **Gaussian** random vector  $\mathbf{X} = \{X_i : i \in \mathbb{Z}^2\}$ .

Joint distribution  $\{\pi(\mathbf{x})\}$ , with full conditionals  $\pi(x_i | \mathbf{x}_{-i})$ ,

 $\Rightarrow \pi(\mathbf{x})$  honours the graph  $\mathcal{G}$  and is a Markov random field w.r.t.  $\mathcal{G}$ .

- Cliquo: any single site or set of mutual neighbours w.r.t.  $\mathcal{G}$ .
- Clique: maximal cliquo.

# Neighbours for 1st–order Markov random field



# Global property for 1st–order Markov random field



# Neighbours for 2nd–order Markov random field



# Global property for 2nd–order Markov random field



# Neighbours for 3rd–order Markov random field



# Neighbours for 4th–order Markov random field



# Neighbours for 5th–order Markov random field



# Cliques for MRF's on rectangular arrays



# Markov random fields on hexagonal arrays



# Neighbours and cliques for MRF's on hexagonal arrays 1st-order 2nd–order

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## Example of irregular regions: Washington State



Besag, Green, Higdon & Mengersen (1995)

## Pairwise difference distributions

- Sites (e.g. pixels)  $i, j, \ldots$ , with associated random variables  $X_i, X_j, \ldots$
- Joint generalized probability density function of  $X_i$ 's:

$$\pi(\mathbf{x}) \propto \exp\{-\sum_{i \heartsuit j} \lambda_{ij} g(|x_i - x_j|)\}, \qquad x_i \in \mathcal{R},$$

where  $i \heartsuit j$  indicates that *i* and *j* are **neighbours**.

At best π(.) is informative about some or all contrasts among X<sub>i</sub>'s.
 NB. Σ<sub>i</sub> c<sub>i</sub>X<sub>i</sub> is a contrast if the constants c<sub>i</sub> satisfy Σ<sub>i</sub> c<sub>i</sub> = 0.

## Gaussian pairwise difference distributions

 $\pi(\mathbf{x}) \propto \exp\{-\sum_{i \heartsuit j} \lambda_{ij} (x_i - x_j)^2\}$ 

•  $\lambda_{ij} > 0$  for all  $i \heartsuit j \implies \sum_{i \heartsuit j} \lambda_{ij} (x_i - x_j)^2$  is positive semidefinite

- $\Rightarrow$  simple **differences** have well–defined distributions
- $\Rightarrow$  variogram  $\nu_{ij} := \frac{1}{2} \operatorname{var} (X_i X_j)$  is well defined.

Künsch (1987), Besag & Kooperberg (1995)

## First-order Gaussian intrinsic autoregressions on $\mathcal{Z}^2$

• Let  $\{X_{u,v} : (u,v) \in \mathbb{Z}^2\}$  be **Gaussian** with conditional means and variances  $E(X_{u,v} | \ldots) = \beta(x_{u-1,v} + x_{u+1,v}) + \gamma(x_{u,v-1} + x_{u,v+1}),$   $\operatorname{var}(X_{u,v} | \ldots) = \kappa > 0,$ where  $\beta, \gamma > 0$  and  $\beta + \gamma = \frac{1}{2}$ . Symmetric special case :  $\beta = \gamma = \frac{1}{4}$ .

#### • Pairwise difference distribution with

 $\pi(\mathbf{x}) \propto \exp\{-\lambda\beta\sum_{u}\sum_{v}(x_{u,v}-x_{u+1,v})^2 - \lambda\gamma\sum_{u}\sum_{v}(x_{u,v}-x_{u,v+1})^2\},\$ where  $\lambda = 1/(2\kappa)$ . All  $\{X_{u,v}-X_{u+s,v+t}\}$  have well-defined distributions.

• Variogram  $\{\nu_{s,t} : s, t \in \mathbb{Z}\}$  is well defined and translation invariant:

$$\nu_{s,t} := \frac{1}{2} \operatorname{var} \left( X_{u,v} - X_{u+s,v+t} \right) = ???$$

- Computational advantage : sparse precision matrix.
- **Disadvantage** : defined w.r.t. regular grid; what are effects of **rescaling**?

