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Optimal design and properties of correlated processes with semicontinuous covariance

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Outline

- Topology-algebra interplay for stochastic processes (continuous and more complex times)
- Semicontinuity of covariance, dependence structures
- Trend and Covariance parameter issues
- Applications (Finance, Image Processing, Geography..)
- Open problems

Which design is good for stochastic processes?

- We employ the D-optimality: to maximize the det(FIM)

  Classical interpretation: (Fedorov, Pázman, Pukelsheim) D-optimum design minimizes the volume of the confidence ellipsoid for θ.

- **We need justification of D-optimality under correlation, since**

  Correlation may lead to unexpected, counter-intuitive even paradoxical effects in the design (e.g. Müller and Stehlík, 2004 & 2009) as well as the analysis (e.g. Smit, 1961) stage of experiments.

- **Justification of D-optimality under correlation**

  a) The inverse of the FIM may well serve **as an approximation of the covariance matrix of MLEs** in special cases (Pázman 2004,2010, Abt and Welch 1998, Zhu and Stein 2005, Zhang and Zimmerman 2005).

  b) Zhu and Stein (2005): Although some simulation and theoretical studies shows the limits of such an approximation of the covariance matrix of the ML estimates, it can still be used as a design criterion **if the relationship between these two are monotone**, since for the purpose of optimal designing **the only correct ordering is important**.

Fisher information (stochastics-optimization-physics)

- (Pearson and Filon 1898, Edgeworth 1908, Fisher 1925, Lehmann and Casella 1998): $\int (\frac{\partial \ln f(x,\vartheta)}{\partial \vartheta})^2 f(x,\vartheta)dx$

  The **Fisher information measures the sensitivity of the distributions P_θ to variations of parameter θ in the neighborhood of θ_0.**

- **Fisher information (deterministic concept1: Hessian)**
  - Inverse problem of finding a model parameter $\hat{r}$ which solves $z = \Phi(\hat{r})$.
  - measurement and model errors $\Rightarrow$ minimizing the LS functional $J(r) = (1/2)||\Phi(r) - z||^2$.
  - Ucinski (2005): then Hessian of J at $\bar{r}$ = the FIM($\sigma = 1$)

- **Fisher information (deterministic concept2: energy, Annealing)** (Luo 2002, Stehlík 2005,..)

- Stehlík 2005: Let us fix the D-optimal design problem with correlated errors. Then $\exists$ Dirichlet problem for Poisson equation, e.g. $\exists$ f and ϕ :

$\ln h$ is the solution of

$$-\Delta u = f, \text{ in } G, \tag{1}$$

$$u = \phi, \text{ in } \Gamma. \tag{2}$$

Furthermore, $\exists$ "abstract" energy $E(r) = -\int_Y |\nabla_r u|^2 e^u dy$, which =FIM.

- If the correlation matrix may be singular, i.e. $\det \Sigma \to 0$, for $r \to r^\star$ then $\nexists$ regular solution of the Dirichlet problem.

Stochastics with continuous time-expect paradoxes!

- **Estimation with variance zero:** *Although every observation possesses non-zero variance it is possible to estimate parameters with variance zero.*

  Example 1: $X = [-1, 1], corr(Y(x_1), Y(x_2)) = 1 - |x_1 - x_2|, x_i \in X$ Example 2: $X = [-1, 1], corr(Y(x_1), Y(x_2)) = \cos(\frac{\pi}{2}(x_1 - x_2))$

  Examples touch the case of singular processes (see Ibragimov Rozanov (1978)). MHD Physics

- **Smit's paradox** (1961) Let $Y(t)$ be a stationary, $\vartheta = EY(t)$ When the process is observable on the interval $[0, T]$, the mean ϑ may be estimated by (unbiased estimators)

  $$\bar{Y}_{N+1} := \frac{1}{N} \sum_{i=0}^{N} Y(kT/N), \quad m_T = \frac{1}{T} \int_0^T Y(t)dt$$

  One might be inclined to expect that $Var(m_T) \leq Var(\bar{Y}_{N+1})$, since *"the estimator m_T utilizes the whole realization rather than a finite number of points"*.

Stochastics with continuous time-expect paradoxes by designing!!

