Imperial College London

Advanced Computational Methods in Statistics: Lecture 3 - MCMC

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London Taught Course Centre
for PhD Students in the Mathematical Sciences
Autumn 2015

Outline

MCMC methods

- Markov Chain Monte Carlo
- Main idea:
  - Want to simulate from a density f or compute functionals of f such as the mean: $\operatorname{E} X = \int x f(x) dx$.
  - Construct a Markov Chain whose stationary distribution is f.

  Note: Usually f need only be known up to a normalising constant.

Most of the material in this lecture is from Robert & Casella (2004).

MCMC and Bayesian Models

- MCMC is the main tool used in (applied) Bayesian statistics!
- Observation y
- Model: $Y \sim g(\cdot|\theta)$, $\theta \sim \pi$
- Mainly interested in the a-posteriori density:
$$\pi(\theta|y) = \frac{g(y|\theta)\pi(\theta)}{m(y)},$$
where $m(y) = \int g(y|\theta)\pi(\theta)d\theta$.
- If θ is high-dimensional - hard to report $\pi(\theta|y)$
$\rightarrow$ report e.g. the posterior mean
$$\mathrm{E}(\theta|y) = \int \theta\pi(\theta|y)dy.$$
- MCMC: construct Markov chain $X_1, X_2, \dots$ with stationary distribution $\pi(\theta|y)$ (evaluation of m is not needed)
run Markov chain for n steps; then $\mathrm{E}(\theta|y) \approx \frac{1}{n}\sum_{i=1}^{n} X_i$

Outline

Definitions

- A sequence $X_0, X_1, X_2, \ldots$ of random variables (random objects) is a Markov chain if for all A and $n \in \mathbb{N}$:

$$\mathrm{P}(X_{n+1} \in A | X_n, \ldots, X_0) = \mathrm{P}(X_{n+1} \in A | X_n).$$

  In words: only the distribution of the current state is relevant for the distribution of the state at the next time.
  Note: discrete time, potentially continuous state.

- It is called (time) homogeneous if for all $t_0 \leq t_1 \leq \cdots \leq t_k$:

$$(X_{t_k}, X_{t_{k-1}}, \ldots, X_{t_1}) | X_{t_0} \sim (X_{t_k - t_0}, X_{t_{k-1} - t_0}, \ldots, X_{t_1 - t_0}) | X_0$$

  The Markov-chains we encounter will be time-homogeneous.
  Example: $k = 2$, $t_2 = 10$, $t_1 = 8$, $t_0 = 7$. For a time homogeneous chain, $(X_{10}, X_8) | X_7 \sim (X_3, X_1) | X_0$.

- transition kernel (corresponding to transition matrix):

$$K(x, B) = \mathrm{P}(X_{n+1} \in B | X_n = x)$$

  Note: $\forall x : K(x, \cdot)$ is a probability measure.

Irreducibility, Recurrence

$\mathcal{X}$ finite: Irreducibility, Recurrence about reaching individual points.
Here: modification for $\mathcal{X}$ continuous.

- $\mathcal{X}$ state space of the Markov chain (X_n)
- $\tau_A = \inf\{n \geq 1 : X_n \in A\}$ (first hitting time of A)
- Let ϕ be a measure.
  (X_n) is ϕ-irreducible if
  $\forall A$ with $\phi(A) > 0$: $\mathrm{P}_x(\tau_A < \infty) > 0$ for all $x \in \mathcal{X}$.
- $\eta_A = \sum_{n=1}^{\infty} 1_A(X_n)$ (number of passages of X_n through A)
- (X_n) is recurrent if
  1. $\exists$ measure ϕ s.t. (X_n) is ϕ-irreducible
  2. $\forall$ A with $\phi(A) > 0$: $\mathrm{E}_x(\eta_A) = \infty$ $\forall$ $x \in A$.
- (X_n) is Harris recurrent if
  1. $\exists$ a measure ϕ s.t. (X_n) is ϕ-irreducible
  2. $\forall A$ with $\phi(A) > 0$: $\mathrm{P}_x(\eta_A = \infty) = 1$ $\forall$ $x \in A$.

(P_x = Prob measure of Markov chain started at x,
E_x = expectation taken w.r.t. P_x)

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(P_x = Prob measure of Markov chain started at x,
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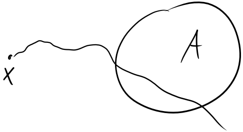
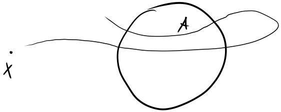
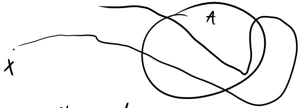
ϕ-irreducible: All sets A with $\phi(A) > 0$ are reached from anywhere.



ϕ-recurrent: The expected number of times a set A with $\phi(A) > 0$ is reached is infinite.



Harris-recurrent: Every set A with $\phi(A) > 0$ is reached infinitely often.



Harris recurrence is much stronger than ϕ-recurrence:

X r.v. with $P(X > t) = \frac{1}{t}$ for $t > 1$.

Then $P(X = \infty) = 0$ but $E(X) = \int_1^\infty \frac{1}{t}\, dt = \log(\infty) - \log(0) = \infty$.

Ergodic Theorems

- Ergodic Theorems= convergence results equivalent to the law of large numbers in the iid case.
- A σ-finite measure π is invariant for the transition kernel $K(\cdot,\cdot)$ (and for the associated chain) if

$$\pi(B) = \int_{\mathcal{X}} K(x,B)\pi(dx), \forall B \in \mathcal{B}(\mathcal{X})$$

  In other words: $X_n \sim \pi \implies X_{n+1} \sim \pi$
- Ergodic Theorem: If (X_n) has a σ-finite invariant measure π then the following two statements are equivalent:
  1. If $f, g \in L^1(\pi)$ with $\int g(x)d\pi(x) \neq 0$ then

$$\frac{\frac{1}{n}\sum_{i=1}^n f(X_i)}{\frac{1}{n}\sum_{i=1}^n g(X_i)} \to \frac{\int f(x)\pi(dx)}{\int g(x)\pi(dx)} \quad (n \to \infty)$$

  2. (X_n) is Harris recurrent

Theorem (Convergence to the Stationary Distribution)

If (X_n) is Harris recurrent and aperiodic with invariant probability measure π then

$$\lim_{n\to\infty} \left\| \int K^n(x,\cdot)\mu(dx) - \pi \right\|_{TV} = 0,$$

for every initial distribution μ, where

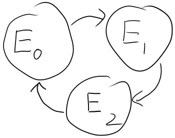
K^n *is the n step transition kernel and*

$\|\mu_1 - \mu_2\|_{\mathrm{TV}} = \sup_A |\mu_1(A) - \mu_2(A)|$ *is the total variation norm.*

(X_n) is periodic if there exist $d \geq 2$ and nonempty disjoint sets $E_0, \ldots, E_{d-1}$ s.t. for all $i = 0, \ldots, d-1$ and all $x \in E_i$:

$$K(x, E_j) = 1 \quad \text{for } j = i + 1 \pmod{d}$$

Otherwise (X_n) is aperiodic.



periodic with $d=3$:

$P(X_{n+1} \in E_1 \mid X_n \in E_0) = 1$

" " E_2 " E_1 "

" " E_0 " E_2 "

Outline

Metropolis-Hastings algorithm

- (target) distribution f
- conditional density q (proposal of new position).

Let X^1 be arbitrary.
For $t = 1, 2, \dots$:

- Let $Y^t \sim q(X^t, \cdot)$
- Let
$$X^{t+1} = \begin{cases} Y^t \text{ with prob } \rho(X^t, Y^t) \\ X^t \text{ with prob } 1 - \rho(X^t, Y^t) \end{cases}$$
where $\rho(x, y) = \min\left(\frac{f(y)q(y,x)}{f(x)q(x,y)}, 1\right)$

Notes:

- f is only needed up to a normalising constant.
- the terms involving q cancel if proposal is symmetric around the current position.

Example - Space-Shuttle O-ring

- Explosion of the Space-shuttle Challenger caused by the failure of an *O-ring* (a ring of rubber used as a sealant)
- Caused by unusually low temperatures (31° F)
- Data from previous flights:

Failure	1	1	1	1	0	0	0	0	0	0	0	0	1	1	0	0	0	1	0	0	0	0	0
Temp	53	57	58	63	66	67	67	67	68	69	70	70	70	70	72	73	75	75	76	76	78	79	81

- Failure= blowby or erosion (diagnosed after the flight)
- More details: see Dalal et al. (1989).

Example - Space-Shuttle O-ring - Model

- Logistic model:

$$P(Y=1) = \frac{\exp(\alpha + x\beta)}{1+\exp(\alpha + x\beta)}$$

  x =temperature

- prior:

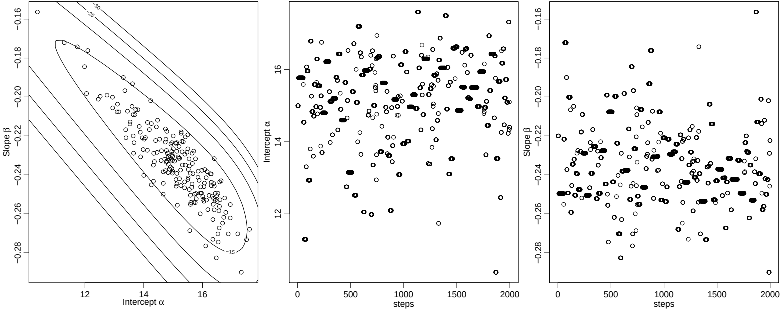
$$\pi(\alpha, \beta) = \frac{1}{b} e^{\alpha} e^{-e^{\alpha}/b}$$

  (flat prior on β, exponential on $\log(\alpha)$)
  choose b st $\mathrm{E}\,\alpha$=MLE of α.

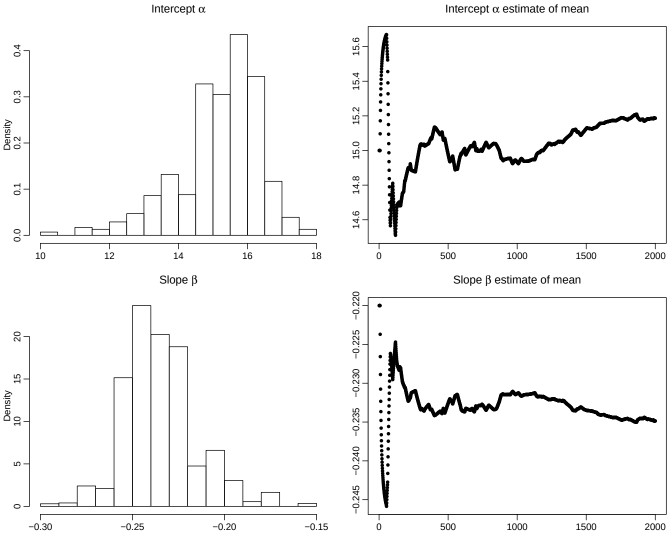
Space-Shuttle O-ring - Independent Proposal

Proposal for the Metropolis Hastings Algorithm

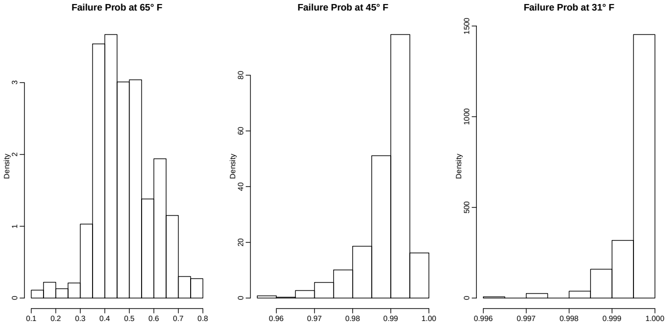
- $\exp(\alpha_{prop}) \sim$ Exponential$(1/b)$
- $\beta_{prop} \sim N(-0.2322, 0.1082)$
- Realisation of the Markov chain:



Posterior Distribution, Mean of posterior



Prediction of Failure Probability



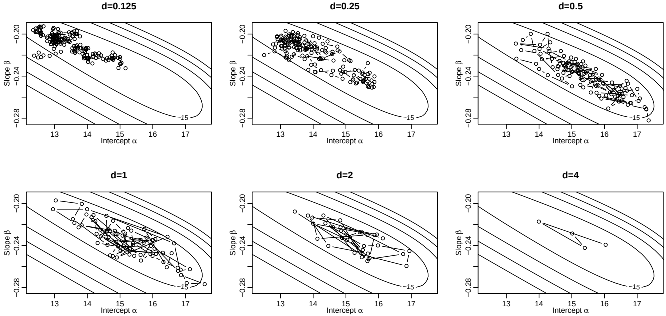
Space-Shuttle O-ring - Random Walk Proposal

Proposal for the Metropolis Hastings Algorithm

- $\alpha_{prop} = \alpha + Z_a, \quad Z_a \sim N(0, \sqrt{0.02d})$
- $\beta_{prop} = \beta + Z_b, \quad Z_b \sim N(0, \sqrt{d})$

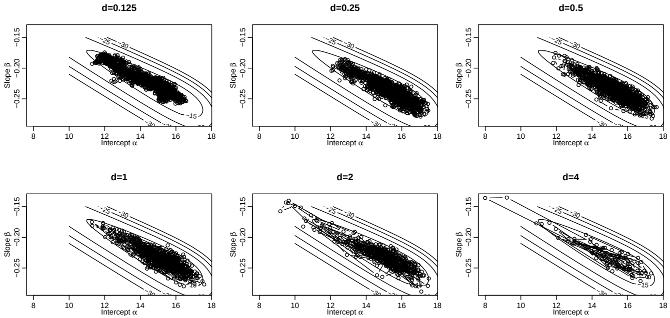
Acceptance prob simplifies: $\rho(x,y) = \min\left(\frac{f(y)\cancel{q(y,x)}}{f(x)\cancel{q(x,y)}}, 1\right)$

First 200 steps:



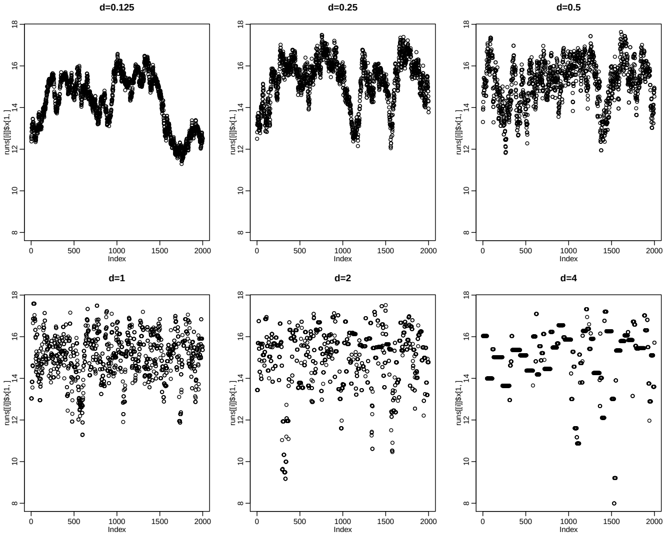
Space-Shuttle O-ring - Random Walk Proposal (cont)

