Markov-chain Monte Carlo for Phase-type Models

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September 2011







Cano & Rios (2006) provide conjugate posterior calculations in the context of analysing repairable systems when stochastic process leading to absorption is observed.

Data

For each absorption time, one has:

- Starting state
- Length of time in each state
- Number of transitions between each state
- Ultimate absorption time



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Model by a Phase-type distribution \implies Bladt et al. (2003) provides a Bayesian MCMC algorithm.



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Definitio	n of Phase-type	Distributions	

An absorbing continuous time Markov chain is one in which there is a state that, once entered, is never left. That is, the n + 1 state intensity matrix can be written:

$$\mathbf{T} = \left(\begin{array}{cc} \mathbf{S} & \mathbf{s} \\ \mathbf{0} & 0 \end{array}\right)$$

where **S** is $n \times n$, **s** is $n \times 1$ and **0** is $1 \times n$, with

$$s = -Se$$

Then, a *Phase-type distribution* (PHT) is defined to be the distribution of the time to entering the absorbing state.

$$Y \sim \operatorname{PHT}(\boldsymbol{\pi}, \mathbf{S}) \implies \begin{cases} F_Y(y) = 1 - \boldsymbol{\pi}^{\mathrm{T}} \exp\{y\mathbf{S}\}\mathbf{e} \\ \\ f_Y(y) = \boldsymbol{\pi}^{\mathrm{T}} \exp\{y\mathbf{S}\}\mathbf{s} \end{cases}$$



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In summary:

• Can simulate chain from

 $\mathbb{P}(\text{path } \cdot \mid Y_i \ge y_i)$

trivially by rejection sampling.

• A Metropolis-Hastings acceptance ratio (ratio of exit rates) exists such that for sufficient draws, the final chain when truncated to time y_i (at which point it absorbs) will be a draw from

 $\mathbb{P}(\text{path } \cdot | Y_i = y_i)$



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Algorithm $\overline{2}$: Gibbs Sampling from Posterior

The Gibbs step achieves the goal of simulating from

 $p(\pmb{\pi}, \mathbf{S} \,|\, \mathbf{y})$

by sampling from

 $p(\boldsymbol{\pi}, \mathbf{S}, \text{paths } \cdot | \mathbf{y})$

through the iterative process

$$\left(\begin{array}{c}p(\boldsymbol{\pi},\mathbf{S} \,|\, \text{paths}\,\cdot,\mathbf{y})\\p(\text{paths}\,\cdot\,|\,\boldsymbol{\pi},\mathbf{S},\mathbf{y})\end{array}\right)$$





• Certain state transitions make no physical sense. (eg $2 \rightarrow 3$ in earlier example)

	State	Meaning		
	1	both PS we	orking	
	2	1 failed, 2 v	vorking	
	3	1 working, 2	2 failed	
	4	subsystem f	failed	
	$\int -2\lambda$	$_{ m f}$ $\lambda_{ m f}$	$\lambda_{ m f}$	0 \
) T	$\lambda_{\rm r}$	$-\lambda_{ m r} - \lambda_{ m f}$	0	λ_{f}
\rightarrow T =	$\lambda_{\rm r}$	0	$-\lambda_{\rm r} - \lambda_{\rm f}$	λ_{f}
	(0	0	0	0 /





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- 3 Where there is no reason to believe distributional differences between parameters, they should (in ideal sense) be constrained to be equal. This is as much to assist with reducing parameter dimensionality.
- **4** Computation time!



In other words, we want an MCMC algorithm fit for performing inference when PHTs used for stochastic rather than statistical modelling.

Stochastic Model

"Stochastic models seek to represent an underlying physical phenomenon of interest, albeit often in a highly idealised way, and have parameters that are physically interpretable." — Isham

Statistical Model

"In contrast, statistical models are descriptive, and represent the statistical properties of data and their dependence on covariates, without aiming to encapsulate the physical mechanisms involved." — Isham



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Stochastic Model \longrightarrow Aslett & Wilson

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Statistical Model \longrightarrow Bladt et al

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Solving I-	III		

- **1** To prohibit a transition $i \to j$,
 - Do not draw S_{ij} from the prior in algorithm 2.
 - Fix S_{ij} at zero when running algorithm 1.
 - Do not draw values for S_{ij} from the full conditional posterior in algorithm 2.
- **2** To account for censoring:
 - In algorithm 1, if y_i is a censored observation, return immediately once rejection sampling from

 $\mathbb{P}(\text{path } \cdot \mid Y_i \ge y_i)$

is complete, ignoring the MH steps. Else, use algorithm 1 as normal.

