

Perfect simulation of repulsive point processes

Mark Huber

Department of Mathematical Sciences, Claremont McKenna College

29 November, 2011



Some repulsive things

Spanish towns

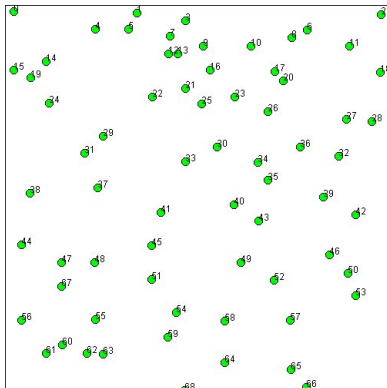


Pine trees

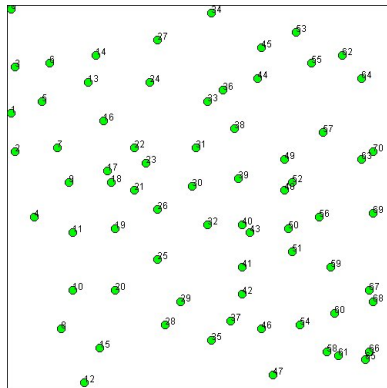


Two data sets

Locations: Spanish towns

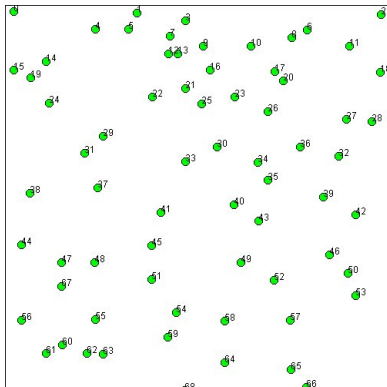


Locations: Swedish pines

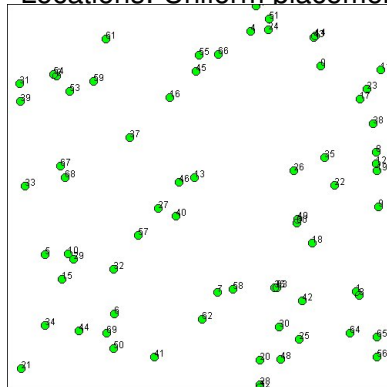


Points farther apart than under uniformity

Locations: Spanish towns



Locations: Uniform placement



Modeling repulsion

Modeling repulsion

Two common modeling approaches

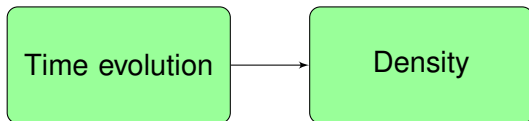
- 1 Give story about how process developed (time evolution)
- 2 Family of densities with respect to Poisson point process (density)

Both based on Poisson point process

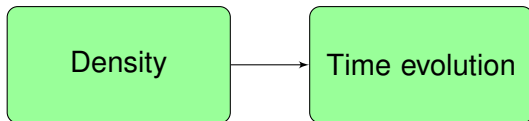
- ▶ # of points has Poisson distribution
- ▶ Given the # of points, place points uniformly independently
- ▶ Mean of Poisson is λ times size of region

Today's talk

Matérn type III process



Strauss process



Strauss process uses density

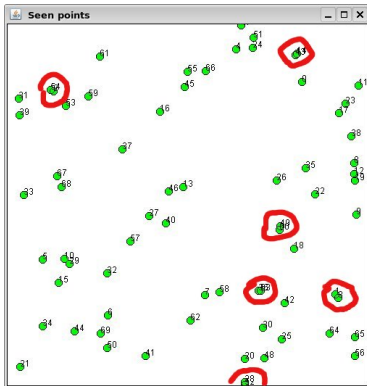
Penalize PPP as follows

- ▶ Distance parameter R
- ▶ Penalty parameter $\gamma \in (0, 1)$
- ▶ Intensity parameter λ
- ▶ For points x , let $r(x) = \#$ of pairs less than R apart
- ▶ For points x , density $f(x) = \gamma^{r(x)} \lambda^{\#x} / Z(\gamma, \lambda)$

Parameter effects

- ▶ Big R spaces points farther apart
- ▶ Small γ means fewer points violate R distance
- ▶ Higher λ means more points

Example of Strauss



$$R = .02$$

$$f(x) = \gamma^6 \lambda^{55} / Z$$

Basic perfect simulation for Strauss

Acceptance rejection

- ▶ Draw a PPP X with intensity λ
- ▶ Find $r(X)$
- ▶ Accept X as Strauss draw with probability $\gamma^{r(X)}$
- ▶ Otherwise, reject and start over

