

On the exact simulation of functionals of stationary Markov chains

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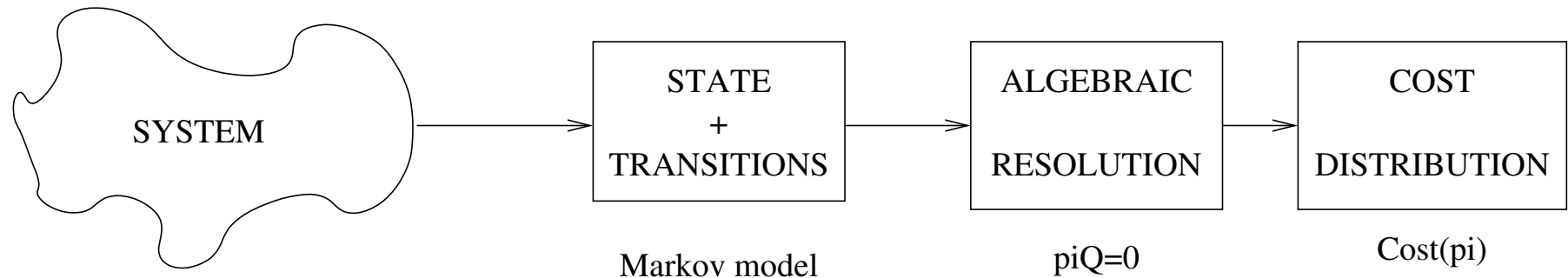


Outline

1. Motivations, simulation of Markov chains
2. Backward coupling techniques
3. Functional backward coupling
4. Implementation
5. Examples
6. Conclusion and future works



Modeling discrete event systems



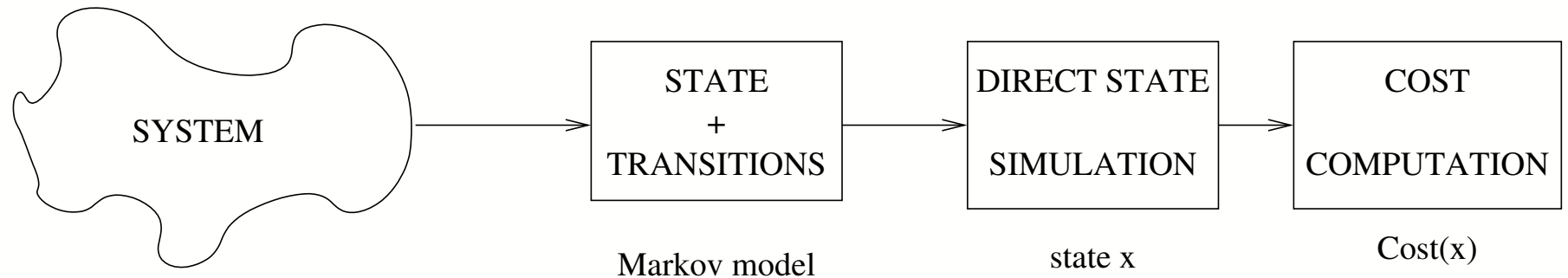
Difficulties:

- complex structure
- large state space
- analytical/numerical method
- approximation/bounding techniques