3 Some routine algebra shows conjugacy can be maintained with constraints, though naturally the parameter updating changes.





Uncensored Case

100 uncensored observations simulated from PHT with

$$\mathbf{S} = \begin{pmatrix} -3.6 & 1.8 & 1.8 \\ 9.5 & -11.3 & 0 \\ 9.5 & 0 & -11.3 \end{pmatrix}$$



Failure Rate



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Toy Exan	nple Results			



100~(25%) censored observations simulated from PHT with

$$\mathbf{S} = \begin{pmatrix} -3.6 & 1.8 & 1.8\\ 9.5 & -11.3 & 0\\ 9.5 & 0 & -11.3 \end{pmatrix}$$



Failure Rate



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The Big	Issue		





















$$\mathbb{P}(Y_i \ge y_i \mid \boldsymbol{\pi}, \mathbf{S}) = 0.09$$

$$p(\boldsymbol{\pi}, \mathbf{S} \mid \text{paths} \cdot, \mathbf{y})$$

$$\mathbb{E}(\text{RS iter.}) = 11$$

$$95\% \text{ CI} = [1, 39]$$























$$\mathbb{P}(Y_i \ge y_i \mid \boldsymbol{\pi}, \mathbf{S}) = 10^{-6}$$

$$p(\boldsymbol{\pi}, \mathbf{S} \mid \text{paths} \cdot, \mathbf{y})$$

$$\mathbb{E}(\text{RS iter.}) = 10^{6}$$

$$95\% \text{ CI} = [25317, 3688877]$$



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The Big	Issue		

- longer chains and MCMC jumps to states for which observations are far in the tails can stall rejection sampling step of MH algorithm.
- **2** states from which absorption impossible wasteful to resample whole chain because state at time y_i unsuitable for truncation.





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The Big	Issue		

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State	Meaning	$\mathbb{P}(\text{state})$	
1	both PS working	$0.9986 \Longrightarrow$	$\mathbb{E}(MH \text{ iter}) = 1429$
2	1 failed, 2 working	0.0007	
3	1 working, 2 failed	0.0007	95% CI = [36, 5267]



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The Big	Issue		

- longer chains and MCMC jumps to states for which observations are far in the tails can stall rejection sampling step of MH algorithm.
- 2 states from which absorption impossible wasteful to resample whole chain because state at time y_i unsuitable for truncation.
- time for MH algorithm to reach stationarity can grow rapidly.





Iterations



Replace rejection sampling + MH with exact conditional sampling.

• Sample a starting state, i, from the probability mass function:

$$\mathbb{P}(Y\{0\} = i \,|\, \boldsymbol{\pi}, \mathbf{S}, Y = y) = \frac{\mathbf{e}_i^{\mathrm{T}} \exp\{\mathbf{S}y\}\mathbf{s} \,\pi_i}{\boldsymbol{\pi}^{\mathrm{T}} \exp\{\mathbf{S}y\}\mathbf{s}}$$

and set t = 0





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and set t = 0

• With probability

$$\mathbb{P}(Y[t,y) = i \cap Y\{y\} = n+1 \mid \mathbf{S}, Y = y, Y\{t\} = i)$$
$$= \frac{\exp\{S_{ii}(y-t)\} s_i}{\mathbf{e}_i^{\mathrm{T}} \exp\{\mathbf{S}(y-t)\}\mathbf{s}}$$

Trinity set Y[t, y) = i and $Y\{y\} = n + 1$ and end the algorithm; College Dublin else continue