First 2000 steps:

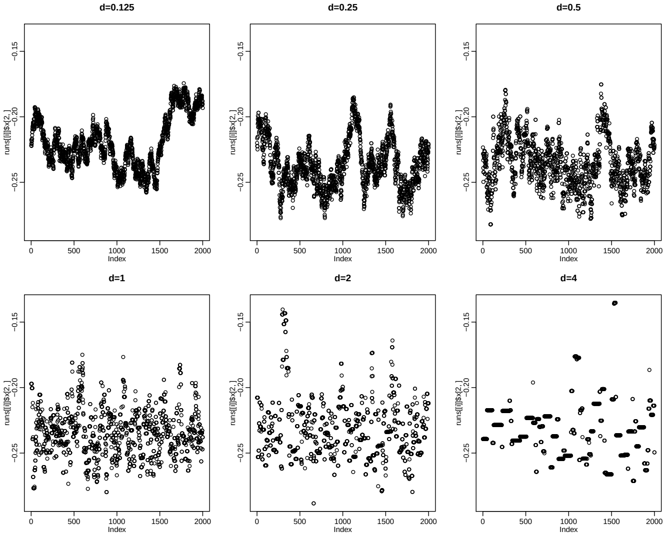


d	0.125	0.25	0.5	1	2	4
Acceptance Rate	0.88	0.762	0.5645	0.3275	0.1655	0.0425

Space-Shuttle O-ring - Random Walk Proposal - Intercept



Space-Shuttle O-ring - Random Walk Proposal - Slope



Sufficient Condition for Stationary Densities

Definition

A Markov chain with transition kernel K satisfies the detailed balance condition with the probability density function f if

$$K(x, y)f(x) = K(y, x)f(y) \quad \forall x, y$$

Remarks

- $K(x, y)f(x)$=mass flowing from x to y.
  $K(y, x)f(y)$=mass flowing from y to x.
- Detailed balance is (up to measure theoretic complications) equivalent to "reversibility":
  A stationary Markov chain (X_n) is *reversible* if
  $(X_{n+1}|X_{n+2} = x) \sim (X_{n+1}|X_n = x)$.

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$$K(x,y)f(x) = K(y,x)f(y) \quad \forall x, y$$

Theorem

Suppose a Markov chain satisfies the detailed balance condition with the pdf f. Then f is the invariant density of the chain.

Proof.

Let $X_n \sim f$. Then $\forall B$:

$$\begin{aligned}\mathrm{P}(X_{n+1} \in B) &= \int_{\mathcal{X}} K(y,B)f(y)dy = \int_{\mathcal{X}}\int_B K(y,x)f(y)dxdy \\ &= \int_{\mathcal{X}}\int_B K(x,y)f(x)dxdy = \int_B \underbrace{\int_{\mathcal{X}} K(x,y)dy}_{=1} f(x)dx = \mathrm{P}(X_n \in B)\end{aligned}$$

Stationary Distribution of the Metropolis-Hastings Alg.

Theorem

Suppose $\bigcup_{x \in \operatorname{supp} f} \operatorname{supp} q(x, \cdot) \supset \operatorname{supp} f$*. Then* f *is a stationary distribution of the chain.*

Proof.

Will verify the detailed balance condition
$K(x, y)f(x) = K(y, x)f(y) \quad \forall x, y.$
Here,

$$K(x, y) = \rho(x, y)q(x, y) + (1 - r(x))\delta_x(y),$$

where $r(x) = \int \rho(x, y)q(x, y)dy$ is the overall acceptance probability at x and δ_x is the Dirac measure at x. Suffices to check

(a) $\rho(x, y)q(x, y)f(x) = \rho(y, x)q(y, x)f(y)$

(b) $(1 - r(x))\delta_x(y)f(x) = (1 - r(y))\delta_y(x)f(y)$

Both sides of (b)=0 for $x \neq y$;
To see (a): $\rho(x, y) = 1$ or $\rho(y, x) = 1$
(Recall: $\rho(x, y) = \min\left(\frac{f(y)q(y,x)}{f(x)q(x,y)}, 1\right)$) □

Ergodicity of the Metropolis Hastings Algorithm

Let (X^t) be the Markov chain of a Metropolis Hastings algorithm.

- (X^t) is f-irreducible if

$$q(x, y) > 0 \text{ for every } (x, y)$$

  Then (X^t) is Harris-recurrent and the Ergodic theorem applies, i.e. $\forall h \in L^1(f)$:

$$\lim_{T\to\infty} \frac{1}{T} \sum_{t=1}^{T} h(X^t) = \int h(x)f(x)dx \quad \text{a.s.}$$

- If (X^t) is also aperiodic then

$$\lim_{n\to\infty} \| \int K^n(x, \cdot)\mu(dx) - f\|_{\mathrm{TV}} = 0,$$

  for every initial distribution μ, where K^n denotes the n step transition kernel.
- (X^t) is aperiodic if the probability of rejecting a step is positive (i.e. $\mathrm{P}(X^t = X^{t+1}) > 0$).

What is a good acceptance rate?

- Independent Proposal Distribution:
  As close to 1 as possible
  (ideally, I would like the proposal distribution to equal the distribution to be simulated)
- Random Walk:
  - too high: support of f is not explored quickly
    In particular if the density is multimodal
  - too low: waste of simulations (proposals outside the range of f)
  - Heuristic: acceptance rate of $1/4$ for high-dimensional models and of $1/2$ for models of dimension 1 or 2.
    See Roberts et al. (1997).

Adaptive Schemes

- Unrealistic to hope for a generic MCMC sampler that works in every possible setting
- Problems: High dimension, disconnected support
- Problems of adaptive schemes (prior states of the Markov Chain are used to tune e.g. the proposal distribution): Markov property gets lost $\rightarrow$ loss of theoretical underpinning
- Article on theoretical underpinning of adaptive MCMC: e.g. Andrieu & Moulines (2006)
- To be on the safe side:
  - Use a burn-in period to tune parameters such as the proposal distribution.
  - The burn-in period should not contribute to expectations/quantiles of the target distribution.

Outline

Gibbs Sampler - Introduction

- Origin of the name "Gibbs sampling":
  Geman & Geman (1984), who brought Gibbs sampling into statistics, used the method for a Bayesian study of Gibbs random fields, which have their name from the physicist Gibbs (1839-1903)
- Main idea:
  - update components of the Markov Chain individually
  - by sampling the component to be updated conditional on the value of the other components.

The Gibbs Sampler

Want to sample from the density $f : \mathbb{R}^p \to [0, \infty)$
f_j=conditional density of $X_j | \{X_i, i \neq j\}$
Let X^0 be some starting value.
For $t = 0, 1, 2, \dots$:

- $X_1^{t+1} \sim f_1(x_1 | X_2^t, \dots, X_p^t)$
- $X_2^{t+1} \sim f_2(x_2 | X_1^{t+1}, X_3^t, \dots, X_p^t)$
- $\dots$
- $X_p^{t+1} \sim f_p(x_p | X_1^{t+1}, \dots, X_{p-1}^{t+1})$

Example - Truncated Normal

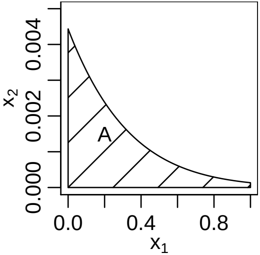
Want to sample from $N(-3,1)$ truncated to $[0,1]$, i.e.

$$f(x) \propto \exp\left(-\frac{(x+3)^2}{2}\right) \mathbb{I}(0 \leq x \leq 1)$$

Consider the uniform distribution g on

$$A = \left\{(x_1, x_2)' : x_1 \in [0,1], 0 \leq x_2 \leq f(x_1)\right\}$$

f is the marginal density of the first component.



Gibbs sampler for g

- $g_1(x_1|x_2) \propto \mathbb{I}(0 \leq x_1 \leq \min(1, -3 + \sqrt{-2\log x_2}))$
- $g_2(x_2|x_1) \propto \mathbb{I}(0 \leq x_2 \leq f(x_1))$

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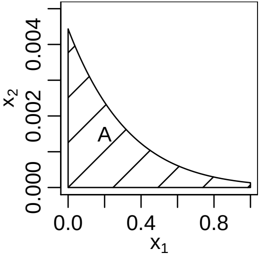

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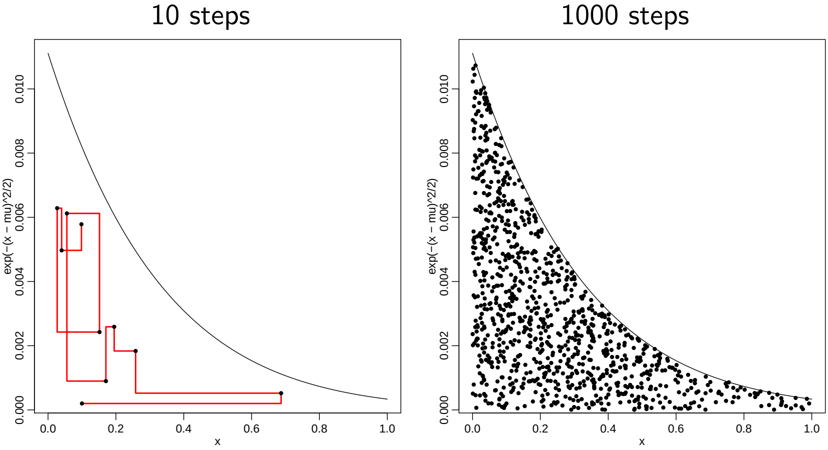

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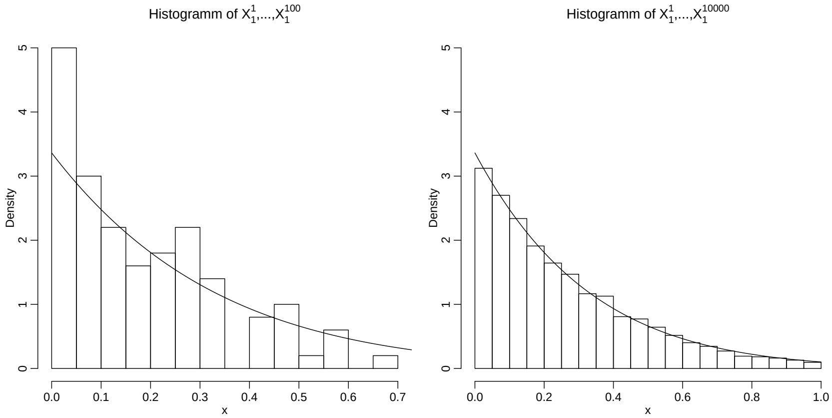


Gibbs-Sampler- Stationary Distribution

- Will show that f is stationary for each of the p steps
- WLOG consider the first step
- Need to show: If $(X_1, X_2, \dots, X_p) \sim f$ and $\tilde{X}_1 \sim f_1(x_1 | X_2, \dots, X_p)$ then $(\tilde{X}_1, X_2, \dots, X_p) \sim f$
- Let $X_{-1} = (X_2, \dots, X_p)$, $x_{-1} = (x_2, \dots, x_p)$.
- Let $p_A := \mathrm{P}((\tilde{X}_1, X_2, \dots, X_p) \in A)$.

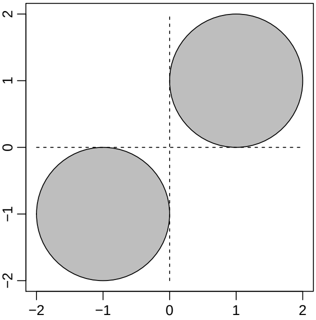
$$p_A = \int \int \mathtt{I}((\tilde{x}_1, x_{-1}) \in A) f_1(\tilde{x}_1 | x_{-1}) d\tilde{x}_1 f(x) dx$$

- Using $\int f(x) dx_1 = \int f_1(x_1 | x_{-1}) f_{-1}(x_{-1}) dx_1 = f_{-1}(x_{-1})$,

$$\begin{aligned} p_A &= \int \int \mathtt{I}((\tilde{x}_1, x_{-1}) \in A) f_1(\tilde{x}_1 | x_{-1}) d\tilde{x}_1 f_{-1}(x_{-1}) dx_{-1} \\ &= \int \int \mathtt{I}((\tilde{x}_1, x_{-1}) \in A) f(\tilde{x}_1, x_{-1}) d\tilde{x}_1 dx_{-1} = \int \mathtt{I}(x \in A) f(x) dx \end{aligned}$$

Gibbs-Sampler- Disconnected Support - Example

- Let D_1 and D_2 be discs in $\mathbb{R}^2$ with radius 1 and and centres $(1, 1)$ and $(-1, -1)$
- Consider the uniform distribution on $D_1 \cup D_2$
- Gibbs Sampler is not an irreducible chain (remains concentrated in the disc it is started in)
- (transformation of coordinates to $x_1 + x_2$ and $x_2 - x_1$ would solve the problem)



Gibbs Sampler - Some Theoretical Results

- If f satisfies the following positivity condition then the resulting Gibbs sampler is f-irreducible.

$$f^{(i)}(x_i) > 0 \forall i \implies f(x_1, \dots, x_p) > 0$$

  ($f^{(1)}, \dots, f^{(p)}$ denote the marginal distributions)
- If a Gibbs sampler is
  - f-irreducible with stationary distribution f and
  - for every x the transition probability $K(x, \cdot)$ is absolutely continuous with respect to f

  then the Gibbs sampler is Harris recurrent. (Tierney, 1994, Corollary 1)
- (Recall: Harris recurrence implies the usual ergodicity results)

BUGS software

- Bayesian inference Using Gibbs Sampling
- “flexible software for the Bayesian analysis of complex statistical models using Markov chain Monte Carlo (MCMC) methods”
- Allows specification of Bayesian models in the BUGS language. MCMC chain is constructed automatically.
- Original version: WinBUGS
- Open source version: OpenBUGS
- Similar: JAGS (based on C, hopefully more portable)

Outline

Introduction

- A variable dimension model is a "model where one of the things you do not know is the number of things you do now know" (Peter Green)
- in other words: the dimension of the parameter space is not fixed.
- can occur in model selection, checking, improvement, ...