# Symmetric first-order intrinsic autoregression



 $256 \times 256$  array

# X-ray mammography (film)



Analysis: Larissa Stanberry Data: Ruth Warren Stephen Duffy

## Spectral density diagram for simple Gaussian time series



First–order Gaussian intrinsic autoregressions on  $\mathcal{Z}^2$ 

• Let  $\{X_{u,v} : (u,v) \in \mathbb{Z}^2\}$  be **Gaussian** with conditional means and variances  $E(X_{u,v} | \ldots) = \beta(x_{u-1,v} + x_{u+1,v}) + \gamma(x_{u,v-1} + x_{u,v+1}),$   $\operatorname{var}(X_{u,v} | \ldots) = \kappa > 0,$ where  $\beta, \gamma > 0$  and  $\beta + \gamma = \frac{1}{2}$ .

•  $\{X_{u,v}\}$  has generalized spectral density function

$$f(\omega,\eta) = \kappa / (1 - 2\beta \cos \omega - 2\gamma \cos \eta)$$

and finite variogram  $\{\nu_{s,t} : s, t \in \mathcal{Z}\}$ 

$$\nu_{s,t} := \frac{1}{2} \operatorname{var} \left( X_{u,v} - X_{u+s,v+t} \right) = \frac{1}{\pi^2} \int_0^{\pi} \int_0^{\pi} \frac{1 - \cos s\omega \, \cos t\eta}{1 - 2\beta \cos \omega - 2\gamma \cos \eta} \, d\omega \, d\eta.$$

- Computational advantage : sparse precision matrix.
- **Disadvantage** : defined w.r.t. regular grid; what are effects of **rescaling**?

## Variety trial for wheat at Plant Breeding Institute, UK



Besag and Higdon (JRSS B, 1999)



Calculating the exact variogram  $\{\nu_{s,t}\}$ 

$$\nu_{s,t} = \frac{1}{2} \operatorname{var} \left( X_{u,v} - X_{u+s,v+t} \right) = \frac{1}{\pi^2} \int_0^{\pi} \int_0^{\pi} \frac{1 - \cos s\omega \, \cos t\eta}{1 - 2\beta \cos \omega - 2\gamma \cos \eta} \, d\omega \, d\eta$$

... but extremely awkward in general, both analytically and numerically.

- Symmetric case  $\beta = \gamma = \frac{1}{4}$  (McCrea & Whipple, 1940; Spitzer, 1964)
- General case  $\beta \neq \gamma$  (Besag & Mondal, 2005)

Obtain **delicate** finite summations for  $\nu_{s,0}$  and  $\nu_{0,t}$ . Then

$$\pi \,(\beta\gamma)^{\frac{1}{2}} \,\nu_{s,s} = 1 + \frac{1}{3} + \frac{1}{5} + \ldots + \frac{1}{2s-1} \\ \nu_{s,t} = -\delta_{s,t} + \beta \,(\nu_{s-1,t} + \nu_{s+1,t}) + \gamma \,(\nu_{s,t-1} + \nu_{s,t+1}) \right\} \quad \Rightarrow \quad \nu_{s,t}$$

## Asymptotic expansion of the variogram

• Exact results for  $\nu_{s,0}$  and  $\nu_{0,t}$  are numerically **unstable** for large s and t; but

$$\pi (\beta \gamma)^{\frac{1}{2}} \nu_{s,s} = 1 + \frac{1}{3} + \frac{1}{5} + \ldots + \frac{1}{2s-1}$$

 $\Rightarrow \quad \nu_{s,t} \approx \text{ logarithm } + \text{ constant } + \dots$ 

cf. de Wijs process (logarithm) + white noise (constant).

• Symmetric case  $\beta = \gamma = \frac{1}{4}$  (Duffin & Shaffer, 1960)

 $\pi \nu_{s,t} = 2\ln r + 3\ln 2 + 2\rho - \frac{1}{6}r^{-2}\cos 4\phi + O(r^{-4}),$ 

where  $r^2 = s^2 + t^2$ ,  $\rho = 0.5772...$  is Euler's constant and  $\tan \phi = s/t$ .

