Biips software: **B**ayesian **i**nference with **i**nteracting **p**article **s**ystems

BAYES 2015

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Basel, May 2015

Outline

Summary

Context

Biips $=$ **B**ayesian **i**nference with **i**nteracting **p**article **s**ystems

Bayesian inference

- Sample from a posterior distribution $p(X|Y) = \frac{p(X,Y)}{p(Y)} = \frac{p(X,Y)}{Z}$
- High dimensional, arbitrary complexity
- Simulation methods: MCMC, SMC...

Motivation

- Last 20 years: success of SMC in many applications
- No general and easy-to-use software for SMC

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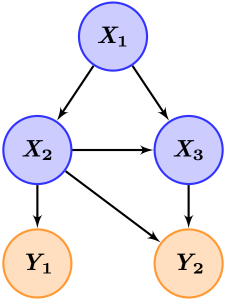
Features

- BUGS language compatible
- Extensibility: custom functions/samplers
- Black-box SMC inference engine
- Interfaces with popular software: Matlab/Octave, R
- Post-processing tools

Summary

Graphical models



Directed acyclic graph

The graph displays a factorization of the joint distribution:

$p(x_{1:3}, y_{1:2})$

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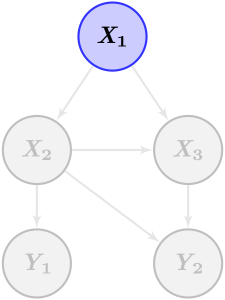

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The graph displays a factorization of the joint distribution:

$$p(x_{1:3}, y_{1:2}) = p(x_1)\ p(x_2|x_1)\ p(y_1|x_2)\ p(x_3|x_1, x_2)\ p(y_2|x_2, x_3)$$

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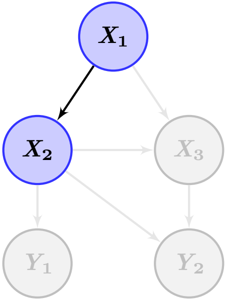

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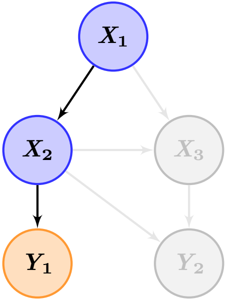

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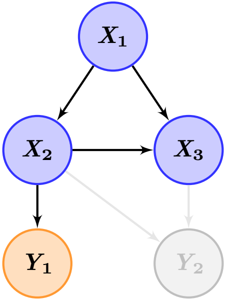

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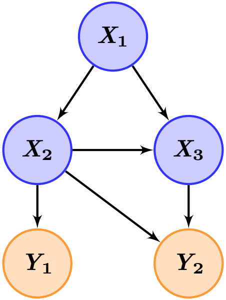

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BUGS language

- S-like declarative language for describing graphical models
- Stochastic relations
- Deterministic relations

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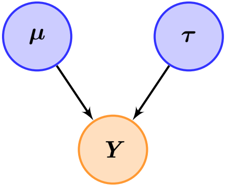
Linear regression:

```
model {
    Y ~ dnorm(mu, tau)
}
```



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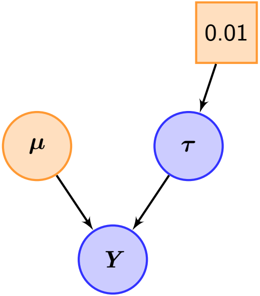

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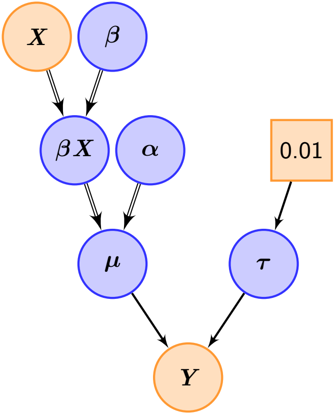

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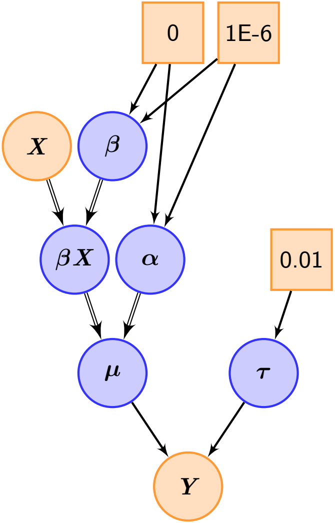

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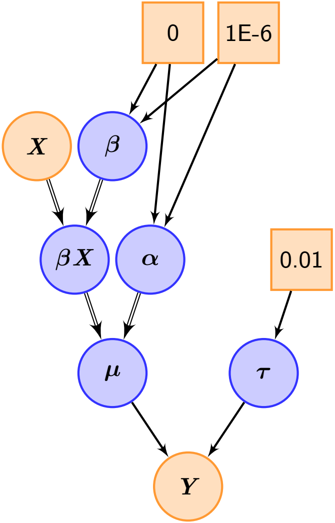


Goal:

Estimate $p(\alpha, \beta, \tau | X, Y)$

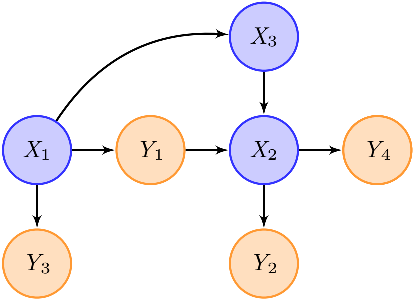
BUGS software using MCMC

BUGS = **B**ayesian inference **U**sing **G**ibbs **S**ampling

- WinBUGS, OpenBUGS, JAGS [Plummer, 2012]
- Expert system automatically derives MCMC methods (Gibbs, Slice, Metropolis, ...) in a 'black-box' fashion
- Very popular among practitioners, applying MCMC methods to a wide range of applications [Lunn et al., 2012]

