Estimation & Dependence in Space
Lecture 3: Random fields and Other Dependent Data

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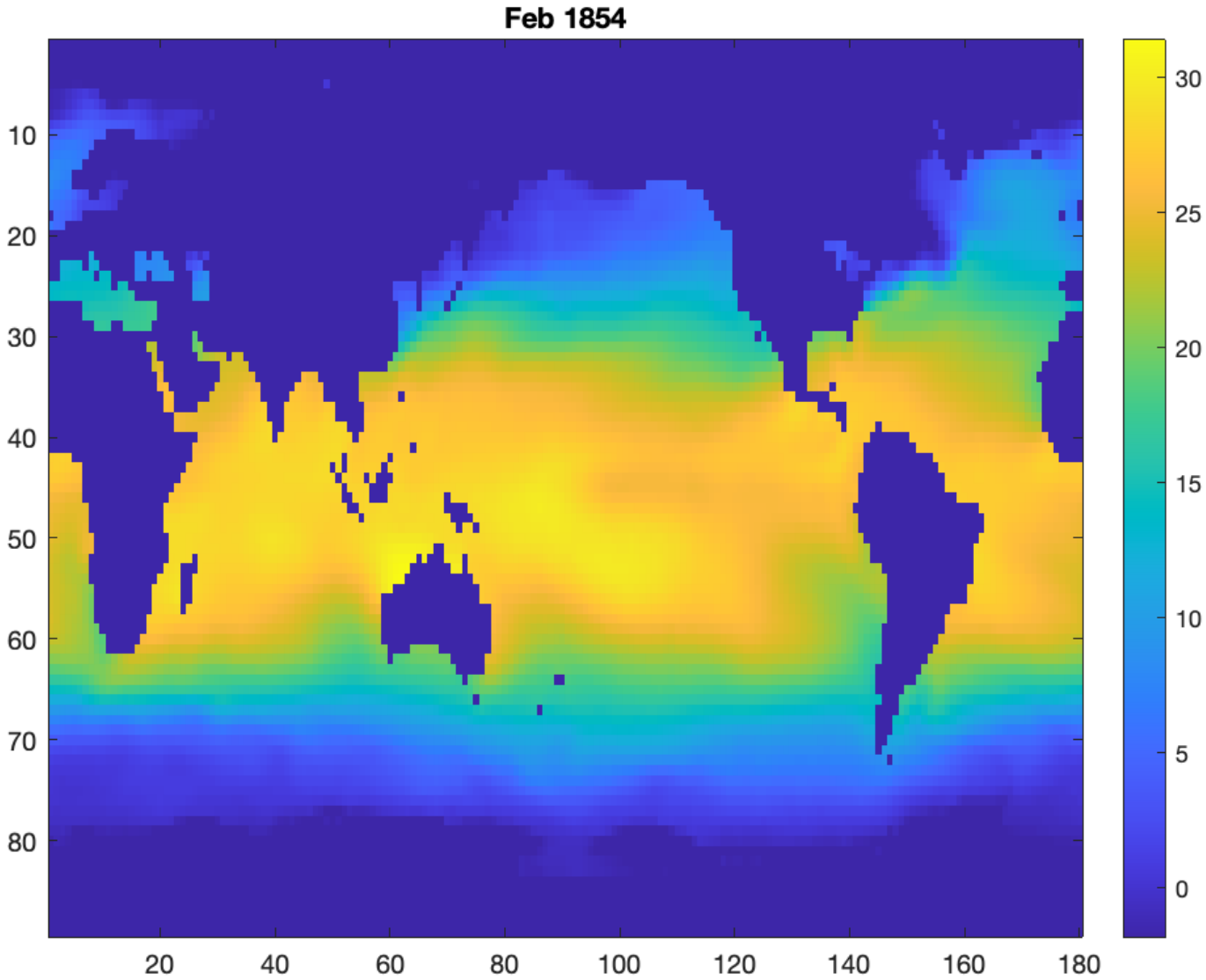
Examples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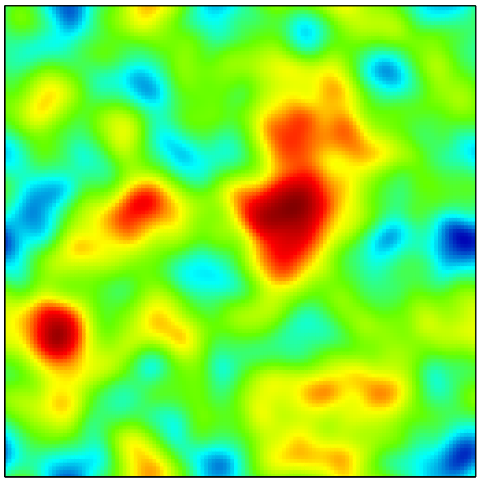
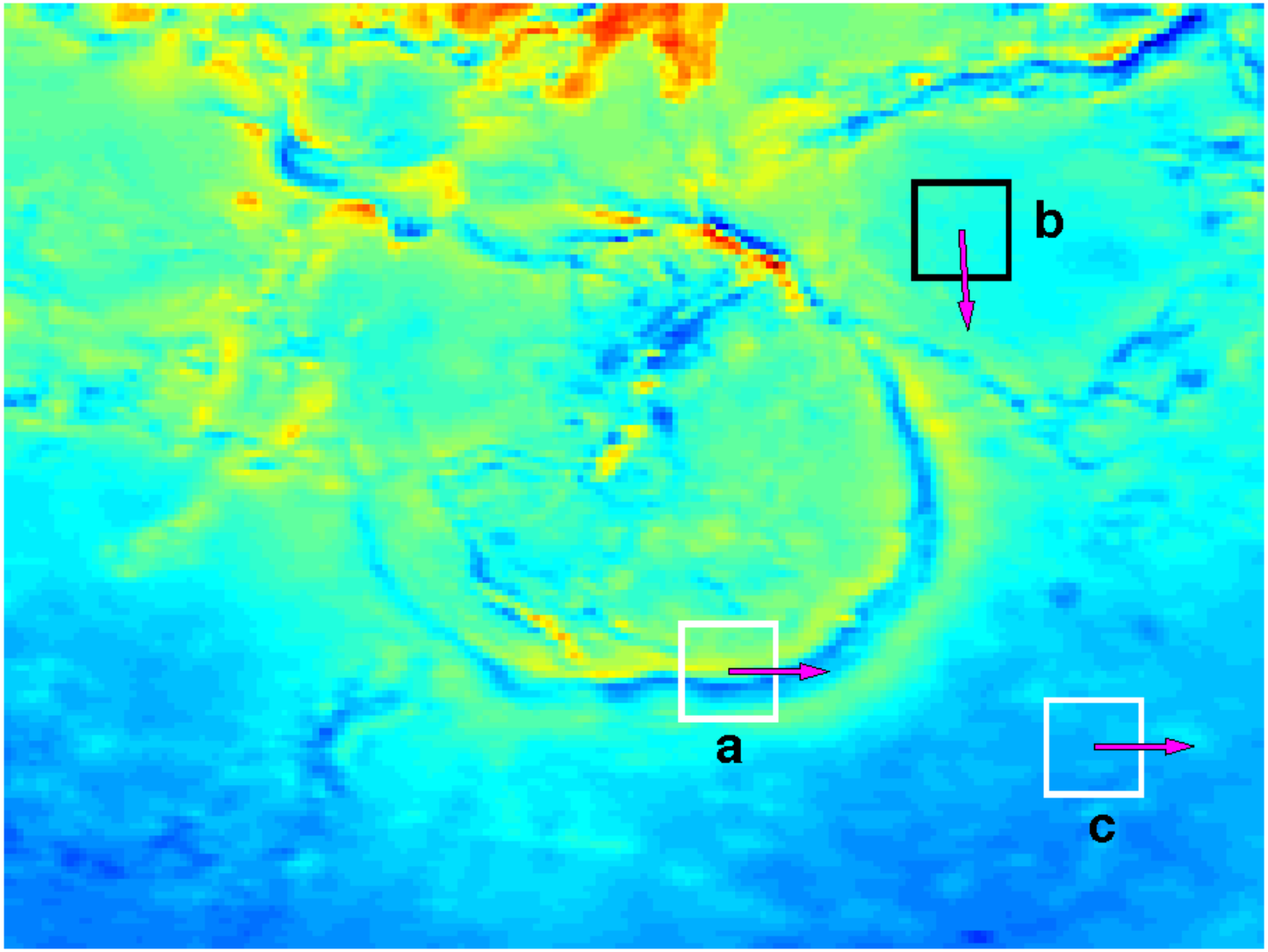
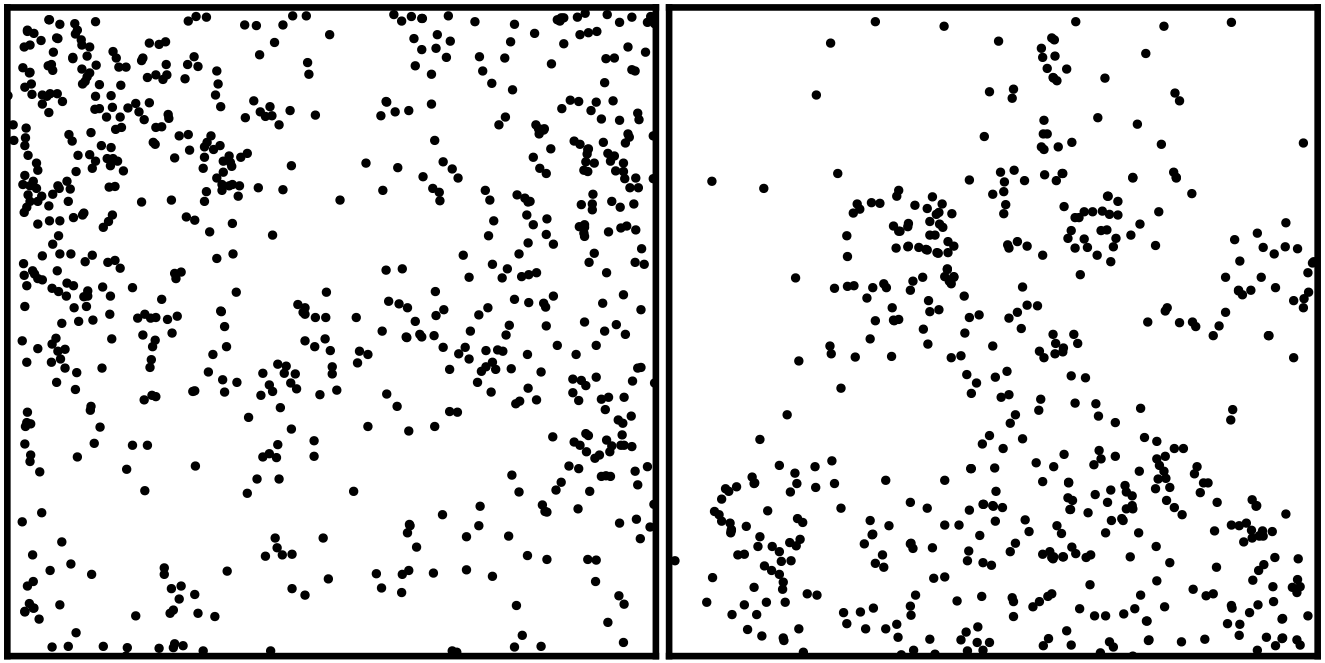