⇒ reduction of the state space



Modeling discrete event systems

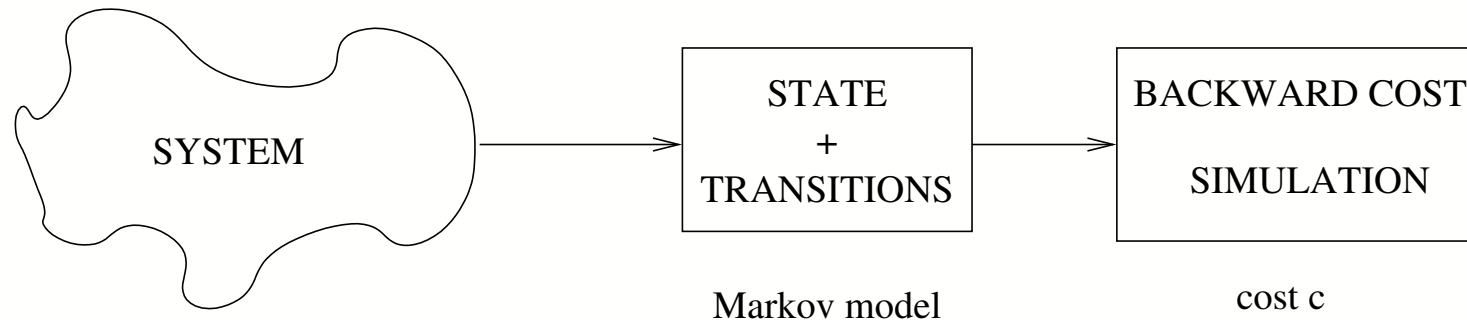


Difficulties:

- stopping criteria : burn in time
- simulation biases $\|\pi_n - \pi_\infty\|$
- estimation biases : confidence intervals $\mathcal{O}\left(\frac{1}{\sqrt{n}}\right)$



Modeling discrete event systems



Properties:

- Exact stopping criteria
⇒ no simulation bias

Constraints:

- N parallel trajectories



Iterated system of functions

\mathcal{X} state space (size n); \mathcal{U} set of external input values

Transition function Φ

$$\begin{aligned}\Phi : \mathcal{X} \times \mathcal{U} &\longrightarrow \mathcal{X} \\ (x, u) &\longmapsto \Phi(x, u)\end{aligned}$$

If $\{U_n\}_{n \in \mathbb{Z}}$ is IID then

$$X_0 = x_0, \quad X_{n+1} = \Phi(X_n, U_{n+1})$$

is a Markov chain (stochastic recursive sequence).

$$\{\Phi(\cdot, u)\}_{u \in [0,1[}$$

is an iterated system of function.

Reciprocally, given a transition matrix Q it is possible to build a family of function $\Phi(\cdot, u)$ such that the associated process is a markov chain with transition matrix Q .

\implies Simulation kernel

Problem : several representation of Q



Representations examples



Transition matrix :

$$P = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix},$$

unique steady-state distribution :

$$\pi = \left(\frac{1}{2}, \frac{1}{2}\right).$$

Φ_a, Φ_b and Φ_c

have the same transition matrix P .

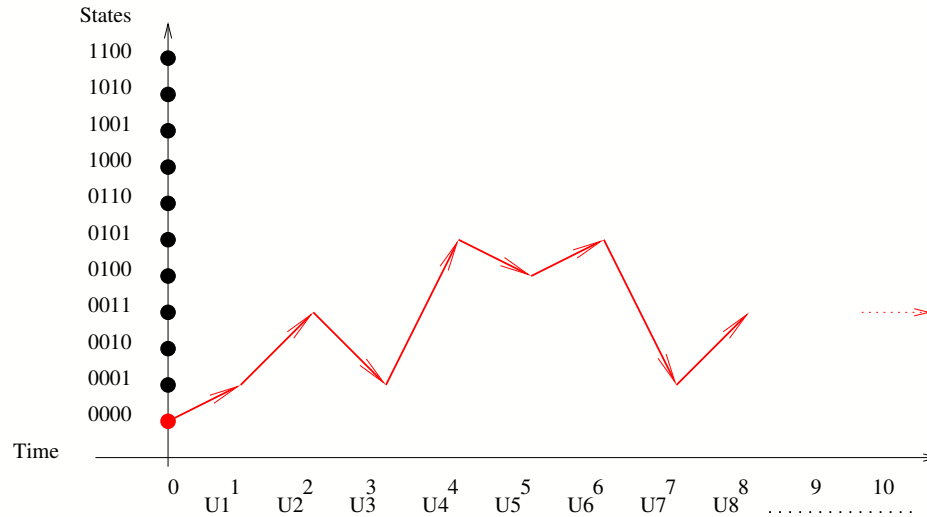
$$\Phi_a(0, u) = \Phi_b(0, u) = \Phi_c(0, u) = \begin{cases} 0 & \text{if } 0 \leq u < \frac{1}{2}; \\ 1 & \text{if } \frac{1}{2} \leq u < 1. \end{cases}$$