Takes too long unless λ small or γ big

Matérn Type I

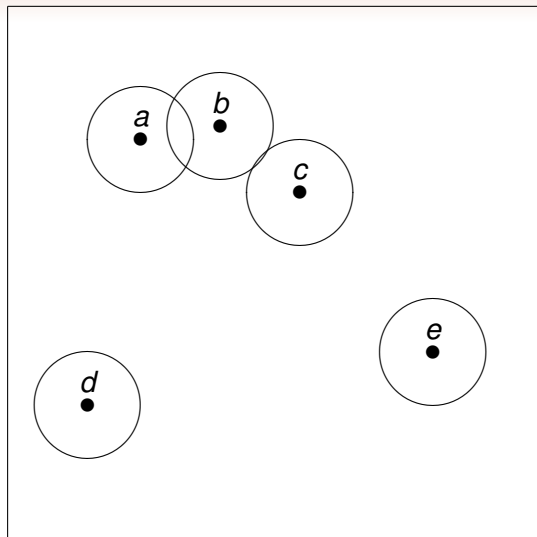
Matérn is a storyteller

- ▶ Introduced three ways of explaining the repulsion
- ▶ Type I, II, and III

Simulate a Matérn Type I as follows

- ▶ First simulate a Poisson point process (PPP)
- ▶ Remove any point within R distance of another point

Matérn Type I example

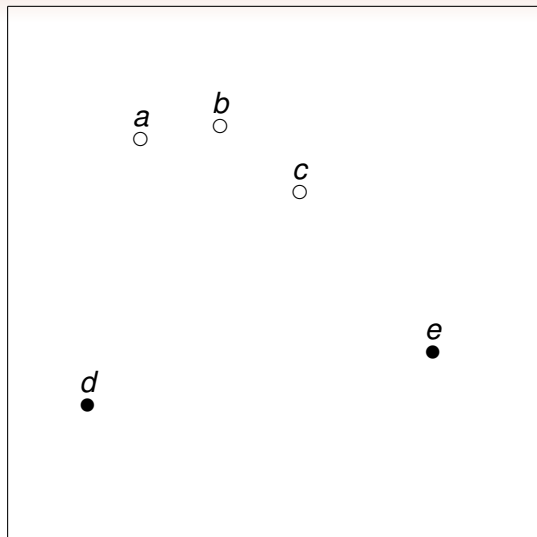


Circles of radius $R/2$

Circles touch =
points eliminated

Points a, b, c eliminated

Type I: After removal



Call *a*, *b*, *c* ghost points

Call *d*, *e* seen points

Ghost points exert
invisible pressure

Type I: Comments

Problems

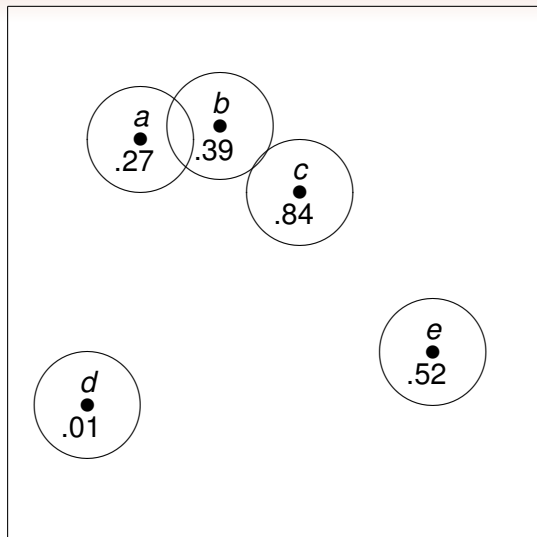
- ▶ Too many eliminations
- ▶ As $\lambda \rightarrow \infty$, # of points $\rightarrow 0$
- ▶ Need method that preserves some points

Matérn Type II: Older points rule!

Simulate a Matérn Type II as follows

- ▶ First simulate a Poisson point process (PPP)
- ▶ Assign each point a birthday in $[0, \infty)$
- ▶ Remove any point within R distance of an *older* point