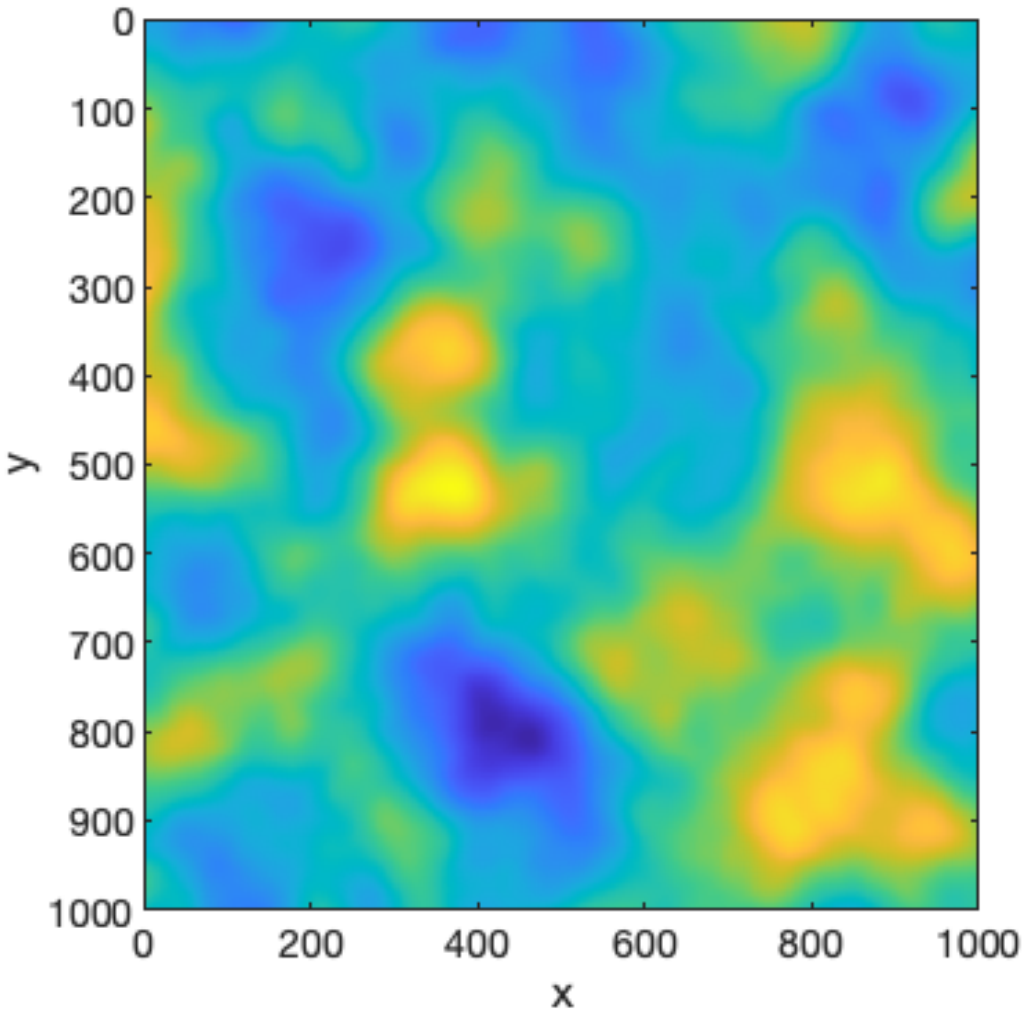
Isotropic, anisotropic & unidirectional random fields.