Bayesian variable dimension model

- A Bayesian variable dimension model is defined as a collection of models ($k = 1, \dots, K$),

$$\mathcal{M}_k = \{f(\cdot|\theta_k); \theta_k \in \Theta_k\},$$

  with a collection of priors on the parameters of these models,

$$\pi_k(\theta_k),$$

  and a prior distribution $\rho_k, k = 1, \dots, K$ on the indices of these models.
- Note: Θ_k may have different dimensions
- In this setting one can compute the posterior probability of models, i.e.

$$p(\mathcal{M}_k|\mathbf{y}) = \frac{\rho_k \int f_k(\mathbf{y}|\theta_k)\pi_k(\theta_k)d\theta_k}{\sum_j \rho_j \int f_j(\mathbf{y}|\theta_j)\pi_j(\theta_j)d\theta_j}$$

Reversible Jump Algorithm

- Want: proper framework for designing moves between models $\mathcal{M}_k$
- Construction of a reversible kernel K on $\Theta = \bigcup_k \{k\} \times \Theta_k$
- Main ideas of Green (1995):
  only consider moves between pairs of models.
  construct "dimension matching" moves.
  accept a move with probability similiar to the Metropolis-Hastings algorithm

Toy Example

(from a tutorial written by Peter Green, see
`http://www.maths.bris.ac.uk/~mapjg/slides/tdtut4.pdf`)

- $x \in \mathbb{R} \cup \mathbb{R}^2$
- $\pi(x)$ is a mixture:
  - x is $U(0,1)$ with probability p_1
  - x is uniform on the triangle $0 < x_2 < x_1 < 1$ with probability $1 - p_1$.
- Three moves:

  (1) within $\mathbb{R}$: $x \to U(\max(0, x-\epsilon), \min(1, x+\epsilon))$
  (2) within $\mathbb{R}^2$: $(x_1, x_2) \to (1 - x_2, 1 - x_1)$
  (3) between $\mathbb{R}$ and $\mathbb{R}^2$

  If $x \in \mathbb{R}$: choose moves (1), (3) with probability $1 - r_1$, r_1
  If $x \in \mathbb{R}^2$: choose moves (2), (3) with probability $1 - r_2$, r_2

Toy Example (cont)

- Trans-dimensional move [(3)]:
  - From $x \in \mathbb{R}$ to $(x_1, x_2) \in \mathbb{R}^2$: draw u from $U(0,1)$, propose (x, u) Accept with probability

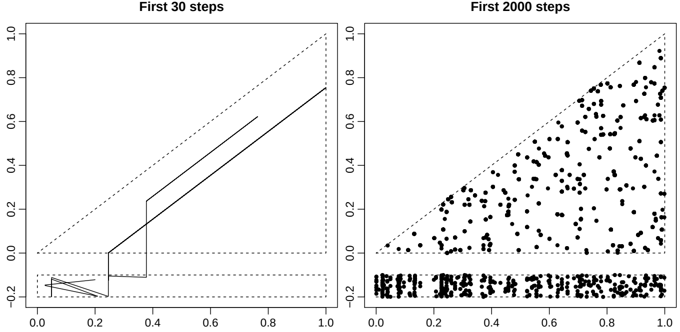
$$\alpha = \min(1, \frac{2(1-p_1)r_2}{p_1 r_1})\mathtt{I}(u < x)$$

  - From $(x_1, x_2) \in \mathbb{R}^2$ to $x \in \mathbb{R}$: propose $x = x_1$

$$\alpha = \min(1, \frac{p_1 r_1}{2(1-p_1)r_2})$$

Toy Example - Results

$p_1 = 0.2,\ r_1 = 0.7,\ r_2 = 0.4,\ \epsilon = 0.3$



Outline

Diagnosing Convergence

- To diagnose convergence to the stationary distribution: plot the parameter ("trace plots").
- Start multiple chains and compare the "within chain variance" to the variance when all chains are thrown together.
- Fundamental problem is mixing - you will never see if you have not explored the entire parameter space.
- No "magic" solution
- Even if you have (somehow) established that the chain is exploring the entire parameter space, there is still the issue of convergence - how long should you run the chain(s)?

Confidence intervals for standard Monte Carlo simulations

- Standard CLT: Suppose $X, X_1, X_2, \dots$ iid with $0 < \mathrm{Var}(X) < \infty$. Then

$$\sqrt{n}\left(\frac{1}{n}\sum_{i=1}^{n} X_i - \mathrm{E}(X)\right) \xrightarrow{d} N(0, \mathrm{Var}(X)) \quad (n \to \infty)$$

- $\mathrm{Var}(X)$ can be reasonably well estimated by the sample variance

$$S^2 = \frac{1}{n-1}\sum_{i=1}^{n}\left(X_i - \frac{1}{n}\sum_{j=1}^{n} X_j\right)^2$$

- Thus an asymptotic $1-\alpha$ confidence interval for $\mathrm{E}(X)$ is

$$\left[\frac{1}{n}\sum_{i=1}^{n} X_i - \frac{1}{\sqrt{n}}cS, \frac{1}{n}\sum_{i=1}^{n} X_i + \frac{1}{\sqrt{n}}cS\right]$$

where c is such that $\Phi(1-c) = \frac{\alpha}{2}$.

CLT for Markov chains

- Suppose $X_1, X_2, \dots$ is a stationary Markov chain. Then, under suitable conditions,

$$\sqrt{n}\left(\frac{1}{n}\sum_{i=1}^{n} X_i - \mathrm{E}(X)\right) \xrightarrow{d} N(0,\sigma^2) \quad (n \to \infty)$$

where

$$\sigma^2 = \mathrm{Var}(X_i) + 2\sum_{k=1}^{\infty} \mathrm{Cov}(X_i, X_{i+k}). \tag{1}$$

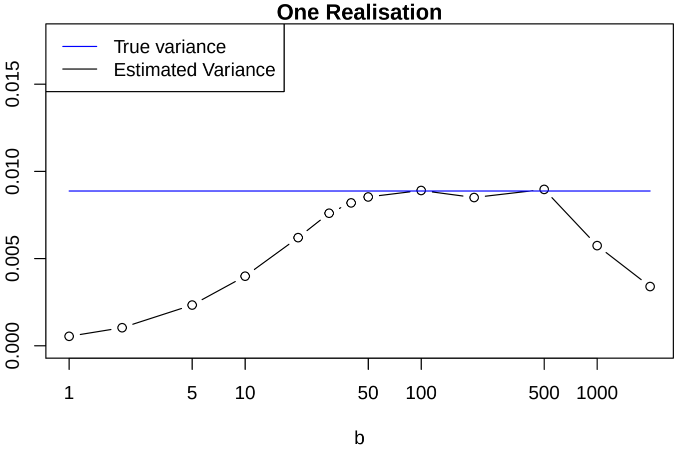
Limiting variance is more complicated.

Batch Means

- Markov chain $X_1, X_2, \ldots$. Interested in $\mu = \mathrm{E}(g(X))$. Assume we want to use the estimator $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} g(X_i)$.
- $$\underbrace{g(X_1)\ \cdots\ g(X_\ell)}_{\hat{\mu}_1}\quad \underbrace{g(X_{\ell+1})\ \cdots\ g(X_{2\ell})}_{\hat{\mu}_2}\quad \cdots,\quad \underbrace{g(X_{n-\ell+1})\ \cdots\ g(X_n)}_{\hat{\mu}_{n/\ell}}$$
  Assuming b divides n, let $\hat{\mu}_k = \frac{1}{b}\sum_{i=(k-1)b+1}^{kb} X_i$.
  Then $\hat{\mu} = \frac{1}{n/b}\sum_{k=1}^{n/b}\hat{\mu}_k$.
- $\hat{\mu}_1$, $\hat{\mu}_2$, ... is again a Markov chain with a similar CLT.
- Pragmatic approach: hope that the autocovariance is much smaller, so that $\hat{\mu}_1, \hat{\mu}_2, \ldots$ can be treated as an iid sample.
- Then construct confidence intervals using $\frac{1}{n/b}S_b^2$ as estimate of the variance of $\hat{\mu}$, where S_b^2 is the sample variance of $\hat{\mu}_1, \ldots, \hat{\mu}_{n/b}$.
- Note: $\frac{1}{n/b}S_b^2$ tends to underestimate the variance of $\hat{\mu}$ (as we are ignoring terms in (1)).

Batch Means - Example AR(1)

- $X_i = 0.9 \cdot X_{i-1} + \epsilon_i$, $\epsilon_i \sim N(0,1)$ independently, $i = 1, \ldots, 10000$.



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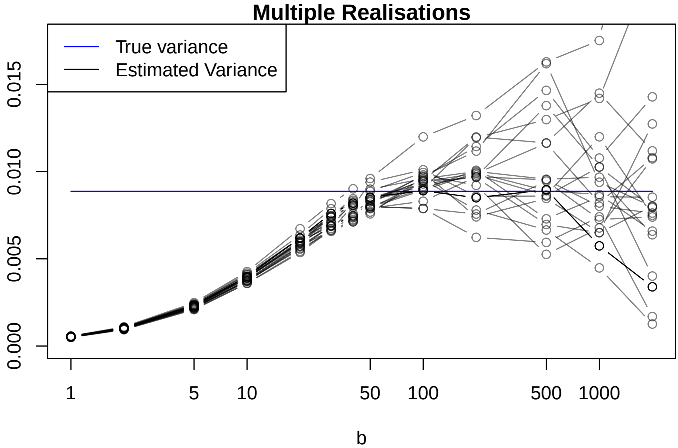

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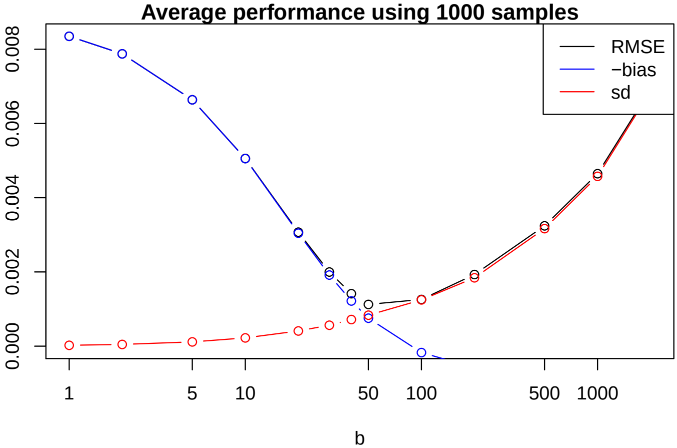


Comments

- Bias-variance trade-off (small batch size: bias, underestimation of the variance, large batch size: variance).
- The batches can also be taken to be overlapping.
- Other approaches try to estimate the coefficients in (1) directly, see e.g. (Brooks et al., 2011, Section 1.10.2)

Outline

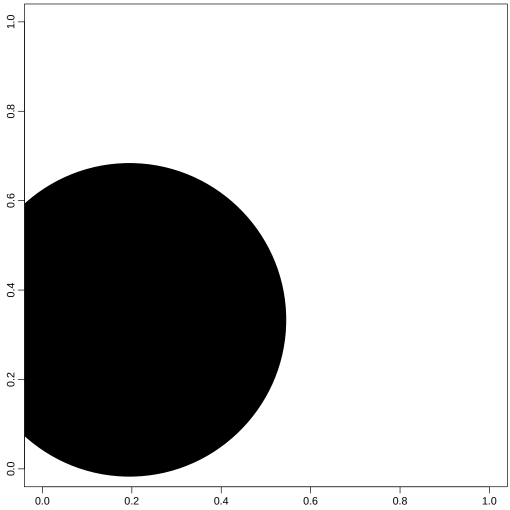
Perfect Sampling - Introduction

- So far: run Markov chain forward
- downside: converge to the stationary distribution only asymptotically
- Perfect Sampling: get a sample from precisely the stationary distribution.
- Methods in this section are not (yet?) in mainstream use

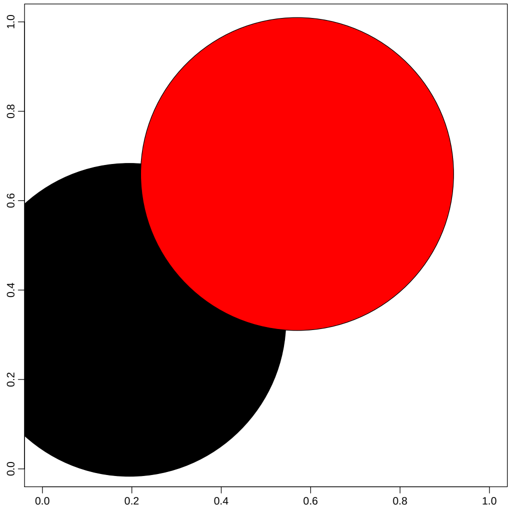
Example - Falling Leaves

- observe the square (0,1)x(0,1)
- leave = circle of radius r=0.35
- centre of falling leaves follows a Poisson distribution (will sample it on (-r,1+r)x(r,1+r))
- Markov chain with state space: leaves seen from the top
- Interested in obtaining a sample from the stationary distribution.