Summary

Ordering of the graph



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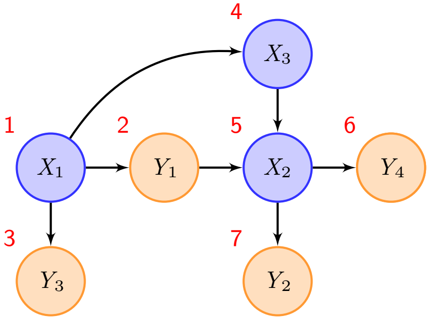
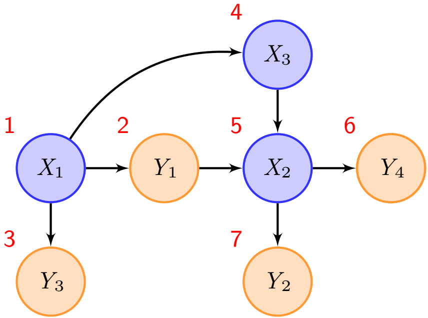
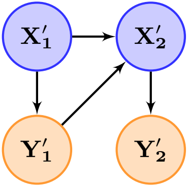


Topological sort (with priority to measurement nodes):
$(X_1, Y_1, Y_3, X_3, X_2, Y_4, Y_2)$

Ordering of the graph



Rearrangement of the directed acyclic graph:



Topological sort (with priority to measurement nodes):

$$(\underbrace{X_1}_{\mathbf{X}'_1}, \underbrace{Y_1, Y_3}_{\mathbf{Y}'_1}, \underbrace{X_3, X_2}_{\mathbf{X}'_2}, \underbrace{Y_4, Y_2}_{\mathbf{Y}'_2})$$

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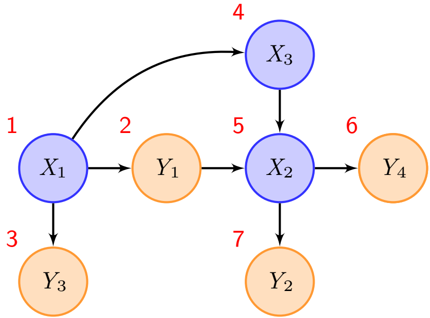

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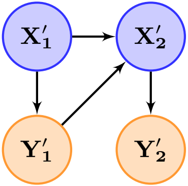


The statistical model decomposes as

$$p(x'_1, x'_2, y'_1, y'_2) = p(x'_1)p(y'_1|x'_1) p(x'_2|x'_1, y'_1)p(y'_2|x'_2)$$

SMC algorithm

More generally, assume that we have sorted variables $(X_1, Y_1, \ldots, X_n, Y_n)$.
The statistical model decomposes as

$$p(x_{1:n}, y_{1:n}) = p(x_1)p(y_1|x_1)\prod_{t=2}^{n} p(x_t|\mathrm{pa}(x_t))p(y_t|\mathrm{pa}(y_t))$$

where $\mathrm{pa}(x)$ denotes the set of parents of variable x.

SMC algorithm

- A.k.a. interacting MCMC, particle filtering, sequential Monte Carlo methods (SMC) ...
- Sequentially sample from conditional distributions of increasing dimension

$$\pi_1(x_1|y_1) \rightarrow \pi_2(x_{1:2}|y_{1:2}) \rightarrow \ldots \rightarrow \pi_n(x_{1:n}|y_{1:n})$$

where, for $t = 1, \ldots, n$

$$\begin{aligned}\pi_t(x_{1:t}|y_{1:t}) &= \frac{p(x_{1:t}, y_{1:t})}{p(y_{1:t})} \\ &= \pi_{t-1}(x_{1:t-1}|y_{1:t-1}) \frac{p(x_t|\text{pa}(x_t))p(y_t|\text{pa}(y_t))}{p(y_t|y_{1:t-1})}\end{aligned}$$

Two stochastic mechanisms:

- **Mutation/Exploration**
- **Selection**

[Doucet et al., 2001, Del Moral, 2004, Doucet and Johansen, 2010]

Standard SMC Algorithm

For $t = 1, \dots, n$

- For $i = 1, \dots, N$
  - Sample: $X_{t,t}^{(i)} \sim q_t$ and let $X_{t,1:t}^{(i)} = (\widetilde{X}_{t-1,1:t-1}^{(i)}, X_{t,t}^{(i)})$
  - Weight: $w_t^{(i)} = \frac{\pi(y_t|\text{pa}(y_t))\pi(x_{t,t}^{(i)}|\text{pa}(x_{t,t}^{(i)}))}{q_t(x_{t,t}^{(i)})}$
  - Normalize: $W_t^{(i)} = \frac{w_t^{(i)}}{\sum_{j=1}^N w_t^{(j)}}$
- Resample: $\{X_{t,1:t}^{(i)}, W_t^{(i)}\}_{i=1,\dots,N} \to \{\widetilde{X}_{t,1:t}^{(i)}, \frac{1}{N}\}_{i=1,\dots,N}$

Outputs

- Weighted particles $(W_t^{(i)}, X_{t,1:t}^{(i)})_{i=1,\dots,N}$ for $t = 1, \dots, n$
- Estimate of the marginal likelihood $\widehat{Z} = \prod_{t=1}^n \left(\frac{1}{N} \sum_{i=1}^N w_t^{(i)} \right)$

SMC algorithm

Marginal distributions

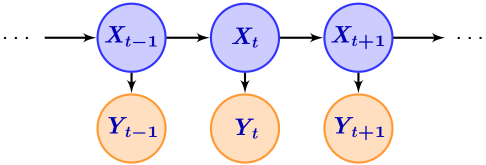
$$\pi_1(x_1|y_1) \quad \rightarrow \quad \pi_2(x_{1:2}|y_{1:2}) \quad \rightarrow \dots \rightarrow \quad \pi_n(x_{1:n}|y_{1:n})$$

Filtering:	$\pi_1(x_1\|y_1)$,	$\pi_2(x_2\|y_{1:2})$,	$\dots$,	$\pi_n(x_n\|y_{1:n})$
Smoothing:	$\pi_1(x_1\|y_{1:n})$,	$\pi_2(x_2\|y_{1:n})$,	$\dots$,	$\pi_n(x_n\|y_{1:n})$