Topography of Venus.



Point patterns of tree locations for hickory and maple.



Matérn random field.

Random Fields

Random field

Stochastic object.

Definition (Random Field)

A random eld $G(\mathbf{x})$ is a stochastic process where $G(\mathbf{x})$ is vector-valued realisation with dimension p and $\mathbf{x}$ has dimension d then G is a $(d;p)$ random eld.

We should mention Kolmogorov's extension theorem, that relates the distribution of a finite sample to that of the process.

Definition (Gaussian Random Field)

A Gaussian random eld $G(\mathbf{x})$ is a collection of p-variate random vectors for each value of $\mathbf{x}$, whose mean function takes the form $_G(\mathbf{x})$ and

$$\Sigma_{GG}(\mathbf{x}_1;\mathbf{x}_2) = \mathrm{E}\left\{(G(\mathbf{x}_1) \quad (\mathbf{x}_1))(G(\mathbf{x}_2) \quad (\mathbf{x}_2))^T\right\};$$

where any p-variate set of samples has a multivariate Gaussian distn.

Isotropic Random field

What is an isotropic Gaussian spatial process?

Definition (Gaussian Homogeneous Random Field)

$G(\mathbf{x})$ is a Gaussian Homogeneous Random Field if it is a Gaussian Random Field, the mean is constant and $\Sigma_{GG}(\mathbf{x}_1;\mathbf{x}_2)$ only depends on $\mathbf{x}_1 \quad \mathbf{x}_2$; or equivalently $\Sigma_{GG}(\mathbf{x}_1;\mathbf{x}_2) = C_{GG}(\mathbf{x}_1 \quad \mathbf{x}_2)$.

Definition (Gaussian Isotropic Homogeneous Random Field)

$G(\mathbf{x})$ is a Gaussian Isotropic Homogeneous Random Field if it is a Gaussian Homogeneous Random Field, the mean is constant and $\Sigma_{GG}(\mathbf{x}_1;\mathbf{x}_2)$ only depends on $k\mathbf{x}_1 \quad \mathbf{x}_2 k$, or equivalently $\Sigma_{GG}(\mathbf{x}_1;\mathbf{x}_2) = C_{GG}(k\mathbf{x}_1 \quad \mathbf{x}_2 k)$.

These assumptions may seem arbitrary. Homogeneity is the spatial equivalent of stationarity; isotropy enforces additional symmetry.

A special class of Matérn random fields

Are there any examples of (Gaussian) random fields? One example is to take with
; ; ^{2} 2 R^+

$$C_{GG}(\mathbf{h}) = \ ^2\frac{2^1}{\Gamma(\ )}\ \ \left(\frac{p}{2}\frac{k\mathbf{h}k}{\ }\right)\ \ K\ \ \left(\frac{p}{2}\frac{k\mathbf{h}k}{\ }\right)\ ; \tag{1}$$

where $K\ (\ )$ is a Bessel function of the second kind.

The Matern model is very popular in geophysics.

It monotonically decays in its argument. The covariance corresponds to the spectral density of

$$S_{GG}(\mathbf{k}) = \ ^2\frac{4\ \ \Gamma(\ \ +1)(2\ \ )}{\Gamma(\ \ )\ ^2}\ \ \left(\frac{2}{\ _2}+4\ \ ^2k\mathbf{k}k^2\right)^{\ \ 1=2}; \quad \mathbf{k}\ 2\ \mathrm{R}^2: \tag{2}$$

It can be hard to estimate both and in this model, see [21], and also [14].

Anisotropic Matérn random fields

Assume you wish to incorporate anisotropy in the Matérn model following [11].

We introducing the deformation matrix $\mathbf{D}$ and replacing $k\mathbf{k}k^2$ by $\mathbf{k}^T\mathbf{D}\mathbf{k}$:

The new spectrum takes the form

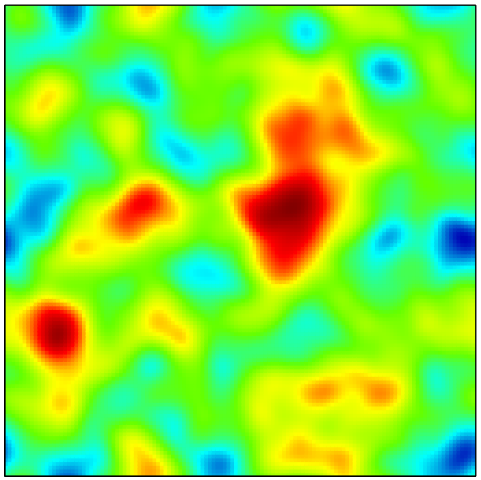
$$S_{GG}(\mathbf{k}) = {}^{2}\frac{4 \ \Gamma(\ +1)(2 \ )}{\Gamma(\ ) \ ^{2}} \ \frac{2}{2} + 4 \ {}^{2}\mathbf{k}^T\mathbf{D}\mathbf{k} \qquad ^{1=2}; \quad \mathbf{k} \ 2 \ \mathrm{R}^2: \tag{3}$$

We assume that the matrix $\mathbf{D}$ admits a spectral representation of

$$\mathbf{D} = \mathbf{R} \qquad \mathbf{R} \ ;$$

where is diagonal.

As $_{\max} = \ _{\min}$ changes the degree of anisotropy changes.



Isotropic ($_{\max} = \ _{\min}$), anisotropic ($_{\max} > \ _{\min}$) & unidirectional ($_{\max} >> \ _{\min}$) random fields.

Probabilistic symmetries

Kallenberg [15, 6] discusses the notion of probabilistic symmetries more broadly.

Note that it consists of the property for the distribution of the infinite dimensional object (stationarity, cyclo-stationarity, contractability, exchangeability, isotropy) and the action itself (temporal shifts, periodic temporal shifts, contractions, permutations, rotations).