- However, there are equidistant designs ξ_n for which

$$Var(\bar{Y}_{N+1}) < Var(m_T).$$

  Example 3: $X = [-1, 1], cov(Y(x_1), Y(x_2)) = \exp(-|x_1 - x_2|)$

$$\xi_5 = \{-1, -0.5, 0, 0.5, 1\}.$$

  We have $Var(\bar{Y}_{N+1}) = 0.529$ and $Var(m_T) = 0.568$

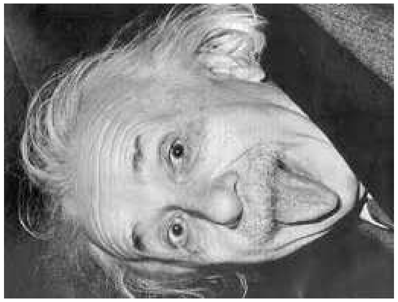
  To explain the paradox: in general, m_T is not the BLUE for ϑ

- **Loss in efficiency by additional observations**

  The variance of $\bar{Y}$ can increase by use of additional observations.

  Example 4: $X = [-1, 1], cov(Y(x_1), Y(x_2)) = \exp(-|x_1 - x_2|)$ $\xi_5 = \{-1, -0.5, 0, 0.5, 1$ are equidistant designs.

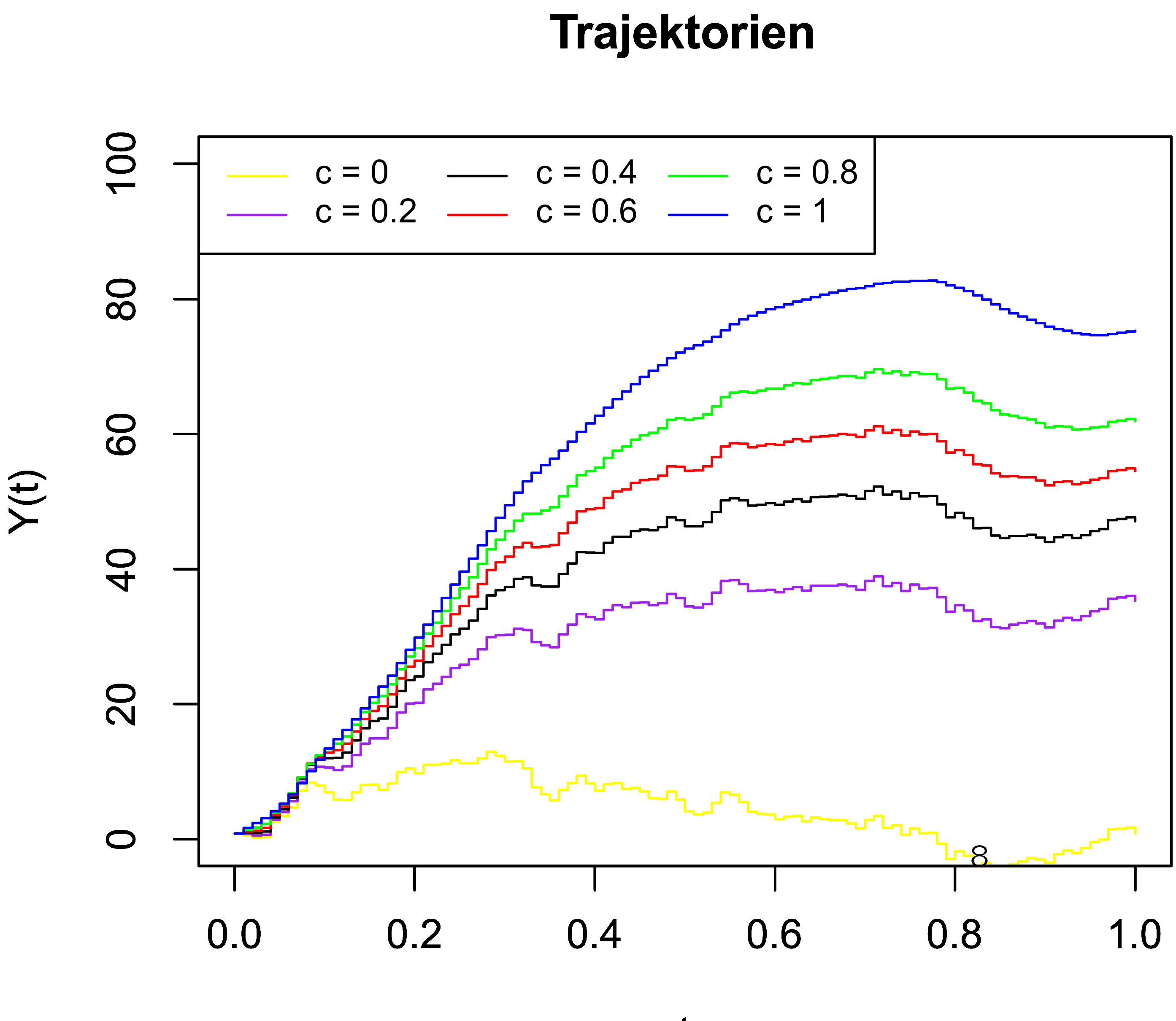
  We have $Var(\bar{Y}(\xi_5)) = 0.529$ and $Var(Y(\xi_9)) = 0.542$. The BLUE-variance is 0.5.



