Stochastic Simulation and Bayesian Inference for Gibbs Fields: The Software-Package ANTS_inFields

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ANTsInFields is a Software Package for Simulation and Statistical Inference on Gibbs Fields. It is intended for mainly two purposes: To support teaching by demonstrating well known sampling and estimation techniques and for assistance in research.

ANTsInFields is available for download from http://www.antsinfields.de
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History

1995–1998: Development of Voyager
Portable and extensible System for simulation and data analysis

1998: Diploma thesis
Parameter estimation on Gibbs fields in the context of statistical Image Analysis

Need for implementation of
- samplers for various Gibbs Fields (Ising Model and extensions)
- parameter estimators on simulated or external data.

today: A\textsc{nts}_\textsc{InFields}
Software for Simulation of and Statistical Inference on Gibbs Fields
Aims / Requirements

Aims

• support teaching
• assistance for research

Requirements

• (really) easy to handle
• interactive visualization turned out to be efficient tool for teaching
• flexibility for research, testing new techniques etc.
• extensibility for implementing new samplers etc.
Realization

• **Strongly object oriented concept**
  allows implementation close to mathematical structure intuitive and self-explaining
  easy implementation of interaction and consistent visualization

• **modular design** for extensibility, reusability

• **command language** for flexibility on intermediate level

**ANTSInFields** is written in Oberon System 3 (ETH Zürich, N.Wirth, Gutknecht, H.Marais, E.Zeller et al.)

**Oberon** is also an **Operating System**. It runs on bare PC Hardware or as Emulation on Windows, MacOS, Linux,… (Portability)

**ANTSInFields** uses the **Voyager extension** (University of Heidelberg, G.Sawitzki, M.Diller, F.Friedrich et al.)
Scope

\textbf{\textit{ANTS}}_{\text{InFields}} \textbf{contains}

- Handling and visualization of 1D, 2D and 3D data
- Gibbs and Metropolis Hastings Algorithms, Simulated Annealing, Exact Sampling (CFTP)
- Bayesian image reconstruction methods
- Parameter estimators on Gibbs fields
- ...

\textbf{\textit{ANTS}}_{\text{InFields}} \textbf{is attached to 2nd Edition of G. Winklers Book}
‘Image Analysis, Random Fields and Dynamic Monte Carlo Methods’, Springer Verlag

\textbf{In progress}: Meta compiler (alpha) for easy implementing of new models

\textbf{Planned}: Interface to R (both command language and procedure calls).

Demonstration: Look and feel, Commands, Panels, Random Numbers
Bayesian Image Restoration

- "true" image
- Prior Distribution
- Markov Kernel
- Posterior Distribution
- Estimate true image using the
- data
- estimate
Random Fields

Notation

\[ E \text{ finite space of states} \]
\[ S \subset \mathbb{Z}^d \text{ finite index set} \]
\[ x = (x_s)_{s \in S} \in E^S \text{ configuration} \]
\[ X := E^S \text{ space of configurations} \]
Gibbs Fields

We consider **Neighbour-Gibbs fields**

\[
\Pi(x) = \frac{\exp(-H(x))}{\sum_{y \in X} \exp(-H(y))},
\]

where \( H \) is of the form

\[
H(x) = \sum_{s \in S} f(x_s, x_{\partial(s)})
\]

with \( \partial(t) \) some neighbourhood of \( t, t \in S \).
Ising Model

Easiest nontrivial case: $E = \{-1, 1\}$, nearest neighbours and isotropy.

An Ising Model with parameters $\beta, h \in \mathbb{R}$ is a Gibbs-Field with energy

$$H(x) = -\beta \sum_{s \sim t} x_s x_t + h \sum_s x_s$$

$h$: global tendency to take value $1$

$\beta$: tendency of neighbours to be alike.
Problems with sampling:

\[ P(X = x) = \frac{\exp(-H(x))}{\sum_{y \in X} \exp(-H(y))} \text{ untractable,} \]

but

\[ P(X_t = x_t | X_s = x_s, s \neq t) = \frac{\exp(x_t(h + \beta \sum_{s \neq t} x_s))}{\cosh(h + \beta \sum_{s \neq t} x_s)} \text{ easy to calculate} \]