We know about intrinsic representations that follow from these assumptions, e.g. the spectral representation, Aldous–Hoover etc.

The representation is useful as it helps us model the intrinsic random object.

There are issues when dealing with finite samples as the symmetry refers to the process, not the finite sample. Cyclo-stationarity and finitely exchangeable (extendable...) sequences are a way to acknowledge finiteness.

Spectral Distribution Theorem

OK, so assuming just homogeneity of the underlying spatial process we get the d-dimensional spectral representation theorem.

Theorem (Spectral distribution theorem [1])

A continuous function $C : \mathrm{R} \nearrow \mathrm{C}$ is non-negative de nite function (i.e. a covariance function) if and only if there exists a nite measure $S^{(I)}(\ )$ on the Borel { eld such that

$$C(\mathbf{x}) = \int_{\mathrm{R}^d} e^{i\mathbf{x}^T\mathbf{k}} dS^{(I)}(\mathbf{k}): \tag{4}$$

For one dimension we characterised the spectral density into three components, we are not doing that here.

Spectral Representation Theorem

We now can use this distribution theorem to obtain:

Theorem (Spectral representation theorem [1])

Let $S^{(I)}(\ )$ be a nite measure and Z a complex $S^{(I)}(\ )$-noise. Then the complex valued random eld

$$Y(\mathbf{x}) = \int_{\mathbb{R}^d} e^{i\mathbf{x}^T\mathbf{k}}\, dZ(\mathbf{k}) \tag{5}$$

has covariance

$$C(\mathbf{x};\mathbf{y}) = \int_{\mathbb{R}^d} e^{i(\mathbf{x}\ \mathbf{y})^T\mathbf{k}}\, dS^{(I)}(\mathbf{k}): \tag{6}$$

and so is a homogeneous random eld. Furthermore, to every mean square continuous, centered, (Gaussian) stationary random eld Y with covariance function C and spectral measure $S^{(I)}(\ )$ there corresponds a complex (Gaussian) $S^{(I)}(\ )$-noise Z such that (5) holds in mean square for each $\mathbf{x}$. In both cases, Z is called the spectral process corresponding to Y.

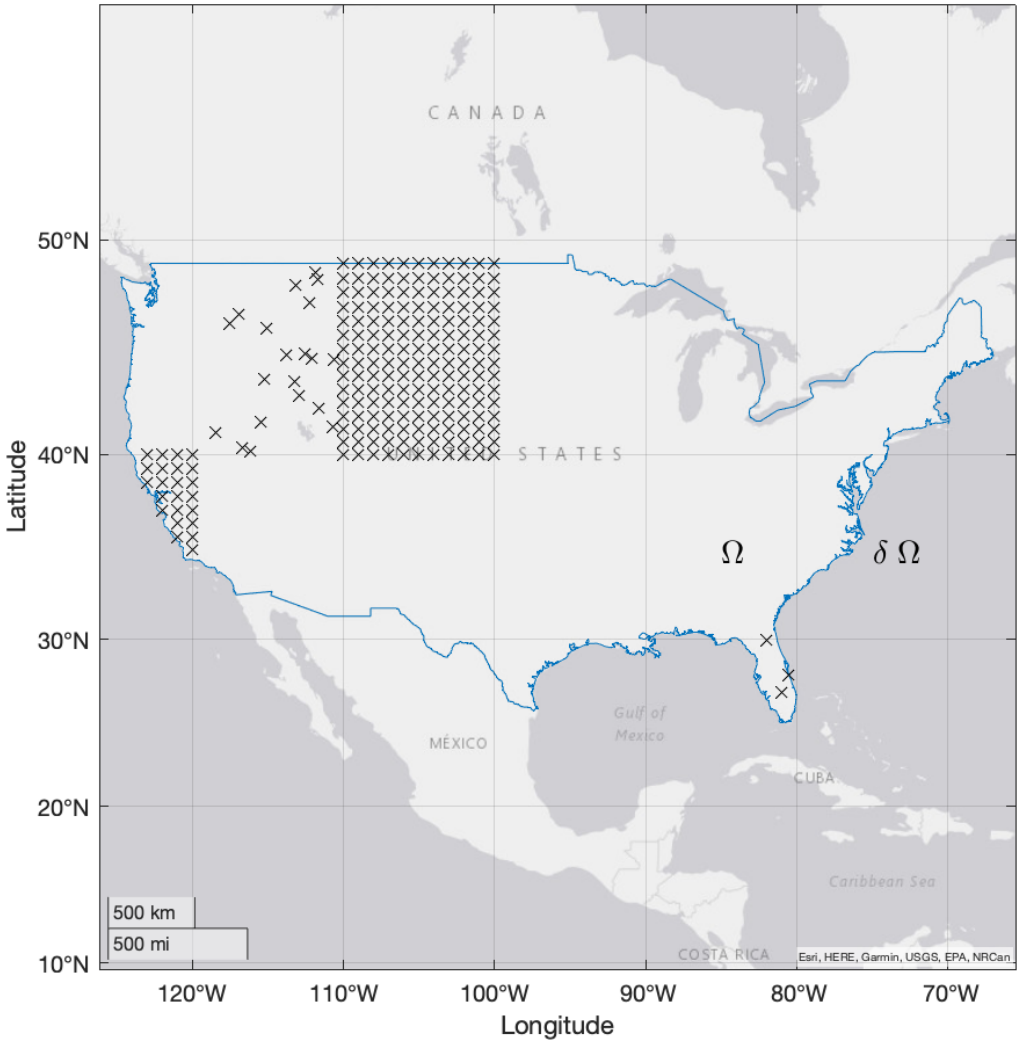
Sampling

Recording spatial phenomena

Any process we record has to be sampled or observed. In signal processing this is called sampling. Signal processing sampling refers to the spatial sampling design, not sampling in the statistical sense of a sampling distribution.

- We can sample spatial regions by the aggregate effect for the region Ω with boundary Ω.
- We can sample spatial regions by putting a regular grid with sampling period $\Delta_1 > 0$ and $\Delta_2 > 0$ in a region Ω.
- We can sample locations uniformly at random inside Ω.
- Ω can be a tensor product of regions, or completely irregular.

Recording spatial phenomena



Asymptotics

Normally we are interested in what happens for large samples of observations. In space this now comes with many potential choices.

- We sample $Y(\mathbf{x})$ at locations $\mathbf{x}_i$ 2 Ω with boundary Ω.
- We assume we observe $Y(\mathbf{x})$ at N points. One potential is to let N ! 1. Gaussian limits should happen.
- We can decide if $j\Omega j$ is fixed or growing with N. This leads to **xed domain** (see [20] or [21]) or **growing domain** asymptotics [13].
- In fixed domain asymptotics we are getting more and more high frequency information about $Y(\mathbf{x})$ (with some caveats).
- In growing domain asymptotics we are getting more highly resolved frequency information.
- Some parameters are not consistently estimated with some choices of sampling domains [20, 21], and asymptotic growth schemes [22].