• General case  $\beta + \gamma = \frac{1}{2}$ ,  $\beta \neq \gamma$  (Besag & Mondal, 2005)

 $4\pi \,(\beta\gamma)^{\frac{1}{2}} \nu_{s,t} = 2\ln r + 3\ln 2 + 2\rho - \frac{1}{6}r^{-2} \{\cos 4\phi - 4(\beta - \gamma)\cos 2\phi\} + O(r^{-4}),$ where  $r^2 = 4\beta s^2 + 4\gamma t^2$  and  $\tan \phi = \gamma^{\frac{1}{2}} s/(\beta^{\frac{1}{2}}t).$  De Wijs process  $\{Y(\mathbf{r})\}$  on  $\mathcal{R}^2$ 

•  $\{Y(\mathbf{r})\}$  is Gaussian and Markov with spectral density function

$$g(\omega,\eta) = \kappa / (\omega^2 + \eta^2)$$

Realizations defined w.r.t. differences between **regional averages**. Generalized functions : **Schwarz space**.

• Integrated de Wijs process  $\{Y(A)\}$ 

$$Y(A) = \frac{1}{|A|} \int_A dY(\mathbf{x}), \qquad A \subset \mathcal{R}^2.$$

• Variogram intensity is logarithmic: process is conformally invariant.

Let  $A, B \subset \mathbb{R}^2$  with |A| = |B| = 1 and  $\phi(\mathbf{x}) := \mathbf{1}_A(\mathbf{x}) - \mathbf{1}_B(\mathbf{x}), \ \mathbf{x} \in \mathbb{R}^2$ .

$$\Rightarrow \quad \nu(A,B) := \operatorname{var} \left\{ Y(A) - Y(B) \right\} = - \int_{\mathcal{R}^2} \int_{\mathcal{R}^2} \phi(\mathbf{x}) \, \phi(\mathbf{y}) \, \log \|\mathbf{x} - \mathbf{y}\| \, d\mathbf{x} \, d\mathbf{y}.$$

• Can incorporate **asymmetry** and more general **anisotropy**.

# Original lattice $\mathcal{L}_1$ with array $\mathcal{D}_1$ and cells A and B

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## Integrated de Wijs process on $\mathcal{D}_1$

• Recall that De Wijs process on  $\mathcal{R}^2$  has **spectral density function** 

$$g(\omega,\eta) = \kappa / (\omega^2 + \eta^2).$$
  
$$\Rightarrow \quad \nu(A,B) = \frac{4\kappa}{\pi^2} \int_0^\infty \int_0^\infty \frac{\sin^2 \omega \, \sin^2 \eta \, \sin^2(s\omega + t\eta)}{\omega^2 \eta^2 \, (\omega^2 + \eta^2)} \, d\omega \, d\eta,$$

where (s,t) denotes the  $\mathcal{L}_1$ -separation of A and B.

• NB. If  $\phi(\mathbf{x})$  and  $\varphi(\mathbf{x})$  are **test functions**, i.e. integrate to zero, then

$$-\int_{\mathcal{R}^2} \int_{\mathcal{R}^2} \phi(\mathbf{x}) \,\varphi(\mathbf{y}) \,\log \|\mathbf{x} - \mathbf{y}\| \,d\mathbf{x} \,d\mathbf{y} \ \equiv \ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\tilde{\phi}(\omega, \eta) \,\tilde{\varphi}(-\omega, -\eta)}{\omega^2 + \eta^2} \,d\omega \,d\eta,$$

where  $\tilde{\phi}$  and  $\tilde{\varphi}$  are **Fourier transforms** of  $\phi$  and  $\varphi$ . Here

$$\phi(\mathbf{x}) = \varphi(\mathbf{x}) = 1_A(\mathbf{x}) - 1_B(\mathbf{x}), \qquad \mathbf{x} \in \mathcal{R}^2.$$



 $256 \times 256$  arrays

# Sublattice $\mathcal{L}_2$ with subarray $\mathcal{D}_2$ and cells A and B



Consider first-order intrinsic autoregression on  $\mathcal{L}_2$  averaged to  $\mathcal{D}_1$ 





## Intrinsic autoregression



averaged over  $2 \times 2$  blocks

 $256 \times 256$  arrays

# Sublattice $\mathcal{L}_4$ with subarray $\mathcal{D}_4$ and cells A and B



Consider first-order intrinsic autoregression on  $\mathcal{L}_4$  averaged to  $\mathcal{D}_1$ 