Type II: Picture

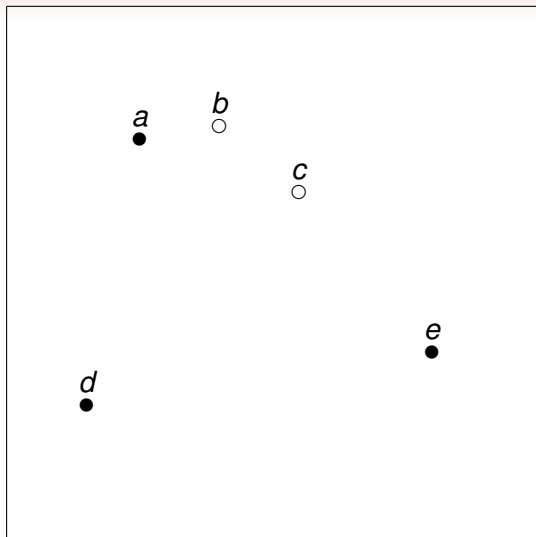


Circles of radius $R/2$

Point a eliminates b

Point b eliminates c

Type II: After thinning



Call *b*, *c* *ghost points*

Call *a*, *d*, *e* *seen points*

Ghost points exert
invisible pressure

Type II: Comments

Better, but not perfect

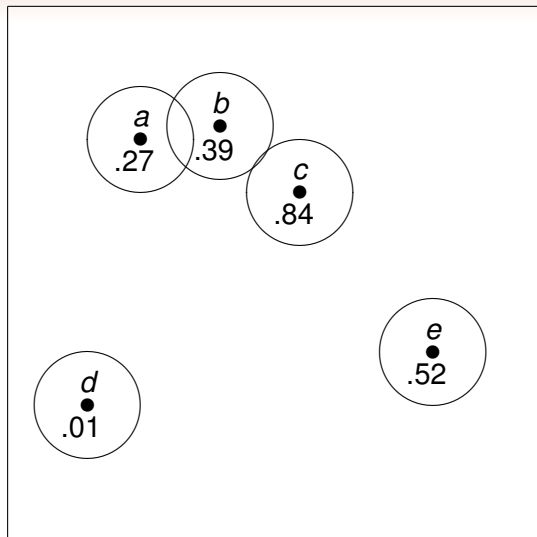
- ▶ First points survive
- ▶ Higher number of points than Type I
- ▶ Why should b take out c if already killed by a ?

Matérn Type III

Simulate a Matérn Type III as follows

- ▶ First simulate a Poisson point process (PPP)
- ▶ Assign each point a birthday in $[0, \infty)$
- ▶ Run time forward
- ▶ Only allow point birth if not within R of older born point

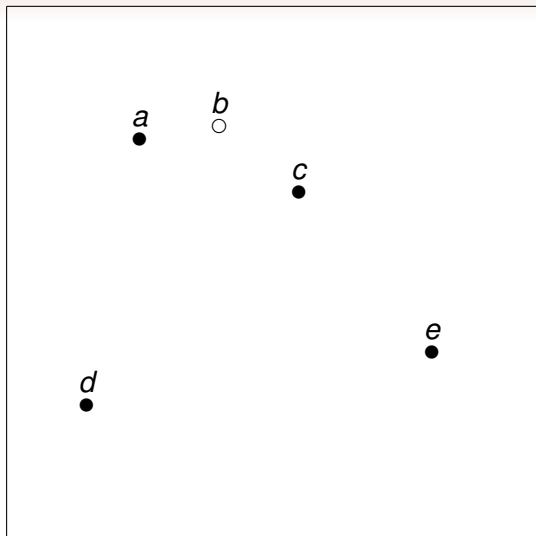
Type III: Picture



Circles of radius $R/2$

Point a eliminates b

Type III: After thinning



Call c *ghost point*

Call a, c, d, e *seen points*

Ghost points exert
invisible pressure

Type III: Comments

The good

- ▶ Very natural story
- ▶ Try to add towns/trees
- ▶ If too close to existing town/tree, dies off

The bad

- ▶ Density not in closed form—nasty high dimensional integral
- ▶ Makes it difficult to do maximum likelihood estimate/posterior

Using Matérn Type III for inference

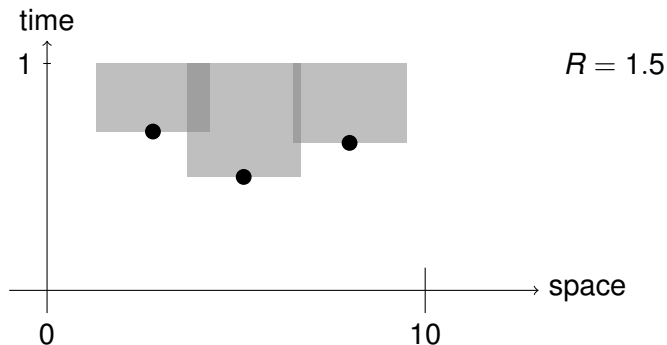
The plan

- ▶ First turn story of Matérn into density (as with Strauss)
- ▶ Build Markov chain for density
- ▶ Build perfect sampler around Markov chain
- ▶ Build product estimator to utilize samples effectively
- ▶ (Those last two are my area of research)