Kriging

Kriging

Kriging is a method for interpolating spatial data.

This is based on knowing the covariance structure that generated the data, so normally this has to be estimated.

Suppose that we observe a random field $fY(\mathbf{x})g$ at locations $\mathbf{x}_1; : : : ; \mathbf{x}_n$ and wish to predict the value of the field at another location, $\mathbf{x}_0$, say.

We collect the observations in vector $\mathbf{Y} = \quad Y(\mathbf{x}_1) \quad ::: \quad Y(\mathbf{x}_n) \quad ^T :$

Thus we take

$$\text{Ŷ}(\mathbf{x}_0) = \quad + \quad ^T \mathbf{Y} :$$

To get a good choice of and we minimize that mean square prediction. We define $(\mathbf{x}_0) = \mathrm{E} f\mathbf{Y}(\mathbf{x}_0)g$, $C_0 = C(\mathbf{x}_0; \mathbf{x}_0)$, $\mathbf{p} = \mathrm{Cov} f\mathbf{Y}; Y(\mathbf{x}_0)g$ and $\mathbf{P} = \mathrm{Cov} f\mathbf{Y}; \mathbf{Y}^T g$. We find

$$= \mathbf{P} \quad ^1\mathbf{p}; \qquad = \quad (\mathbf{x}_0) \qquad ^T\mathbf{p} :$$

This determines our predictor $\text{Ŷ}(\mathbf{x}_0)$ if the covariance is known, otherwise a covariance family is chosen and its parameters estimated.

Spectral Inference

Inference

Our first idea for making inferences might be to evaluate the log-likelihood. As long as the models we are interested in have a covariance function $C(h; \ )$, enumerating the covariance matrix of the sample $C(\ )$ we can (theoretically) evaluate:

$$`(\ ) = \frac{1}{2} \log|C(\ )| \quad \frac{1}{2}(Y \quad)^T C^{1}(\ )(Y \quad): \qquad (7)$$

We can then for Gaussian data determine the maximum likelihood estimator [16].

Unfortunately the matrix inversion is prohibitive.

We need an appropriate choice of quasi{likelihood.

Inference I

We can transform this log-likelihood to the spectral domain.

This means we replace the log-likelihood of (7) with an approximation.

This approximation is based on the form of circulant matrices, but using an approximation rather than the exact form.

We could also look at the exact likelihood of the DFT of a Gaussian sampl This would have a di erent variance, and some covariance.

We start by de ning the tapered DFT:

$$J_l(k) = \sum_{x \in D} h_l(x) e^{-i x^T k}: \tag{8}$$

The l notation is used for non-parametric estimation, and will be replaced b a 0 in this section.

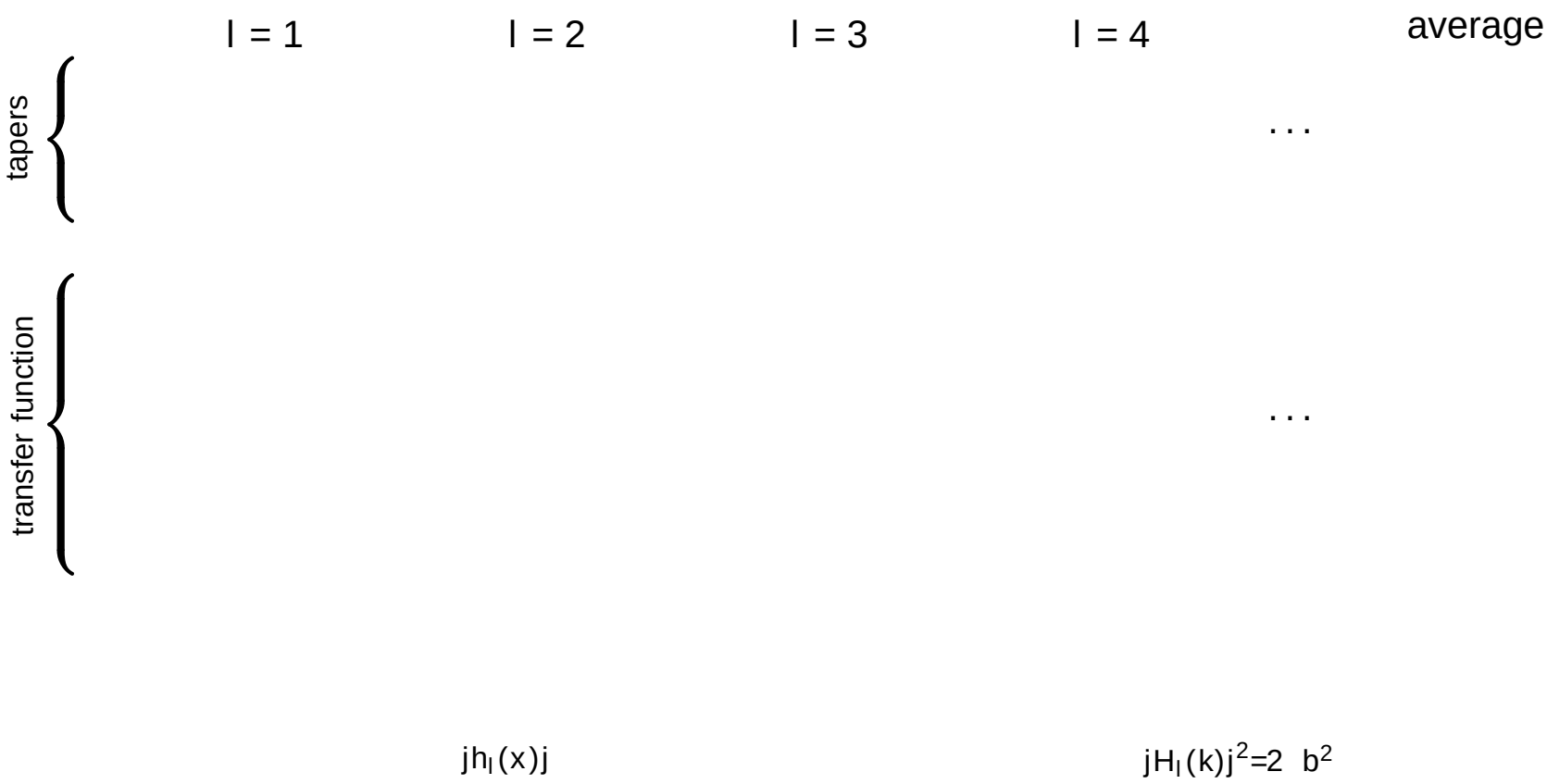


Figure: Irregular region spatial tapering from [12].

