National Research Center
for Environment & Health

Institute of Biomathematics
& Biometry

Mathematical Modelling in Ecology and the Biosciences

Stochastic Simulation and Bayesian Inference for Gibbs Fields: The Software-Package ANTS$_{\text{InFields}}$

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The Software Package ANTS$_{\text{InFields}}$

ANTS$_{\text{InFields}}$ 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.

ANTS$_{\text{InFields}}$ 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: ANTS$_{\text{InFields}}$

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

ANTS$_{InFields}$ 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**
- **. . .**

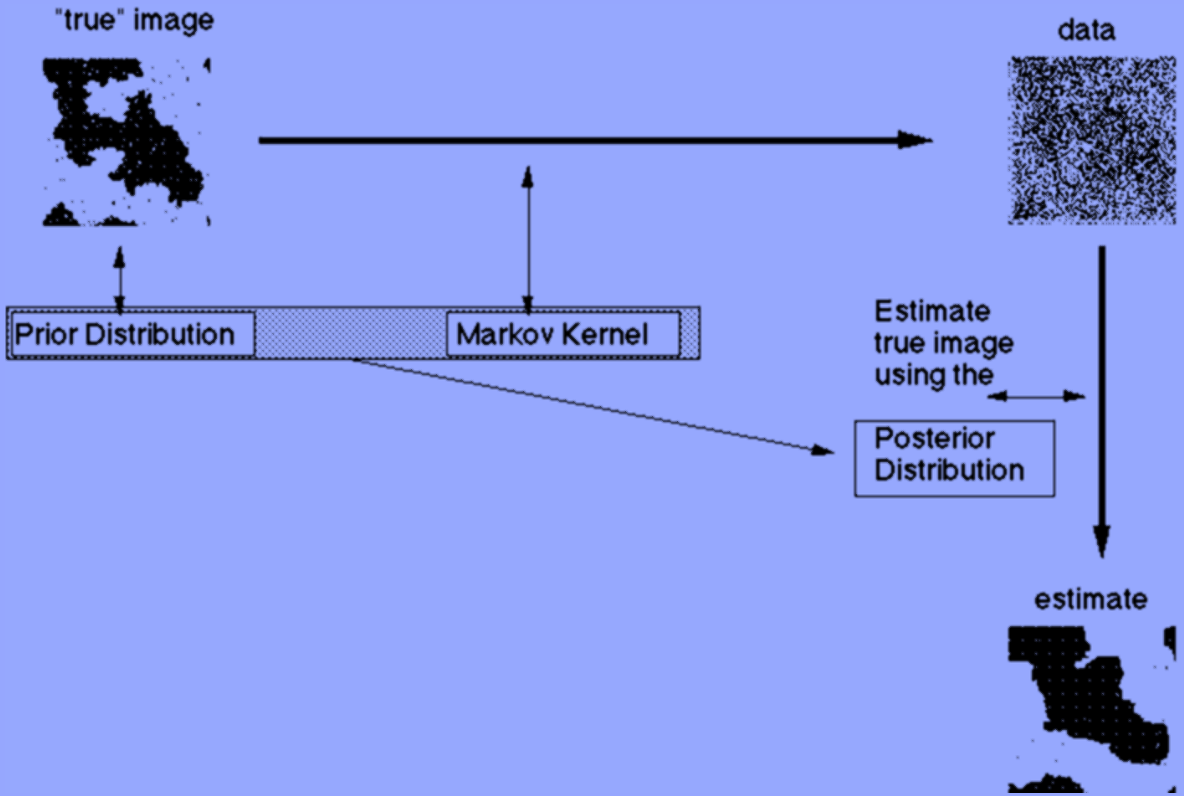
ANTS$_{InFields}$ is attached to 2nd Edition of G. Winklers Book ‘Image Analyis, Random Fields and Dynamic Monte Carlo Methods’, Springer Verlag

In progress: Meta compiler (alpha) for easy implementing of new models

Planned: Interface to R (both command language and procedure calls).