Matérn Type III: Time evolution to density

Casting shadows

The seen points cast a shadow across time



Any ghost points must lie in shaded region
More shadow = more space for ghost points

From shadows to density

Poisson process in spacetime

- ▶ Looks like PPP conditioned so that no points lie in shadow
- ▶ Parameters $\theta = (\lambda, R)$, region S
- ▶ Let $A_\theta(x, t)$ be the area of the shadow in spacetime
- ▶ For seen points x with no shadow violations:

$$f_{\text{seen points}}(x, t|\theta) = C\lambda^{\#x} \exp(\lambda A_\theta(x, t))$$

Larger shadow means more likely

Alternate way of drawing Matérn Type III process

- ▶ Fix points in x
- ▶ Draw new PPP y to add to x
- ▶ If all of y lies in shadow of x , accept x as Matérn Type III
- ▶ Otherwise draw new y and repeat

Acceptance/rejection leads to density

What is chance of accepting a given y ?

- ▶ Let $|S|$ be size of region, $A_\theta(x, t)$ size of shadow
- ▶ Probability no points outside of shadow

$$\exp(-\lambda(|S| - A_\theta(x, t))) = \exp(\lambda A_\theta(x, t)) \exp(-\lambda|S|)$$

The problem of unknown time of birth

Big problem

- ▶ We do not see the t values!
- ▶ To get the density for just x integrate out t :

$$g(x|\theta) = C\lambda^{\#x} \int_{t \in [0,1]^{\#x}} \exp(\lambda A_{\theta}(x, t))$$

- ▶ Doing this integral directly extremely nasty
- ▶ Even calculating $A_{\theta}(x, t)$ hard

Monte Carlo methods to the rescue!

Given seen points x , want to approximate $g(x|\theta)$

- ▶ Monte Carlo approach: treat t values as auxiliary variables
- ▶ Given x : randomly choose t from $f(x, t|\theta, x)$
- ▶ Allows use to estimate $g(x|\theta)$

How to draw time stamps given locations?

Markov chain Monte Carlo (MCMC)

- 1 Build chain so stationary distribution = target distribution
- 2 Under mild conditions (ϕ -irreducibility, aperiodicity) limiting distribution will equal stationary distribution
- 3 Run chain “for a long time” to mix, then get samples

Metropolis protocol for building Markov chain

One step of Metropolis

- 1 Propose moving from (x, t) to (x, t')
- 2 Accept move with probability

$$\min \left\{ \frac{f(x, t'|\theta)}{f(x, t|\theta)}, 1 \right\}$$

- 3 Otherwise stay where you are

Even better...

Perfect simulation techniques

- ▶ For some Markov chains, possible to do better
- ▶ Can draw exactly from stationary distribution
- ▶ Without worrying about mixing time

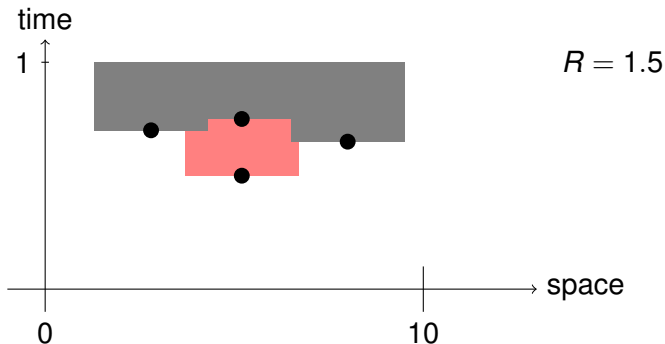
Perfect sampling protocol

- ▶ Coupling from the past (Propp & Wilson 1994)
- ▶ CFTP converts Markov chains to perfect samplers
- ▶ A good property of Markov chain: monotonicity
- ▶ Monotonicity not necessary for CFTP, is sufficient

Is Metropolis for Matérn type III monotonic?

Propose changing time stamp for one point in x

- ▶ How does the shadow change?



- ▶ Probability accept move = $\exp(-\text{area of shadow change})$

How to flip an $\exp(-\mu)$ coin

Fun facts about Poisson point processes

- ▶ For $X \sim \text{PPP}(B)$, $\mathbb{P}(\#X = 0) = \exp(-\mu(B))$
- ▶ For regions $A \subset B$, $X \sim \text{PPP}(B)$ then $X \cap A \sim \text{PPP}(A)$