Example

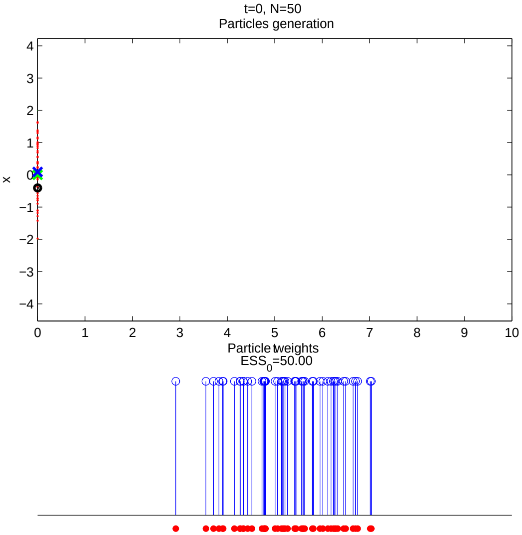
Hidden Markov model/State space model

$$
\begin{aligned}
x_0 &\sim \mathcal{N}(0,1) \\
x_t | x_{t-1} &\sim \mathcal{N}(x_{t-1}, 1), \quad t = 1, ..., 10 \\
y_t | x_t &\sim \mathcal{N}(x_t, 1), \quad t = 1, ..., 10
\end{aligned}
$$



- Linear Gaussian model
- Goal: estimate $p(x_{1:t}|y_{1:t})$
- Analytic solution given by Kalman equations

Example: hidden Markov/state space model



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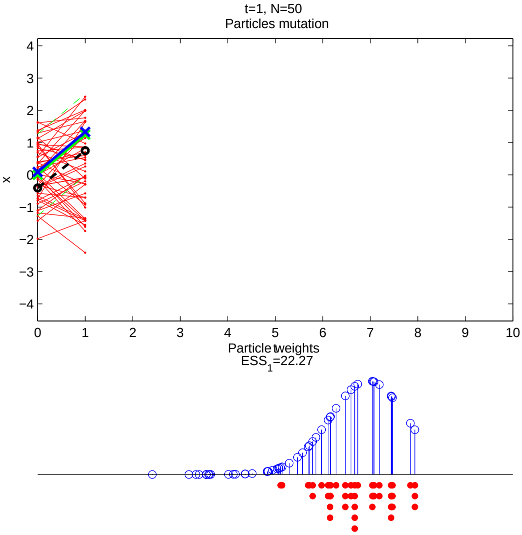

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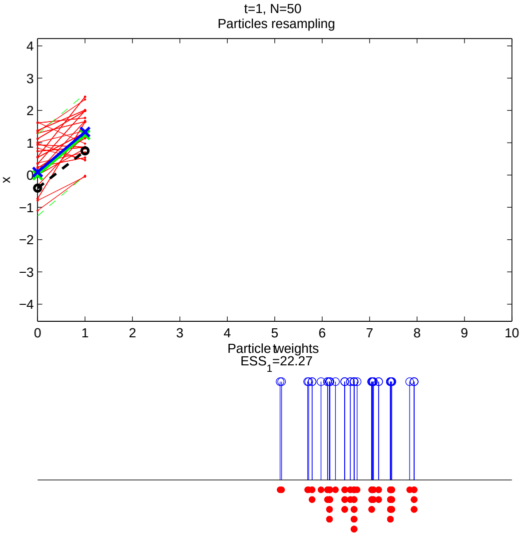

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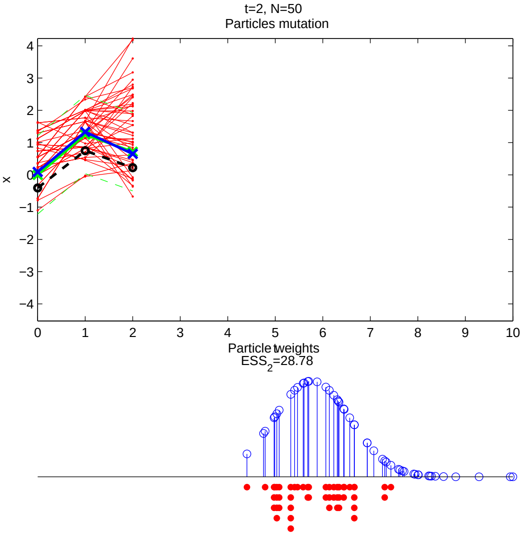

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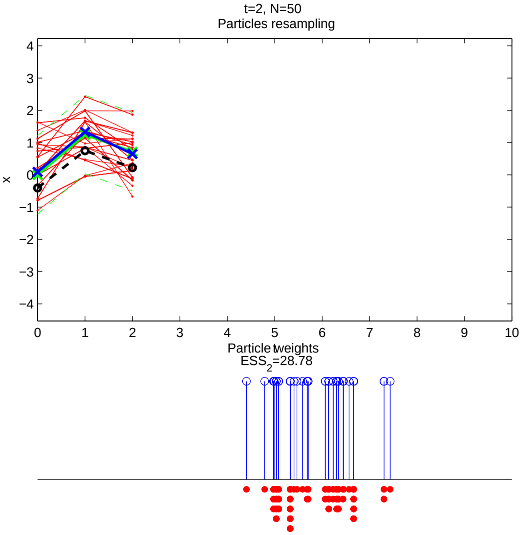

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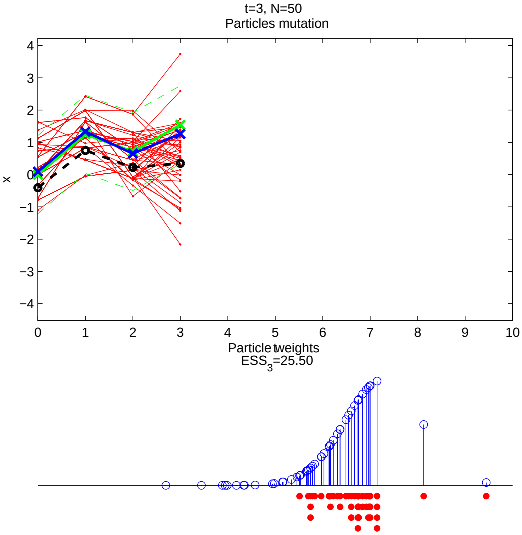