Demonstration: Look and feel, Commands, Panels, Random Numbers

Bayesian Image Restoration

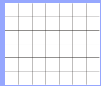


Random Fields

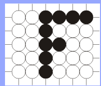
Notation

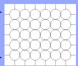
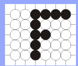
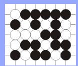
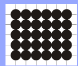
E **finite space of *states*** $\{\bullet, \circ\}$

$S \subset \mathbb{Z}^d$ **finite *index set***



$x = (x_s)_{s \in S} \in E^S$ ***configuration***



$\mathbf{X} := E^S$ ***space of configurations*** $\{$  $, \ldots,$  $, \ldots,$  $, \ldots,$  $\}$

Gibbs Fields

We consider Neighbour-Gibbs fields

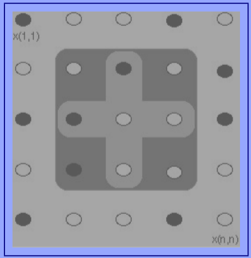
$$\Pi(x) = \frac{\exp(-H(x))}{\sum_{y \in \mathbf{X}} \exp(-H(y))},$$

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, $t \in S$.

$$\partial =$$



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

β**: tendency of neighbours to be alike.**

Problems with sampling:

$$\mathbb{P}(X = x) = \frac{\exp(-H(x))}{\sum_{y \in \mathbf{X}} \exp(-H(y))} \text{ untractable},$$

but

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

Solution

$\rightarrow$ **MCMC techniques like**

- **Gibbs Sampler**
- **Metropolis Hastings Algorithm**
- **Exact Sampling**

Markov Chains

An irreducible Markov Chain with a stationary distribution μ is ergodic and fulfills

(a)

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

(b)

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

if

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

where

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

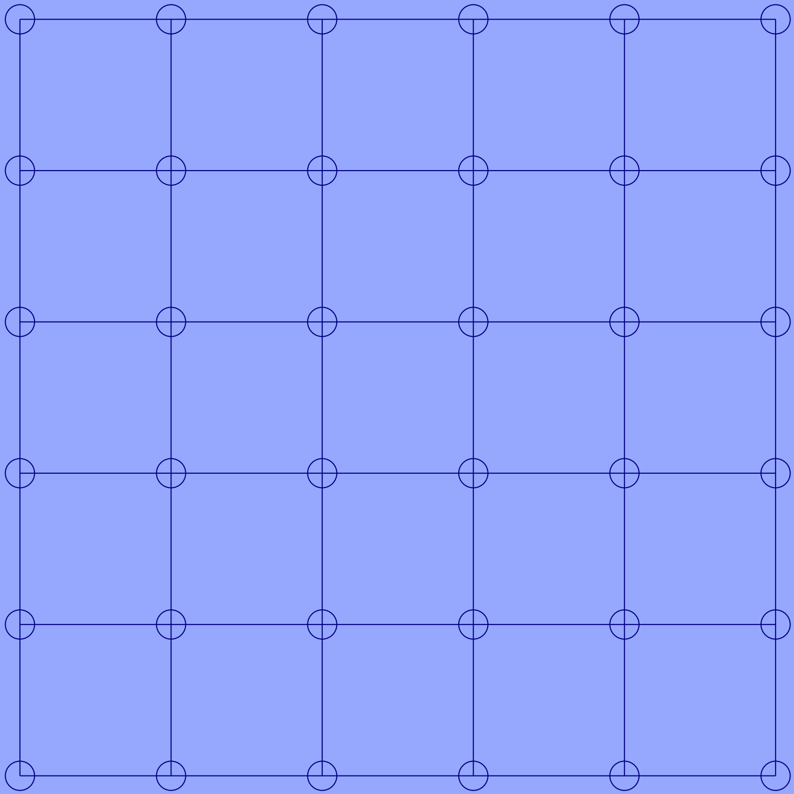
Demonstration: Reflected Markov Chain

Algorithm for the Gibbs Sampler:

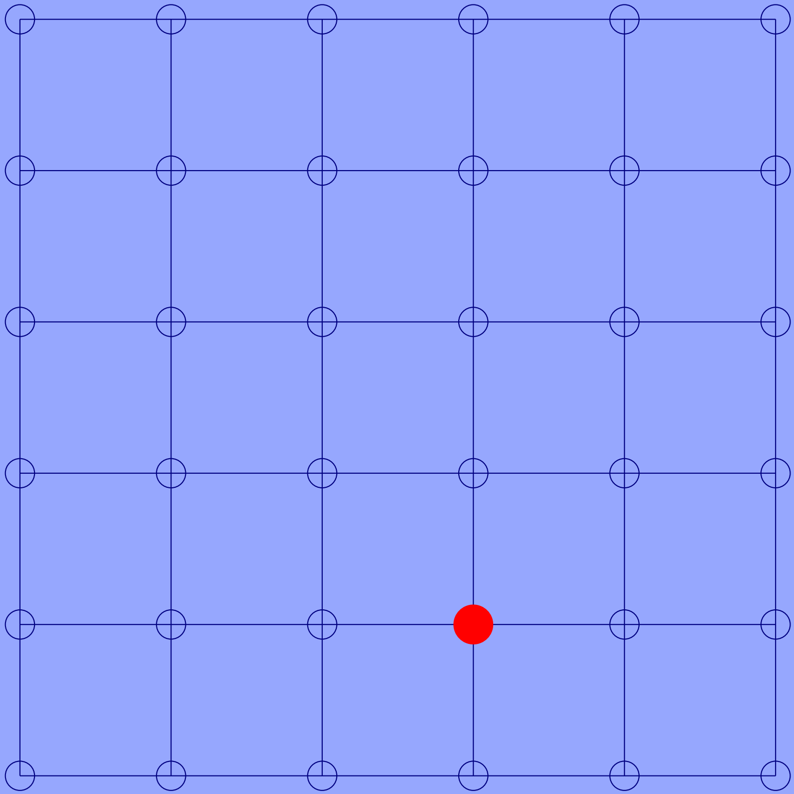
1. $0 \mapsto n$
2. Sample $x^{(0)}$ from initial distribution, say uniform distribution on X
3. Apply K_t on $x^{(n)}$ for all $t \in S$
   i.e. sample from local characteristics Π_1 in each point
4. copy $x^{(n)}$ to $x^{(n+1)}$
5. $n + 1 \mapsto n$
6. Return to step 3 until close enough to Π.