Solution
→ MCMC techniques like

- Gibbs Sampler
- Metropolis Hastings Algorithm
- Exact Sampling
Markov Chains

An irreducible Markov Chain with a stationary distribution $\mu$ is ergodic and fulfills

(a) 

$$P^t(i, j) \xrightarrow{t \to \infty} \mu(j)$$

(b) 

$$\bar{f}_n \xrightarrow{n \to \infty} \mathbb{E}_\mu(f(X))) \text{ in } L^2$$

if

$$\mathbb{E}_\mu(f(X)) < \infty,$$

where

$$\bar{f}_n = \frac{1}{n} \sum_{i=1}^{n} f(x_i)$$

Demonstration: Reflected Markov Chain
Algorithm for the Gibbs Sampler:

1. $0 \mapsto n$

2. Sample $x^{(0)}$ from initial distribution, say uniform distribution on $X$

3. Apply $K_t$ on $x^{(n)}$ for all $t \in S$
   i.e. sample from local characteristics $\Pi_1$ in each point

4. copy $x^{(n)}$ to $x^{(n+1)}$

5. $n + 1 \mapsto n$

6. Return to step 3 until close enough to $\Pi$.

Algorithm is a realization of a Markov chain with stationary distribution $\Pi$
A sweep
Visiting schedule
Visiting schedule
Visiting schedule
Visiting schedule
Visiting schedule
Visiting schedule
Visiting schedule
Visiting schedule: Whole sweep finished
Demonstrations

- Ising Model, Gibbs Sampler

- Ising Model + Channel noise, MMSE

\[ H(x, y) = -\beta \sum_{s \sim t} x_s x_t + h \sum_s x_s + \frac{1}{2} \ln \left( \frac{p}{1 - p} \right) \sum_s x_s y_s \]

- Cooling Schemes, Simulated Annealing, ICM

- Grey-valued “Ising Model” (Potts and others)

\[ H(x) = \beta \sum_{s \sim t} \varphi(x_s, x_t) + h \sum_s x_s \]
• Sampling from arbitrary Posterior Distributions

\[ H(y, x) = \beta \sum_{x \sim t} \varphi(x_s, x_t) + h \sum_s x_s + \sum_s \vartheta(x_s, y_s), \]

• Φ-Model, Texture Synthesis

\[ H(x) = \sum_i \beta_i \sum_{s \sim t} \varphi(x_s, x_t) + h \sum_s x_s \]
Estimating (Hyper-)Parameters

Assume observations on $\bar{\Lambda} = \Lambda + \partial \Lambda$

(Conditional) Maximum-Likelihood estimator (MLE)

$$\hat{\theta}_n := \arg \min_\theta - \log(\mathbb{P}_\theta(X_t = x_t, t \in \Lambda | X_s = x_s, s \in \partial \Lambda))$$

$$= \arg \min_\theta (\log Z_\Lambda(x_{\partial \Lambda}) - H_\Lambda(x_\Lambda | x_{\partial \Lambda}))$$

Problem: $Z_\Lambda$ not computable.
Solution: Subsampling method (Younes(88), Winkler(01))

Alternative approach: Estimators regarding only the conditional distributions $\mathbb{P}_\theta(X_t = x_t | X_s, s \in \partial(t))$ like:
Coding, Maximum-Pseudolikelihood, Minimal least squares, Minimum Chi Square estimator etc.
Coding Estimator (CE)

With

\[ \Lambda_+ = \{ t \in \Lambda \mid t_1 + \ldots + t_d \text{even} \} \]

the MLE on \( \Lambda_+ \) becomes:

\[ \hat{\theta}_n = \arg \min_{\theta} - \log(\mathbb{P}(X_t = x_t, t \in \Lambda_+|X_s = x_s, s \in \partial \Lambda_+)) \]

\[ = \arg \min_{\theta} - \log \sum_{t \in \Lambda_+} \mathbb{P}_\theta(X_t = x_t|X_s, s \in \partial(t)). \]

Maximum-Pseudolikelihood Estimator (MPLE)

Coding Estimator with replacement: \( \Lambda_+ \rightarrow \Lambda. \)

\[ \hat{\theta}_n = \arg \min_{\theta} - \log \sum_{t \in \Lambda} \mathbb{P}_\theta(X_t = x_t|X_s, s \in \partial(t)) \]

Demonstration: Estimating Parameters