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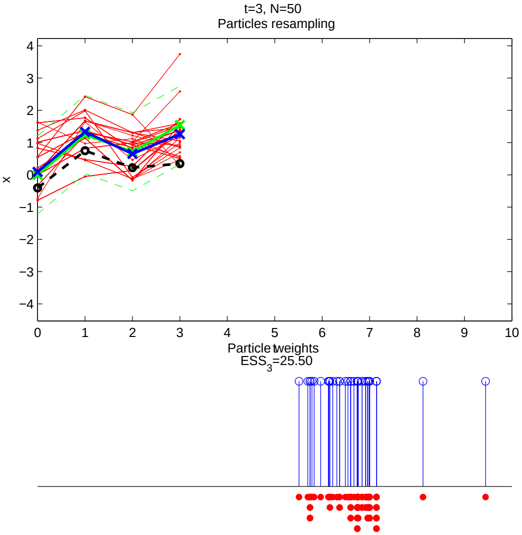

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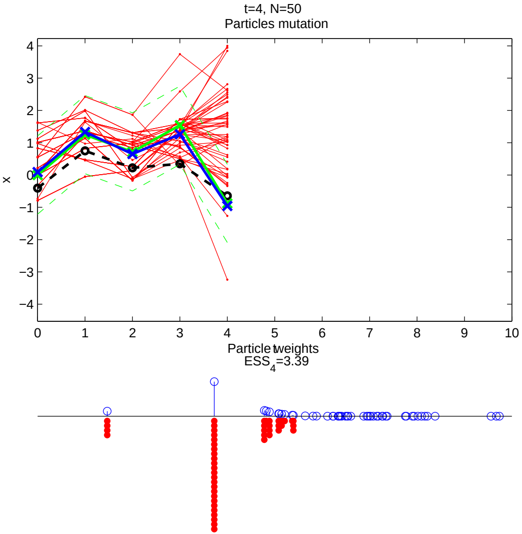

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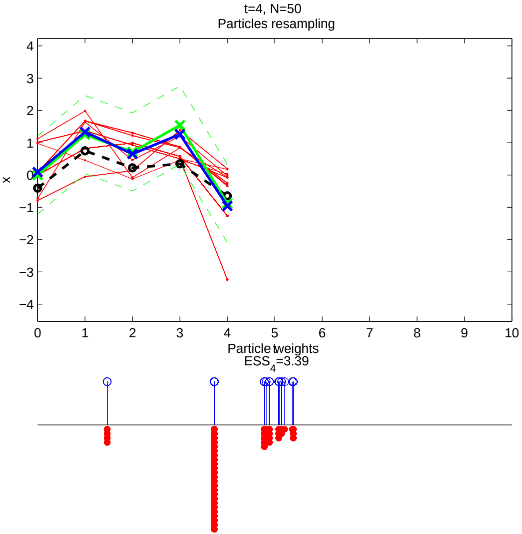

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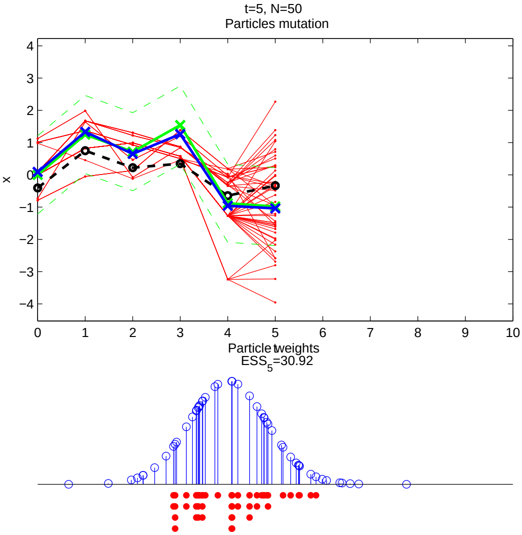

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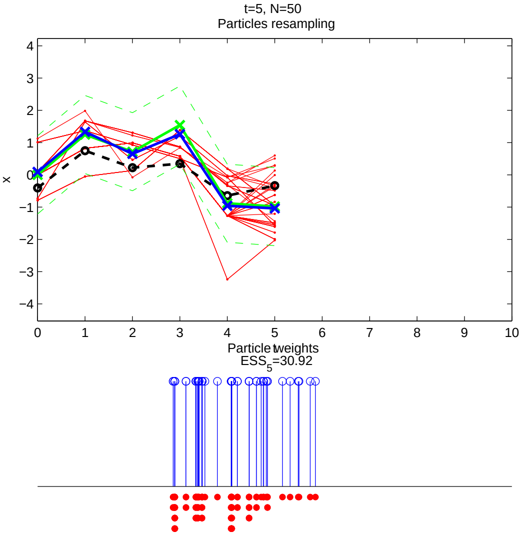

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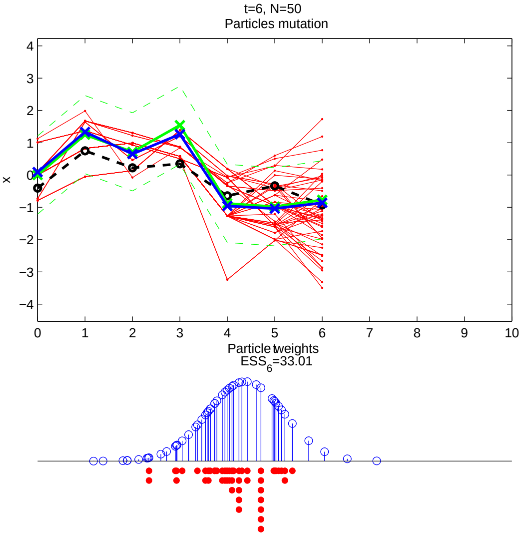