Algorithm is a realization of a Markov chain with stationary distribution Π

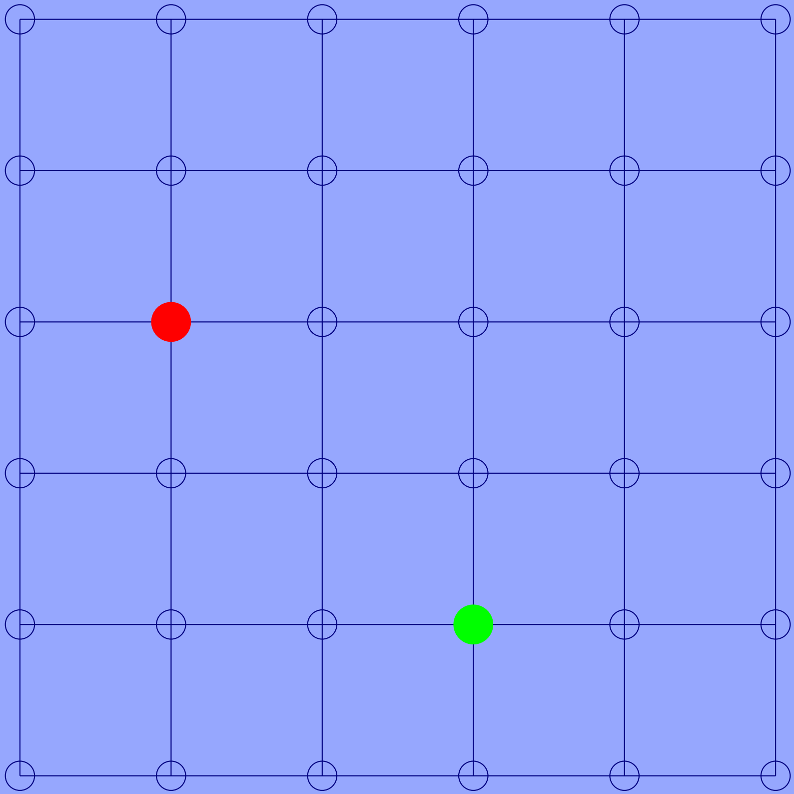
A sweep



Visiting schedule



Visiting schedule



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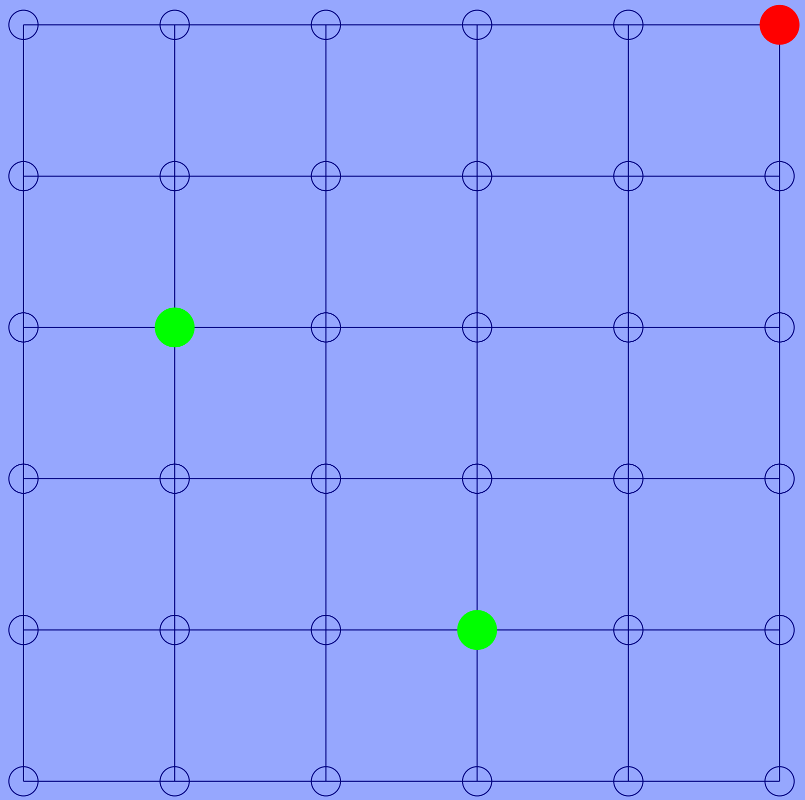