Stochastics with continuous time-expect paradoxes!!

- Is time continuous?
  - **measurable systems:** no, since *Planck time* is the smallest unit of time, and we cannot measure anything smaller!! The Planck time is defined as:
    $t_P \equiv \sqrt{\frac{\hbar G}{c^5}} \approx 5.39124(27) \times 10^{-44}$ s
  - **Idealistic physics:** there is a quantum of time, the *chronon*. But replacing General Relativity of spacetime model (1916) with the quantum one is still not done!

- *Ornstein-Uhlenbeck process (1930)* (X_t: stationary, zero-mean Gaussian process), $dX_t = -rX_t dt + \sqrt{2r} dW_t, X_0 \sim N(0, \frac{\sigma^2}{2\alpha})$. with exponential correlation of the form $\rho(s,t) = \exp(-r|s-t|)$,


Trajektorien
c = 0
c = 0.2
c = 0.4
c = 0.6
c = 0.8
c = 1
Y(t)
0
20
40
60
80
100
0.0
0.2
0.4
0.6
0.8
1.0

The isotropic stationary process

- $Y(x) = \theta + \varepsilon(x)$.
  Design points $x_1, ..., x_N$ are taken from a compact
  $E(Y(x)) = \theta$ is unknown.
  Covariance structure $C(d, r)$ depends on parameter r.

- **Case 1** We are interested only in the trend parameters θ
  Case 2 We are interested only in the covariance parameters r
  Case 3 We are interested in both θ, r

- **Fisher information matrices**
  $M_\theta(n) = 1^T C^{-1}(r) 1$ and (see Pázman (2004) and Xia et al. (2006)) $M_r(n) = \frac{1}{2} tr \left\{ C^{-1}(r) \frac{\partial C(r)}{\partial r} C^{-1}(r) \frac{\partial C(r)}{\partial r^T} \right\}$. For both parameters $M(n)(\theta, r) = \begin{pmatrix} M_\theta(n) & 0 \\ 0 & M_r(n) \end{pmatrix}$.

abc: regularity assumptions on covariance (Stehlík 2009)

- *But how erratic may covariance function be?*

- **Measurable functions?**: discontinuous covariance function should be measurable. Crum (1956): measurable covariance function C admits decomposition $C = C_0 + C_1$; C_0 is a continuous covariance and C_1 vanishes Lebesgue-a.s.

- Crum (1956): if C is isotropic and positive definite on $R^m; m > 1$ then C is continuous except perhaps at $d = 0$. However, for m = 1 the latter is not true anymore: $C(q) = 1$ for all rationals 0 otherwise, which is positive definite, isotropic and discontinuous on Q

- **Idea:** semicontinuous maps of OU covariance

  the class of non negative definite functions $C_r(d) : \Omega \times R^+ \to R$ such that

  a) $C_r(d) \geq 0$ for all $r \in \Omega$ and $0 < d < +\infty$,

  b) $\forall r$ mapping $d \to C_r(d)$ is semicontinuous, non increasing on R^+

  c) $\lim_{d \to +\infty} C_r(d) = 0$ and $\frac{\partial C(r)}{\partial r}$ exists for all $r \in \Omega^\star \subseteq \Omega$.

abc: regularity assumptions on covariance

- **Example 1.**

  The power exponential correlation family $C(d,r) = \sigma^2 \exp(-rd^p)$, $0 < p \leq 2$, $r > 0$. This family is by far the most popular family of correlation models in the computer experiments literature (see Santner et al. (2003)).