Non-parametric inference

We can de ne raw spectral estimates from the multitaper method. The simplest multitaper estimate is

$$\hat{S}^{(mt)}(k) = \frac{1}{K}\sum_{l=0}^{K-1} \hat{S}_l^{(d)}(k):$$

We can determine its expectation:

$$\begin{aligned} E\left\{\hat{S}^{(mt)}(k)\right\} &= \frac{1}{K}\sum_{l=0}^{K-1} E\left\{\hat{S}_l^{(d)}(k)\right\} \\ &= \frac{1}{K}\sum_{l=0}^{K-1}\int_{-\frac{1}{2}}^{\frac{1}{2}} H_l(f - f')S(f')df' \\ &= \int_{-\frac{1}{2}}^{\frac{1}{2}} \overline{H}(f - f')S(f')df' \end{aligned}$$

We call $\overline{H}(k) = \frac{1}{K}\sum_{l=0}^{K-1} H_l(k)$ the average kernel.

We can note that

$$\mathrm{Var}\left\{\hat{S}^{(mt)}(k)\right\} \approx \frac{S^2(k)}{K}$$

As the dimensions increase, the number of degrees of freedom balloon, ar
so bias inevitably dwarfs variance.

Parametric Inference II

We de ne the Whittle log-likelihood:

$$\grave{}_W(\ ) = \sum_{k2J} \log|S(k)| + \frac{|J_0(k)|^2}{S(k)} \quad : \tag{9}$$

This approximates the Gaussian likelihood with $N \log N$ computation time.

As long as $f J_0(k)g$ is jointly Gaussian, then we just need the mean and covariance.

Guillaumin et al. [13] showed there was no loss of rate by ignoring the covariances.

The main problem for $d = 2$ and higher is that $E|J_0(k)|^2 g \neq S(k)$ (even for large samples). The boundary bias for large samples is the dominant error (not the variance). The trick is to replace $S(k)$ by its e ective equivalent $\overline{S}(k)$, leading to a rate-optimal procedure with $N \log N$ computation time.

This method also works for inhomogeneous spatial models, as long as the spatial covariance $C(h; \ )$ can be enumerated, and the sampled process satis es Signi cant Correlation Contribution.

This ensures the correlation is not too strong,

The di erence of the sampled spectra over all frequencies is signi cant.

[13] states these conditions formally.

It is important to appreciate the di erences between one dimension and higher. It is necessary to replace $S(k)$ with the expected periodogram

$$\overline{S}_n(k; \ ) = \frac{(2 \ )^d}{\sum_{s2J} g_s^2} f f_X(\ ; \ ) \ F_n(\ ) g(k) \qquad (10)$$

$$= \frac{(2 \ )^d}{\sum_{s2J} g_s^2} \int_{\mathbb{R}^d} f_X(k \ k^0; \ ) F_n(k^0) \, dk^0;$$

where

$$F_n(k) = n^{-1} \sum_{s2J} g_s \exp(i k \ s)^2 ; \qquad k 2 \mathbb{R}^d : \qquad (11)$$

Intrinsic Random Functions

Intrinsic random functions

When we discussed the characteristics of temporal processes we talked ab three typical non-stationary mechanisms: 1) time-inhomogeneity, 2) integrated processes, and 3) frequency coupling.

We never discussed integrated processes, just the other two yesterday.

Integrated processes or di erence stationary processes have too much correlation to be stationary. Some of the fractionally integrated processes also are non-stationary (FARIMA and fBM).

They are common models for time series in econometrics (unit root models for instance), and part of de ning two nonstationary time series whose di erence is stationary (co-integration).

Intrinsic random functions II

An intrinsic random function is a special case of Gelfand's [4, 5] generalize processes with stationary increments, see also Matheron [17].

They can (informally) be thought of as an aggregation of polynomials with random coe cients and the sum of zero mean stationary processes.

In this instance we do not wish to compute the mean and second order statistics, as the variance of the Intrinsic Random Function is not nite.

Instead we normally assume that

$$\text{Varf}\, Y(x_0 + h) \quad Y(x_0)g$$

is nite. It stops being reasonable to calculate the auto-covariance sequenc

Instead for such processes we calculate the semi-variogram [7]:

$$_h(x) = \frac{1}{2} E^{n} (Y(x + h) \quad Y(x)g)^{2} \; ^{o} : \tag{12}$$

A random eld satisfying the intrinsic hypothesis (characterised by its variogram) is said to follow the intrinsic scheme [7].

Intrinsic random functions III

If $Y(x)$ is second-order stationary (homogeneous) then we have

$$_h(x) = \quad (0) \qquad ((h));$$

which is independent of x.

The semi-variogram is bounded as $_h(x) \quad 2\ (0)$:

Even if a semi-variogram satis es the bounds of Cauchy{Schwarz, non-negativity and its upper bound, there may be no corresponding process [7].

Why do we care about such processes? Many phenomena in geophysics a \red", e.g. have a spectral density supported on low frequencies, and a slo varying trend added.

Topography of North America.

Other probabilistic symmetries

Other probabilistic symmetries

We have discussed translation invariance, and how that leads to the spect representation theorem.

We discussed permutation invariance and exchangeability, which lead to th de Finetti representation in 1-d arrays (sequences).

Other stochastic process representations include the Chaotic representatio theorem for Lévy processes and the predictable representation of Lévy processes [18].

We are now (brie y) going to discuss random graphs.

Graphs or network data structures

A network represents interactions between entities (nodes or vertices), where the presence of an interaction is indicated by an edge.

A network (or graph) G is a pair $G = (V, E)$ of sets so that $E \subseteq [V]^2$. We refer to the elements of V as the vertices (or nodes) of the graph, and E are the edges of G, written as $V(G)$ and $E(G)$.

A vertex v is incident with an edge e if $v \in e$.

Two vertices are adjacent or neighbours if connected by an edge.