## Integrated de Wijs process



## Intrinsic autoregression



averaged over  $4 \times 4$  blocks

 $128 \times 128$  arrays

## Sublattice $\mathcal{L}_8$ with subarray $\mathcal{D}_8$ and cells A and B



Consider first-order intrinsic autoregression on  $\mathcal{L}_8$  averaged to  $\mathcal{D}_1$ 

## First-order intrinsic autoregressions on $\mathcal{L}_m$ averaged to $\mathcal{D}_1$

- $\mathcal{L}_1$  denotes original **lattice** at unit spacing.
  - $\mathcal{L}_m$  denotes corresponding sublattice at spacing 1/m: m = 2, 3, ... $\mathcal{L}_m$  partitions  $\mathcal{R}^2$  into subarray  $\mathcal{D}_m$  of cells, each of area  $1/m^2$ .
- $\{X_{u,v}^{(m)}\}$  denotes symmetric first-order intrinsic autoregression on  $\mathcal{L}_m$ .
- Define sequence of averaging processes  $\{Y_m(A)\}$  on cells  $A \in \mathcal{D}_1$  by

$$Y_m(A) = \frac{1}{m^2} \sum_{(u,v) \in A} X_{u,v}^{(m)}.$$

All contrasts have well–defined distributions with zero mean and finite variance.

• What happens to  $\{Y_m(A)\}$  as  $m \to \infty$ ?

Limiting behaviour of  $\{Y_m(A)\}$  as  $m \to \infty$  (Besag & Mondal, 2005)

$$Y_m(A) = \frac{1}{m^2} \sum_{(u,v) \in A} X_{u,v}^{(m)}, \qquad A \in \mathcal{D}_1,$$

with **variogram** for  $A, B \in \mathcal{D}_1$  separated by (s, t)

the variogram of an integrated de Wijs process  $\{Y(A) : A \in \mathcal{D}_1\}$ .

**Result generalizes** rigorously to any non-empty  $A, B \subset \mathcal{R}^2$ .

In practice, m = 2 or 4 adequate because of rapid convergence.

## Spectral density diagram for simple Gaussian time series



## Spectral density diagram for 2-d Gaussian intrinsic processes



Extends to asymmetric case and some higher-order autoregressions.

# Cotton picking time in NSW, Australia



# (Virtually) de Wijs analysis of 500,000 cotton plots



Debashis Mondal, 2005

## Higher–order intrinsic autoregressions

• Let  $\{X_{u,v}: (u,v) \in \mathbb{Z}^2\}$  be **Gaussian** with conditional means and variances

$$\mathbf{E}\left(X_{u,v}\mid\ldots\right) = \sum_{k,l} \beta_{k,l} x_{u-k,v-l}, \qquad \operatorname{var}\left(X_{u,v}\mid\ldots\right) = \kappa > 0,$$

where (i)  $\beta_{0,0} = 0$  (ii)  $\beta_{k,l} \equiv \beta_{-k,-l}$  (iii)  $\sum_{k,l} \beta_{k,l} = 1$  (iv) ...

•  $\{X_{u,v}\}$  has generalized spectral density function

$$f(\omega,\eta) = \kappa / \{1 - \sum_{k,l} \beta_{k,l} \cos(\omega k + \eta l)\}.$$

• Autoregression is simple if variogram  $\{\nu_{s,t} : s, t \in \mathcal{Z}\}$  exists  $\Rightarrow$ 

$$\nu_{s,t} = \frac{1}{2} \operatorname{var} \left( X_{u,v} - X_{u+s,v+t} \right) = \frac{1}{\pi^2} \int_0^{\pi} \int_0^{\pi} \frac{1 - \cos s\omega \, \cos t\eta}{1 - \sum_{k,l} \, \beta_{k,l} \cos \left(\omega k + \eta l\right)} \, d\omega \, d\eta.$$

Generalizations of limiting behaviour

Second–order intrinsic autoregressions

$$E(X_{u,v} \mid \ldots) = \beta_{10} (x_{u-1,v} + x_{u+1,v}) + \beta_{01} (x_{u,v-1} + x_{u,v+1}) + \beta_{11} (x_{u-1,v-1} + x_{u+1,v+1}) + \beta_{-11} (x_{u-1,v+1} + x_{u+1,v-1})$$

with  $\beta_{10} + \beta_{01} + \beta_{11} + \beta_{-11} = \frac{1}{2}$  etc.