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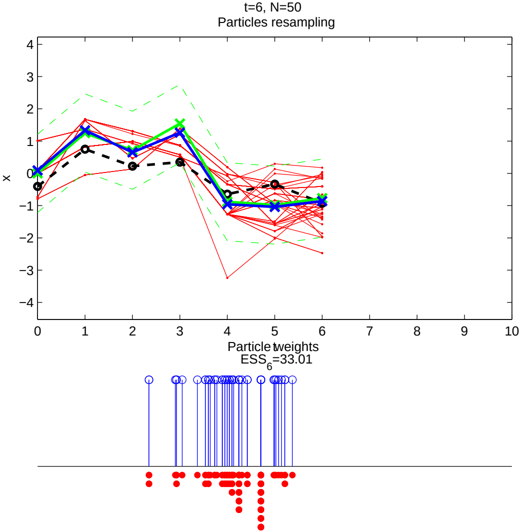

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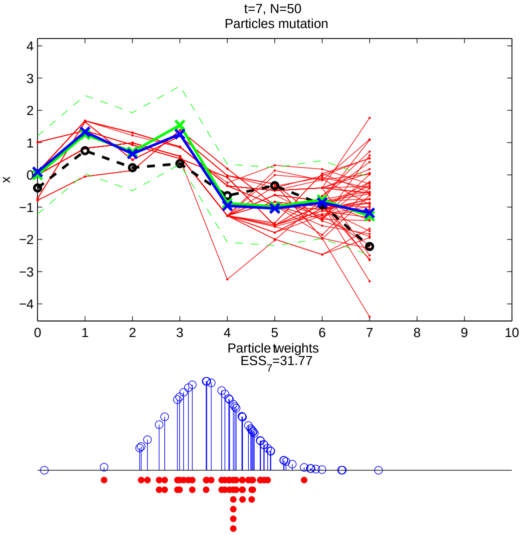

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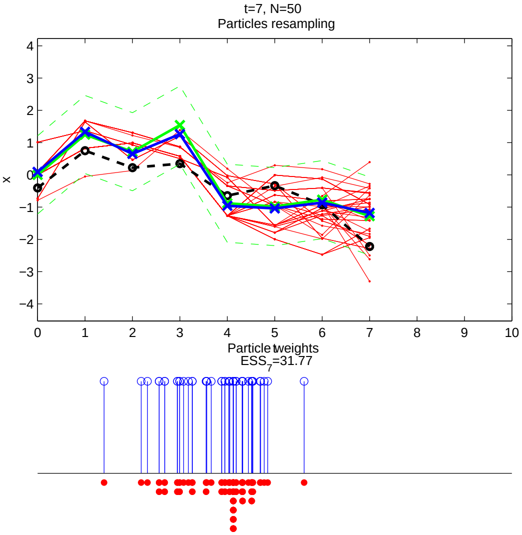

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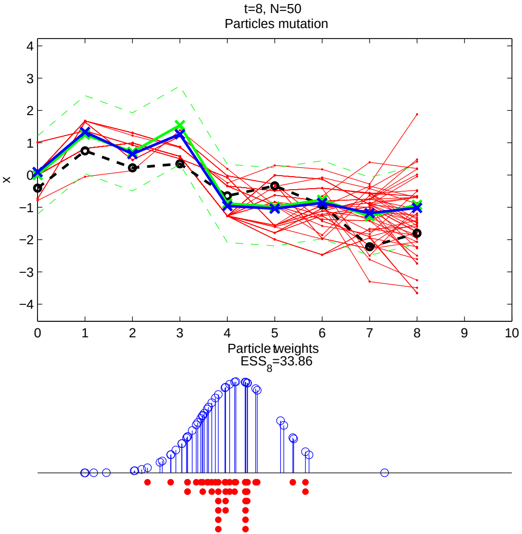

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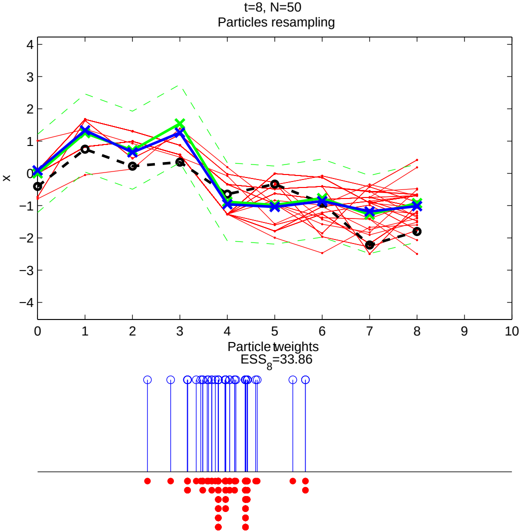

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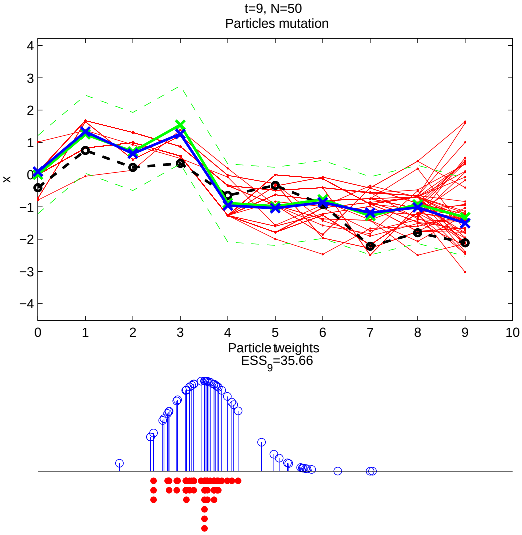