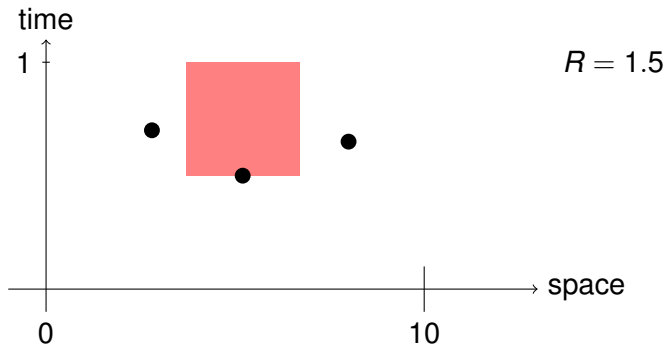
To check if move in Metropolis

- ▶ Draw PPP(largest possible change in shadow)
- ▶ If PPP restricted to actual change in shadow empty, move
- ▶ Otherwise, stay at current time stamp

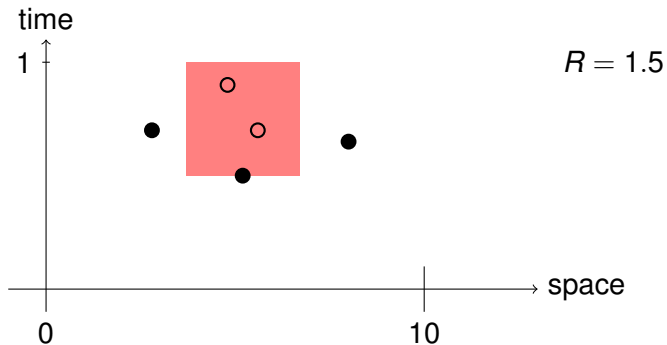
Using PPP to flip exponential coins:

- ▶ First appears in Beskos, Papaspiliopoulos, Roberts (2006)
- ▶ Perfect simulation of diffusions

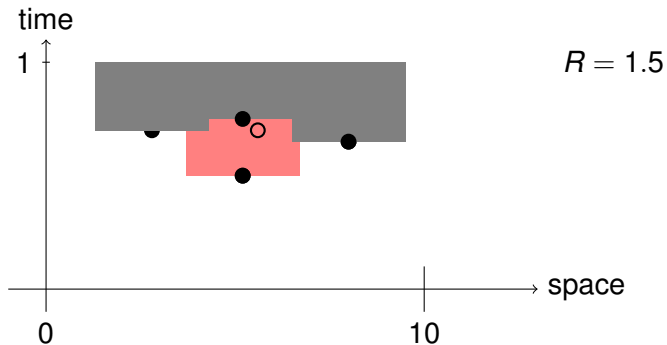
Example



Example



Example



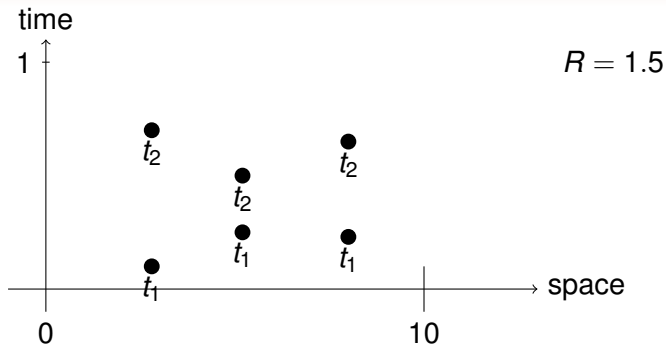
Monotonicity of Markov chain step

For $t_1 \leq t_2$:

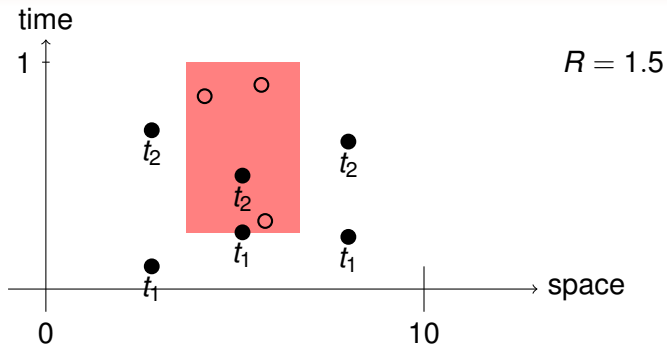
- ▶ Run one step of Markov chain for t_1 and t_2
- ▶ Use same auxiliary PPP in change of shadow
- ▶ Then after step, still have $t_1 \leq t_2$

Immediately gives us perfect sampling!