- Diagonally symmetric : β<sub>10</sub> = β, β<sub>01</sub> = γ, β<sub>11</sub> = ½δ = β<sub>-11</sub>
  ν<sub>m</sub>(A, B) → variogram of asymmetric integrated de Wijs process.
  i.e. limiting spectral density ∝ 1/{(β + δ) ω<sup>2</sup> + (γ + δ) η<sup>2</sup>)}.
  NB. includes first-order case with δ = 0 but β ≠ γ.
- Diagonally antisymmetric :  $\beta_{10} = \beta$ ,  $\beta_{01} = \gamma$ ,  $\beta_{11} = \frac{1}{2}\delta = -\beta_{-11}$   $\nu_m(A, B) \rightarrow \text{variogram of anisotropic integrated de Wijs process.}$ i.e. limiting spectral density  $\propto 1/(\beta\omega^2 + 2\delta\omega\eta + \gamma\eta^2)$ .

# Extreme special case

$$E(X_{u,v} \mid \ldots) = \frac{1}{4} (x_{u-1,v} + x_{u+1,v}) - \frac{1}{4} (x_{u,v-1} + x_{u,v+1})$$
  
+  $\frac{1}{4} (x_{u-1,v-1} + x_{u+1,v+1}) + \frac{1}{4} (x_{u-1,v+1} + x_{u+1,v-1})$ 







 $128\times 128$  averaged over  $2\times 2$  blocks

Generalizations of limiting behaviour

Third–order intrinsic autoregressions

• Symmetric simultaneous intrinsic autoregression (cf. Whittle, 1954)

$$X_{u,v} = \frac{1}{4} \left( X_{u-1,v} + X_{u+1,v} + X_{u,v-1} + X_{u,v+1} \right) + Z_{u,v}$$

where  $\{Z_{u,v}\}$  is Gaussian white noise  $\Rightarrow$ 

$$E(X_{u,v} \mid \ldots) = \frac{2}{5} (x_{u-1,v} + x_{u+1,v} + x_{u,v-1} + x_{u,v+1}) - \frac{1}{10} (x_{u-1,v-1} + x_{u+1,v+1} + x_{u-1,v+1} + x_{u+1,v-1}) - \frac{1}{20} (x_{u-2,v} + x_{u+2,v} + x_{u,v-2} + x_{u,v+2})$$

Requires higher-order differences or contrasts for well-defined distributions. Limiting process corresponds to thin-plate smoothing spline i.e. limiting spectral density  $\propto 1/(\omega^2 + \eta^2)^2$ .

# Generalizations of limiting behaviour

Third–order intrinsic autoregressions

• Locally quadratic intrinsic autoregression (Besag and Kooperberg, 1995)

$$E(X_{u,v} \mid \ldots) = \frac{1}{4} (x_{u-1,v} + x_{u+1,v} + x_{u,v-1} + x_{u,v+1}) + \frac{1}{8} (x_{u-1,v-1} + x_{u+1,v+1} + x_{u-1,v+1} + x_{u+1,v-1}) - \frac{1}{8} (x_{u-2,v} + x_{u+2,v} + x_{u,v-2} + x_{u,v+2})$$

Requires genuine **two-dimensional differences** for well-defined distributions.

Limiting spectral density  $\propto 1/(\omega^4 - \omega^2 \eta^2 + \eta^4)$ .

## Wrap up

- Gaussian Markov random fields are alive and well!!
- Precision matrix of Gaussian MRF's sparse  $\Rightarrow$  efficient computation.
- Regional averages of Gaussian MRF's  $\xrightarrow{\text{rapid}}$  continuum de Wijs process.
- **Reconciliation** between Gaussian MRF and original geostatistical formulation.
- Empirical evidence for de Wijs process in agriculture :
   P. McCullagh & D. Clifford (2006), "Evidence of conformal invariance for crop yields", *Proc. R. Soc. A*, 462, 2119–2143.

Consistently selects de Wijs within Matérn class of variograms (25 crops!).

• de Wijs process also alive and well and can be fitted via Gaussian MRF's.