- **Example 2.**

  The Matérn class of covariance functions

$$\text{cov}(d, \phi, v) = \frac{1}{2^{v-1}\Gamma(v)}\left(\frac{2\sqrt{v}d}{\phi}\right)^v K_v\left(\frac{2\sqrt{v}d}{\phi}\right)$$

  (see e.g. Handcock and Wallis (1994)). Here ϕ and v are the parameters and K_v is the modified Bessel function of the third kind and order v.

abc: regularity assumptions on covariance

- A **topological space** (X, T) is a set X together with T (a collection of subsets of X) satisfying the following axioms:

  1. The empty set and X are in T. 2. T is closed under arbitrary union. 3. T is closed under finite intersection.

  The collection T is called a topology on X

- **Semicontinuity** A survey: Neubrunn (1988)

  1) A set A is **semiopen** if $\exists$ open set $B : B \subset A \subset \bar{B}$.

  2) A set V is **semineighbourhood** of the point x if $\exists$ semiopen set A : $x \in A \subset V$.

  B) A function $f : X \to Y$ is **semicontinuous** at a point $x \in X$ if $\forall$ open $V : f(x) \in V$ $\exists$ semineighbourhood U of $x : f(U) \subset V$.

- **abc class representation theorem** (Stehlík 2009)

  Let C be abc. Then $C_r(d) = \sigma^2 \exp(-\psi_r(d))$, where $\psi_r : [0, +\infty) \to R \cup \{+\infty\}$ is: semicontinuous, non decreasing, $\lim_{d \to +\infty} \psi_r(d) = +\infty$.

abc: regularity assumptions on covariance (Stehlík 2009)

- **Examples**

  Two extremal situations

  1) $C_r(d) = f(rd)$ where f is non increasing, semicontinuous (max. countable number of jumps,

e.g. for appropriately chosen c, D the covariance defined at R^+

$$C(d) = \begin{cases} \sigma^2, & \text{for } d = 0, \\ c\sigma^2, & \text{for } 0 < d \leq D, \\ 0, & \text{else} \end{cases} \tag{3}$$

which is the prolongation of the covariance given by $c \in [0, 1]$, $D, d \in [0, 2]$ in Müller and Pázman (1999). Also compactly supported corr. functions (Stein 2002, Gneiting et al. 2006,..)

2) smooth correlation functions (OU, The Matérn class,..)

Motivation for semicontinuity of Covariance

- **Motivation:** feasibility of wavelets in multi-resolution representation of images containing edges (Mallat-Hwang 92, Korostelev-Müller-Tsybakov 95, Ingster, Tsybakov, and Verzelen 2010)

- If G-field has Cont. covariance: 0-1 Law:

$$P\{X_t \ is \ continuous \ \forall t \in T\} = 0 or 1$$

- **Problem:** *representation of G-random field with discontinuities,* i.e. What happens when X_t has a discontinuous covariance? **No general results available**-similar to DE with *singularities*–

Closeness of abc class: topological case (Stehlík 2009)

- **Strong convergence, Kupka-Toma 1995**

  Let X be an arbitrary set and Y be a topological space. Let $\{f_\gamma, \gamma \in \Gamma\}$ be a net of functions from X to Y. Let π be an open cover of Y. We say, that a net $\{f_\gamma, \gamma \in \Gamma\}$ converges to a function f π-uniformly, iff

  $$\exists \gamma_0 \in \Gamma \ \forall x \in X \ \forall \gamma \geq \gamma_0 \ \exists O \in \pi : \ (f(x), f_\gamma(x)) \in O \times O.$$

  We say that the net $\{f_\gamma, \gamma \in \Gamma\}$ converges to the function f strongly, iff it converges to f π-uniformly for every open cover of Y.

- **Closeness of abc class: topological case** $\{X_\gamma\}$ be a net of isotropic r. fields with abc covariances K_γ

  $K_n : TopSpace \rightarrow Regular, FullynormalTopSpace$

  $K_\gamma \rightarrow K$ (strongly)

  Then K is abc.