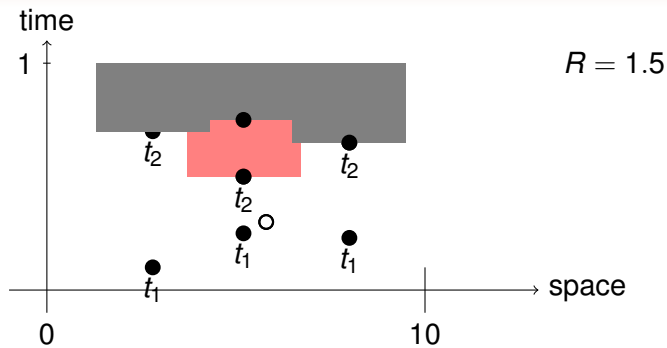
Example of Monotonicity



Example of Monotonicity

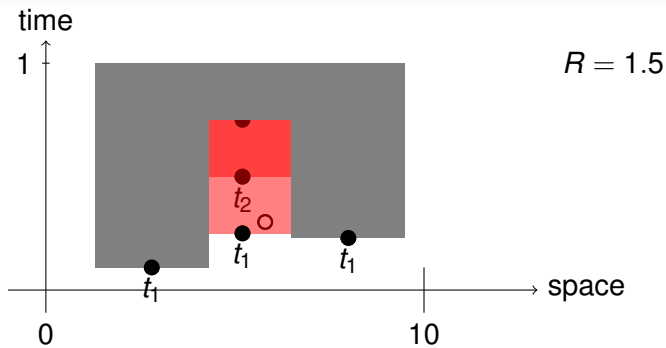


Example of Monotonicity



t_2 accepts move

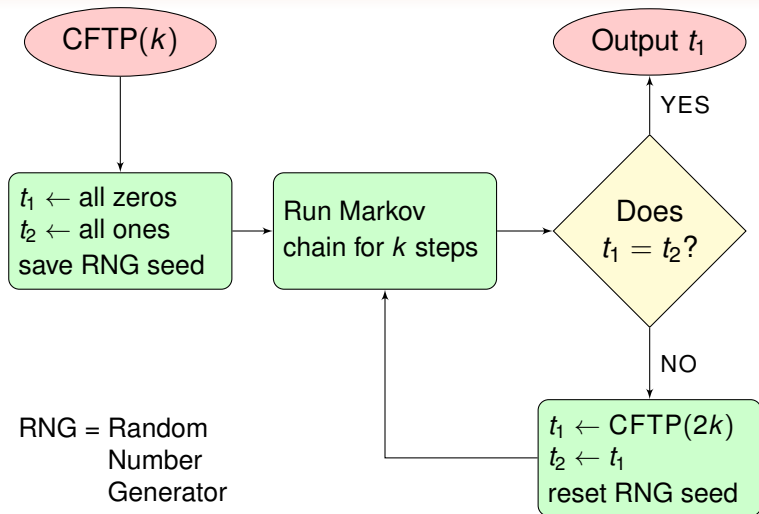
Example of Monotonicity



t_2 accepts move

t_1 rejects move

Monotonic CFTP flowchart



Monotonic CFTP details

Running CFTP(k)

- 1 Set t_1 to all 0's, t_2 to all 1's
- 2 Save seed to random number generator
- 3 Take k steps in the Markov chain
- 4 If $t_1 = t_2$, then set T_k to be this common value
- 5 Else
 - 1 Get T_0 by calling CFTP($2k$) recursively
 - 2 Reset seed to random number generator to what it was in step 2
 - 3 Get T_k by taking k steps in the Markov chain
- 6 Output T_k

What's the point?

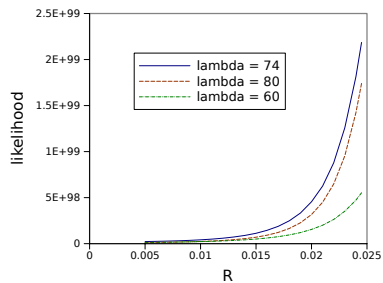
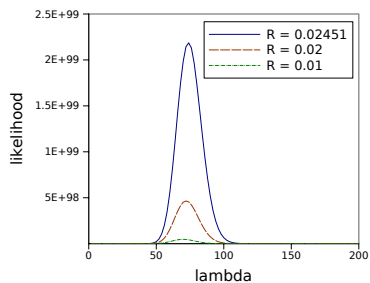
Why do we need samples?