Time running forwards



Time running forwards



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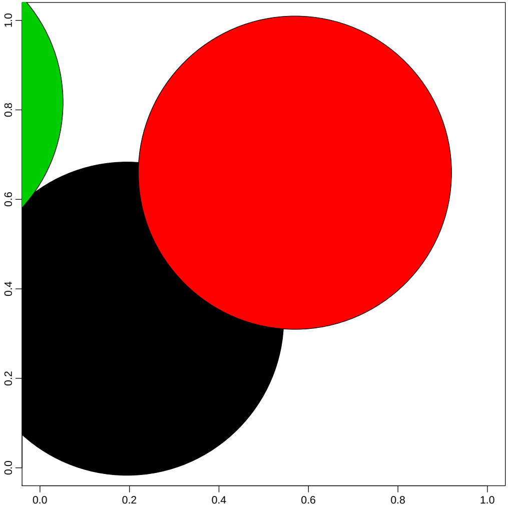

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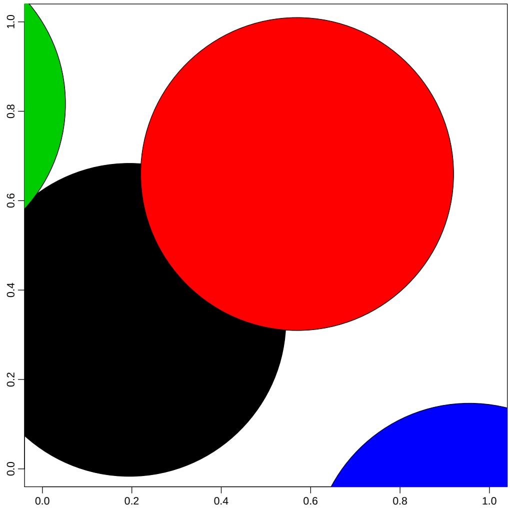

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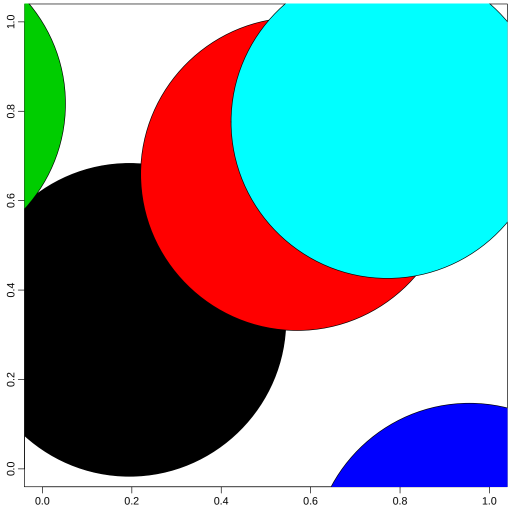

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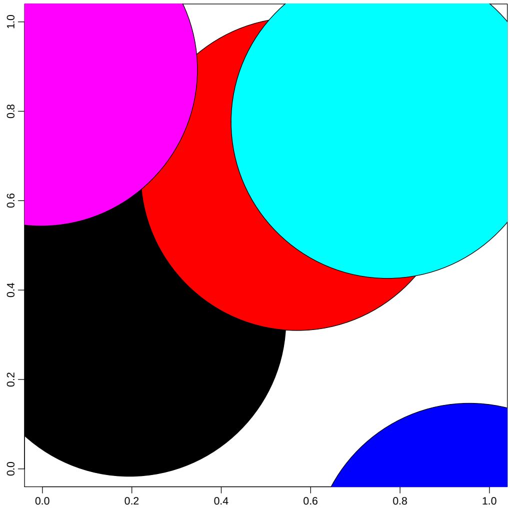

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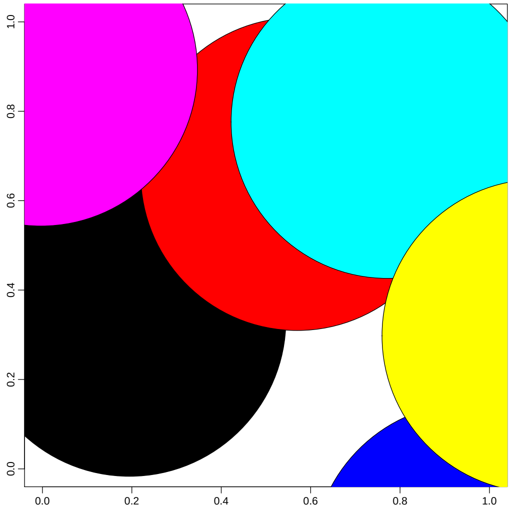

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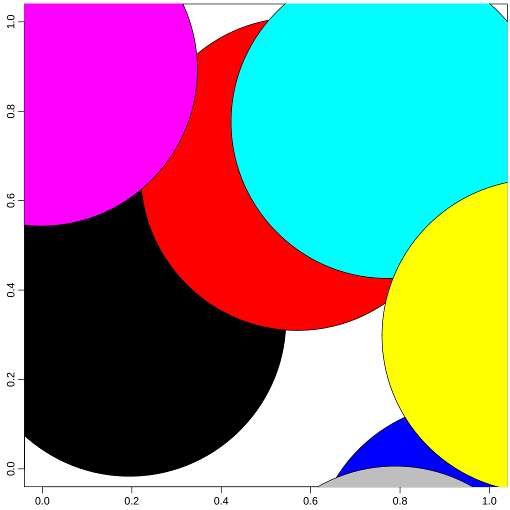

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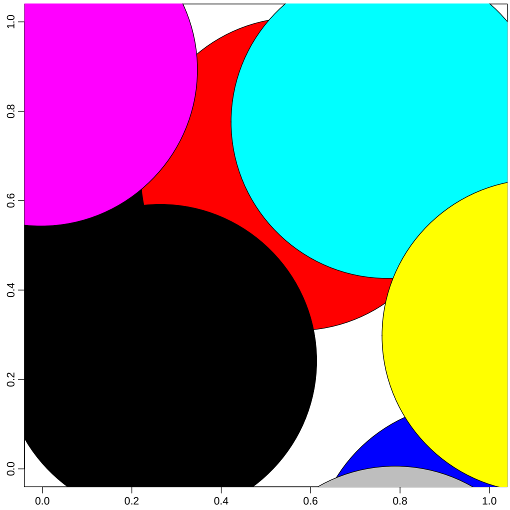

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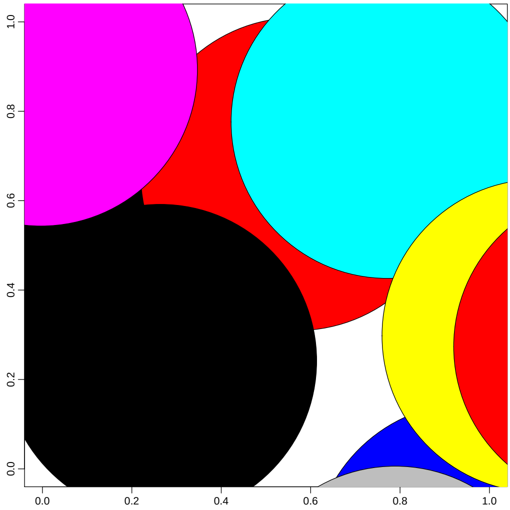

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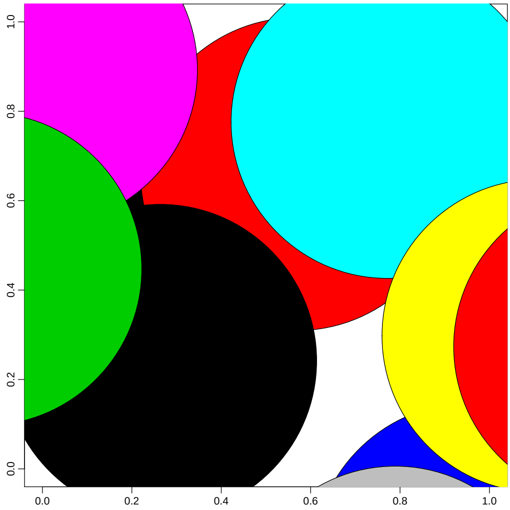

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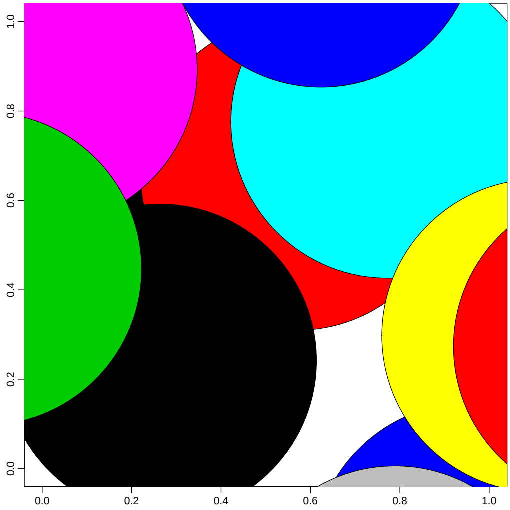

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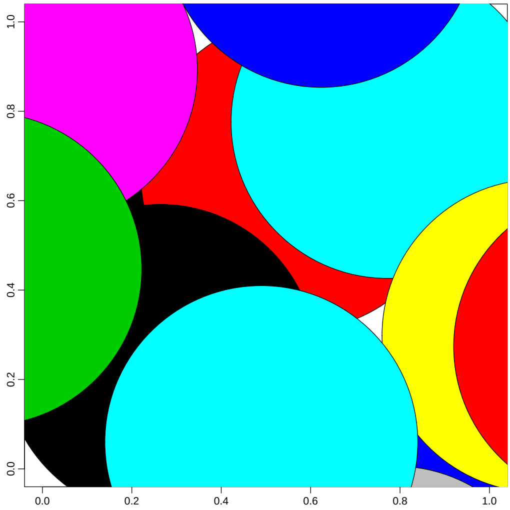

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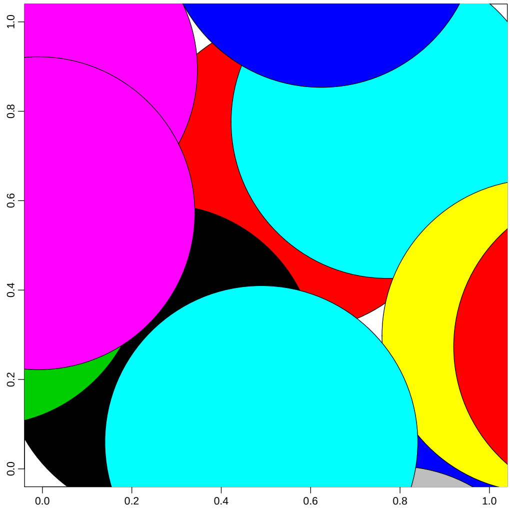

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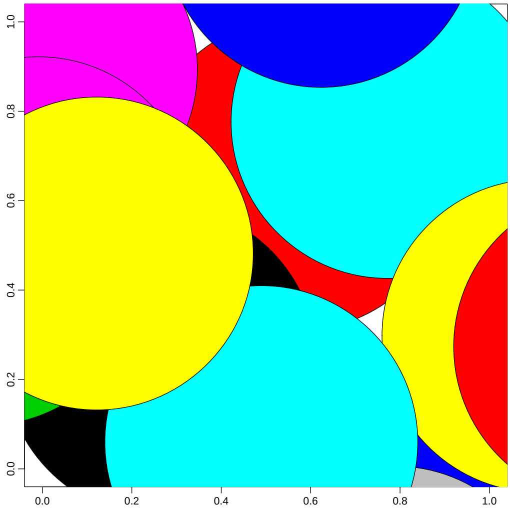

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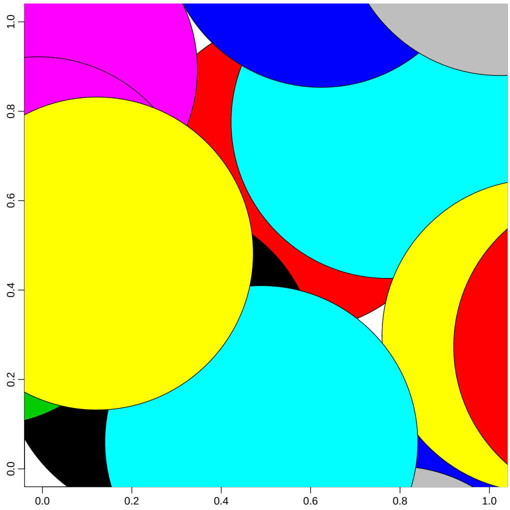

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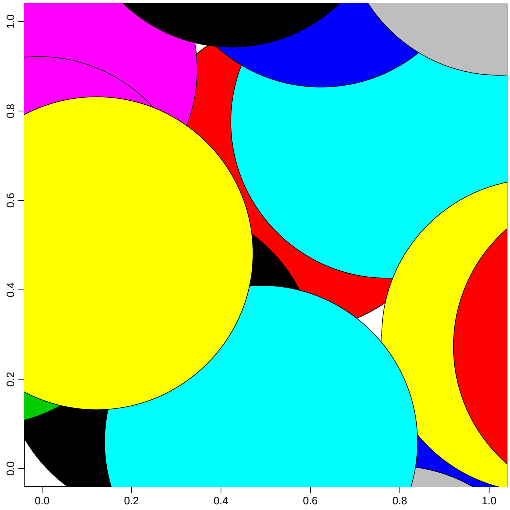

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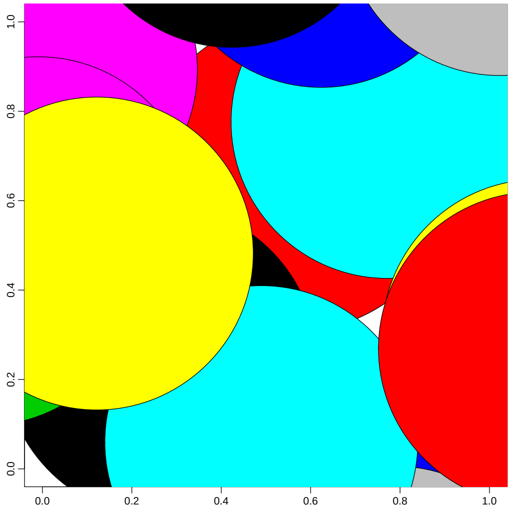

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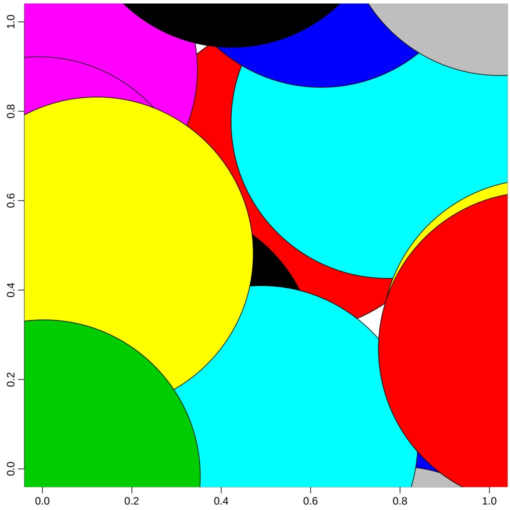

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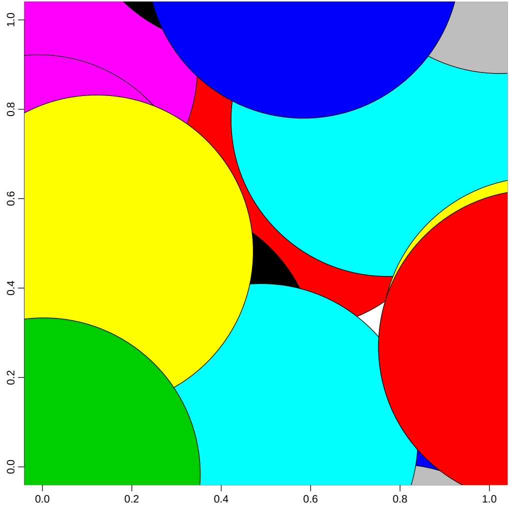