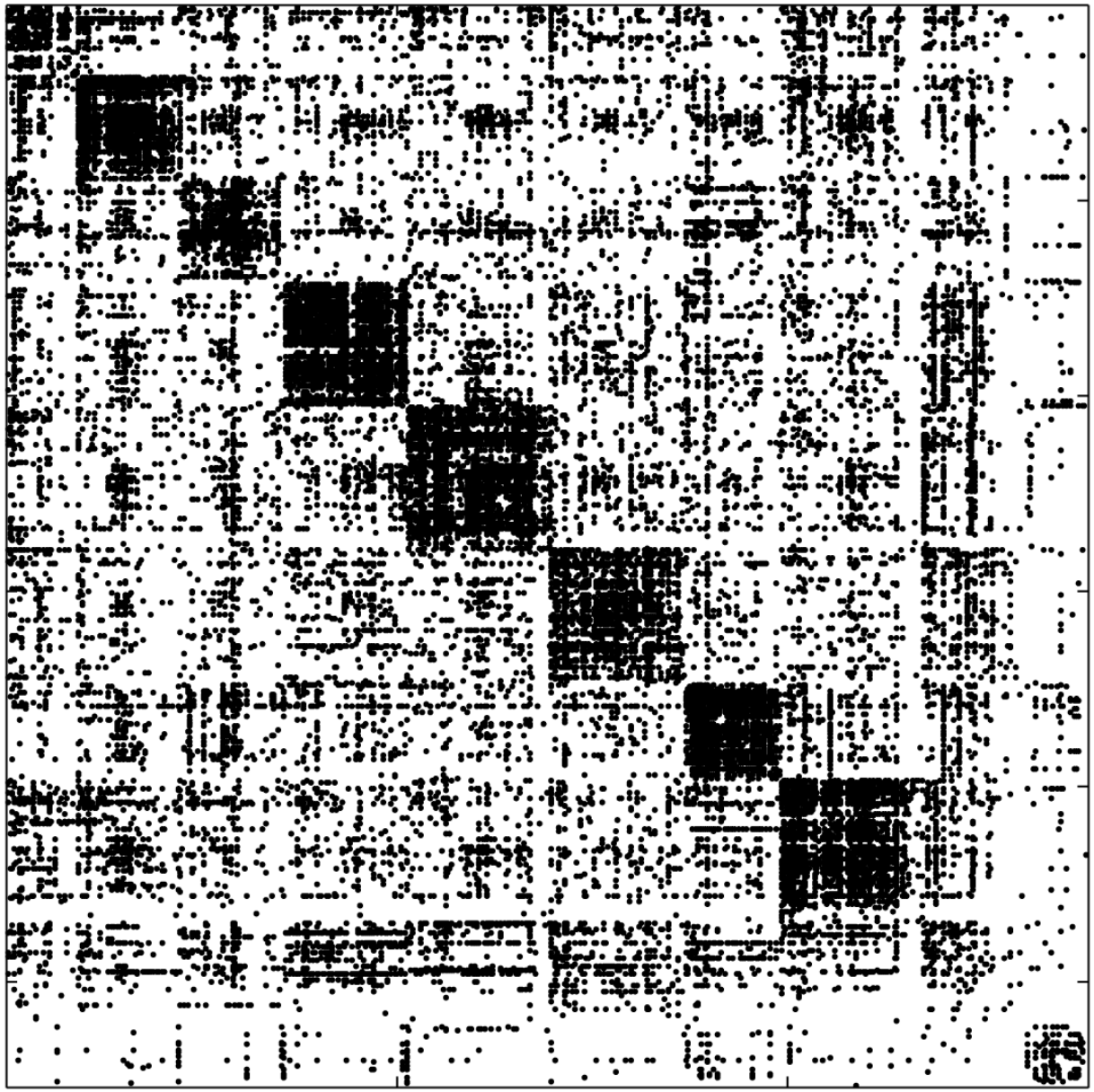
Labelled graphs or networks.

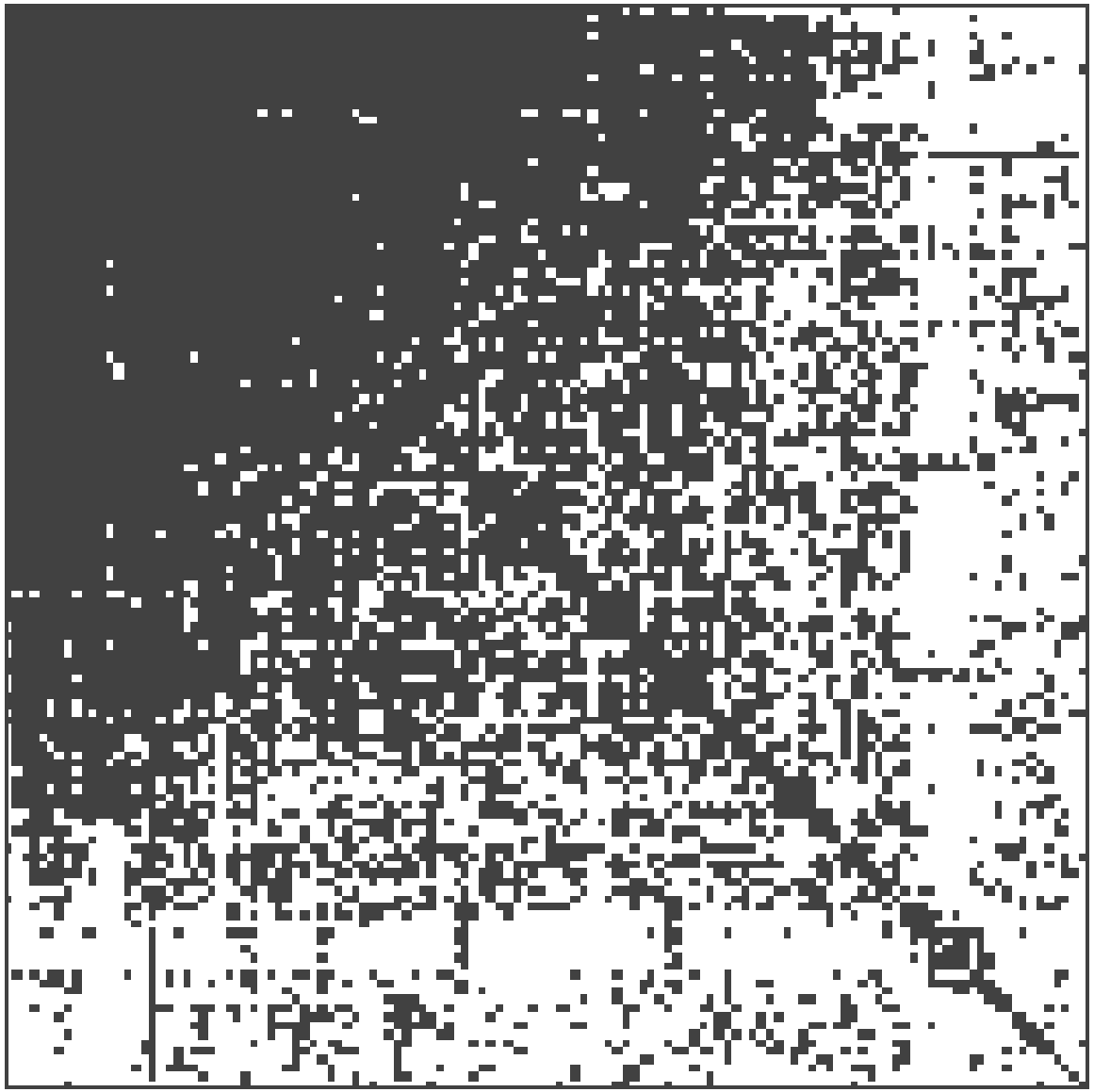
We write a network or a graph as G, which is usually represented by an adjacency matrix A. The edge variable A_{ij} where if node i and node j are linked A_{ij} takes the value unity, otherwise it takes the value zero.