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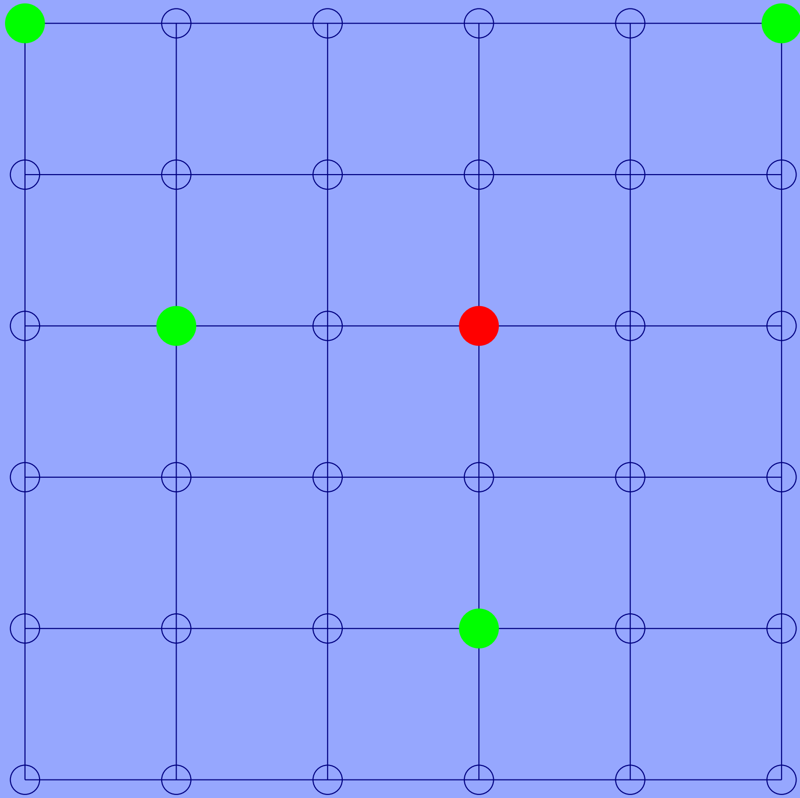

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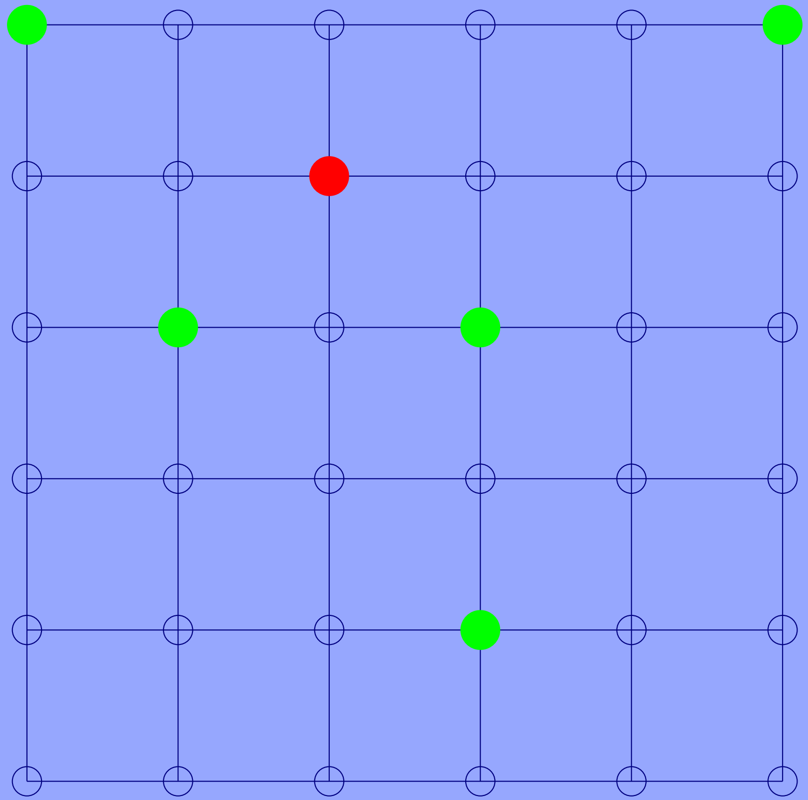