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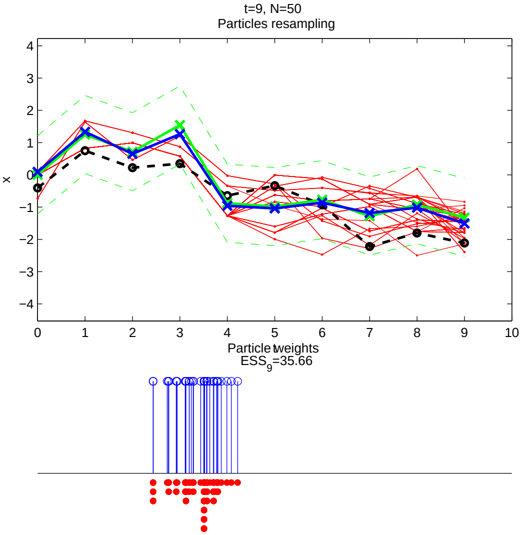

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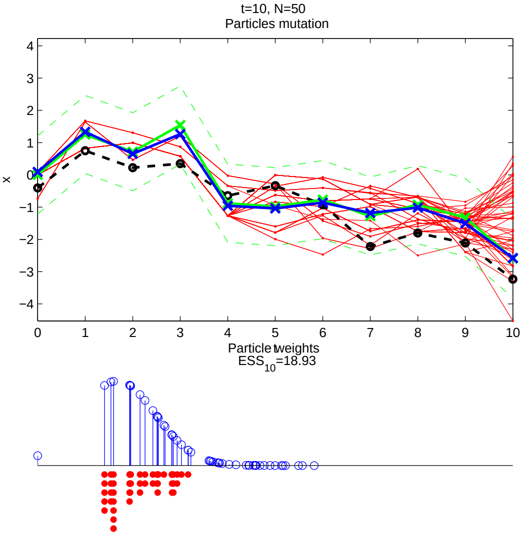
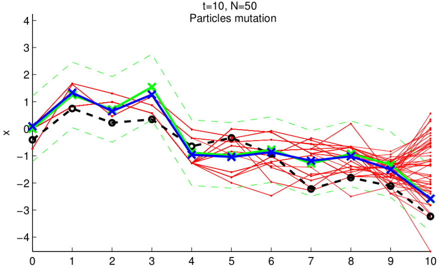


Limitations and diagnosis of SMC algorithms



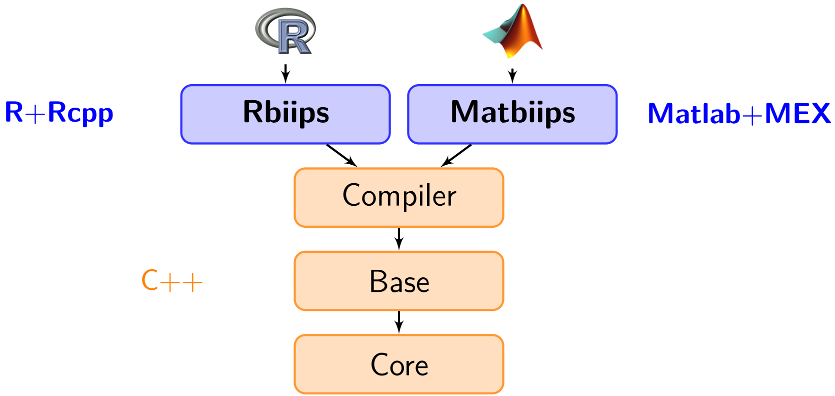
For a given $t \leq n$, for each unique value $X_{n,t}'^{(k)}$, $k = 1, \ldots, K_{n,t}$, let $W_{n,t}'^{(k)} = \sum_{i|X_t^{(i)}=X_t'^{(k)}} W_n^{(i)}$ be its associated total weight. A measure of the quality of the approximation of the posterior distribution $p(x_{t:n}|y_{1:n})$ is given by the smoothing effective sample size ($\mathbf{SESS}$):

$$\mathbf{SESS}_t = \frac{1}{\sum_{k=1}^{K_{n,t}} \left(W_{n,t}'^{(k)}\right)^2} \tag{1}$$

with $1 \leq \mathbf{SESS}_t \leq N$.

Summary

Technical implementation



- Interfaces: Matlab/Octave, R
- Multi-platform: Windows, Linux, Mac OSX
- Free and open source (GPL)

Example: Stochastic kinetic Lotka-Volterra model

- Evolution of two species $X_1(t)$ (prey) and $X_2(t)$ (predator) at time t
- Continuous-time Markov jump process described by three reaction equations:

$$
\begin{aligned}
X_1 &\xrightarrow{c_1} 2X_1 && \text{prey reproduction,}\\
X_1 + X_2 &\xrightarrow{c_2} 2X_2 && \text{predator reproduction,}\\
X_2 &\xrightarrow{c_3} \emptyset && \text{predator death}
\end{aligned}
$$

where $c_1 = 0.5$, $c_2 = 0.0025$ and $c_3 = 0.3$.

$$
\begin{aligned}
&\Pr(X_1(t+dt) = x_1(t)+1, X_2(t+dt) = x_2(t) | x_1(t), x_2(t))\\
&= c_1 x_1(t) dt + o(dt)\\
&\Pr(X_1(t+dt) = x_1(t)-1, X_2(t+dt) = x_2(t)+1 | x_1(t), x_2(t))\\
&= c_2 x_1(t) x_2(t) dt + o(dt)\\
&\Pr(X_1(t+dt) = x_1(t), X_2(t+dt) = x_2(t)-1 | x_1(t), x_2(t))\\
&= c_3 x_2(t) dt + o(dt)
\end{aligned}
$$

[Boys et al., 2008]

Gillespie algorithm

R function to forward simulate from the LV model with Gillespie algorithm

```
lotka_volterra_gillespie <- function(x, c1, c2, c3, dt) {
  z <- matrix(c(1, -1, 0, 0, 1, -1), nrow=2, byrow=TRUE)
  t <- 0
  while (TRUE) {
    rate <- c(c1*x[1], c2*x[1]*x[2], c3*x[2])
    sum_rate <- sum(rate);
    # Sample the next event from an exponential distribution
    t <- t - log(runif(1))/sum_rate
    if (t>dt)
      break
    # Sample the type of event
    ind <- which((sum_rate*runif(1)) <= cumsum(rate))[1]
    x <- x + z[,ind]
  }
  return(x)
}
```