• Sample the sojourn time in the current state, δ , before a non-absorbing move from

$$p(\delta = d | \mathbf{S}, Y = y, Y[t, t + \delta) = i, Y\{t + \delta\} \in \{1, \dots, n\} \setminus i)$$
$$= \frac{\mathbf{p}_i^{\mathrm{T}} \exp\{\mathbf{S}(y - t - d)\}\mathbf{s} \ (-S_{ii})\exp(S_{ii}d)}{\int_0^{y - t} \mathbf{p}_i^{\mathrm{T}} \exp\{\mathbf{S}(y - t - \delta)\}\mathbf{s} \ (-S_{ii})\exp(S_{ii}\delta) \ d\delta}$$

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and set Y[t, t+d) = i

• Sample a state move, $i \rightarrow j$, from

$$\mathbb{P}(Y\{t+d\} = k \mid \mathbf{S}, Y = y, Y[t, t+d) = i, Y\{t+d\} \in \{1, \dots, n\} \setminus i)$$

$$\propto S_{ik} \exp\{\mathbf{S}(y-t-d)\}\mathbf{s}$$

and set $Y\{t+d\} = j$





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and set $Y\{t+d\} = j$ College Update t = t + d and i = j, then loop to second step Introduction
ooPhase-type Distributions
ooBayesian Inference for PHT
ooooooComputational Issues
ooooooTail Depth Performance Improvement











This shows the new method keeping pace in 'nice' problems and significantly outperforming otherwise.

$\mathbf{T} = \begin{pmatrix} -3 & 1 & 1 & 1 \\ 1 & -3 & 1 & 1 \\ 1 & 1 & -3 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$			$\mathbf{T} = \begin{pmatrix} -2 & 0.0 \\ 1 & -3i \\ 299 & 0 \\ 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 1.99 & 0 \\ 00 & 0 & 299 \\ -300 & 1 \\ 0 & 0 \end{pmatrix}$
<u>No</u> problems i-iii		<u>All</u> problems i-iii		
	MH	ECS	MH	ECS
\overline{t}	$1.6 \ \mu s$	$7.2 \ \mu s$	10.2 hours	0.016 secs
s_t	$104 \ \mu s$	$19 \ \mu s$	9.4 hours	0.015 secs





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ſ	$\Gamma = \begin{pmatrix} -3\\1\\1\\0 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 & 1 \\ -3 & 1 & 1 \\ 1 & -3 & 1 \\ 0 & 0 & 0 \end{pmatrix}$	$\mathbf{T} = \begin{pmatrix} -2 & 0.0 \\ 1 & -3i \\ 299 & 0 \\ 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 1.99 & 0 \\ 00 & 0 & 299 \\ -300 & 1 \\ 0 & 0 \end{pmatrix}$	
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 $2,300,000 \times \text{faster on average in hard problem}$



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Future V	Vork		

- At the moment, further speedup simulating the latent process might only be possible though extra efficiencies in computing the matrix exponential. Tough problem, see Moler & Van Loan (2003).
- Beyond this, of interest is whether it is possible to ascertain exact/approximate distributions for the sufficient statistics:

$\mathbf{N} = N_{ij}$	matrix of no. transitions $i \rightarrow j$
$\mathbf{z} = z_i$	vector of total time spent in state i
$\mathbf{B} = B_i$	vector of no. times started in state

of a CTMC, given the generator matrix. This may allow these to be sampled directly rather than indirectly as here?

• Can we combat the creep of increasing autocorrelation for these constrained models?



Phase-typ	oe Distributions	Bayesian	Inference for PHT	Computational Issues
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Bladt, M., Gonzalez, A. & Lauritzen, S. L. (2003), 'The estimation of phase-type related functionals using Markov chain Monte Carlo methods', *Scandinavian Journal of Statistics* 2003(4), 280–300.

Cano, J. & Rios, D. (2006), 'Reliability forecasting in complex hardware/software systems', Proceedings of the First International Conference on Availability, Reliability and Security (ARES'06).

Moler, C. & Van Loan, C. (2003), 'Nineteen dubious ways to compute the exponential of a matrix, twenty-five years later', *SIAM Review* **45**(1), 3–49.