- ▶ Ability to sample gives approximation of nasty integral
- ▶ Use TPA or IS+TPA to go from samples to integral

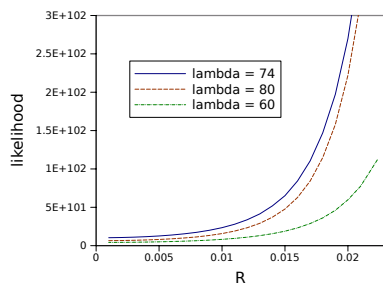
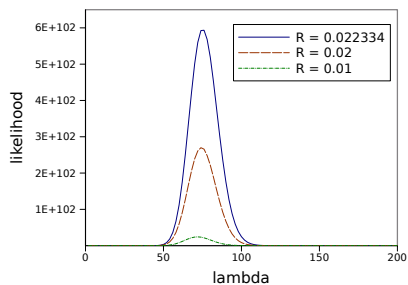
Once you have that integral

- ▶ Gives density of data under Matérn model
- ▶ Basis for maximum likelihood
- ▶ ...or posterior analysis

Results: towns



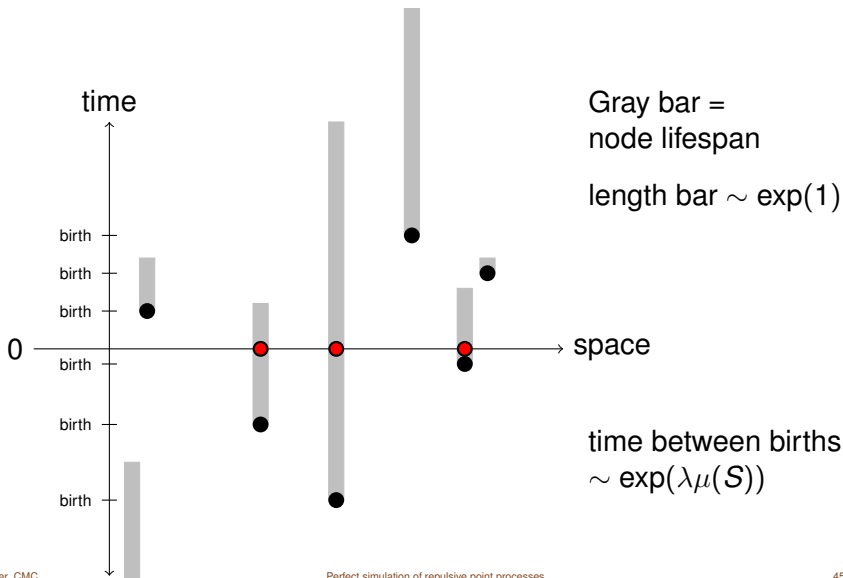
Results: trees



Strauss: Density to time evolution

Preston (1977) Birth-Death Chains

Adding time dimension to Poisson point process



Preston Birth-Death Chains

Points are born, and later die

- ▶ Rate of births is λ times area of region
- ▶ Each point dies at rate 1
- ▶ (Rate is parameter of exponential random variable)

Points alive at time 0 form PPP

Preston for Strauss

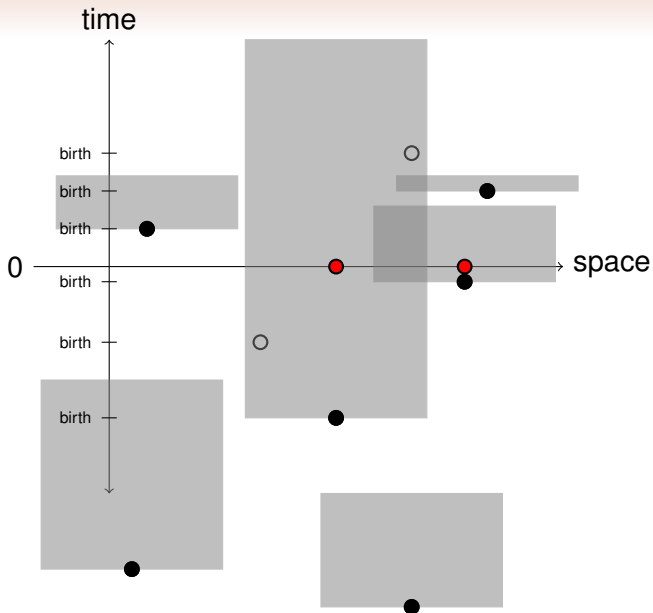
Recall Strauss density

- ▶ Penalty γ for pair of points within distance R

When point is born...

- ▶ If point within distance R of point already born...
- ▶ ...point only born with probability γ

Picture for Strauss $\gamma = 0$



Observations

Red points

- ▶ Strauss process subset of earlier points
- ▶ Kendall and J. Møller (2000): can find red points by looking backwards in time