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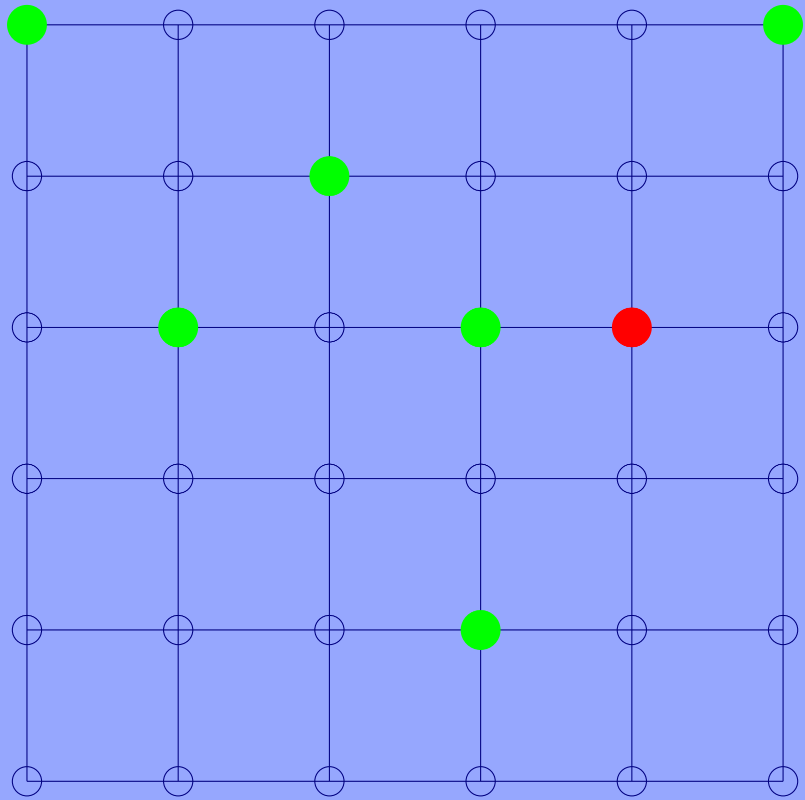
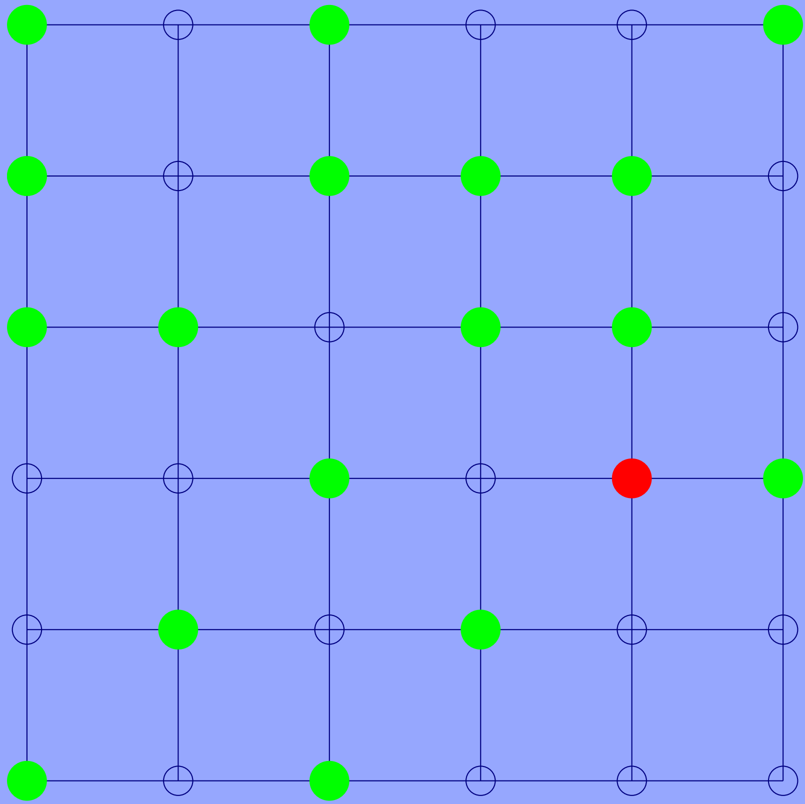
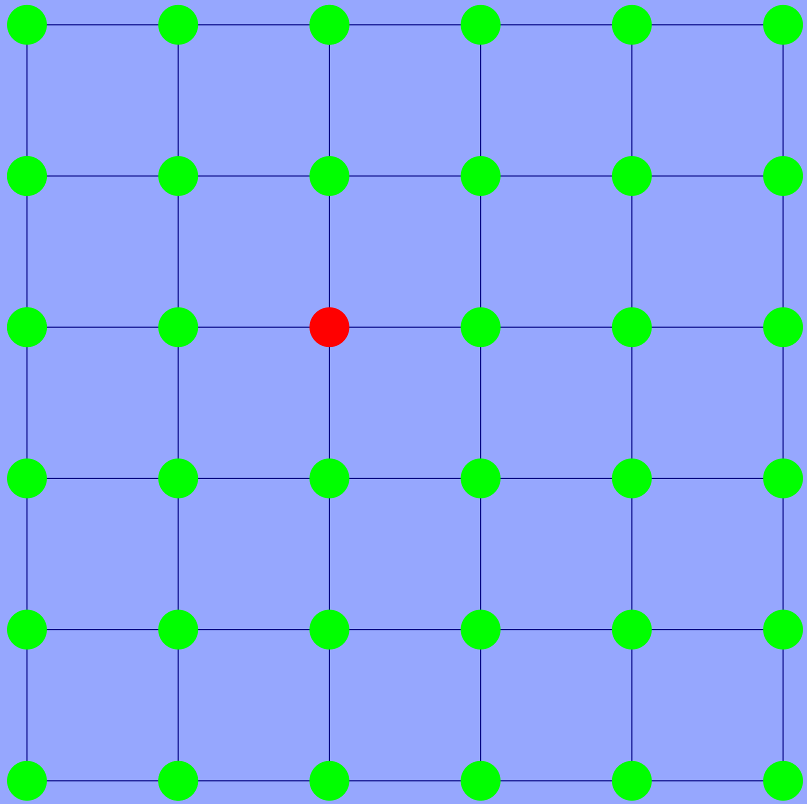