[Gillespie, 1977, Golightly and Gillespie, 2013]

Add a custom sampler to the BUGS language

Rbiips

```
biips_add_distribution(name = 'LV',
                       n_param = 5,
                       fun_dim = lotka_volterra_dim,
                       fun_sample = lotka_volterra_gillespie
                       )
```

Example: Stochastic kinetic Lotka-Volterra model

- We observe at some time $t = 1, 2, \ldots, t_{\max}$ the number of preys with some additive noise

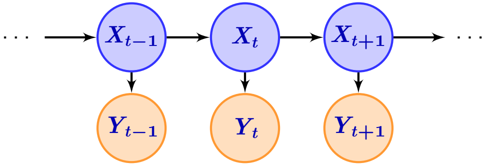
$$Y(t) = X_1(t) + \epsilon(t), \quad \epsilon(t) \sim \mathcal{N}(0, \sigma^2)$$

- Objective: approximate $\Pr(X_1(t), X_2(t) | Y(1), \ldots, Y(t_{\max}))$ at $t = 1, \ldots, t_{\max}$.

Example: Stochastic kinetic Lotka-Volterra model

stoch_kinetic_gill.bug

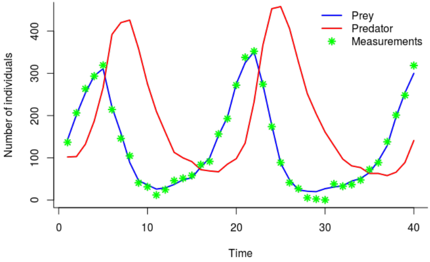
```
model
{
  x[,1] ~ LV(x_init, c[1], c[2], c[3], 1)
  y[1] ~ dnorm(x[1,1], 1/sigma^2)
  for (t in 2:t_max)
  {
    x[,t] ~ LV(x[,t-1], c[1], c[2], c[3], 1)
    y[t] ~ dnorm(x[1,t], 1/sigma^2)
  }
}
```



Model compilation

Rbiips

```
data <- list(t_max = 40, c = c(.5, .0025, .3),
             x_init = c(100, 100), sigma = 10)
model <- biips_model(model_file = 'stoch_kinetic_gill.bug',
                     data = data,
                     sample_data = TRUE)
data <- model$data()
```



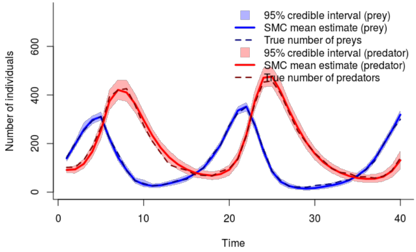
Ground truth and data

SMC samples

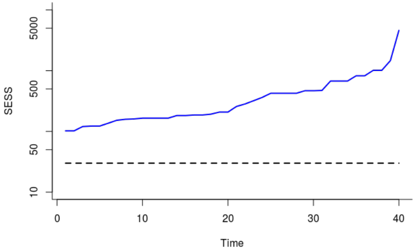
Rbiips

```
out_smc <- biips_smc_samples(model, variable_names = 'x',
                             n_part = 10000, type = 'fs')

diag_smc <- biips_diagnosis(out_smc)
summ_smc <- biips_summary(out_smc, probs=c(.025, .975))
x_s_mean <- summ_smc$x$s$mean
x_s_quant <- summ_smc$x$s$quant
```



(a) Estimates

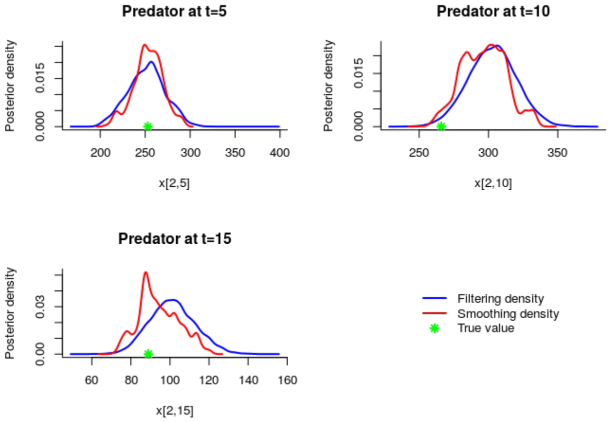


(b) Smoothing effective sample size

Kernel density estimates

Rbiips

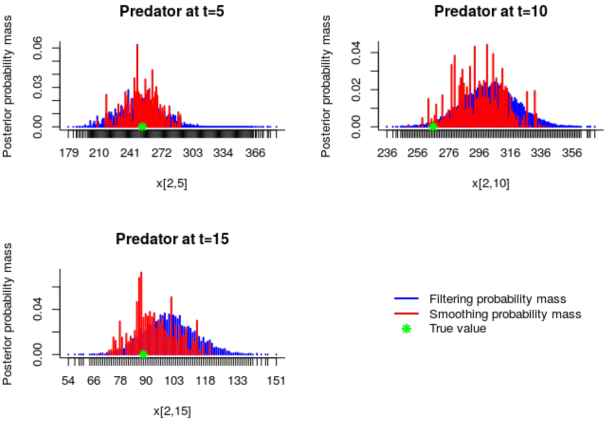
```
kde_smc <- biips_density(out_smc)
```



Probability mass estimates

Rbiips

```r
tab_smc <- biips_table(out_smc)
```



Summary

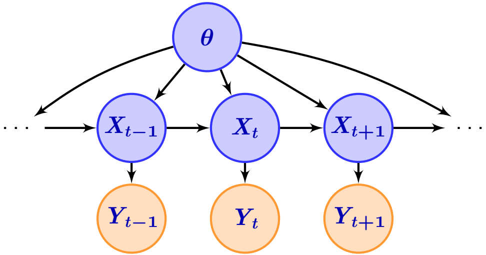
Particle MCMC

Recent algorithms that use SMC algorithms within a MCMC algorithm

- Particle Independant Metropolis-Hastings (PIMH)
- Particle Marginal Metropolis-Hastings (PMMH)

[Andrieu et al., 2010]

Static parameter estimation



Due to the successive resamplings, SMC estimations of $p(\theta|y_{1:n})$ might be poor.