Adding a Swap move

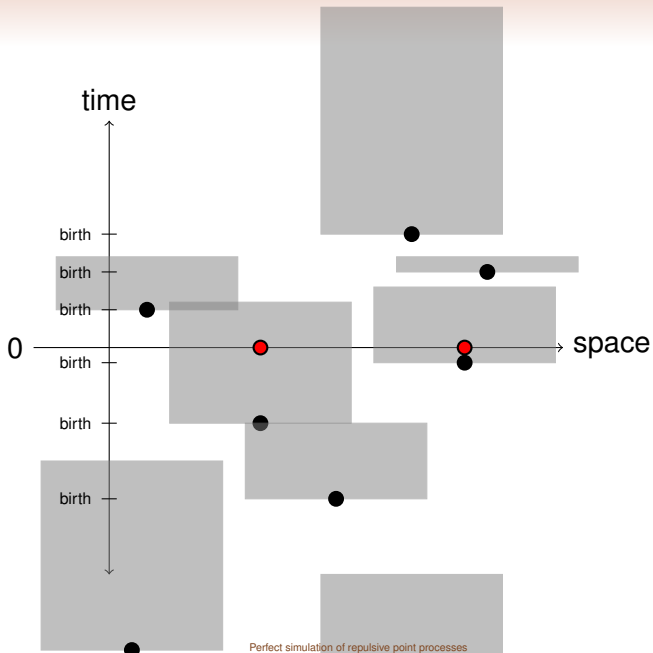
Swap move

- ▶ Broder (1986): swap move for perfect matchings
- ▶ Dyer and Greenhill (2000): swap move for independent sets of graphs

Adding Swaps to Preston

- ▶ Huber (2011)
- ▶ When point not born, give chance to swap
- ▶ If only blocked by one point...
- ▶ ...remove blocker, allow birth

Picture with swap



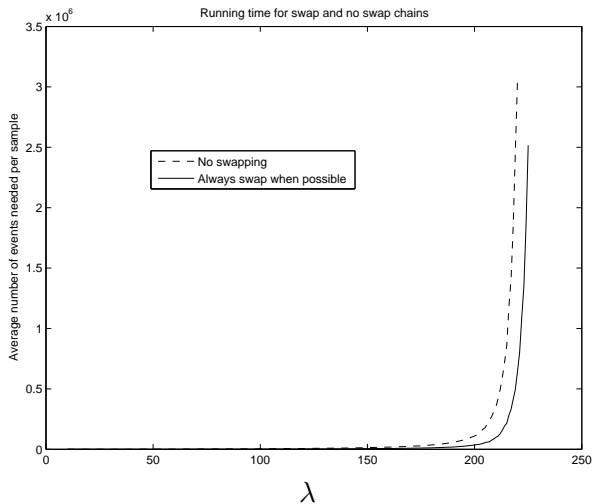
Swap move helps chain mix better

Easier to find red points

- ▶ Verified experimentally on plane
- ▶ Points affect fewer points in future
- ▶ Need to be blocked by at least two points to affect future
- ▶ So effect of point on later points cut in half

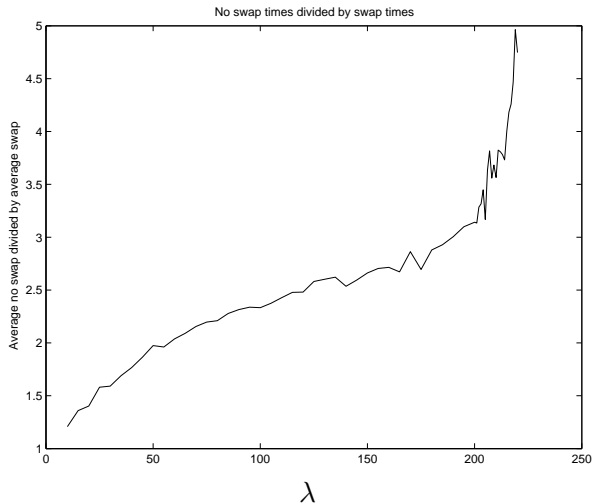
Running times with swap

Strauss model on $S = [0, 1]^2$, $\gamma = 0.5$, $R = .05$



Running times with swap

Time for no swap divided by time for swap



Conclusions




For Matérn type III models

- ▶ Built a density (not in closed form)
- ▶ Can approximate density using perfect MCMC methods
- ▶ Allows MLE or posterior analysis

For Strauss process

- ▶ Already had a density (but not in closed form)
- ▶ Added new type of Markov chain move
- ▶ Seems to speed up chain in practice

References

-  HUBER, M.L. (2011).
Spatial Birth-Death-Swap Chains.
Bernoulli (forthcoming paper, available online)
-  HUBER, M.L. AND R.L. WOLPERT (2009).
Likelihood based inference for Matérn type III repulsive point processes.
Advances in Applied Probability **41**, 958–977.
-  MATÉRN, B. (1986).
Spatial Variation, vol. 36 of *Lecture Notes in Statistics*.
New York, NY: Springer-Verlag, 2nd ed.
(first edition published 1960 by Statens Skogsforsningsinstitut, Stockholm).