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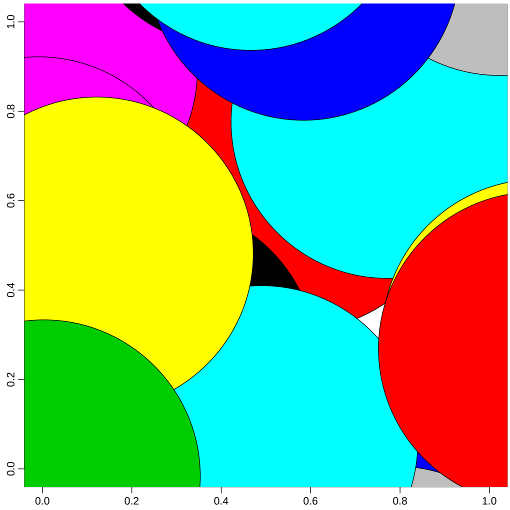

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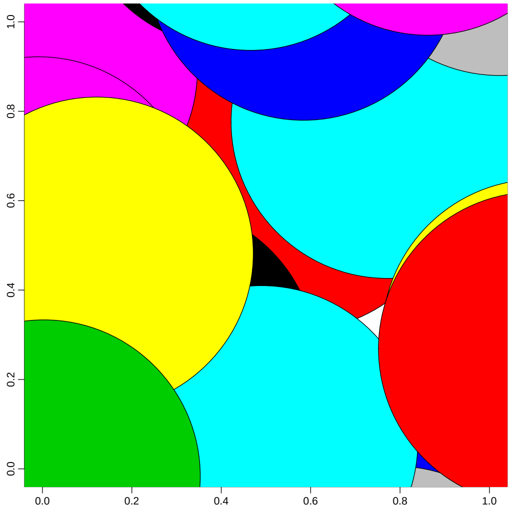

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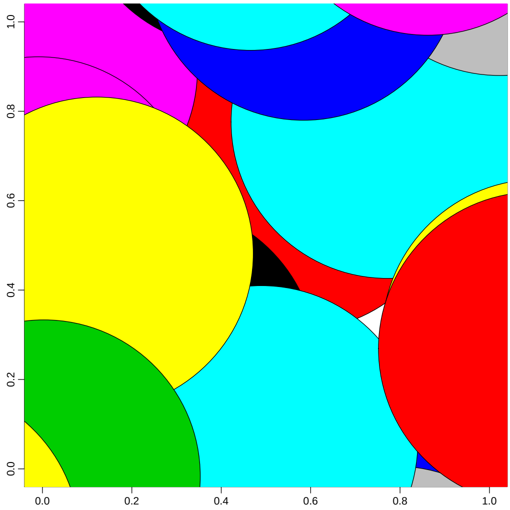

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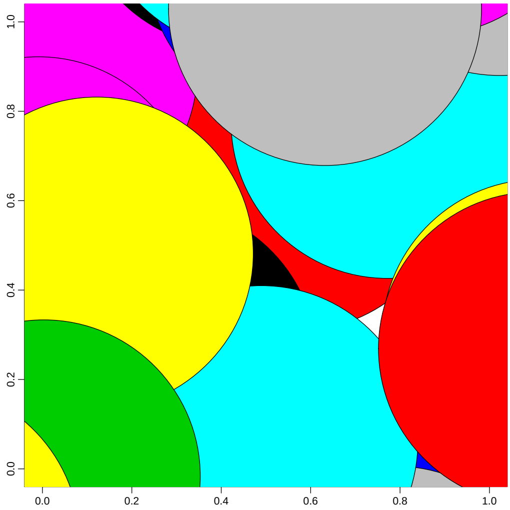

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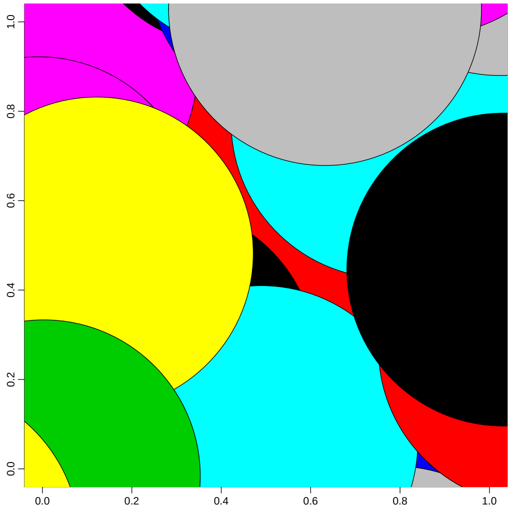

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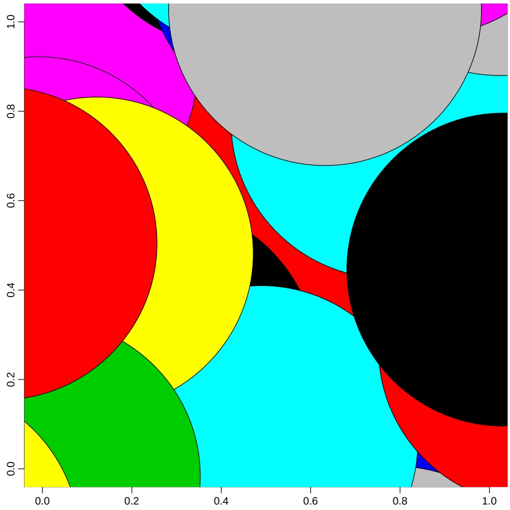

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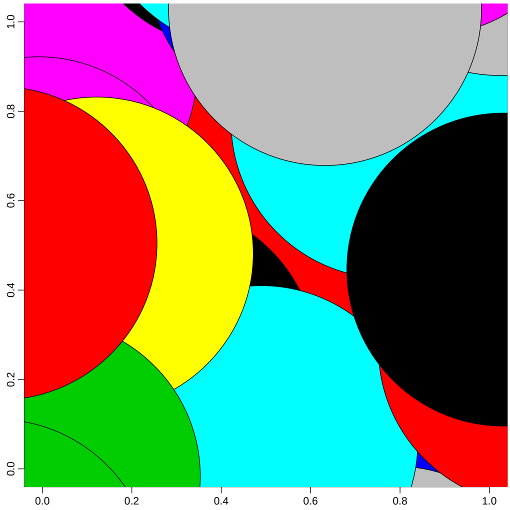

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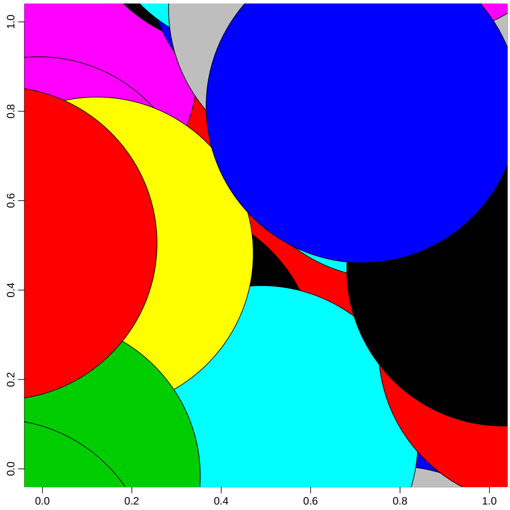

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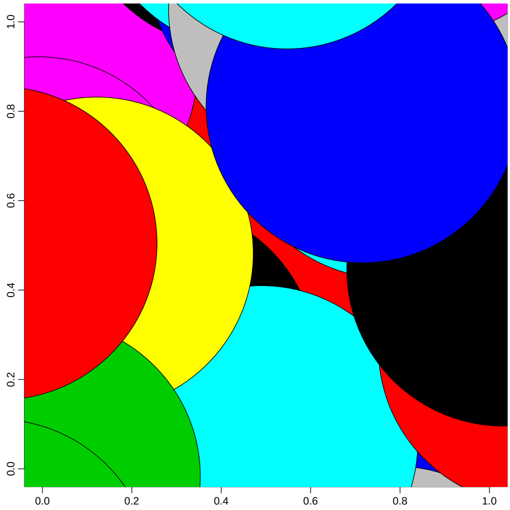

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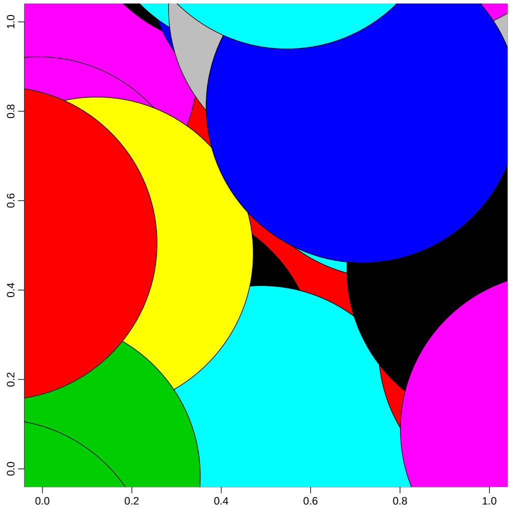

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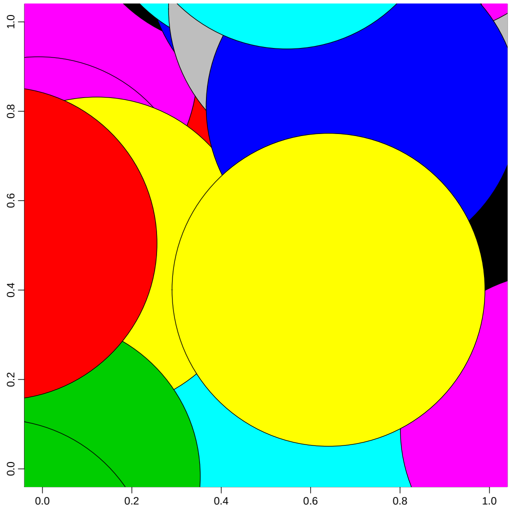

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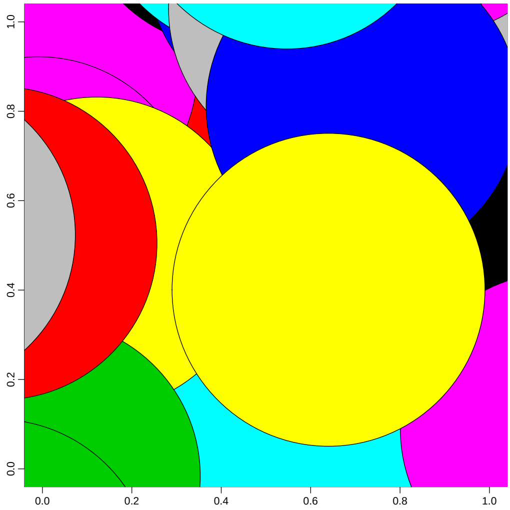

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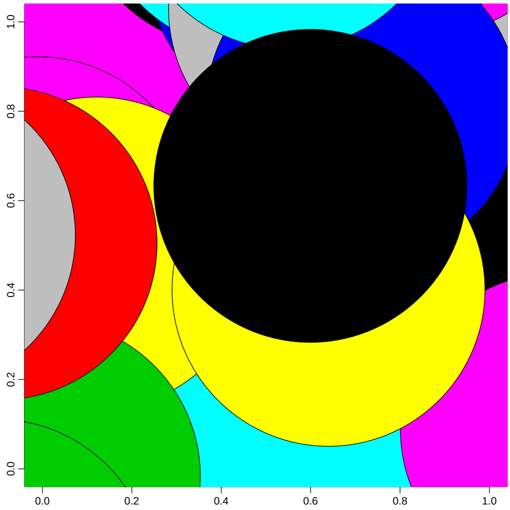

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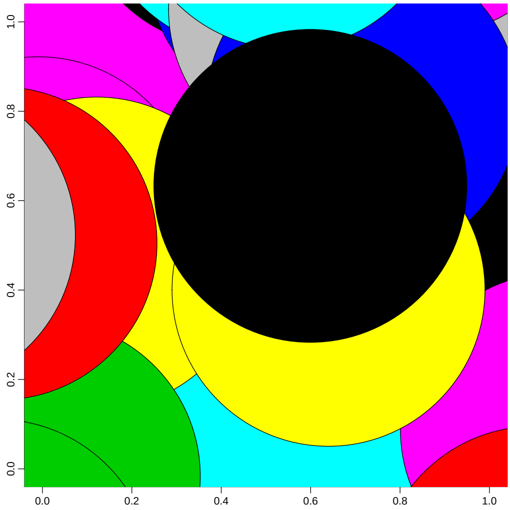

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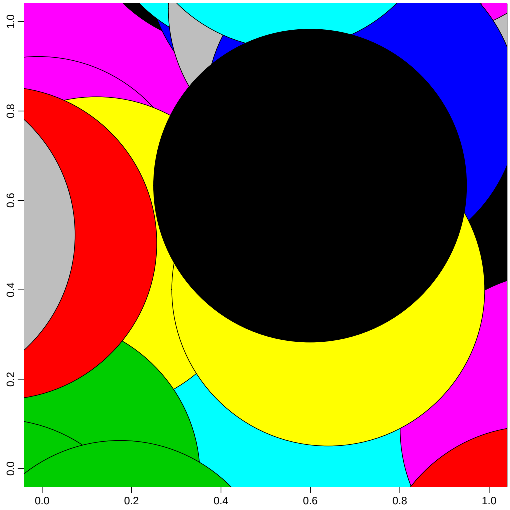

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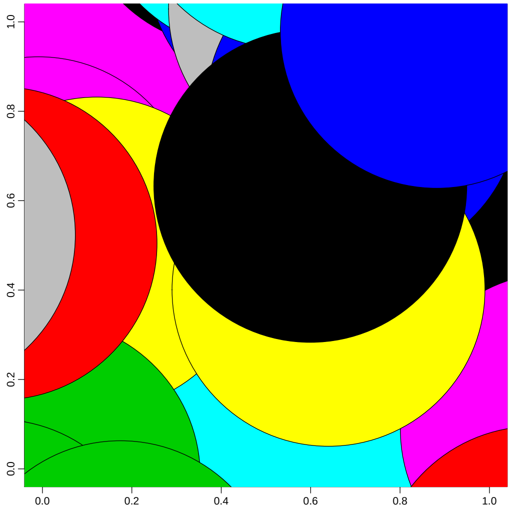

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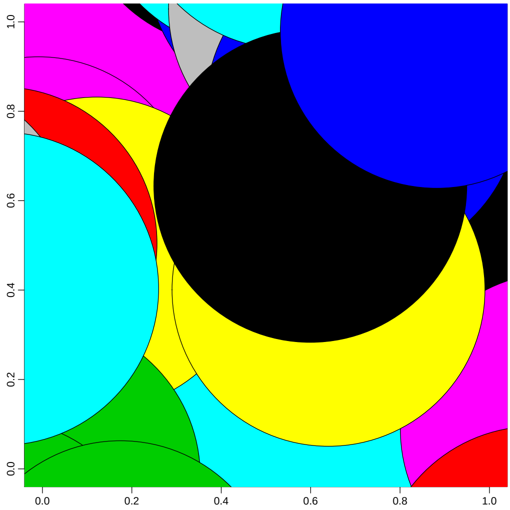