The PMMH splits the variables in the graphical model into two sets:

- a set of variables X that will be sampled using a SMC algorithm
- a set $\theta = (\theta_1, \ldots, \theta_p)$ sampled with a MH proposal

Standard PMMH algorithm

Set $\widehat{Z}(0) = 0$ and initialize $\theta(0)$

For $k = 1, \ldots, n_{\text{iter}}$,

- Sample $\theta^\star \sim \nu(.|\theta^{(k-1)})$
- Run a SMC to approximate $p(x_{1:n}|y_{1:n}, \theta^\star)$ with output $(X_{1:n}^{\star(i)}, W_n^{\star(i)})_{i=1,\ldots,N}$ and $\widehat{Z}^\star \approx p(y_{1:n}|\theta^\star)$
- With probability

$$\min\left(1, \frac{\nu(\theta^\star|\theta(k-1))p(\theta^\star)\widehat{Z}^\star}{\nu(\theta(k-1)|\theta^\star)p(\theta(k-1))\widehat{Z}(k-1)}\right)$$

  set $X_{1:n}(k) = X_{1:n}^{\star(\ell)}$, $\theta(k) = \theta^\star$ and $\widehat{Z}(k-1) = \widehat{Z}^\star$, where $\ell \sim \text{Discrete}(W_n^{\star(1)}, \ldots, W_n^{\star(N)})$
- otherwise, keep previous iteration values

Outputs

- MCMC samples $(X_{1:n}(k), \theta(k))_{k=1,\ldots,n_{\text{iter}}}$

Example: Stochastic kinetic Lotka-Volterra model

stoch_kinetic_gill.bug

```
model
{
  logc[1] ~ dunif(-7,2)
  logc[2] ~ dunif(-7,2)
  logc[3] ~ dunif(-7,2)
  c[1] <- exp(logc[1])
  c[2] <- exp(logc[2])
  c[3] <- exp(logc[3])
  ...
}
```

Run a PMMH algorithm

Rbiips

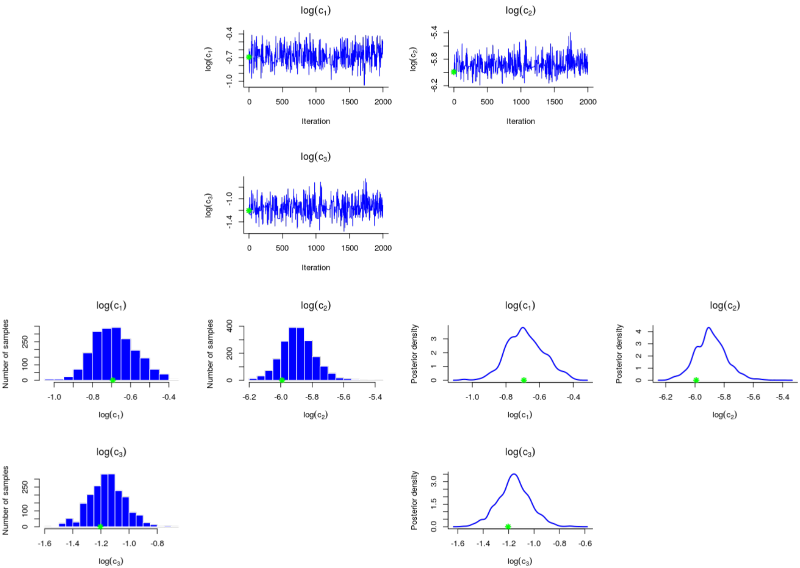
```
# create a pmmh object
obj_pmmh = biips_pmmh_init(model,
                           param_names = c('logc[1]',
                                           'logc[2]',
                                           'logc[3]'),
                           inits = list(-1, -5, -1),
                           latent_names = 'x')

# adaptation and burn-in iterations
biips_pmmh_update(obj_pmmh, n_iter = 2000, n_part = 100)

# samples
out_pmmh = biips_pmmh_samples(obj_pmmh, n_iter = 20000,
                              n_part = 100, thin = 10)

summ_pmmh = biips_summary(out_pmmh, probs = c(.025, .975))
kde_pmmh = biips_density(out_pmmh)
```

Posterior samples



Conclusion

- BUGS language compatible
- Extensibility: custom functions/samplers
- Black-box SMC inference engine
- Interfaces with popular software: Matlab/Octave, R
- Post-processing tools
- And more: backward smoothing algorithm, particle independent Metropolis-Hastings algorithm, sensitivity analysis, some optimal/conditional samplers (Gaussian-Gaussian, beta-Bernoulli, finite discrete)

http://alea.bordeaux.inria.fr/biips

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Paper
Examples
Rbiips doc

Bayesian inference with interacting Particle Systems

What is Biips?

Biips is a general software for **Bayesian inference with interacting particle systems**, a.k.a. sequential Monte Carlo (SMC) methods. It aims at popularizing the use of these methods to non-statistician researchers and students, thanks to its automated "black box" inference engine.

It borrows from the BUGS/JAGS software, widely used in Bayesian statistics, the statistical modeling with graphical models and the language associated with their descriptions.

Features

- BUGS language compatible
- SMC techniques for filtering and smoothing
- Static parameter estimation using particle MCMC
- Core developped in C++
- R, Matlab/Octave interfaces
- Easy language extensions with custom R and Matlab functions
- Multi-platform: Linux, Windows, Mac
- Free and open source (GPL)

[Todeschini et al., 2014]

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THANK YOU

http://alea.bordeaux.inria.fr/biips