Behavior of $M_\theta(n)$ and $M_r(n)$

- $LB(n,\mathcal{D}) := n \inf_x \frac{x^T C^{-1} x}{x^T x}, \quad UB(n,\mathcal{D}) := n \sup_x \frac{x^T C^{-1} x}{x^T x}.$

- **Theorem** (Stehlík, 2009)

  i) Let $C_r(d)$ be a covariance structure satisfying abc. Then for any design $\{x, x+d_1, x+d_1+d_2, ..., x+d_1+...+d_{n-1}\}$ and for any subset of distances $d_{i_j}, j = 1, ..., m$

  - **increasing domain asymptotics:** the LB, UB, FIM(DOD) are non decreasing with inter-distances of points d_i of the design
  - **equidistant design is optimal** for θ in abc on every compact design space X, more precisely for $X = [0,1]$ any point $(d_1, ..., d_{n-1})$ of a set $\otimes_{i=1}^{n-1} \psi_r^{-1}(1/L)$ such that $\sum d_i = 1$ is a set of optimal inter- distances
  - by stationary OU there exist no admissible design for parameter r (i.e. optimal design for r is collapsing), however, in abc class **not necessarily** (nugget effect,..)

- **Case 3: both r and θ of interest, OU Processes**

  The optimal designs for θ and r in any given compact interval: trade-offs between collapsing and equidistant design

  Compromises e.g.Zagoraiou and Antognini (2009): geometric progressive designs for the case of OU.) However, sometimes (e.g. Müller and Stehlík, 2009) compound designs may be a better solution.

- **Case 1: only θ of interest, OU Processes**

  Kiseľák and Stehlík (2008): *The equidistant design for parameter θ is optimal for stationary Ornstein Uhlenbeck Process.*

  Extension of Dette, Kunert and Pepelyshev (2008): for $r \to 0$ the exact n-point D-optimal design in the linear regression model with exponential covariance converges to the equally spaced design.

- **Case 2: only r of interest**

  "It seems to be artificial, that the first moment $E(Y(x))$ is assumed to be unknown whereas the more complicated second one is assumed to be known..." Näther (1985)

  Issue: *bias reduction* for ML estimator of r (Rodríguez-Díaz et al. 2010)

- Kiseľák and Stehlík (2008):

  (a) for all possible combinations of parameters of interest, i.e. $\{\theta\}, \{r\}$ and $\{\theta, r\}$, the interval over which observations are to be made **should be extended as far as possible** *(increasing domain asymptotics)*

  (b) However doubling the number of observation points in a given interval *(infill domain asymptotics)*, when the only parameter θ is of interest and there are already a large number of such points, gives practically no additional estimation information. When $\{r\}$ or $\{\theta, r\}$ are the sets of interest, doubling gives the double information.

- Exact designs (other authors):
  - Zagoraiou and Baldi Antognini, 2009: stationary 1dimOU process
  - Harman and Štulajter 2009: a special nonstationary 1dimOU process
  - Harman and Štulajter 2011: 1dimB motion with a quadratic drift
  - Baldi Antognini and Zagoraiou, 2010: for prediction of 1dimOU process

Optimal designs for parameters of shifted OU sheets (Baran and Stehlík 2011)

- stationary process $Y(s,t) = \theta + \varepsilon(s,t)$
- design points taken from a compact $\mathcal{X} = [a_1, b_1] \times [a_2, b_2]$
- $\varepsilon(s,t),\ s,t \in \mathbb{R}$, is a stationary Ornstein-Uhlenbeck sheet (a zero mean Gaussian process with covariance $\mathsf{E}\,\varepsilon(s_1,t_1)\varepsilon(s_2,t_2) = \frac{\widetilde{\sigma}^2}{4\alpha\beta}\exp\left(-\alpha|t_1-t_2| - \beta|s_1-s_2|\right)$, where $\alpha > 0,\ \beta > 0,\ \widetilde{\sigma} > 0$).
- $\varepsilon(s,t)$ can also be represented as $\varepsilon(s,t) = \frac{\widetilde{\sigma}}{2\sqrt{\alpha\beta}} e^{-\alpha t - \beta s}\mathcal{W}(e^{2\alpha t}, e^{2\beta s})$,

  where $\mathcal{W}(s,t),\ s,t \in \mathbb{R}$, is a a standard Brownian sheet (Baran *et al.*, 2003)
- **Condition D** *The design points* $\{(s_1,t_1),(s_2,t_2),\ldots,(s_n,t_n)\} \subset \mathcal{X},\ n \in \mathbb{N}$, *are not overlapping (observations without repetitions), moreover* $s_1 \le s_2 \le \ldots \le s_n$ *and* $t_1 \le t_2 \le \ldots \le t_n$ *hold.*