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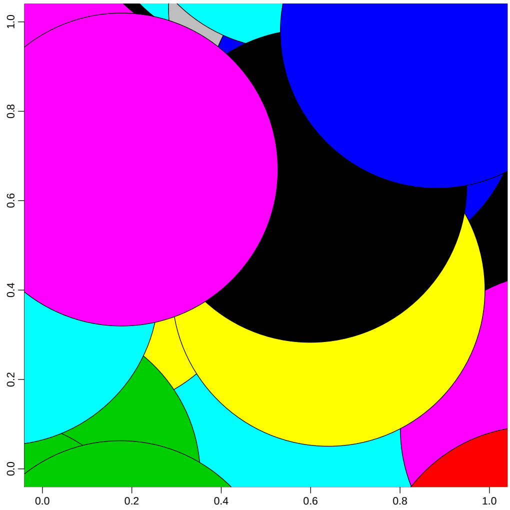

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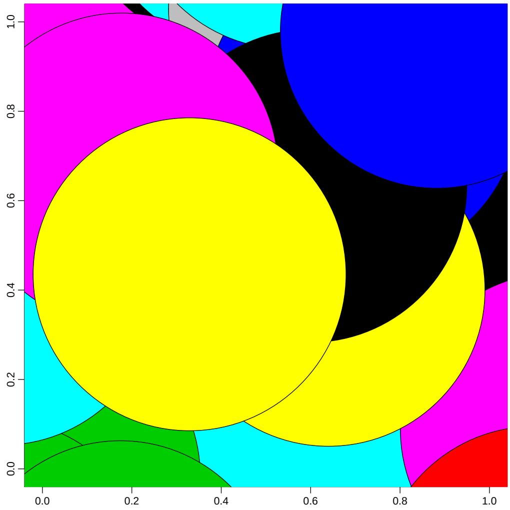

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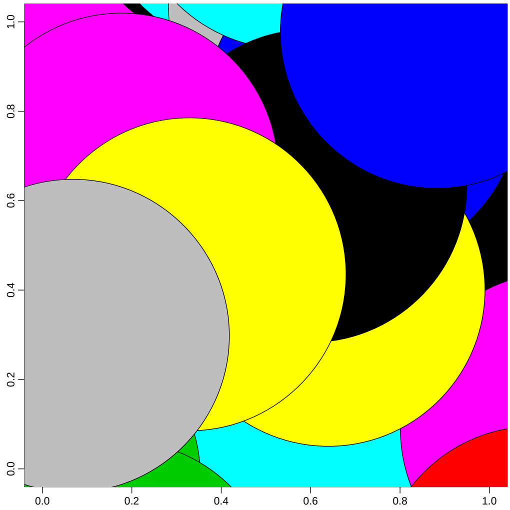

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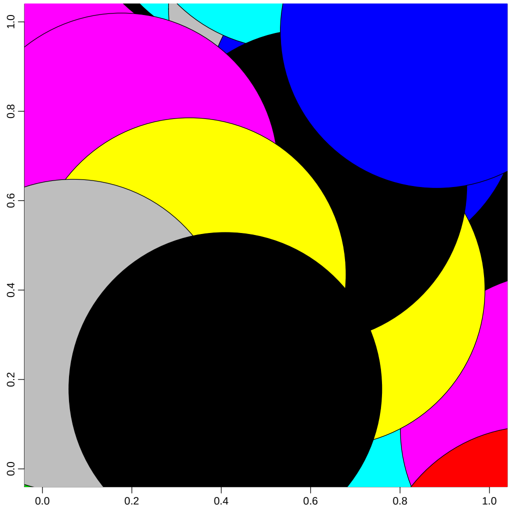
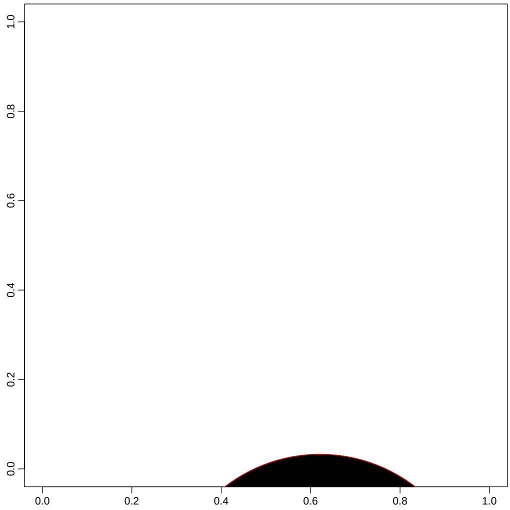


Comments

- Not clear how long to run the chain.
- At best, we can get a sample from an approximation to the distribution of interest.
- This is essentially a problem for all MCMC algorithms so far.

Time running backwards



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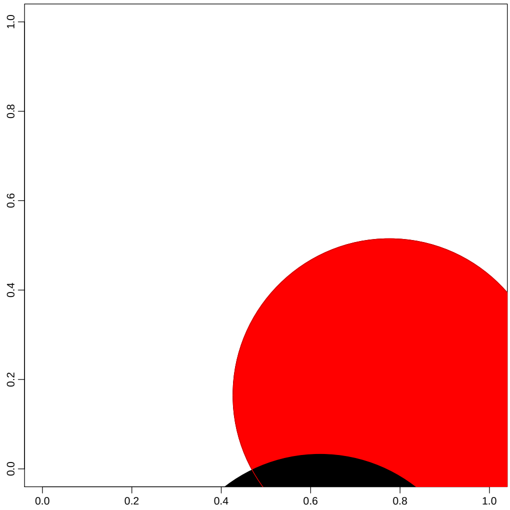

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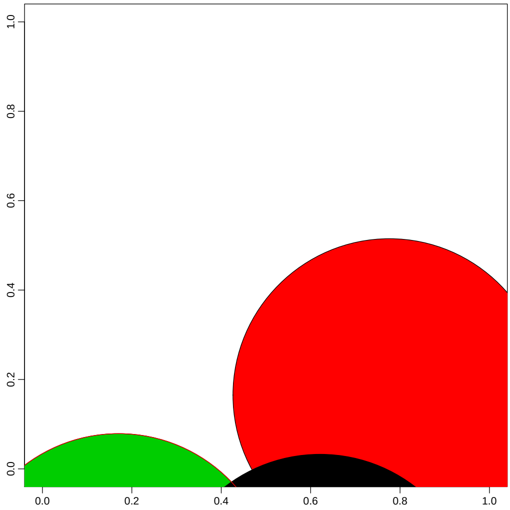

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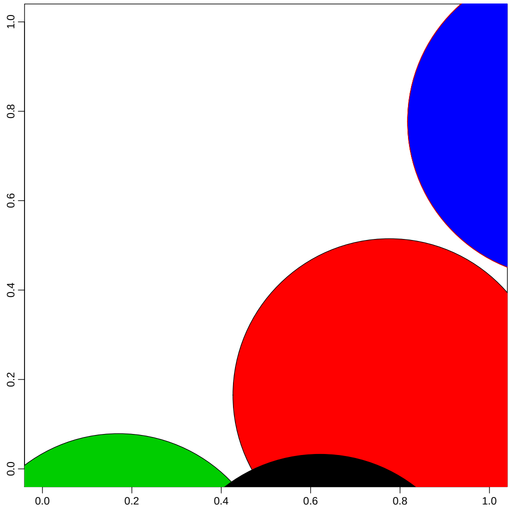

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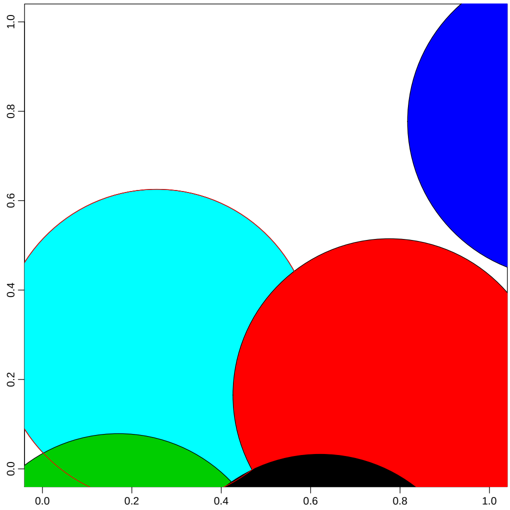

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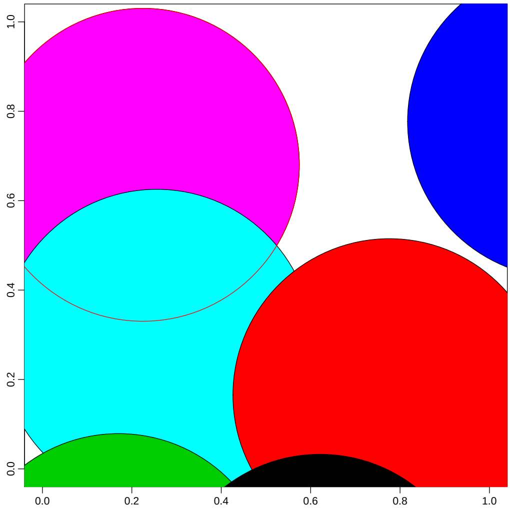

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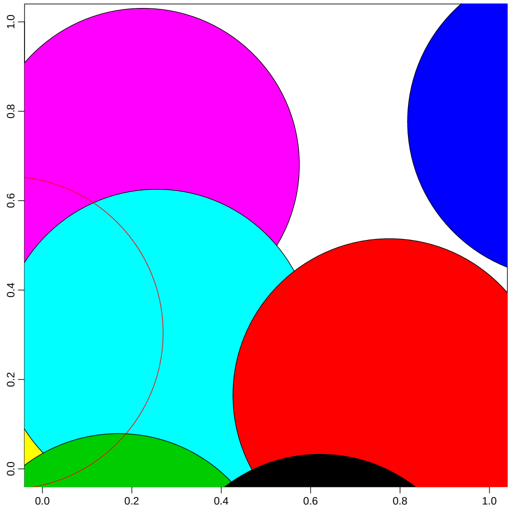

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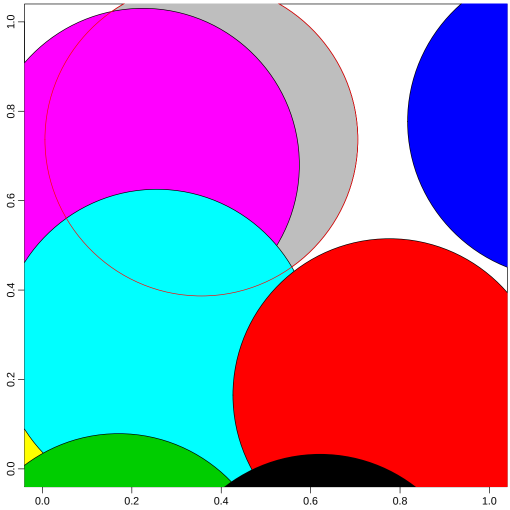

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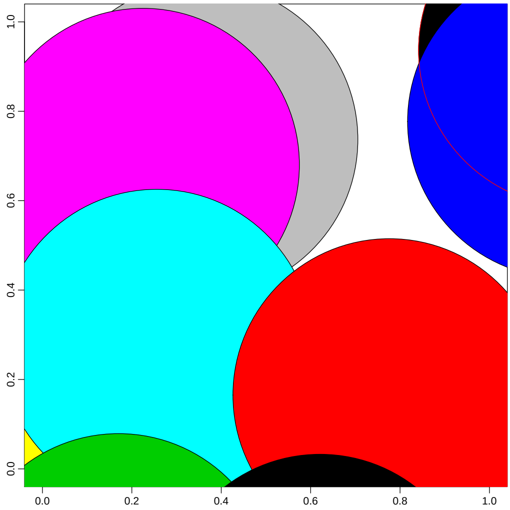

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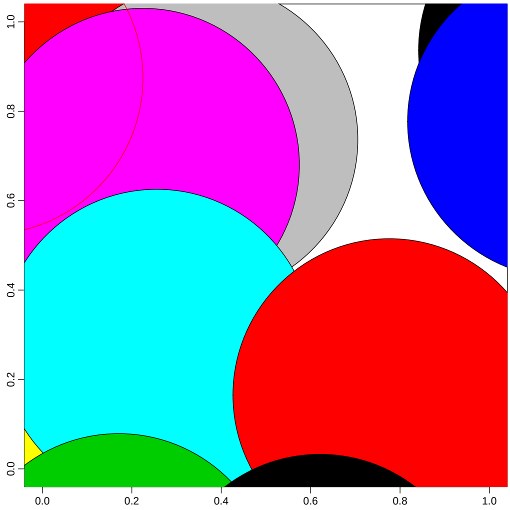

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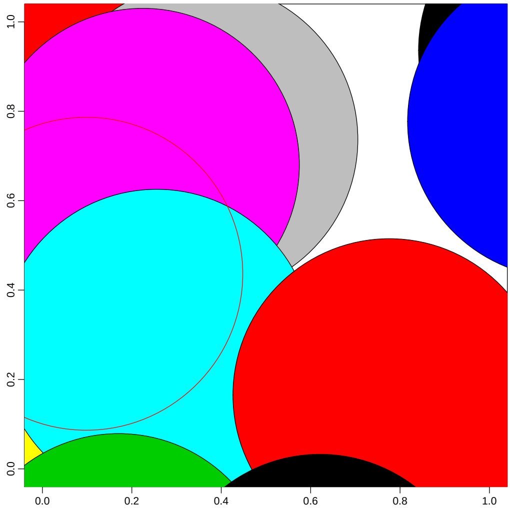

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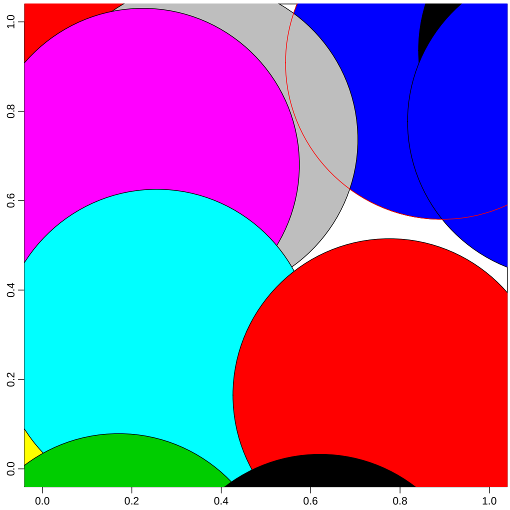