Visiting schedule



Visiting schedule: Whole sweep finished



Demonstrations

- **Ising Model, Gibbs Sampler**

- **Ising Model + Channel noise, MMSE**

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

- **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**

$$H(x) = \sum_i \beta_i \sum_{\substack{s \sim t \\ i}} \varphi(x_s, x_t) + h \sum_s x_s$$

Estimating (Hyper-)Parameters

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

(Conditional) Maximum-Likelihood estimator (MLE)

$$\begin{aligned}\widehat{\theta}_n &:= \arg\min_{\theta} - \log(\mathbb{P}_\theta(X_t = x_t, t \in \Lambda | X_s = x_s, s \in \partial\Lambda)) \\ &= \arg\min_{\theta}(\log Z_\Lambda(x_{\partial\Lambda}) - H_\Lambda(x_\Lambda \mid x_{\partial\Lambda}))\end{aligned}$$

Problem: Z_Λ 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

$$\Lambda_+ = \{t \in \Lambda \mid t_1 + \ldots + t_d \, \textbf{even}\}$$

the MLE on Λ_+ becomes:

$$\begin{aligned} \widehat{\theta}_n &= \arg\min_\theta - \log(\mathbb{P}(X_t = x_t, t \in \Lambda_+ | X_s = x_s, s \in \partial\Lambda_+)) \\ &= \arg\min_\theta - \log \sum_{t \in \Lambda_+} \mathbb{P}_\theta(X_t = x_t | X_s, s \in \partial(t)). \end{aligned}$$

Maximum-Pseudolikelihood Estimator (MPLE)

Coding Estimator with replacement: $\Lambda_+ \longrightarrow \Lambda$.

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

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