Optimal designs for parameters of shifted OU sheets (Baran and Stehlík 2011)

- the Fisher information matrix on $r = (\alpha, \beta)^\top$ has the form $M_r(n) = \begin{pmatrix} M_\alpha(n) & M_{\alpha,\beta}(n) \\ M_{\alpha,\beta}(n) & M_\beta(n) \end{pmatrix}$ where $\mathsf{M}_\alpha(n) := \frac{1}{2}\left\{C^{-1}(n,r)\frac{\partial C(n,r)}{\partial \alpha}C^{-1}(n,r)\frac{\partial C(n,r)}{\partial \alpha}\right\}$ $M_{\alpha,\beta}(n) := \frac{1}{2}\left\{C^{-1}(n,r)\frac{\partial C(n,r)}{\partial \alpha}C^{-1}(n,r)\frac{\partial C(n,r)}{\partial \beta}\right\}$, and $C(n,r)$ is the covariance matrix of the observations $\{Y(s_i,t_i),\ i = 1,2,\ldots,n\}$.

- Let us observe in points $\{(s_i,t_i),\ i = 1,2,\ldots,n\}$ satisfying condition D. Then $\mathsf{M}_\alpha(n) = \sum_{i=1}^{n-1} \frac{d_i^2 q_i^2(1+q_i^2)}{(1-q_i^2)^2}$, $\quad M_{\alpha,\beta}(n) = \sum_{i=1}^{n-1} \frac{d_i \delta_i q_i^2(1+q_i^2)}{(1-q_i^2)^2}$, where $d_i := s_{i+1} - s_i,\ \delta_i := t_{i+1} - t_i$ and $q_i := \exp(-\alpha d_i - \beta \delta_i),\ \ i = 1,2,\ldots n-1$.

Stochastics with fractal time!

- Nottale 1991: *Is space-time fractal?* Time is not linear, is synchronic,
  - **Lipschitz aggregation operators in topological spaces: Stehlík (2011)**
  - **Motivation:** When working with mathematical objects and notions, we often use more structural properties than it is needed! Sometimes it gives us the advantage of simplicity but sometimes it is dangerous: (Gaussian copula, `The formula that felled Wall Street`, by Sam Jones, Financial Times, April 24, 2009.

Markov operators, Continuity of Markovian transition+OU

- Olsen et al. (1996): related copulas to Markovian transition operators.

- Let X, Y be topological spaces and $P(X), P(Y)$ corresponding spaces of Borel probability measures. The translation of a measure $\mu \in P(X)$ to $P(Y)$ via Markov Kernel K is defined as

  $$\mu(K)(B) = \int_X K(x,B)\mu(dx), B \in B(X)$$

  where $K : X \times B(Y) \to [0,1]$ satisfies

  i) $x \to K(x,B)$ is a Borel measurable for all $B \in B(Y)$

  ii) $K(x,.)$ is a Borel probability measure on Y

  Let us consider a net of Markov kernels K_γ and functions $f_\gamma : P(X) \to P(Y), f_\gamma(\mu) = \mu(K_\gamma)$

- Stehlík and Hlubinka, 2005: Let K_γ be a net of strongly convergent Markov kernels from X to $P(X)$ with a limit K. Then the net $f_\gamma(\mu) = \mu(K_\gamma)$ is strong convergent and its limit is $f(\mu) = \mu(K)$.

Thank you for your attention!

Open problems:

– Usage of topological filter technique (comment from Prof. Klement)

– **Monte Carlo type methods**

  * computer experiments setting: Space-Filling Designs (SFDs)

  * Franco et al. (2008): A new SFD : by the Strauss process: both a Markov point process and an exponential family (Strauss 1975).The Strauss processes based designs are implemented into package 'DiceDesign'.

  * Stoyan et al. (1995): Gibbs point processes describe very large systems in the theories of statistical physics, e.g. mutual behavior and arrangement of particles in some material at different temperatures. The probability density function wrt the Lebesgue measure is

$$\frac{1}{Z}\text{exp}(-U(x)), \tag{4}$$

    where Z is a normalizing constant, U is the energy function.

– **Open problem: Strauss process driven by Energy=FIM**

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