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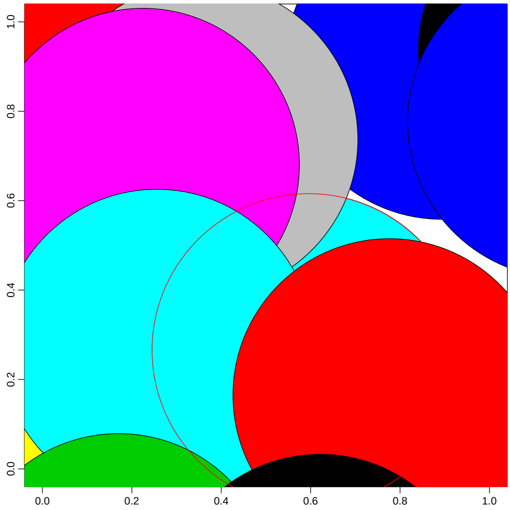

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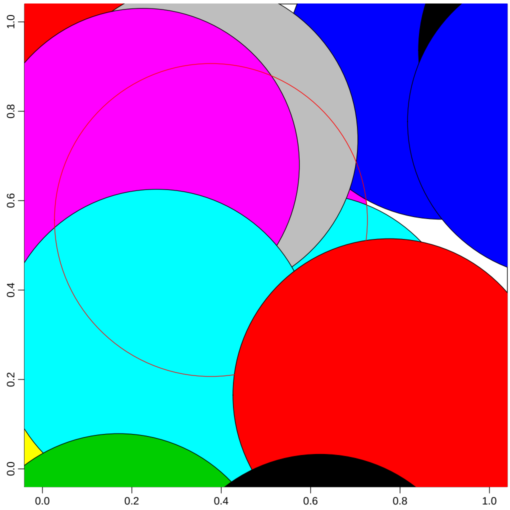

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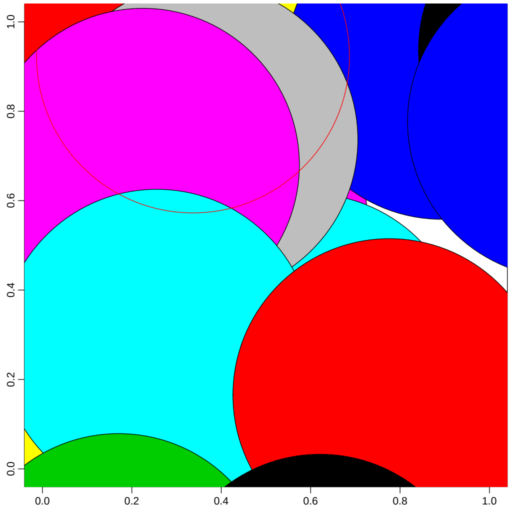

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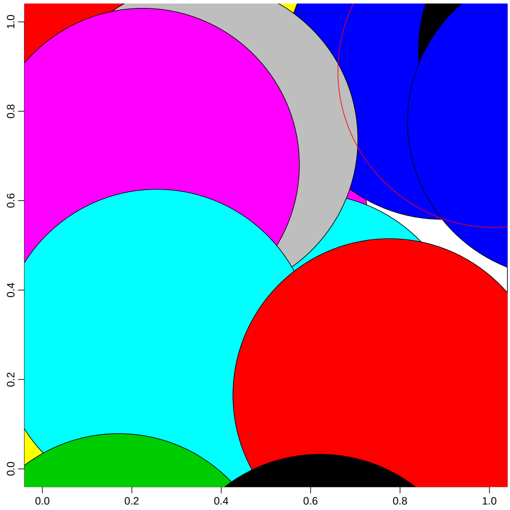

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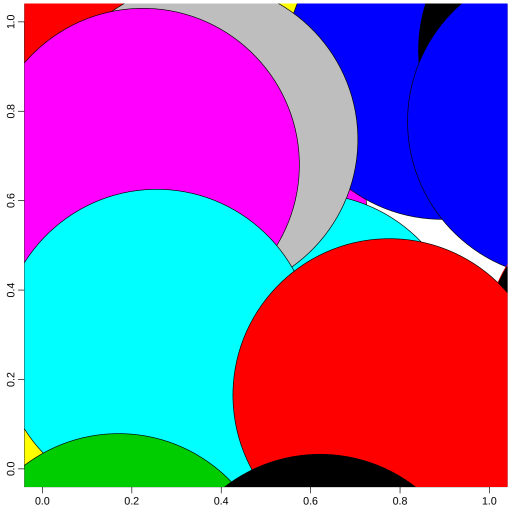

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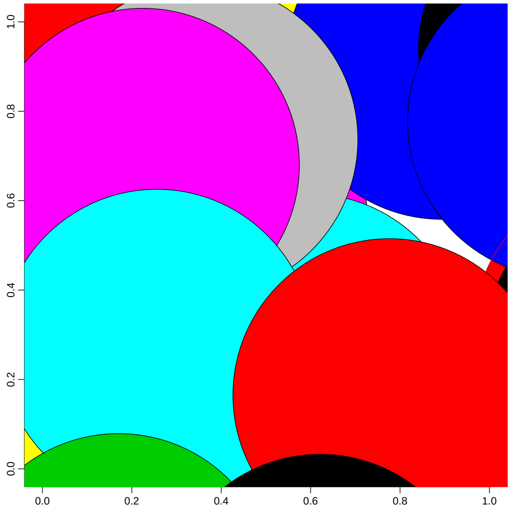

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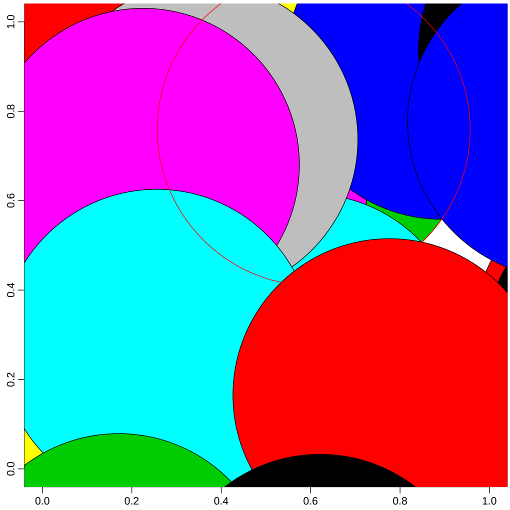

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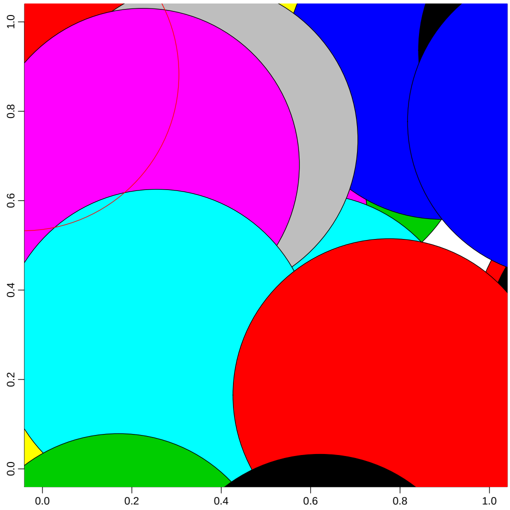

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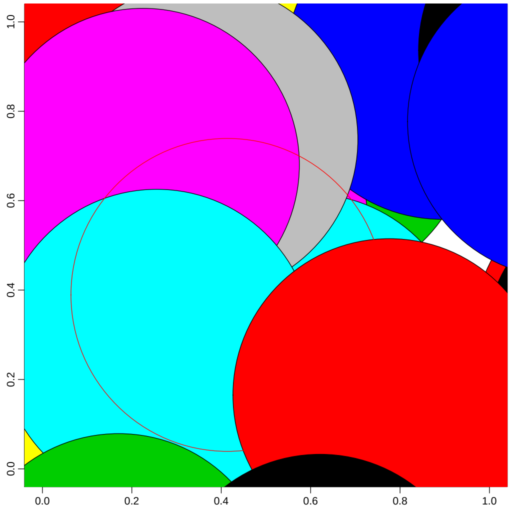

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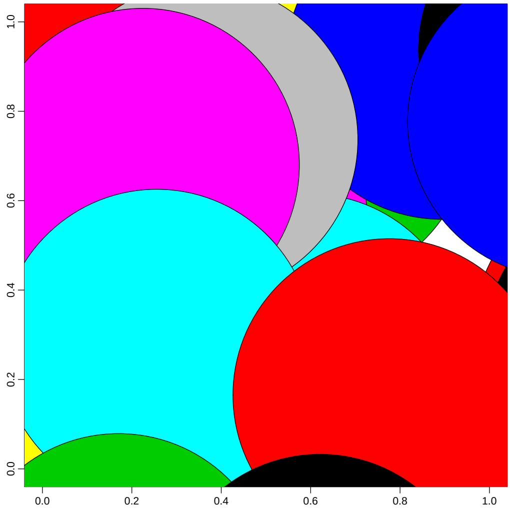

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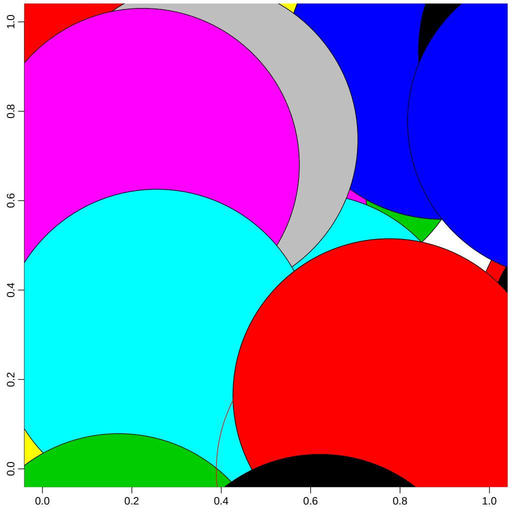

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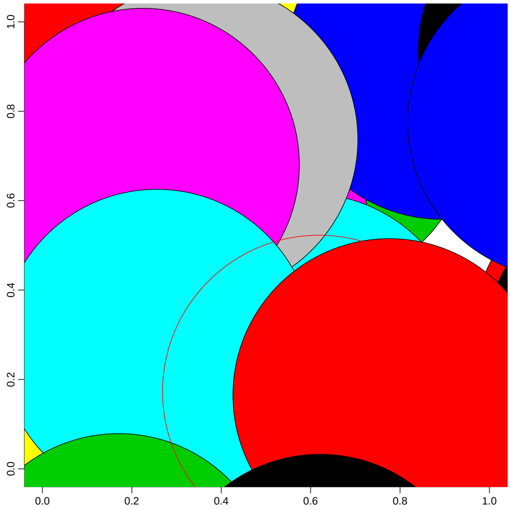

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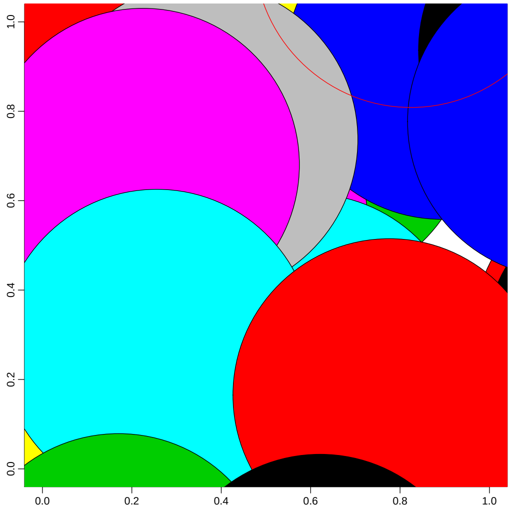

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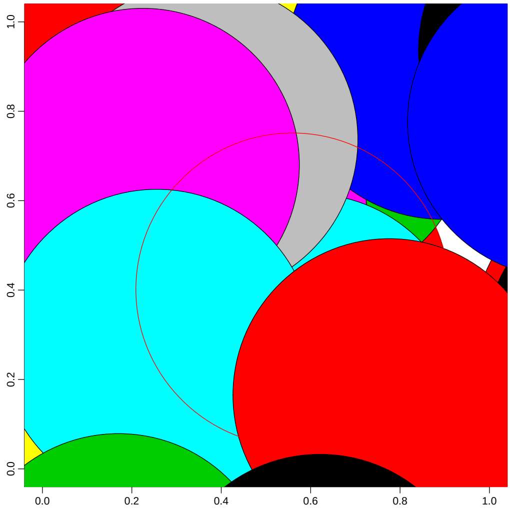

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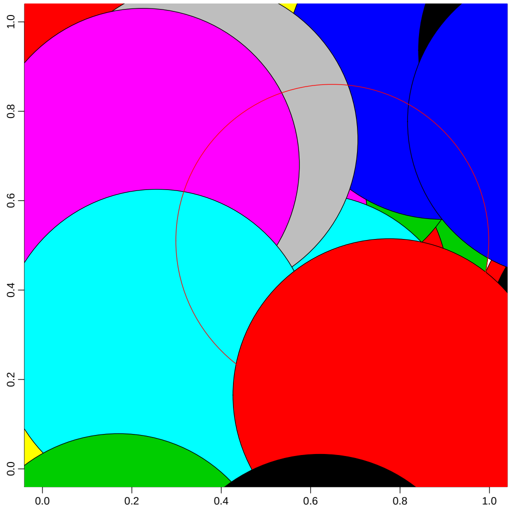

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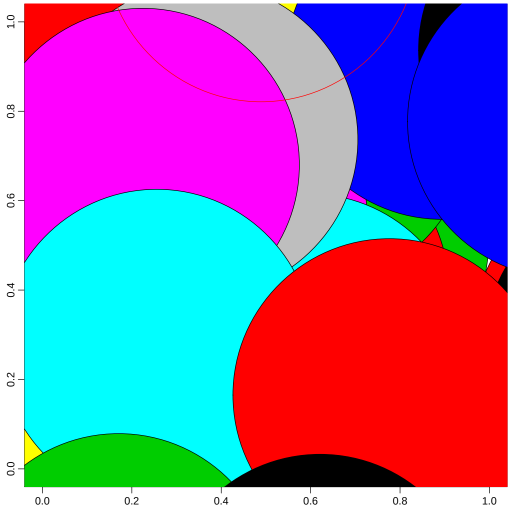

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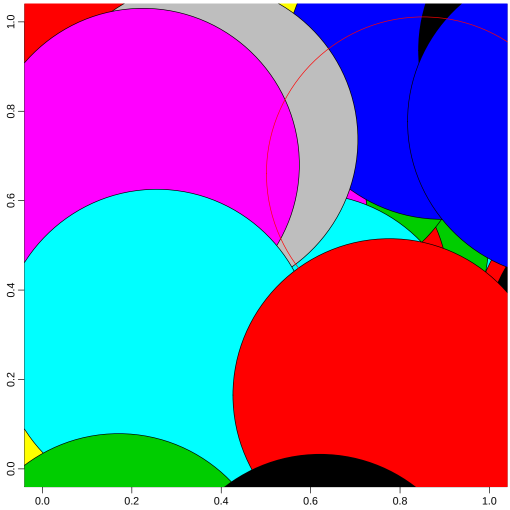