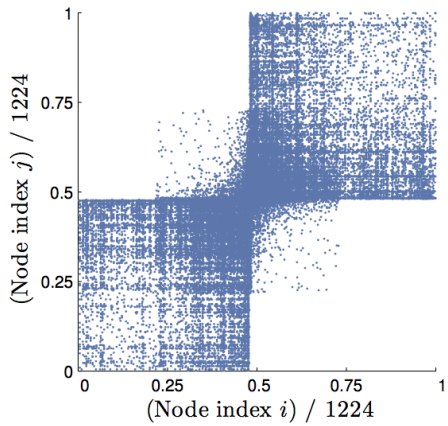
A network can also be represented by a list of edges, an edge list just specifies the existing edges, e.g. $\{(1, 15), (1, 32), \ldots\}$.

We normally assume that $|V(G)| = n$ if not specified otherwise.

A graph $H = (V(H), V(H))$ is a subgraph of G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$.



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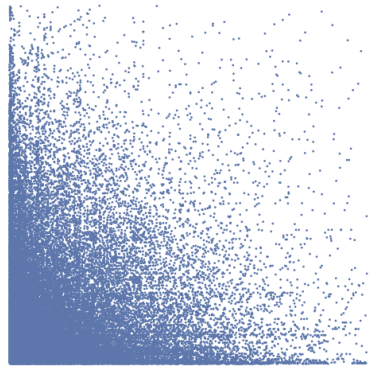

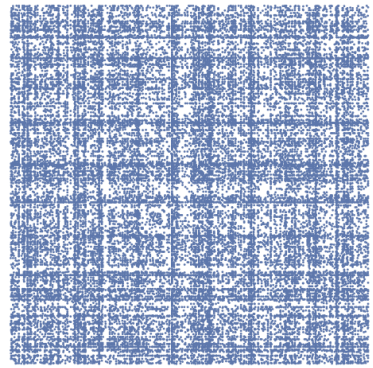

Most of the common network models fall in a more general framework of permutation invariance. Namely, that for most of the enumerated model the value of i or j contain no information about the model structure. Thus if we introduce a permutation that remaps all indices, the nature of the model should not change.

Permutation invariance is a stochastic invariance. What other examples have you met? (hint: translation & rotation invariance). With what property of a stochastic process?

Let Π be a permutation on the ordering so that $\Pi(f1;:::;ng) = f\ (1);:::;\ (n)g$, and let the repermuted adjacency matrix be A^{Π}.

Definition

Permutation-invariance of the distribution holds when $\Pr(A = a) = \Pr(A^{\Pi} = a)$ *for any permutation and any adjacency matrix A. That is, permuting the adjacency matrix does not change its distribution. Then we say that the distribution is permutation-invariant.*

Furthermore this can be related to the underlying array.

Definition

Let E be a suitable space. A sequence of E-valued random variables $(X_n)_{n2\mathbb{N}}$ is exchangeable if

$$(X_n)_n \stackrel{d}{=} (X_{\Pi(n)})_n \quad 8\Pi\ 2\ \mathrm{Sym}(\mathbb{N});$$

where Sym([n]) *is the group of all permutations of* [n] *and* Sym(N) *is the group of all permutations of* N.

Note that this is really an assertion about the measure which is the joint law of the r.v.s (X_n): it is invariant under the action of Sym(N) by the permutation of coordinates. When $E = f0; 1g$ these were studied by de Finetti in the 1930's; for more general E see results by Hewitt and Savage in the 1950's.

Exchangeability

Definition (Exchangeable arrays)

More generally, for any k 1 we can consider an array of E-valued r.v.s $(X_e)_{e \in \mathrm{N}^{(k)}}$ *indexed by size-k subsets of* N, *and say it is (jointly) exchangeable if* $(X_e)_e \stackrel{d}{=} (X_{\Pi(e)})_e$ $\forall \Pi \in \mathrm{Sym}(\mathrm{N})$, *where if* $e = \{n_1, \ldots, n_k\}$ *then* $\Pi(e) := \{\Pi(n_1), \ldots, \Pi(n_k)\}$.

General arrays were studied by Hoover, Aldous, Fremlin and Talagrand and Kallenberg. Finite exchangeability simply puts e in a finite space. A finite $n \quad m$ random matrix $\mathbf{A}$ is row-column exchangeable if for n-permutation and m-permutations

$$\begin{aligned} &\Pr\{A_{11} \in N_{11}, A_{12} \in N_{12}, \ldots, A_{nm} \in N_{nm}\} \\ &= \Pr\{A_{(1)(1)} \in N_{11}, A_{(1)(2)} \in N_{12}, \ldots, A_{(n)(m)} \in N_{nm}\}, \end{aligned}$$

for all Borel sets $N_{11}, \ldots, N_{nm}$.

For $r > n$ and $q > m$ the matrix $\mathbf{A}$ is called $(r; q)$-extendible if there are matrices $\mathbf{T}$, $\mathbf{Z}$ and $\mathbf{W}$ with

$$\mathbf{T} = (A_{ij}); \quad i = 1; : : : ; n; \quad j = m + 1; : : : ; q \tag{13}$$

$$\mathbf{Z} = (A_{ij}); \quad i = n + 1; : : : ; r; \quad j = 1; : : : ; m \tag{14}$$

$$\mathbf{W} = (A_{ij}); \quad i = n + 1; : : : ; r; \quad j = m + 1; : : : ; q; \tag{15}$$

such that

$$\mathbf{A} = \begin{matrix} \mathbf{A} & \mathbf{T} \\ \mathbf{Z} & \mathbf{W} \end{matrix};$$

is row-column exchangeable. A matrix that is $(r; q)$ extendible for all $r > n$ and $q > m$ is called infinitely extensible.

Theorem (Aldous Hoover)

An array $\mathbf{A}$ *is jointly exchangeable, i it has the same distribution as*

$$A_{ij} = f(\ ; \ _i; \ _j; \ _{ij}); \ 1 \quad i < j;$$

with $f : \mathrm{R}^4 \ 7! \ \mathrm{R}$ *and some iid random uniform variables* , $_i$ *and* $_{ij}$.

Exchangeable arrays

We can also express this theorem as:

Theorem (Aldous–Hoover)

An array $\mathbf{A}$ *is jointly exchangeable, i it has the same distribution as*

$$A_{ij} \overset{iid}{=} \text{Bern}(f(\ _i;\ _j));\ 1 \quad i < j;$$

with $f : \mathrm{R}^2 \mapsto [0;1]$ *and some iid random uniform variables* $\ ,\ _i$.

With only one realization; can only estimate for one usually using stochastic block model. Let us thus remove that notation.

With additional smoothness assumptions on $f(x;y)$ such as Hölder( ); various averaging strategies for estimation has been proposed using the stochastic blockmodel e.g. Olhede & Wolfe (2014), Chatterjee (2015), Gao et al (2015) etc.

Probabilistic invariances

This set of lectures covered structured and dependent data.

We started out with 1 dimensional shift invariance, and studied stationary sequences.

We acknowledged that they may have been sampled a process with countably many entries.

We then looked at 2 dimensional shift invariance, and adding on rotational invariance.

Finally we explored permutation invariance for symmetric arrays.

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