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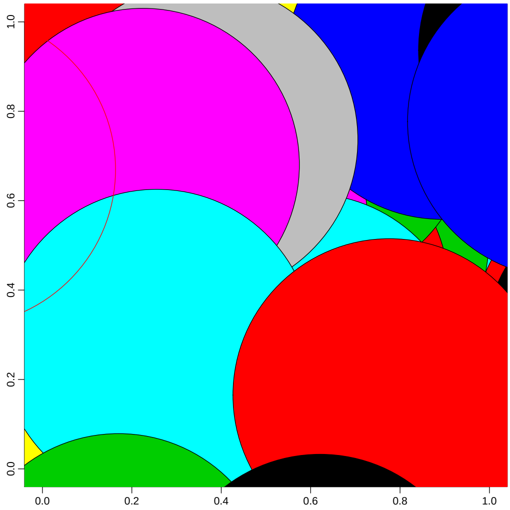

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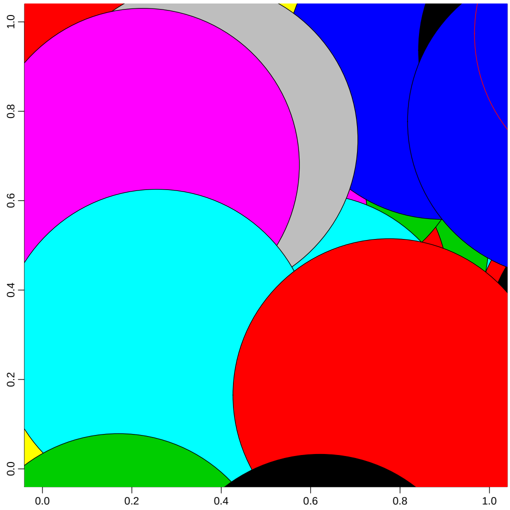

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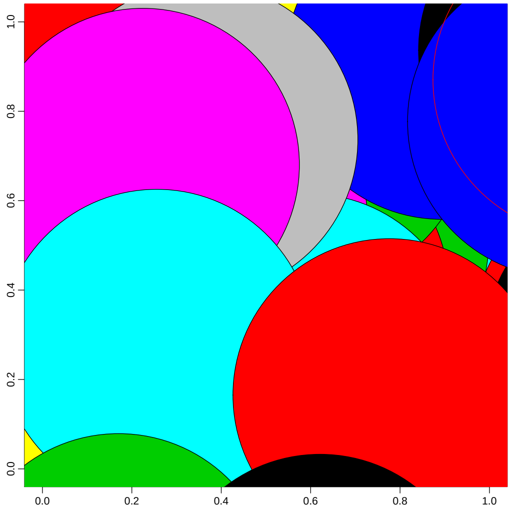

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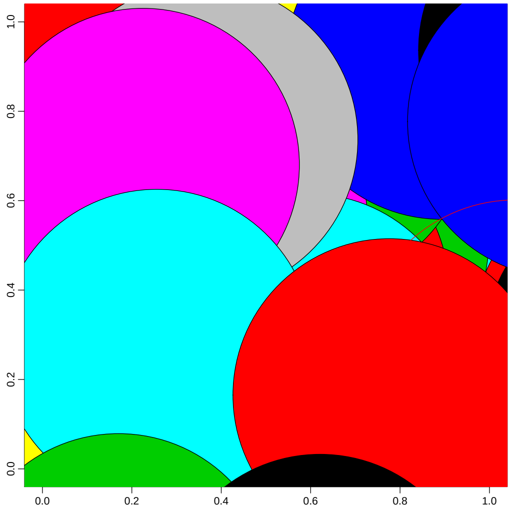

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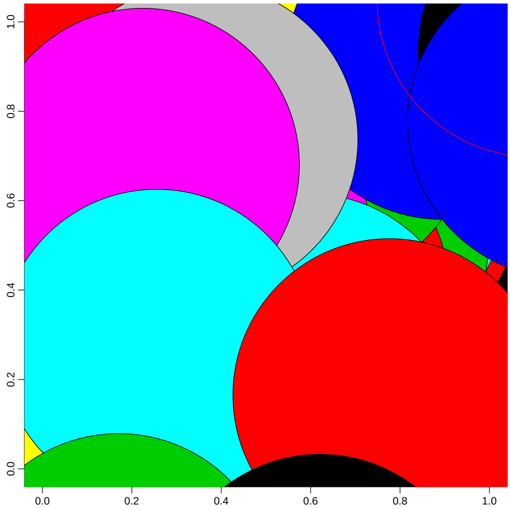

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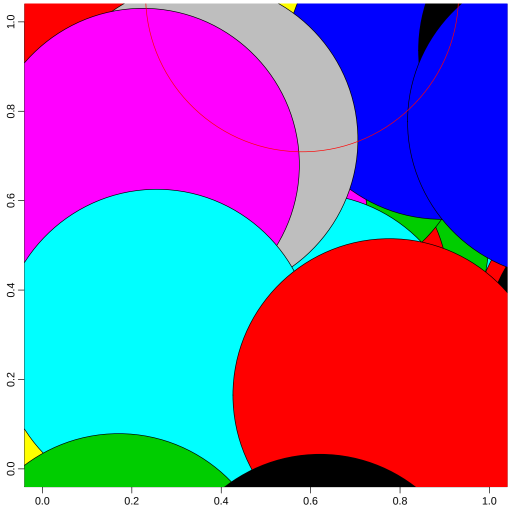

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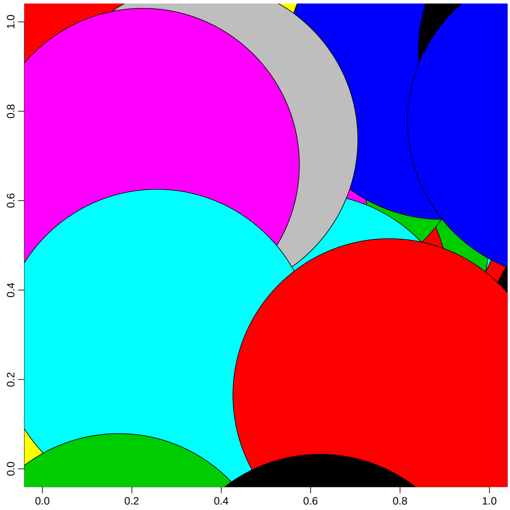

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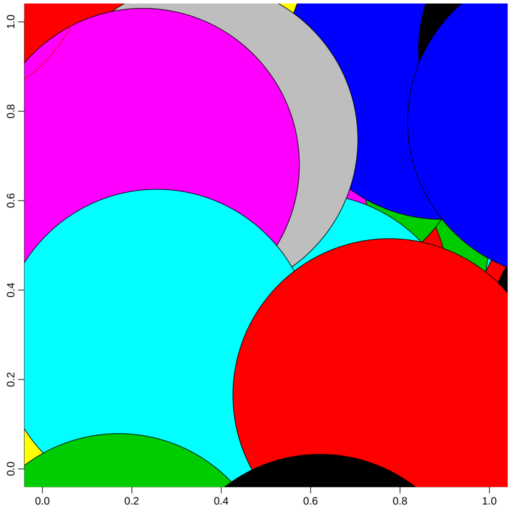

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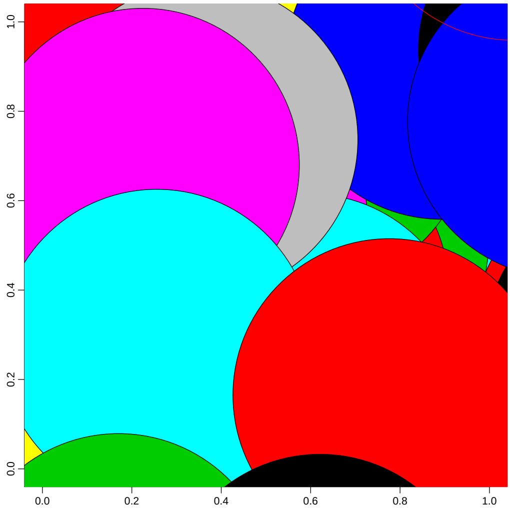

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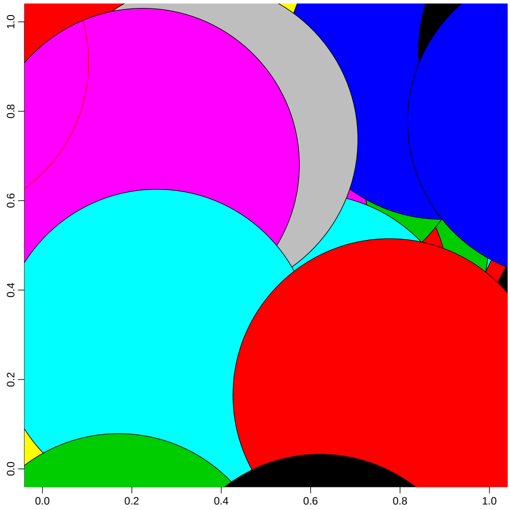

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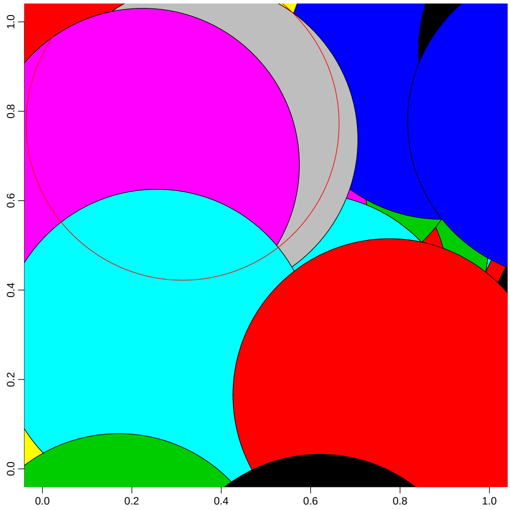

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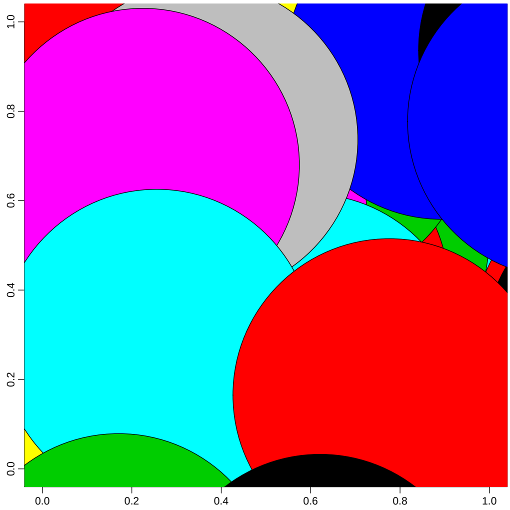
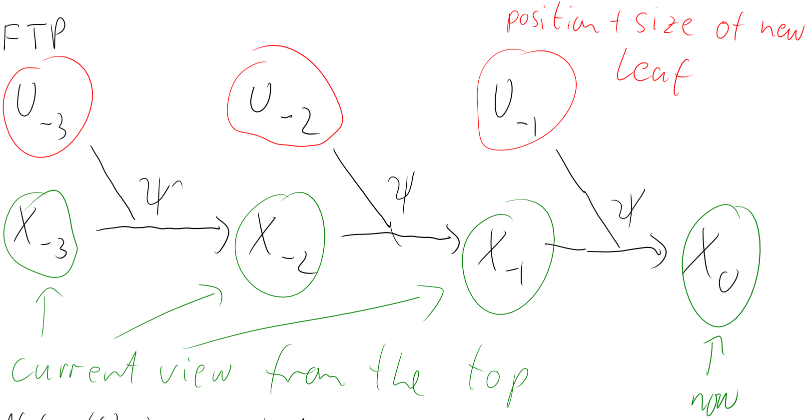


CFTP



Note: $(U_t)_{t\in\mathbb{Z}}$ iid

If ψ is suitably constructed, can assume $U_i \sim U[0,1]$

Coupling From the Past (CFTP)

- Propp & Wilson (1996), generates realisations from the stationary distribution of a Markov chain
- The transition of Markov chains can be represented as
$$X_{t+1} = \psi(X_t, U_t)$$
where U_t are iid.
- Suppose (X_t) is a Markov Chain with stationary distribution f.
- Algorithm:
  - Generate $U_{-1}, U_{-2}, \dots$.
  - Let $\psi_t(\cdot) = \psi(\cdot, u_t)$ and
$$\phi_t(x) = \psi_{-t}(\psi_{-t+1}(\dots\psi_{-1}(x)\dots)$$
  - Determine T such that ϕ_T is constant by looking at $\phi_1, \phi_2, \phi_4, \phi_8, \dots$
  - Take $\phi_T(x)$ (for any x) as a realisation from f.

Using Monotonicity Structure

- Computationally intensive to verify if ϕ_T is constant
- Suppose $\psi(x, u)$ is monotonic in x, i.e.:
  - there exists an ordering $\preceq$ on the state space $\mathcal{X}$ such that $x \leq y \implies \psi(x, u) \leq \psi(y, u)$.
  - there exists a largest element $\overline{x}$ (and a smallest element $\underline{x}$) of $\mathcal{X}$ wrt $\preceq$
- Then it suffices to check if the chains started at $\underline{x}$ and $\overline{x}$ at time $-T$ have coupled before time t, i.e. if $\phi_T(\underline{x}) = \phi_T(\overline{x})$.

Forward Coupling

- Problem with Coupling from the Past:
  Algorithm cannot be interrupted
- Fill (1998) Forward-backward coupling algorithm:
- Main idea: Chain is run backward from a fixed time horizon T (in the future) and an arbitrary starting value X^T to time $0 \to X^0$.
- If coupling has occurred between 0 and T then X_0 is the sample otherwise increase T and begin again

Outline

Some Remarks

- MCMC not straightforward to parallelise - approaches
  - Could use parallel chains
  - Could use the conditional structure of the statistical model to parallelise the individual MCMC steps

  Can use parallel chains to facilitate jumps between different modes of the target density.
- Recent extensive treatment of MCMC methods: Brooks et al. (2011)
  (many examples and useful lists of references)
- Overview over R-packages for Bayesian computations:
  `http://cran.r-project.org/web/views/Bayesian.html`

Part I

Appendix

Topics in the coming lectures:

- Bootstrap
- Particle Filtering

References I

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