$$\Phi_a(1, u) = \begin{cases} 0 & \text{if } 0 \leq u < \frac{1}{2}; \\ 1 & \text{if } \frac{1}{2} \leq u < 1. \end{cases}$$

$$\Phi_b(1, u) = \begin{cases} 0 & \text{if } 0 \leq u < \frac{1}{4} \text{ or } \frac{3}{4} \leq u < 1; \\ 1 & \text{if } \frac{1}{4} \leq u < \frac{3}{4}. \end{cases}$$

$$\Phi_c(1, u) = \begin{cases} 0 & \text{if } \frac{1}{2} \leq u < 1; \\ 1 & \text{if } 0 \leq u < \frac{1}{2}. \end{cases}$$

Forward simulation



Forward simulation

$x \leftarrow x_0;$

repeat

$u \leftarrow \text{Random};$

$x \leftarrow \Phi(x, u);$

until stopping criterium

return x

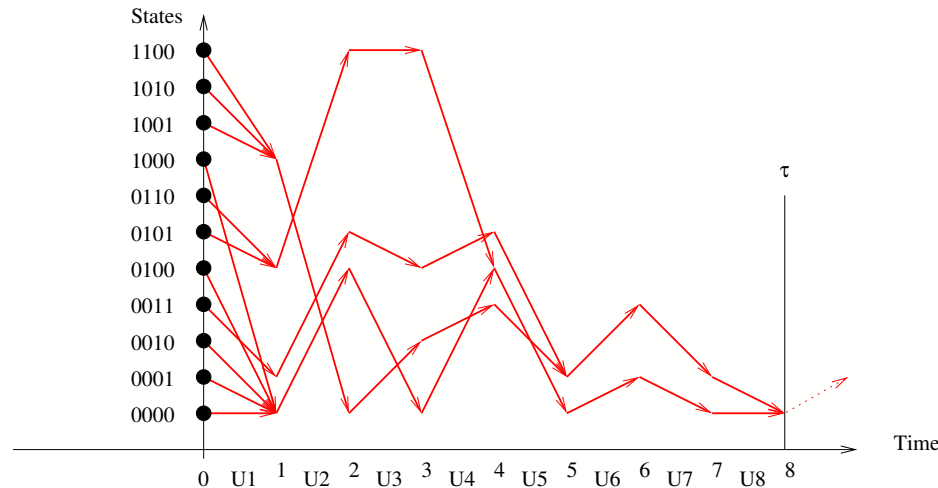
compute statistics

Problems :

- choice of the initial state
- choice of stopping criterium
- error computation (bias)

Forward coupling simulation

Forward coupling algorithm



for all $x \in \mathcal{X}$ **do**

$y(x) \leftarrow x$

end for

repeat

$u \leftarrow \text{Random};$

for all $x \in \mathcal{X}$ **do**

$y(x) \leftarrow \Phi(y(x), u);$

end for

until All $y(x)$ are equal

return $y(x)$

Problems :

- generated state $y(x)$

does not follow the stationary distribution

Coupling time τ

$$\tau = \min\{n \in \mathbb{N}, |\Phi(\Phi(\dots(\Phi(\mathcal{X}, U_1), \dots), U_{n-1}), U_n)| = 1\}$$

- Is τ almost surely **finite** ? $\mathbb{P}(\tau < +\infty) = 1$?

Backward coupling simulation

Idea :

Propp & Wilson(1996)

- reverse time
- run N parallel trajectories
- wait for coupling.

$$\mathcal{Z}_n = \Phi(\Phi(\cdots(\Phi(\mathcal{X}, U_{-n+1}), \cdots), U_{-1}), U_0).$$

potential set of reachable states at step n

```
for all  $x \in \mathcal{X}$  do
   $y(x) \leftarrow x$ 
end for
repeat
   $u \leftarrow \text{Random};$ 
  for all  $x \in \mathcal{X}$  do
     $y(x) \leftarrow y(\Phi(x, u));$ 
  end for
until All  $y(x)$  are equal
return  $y(x)$ 
```



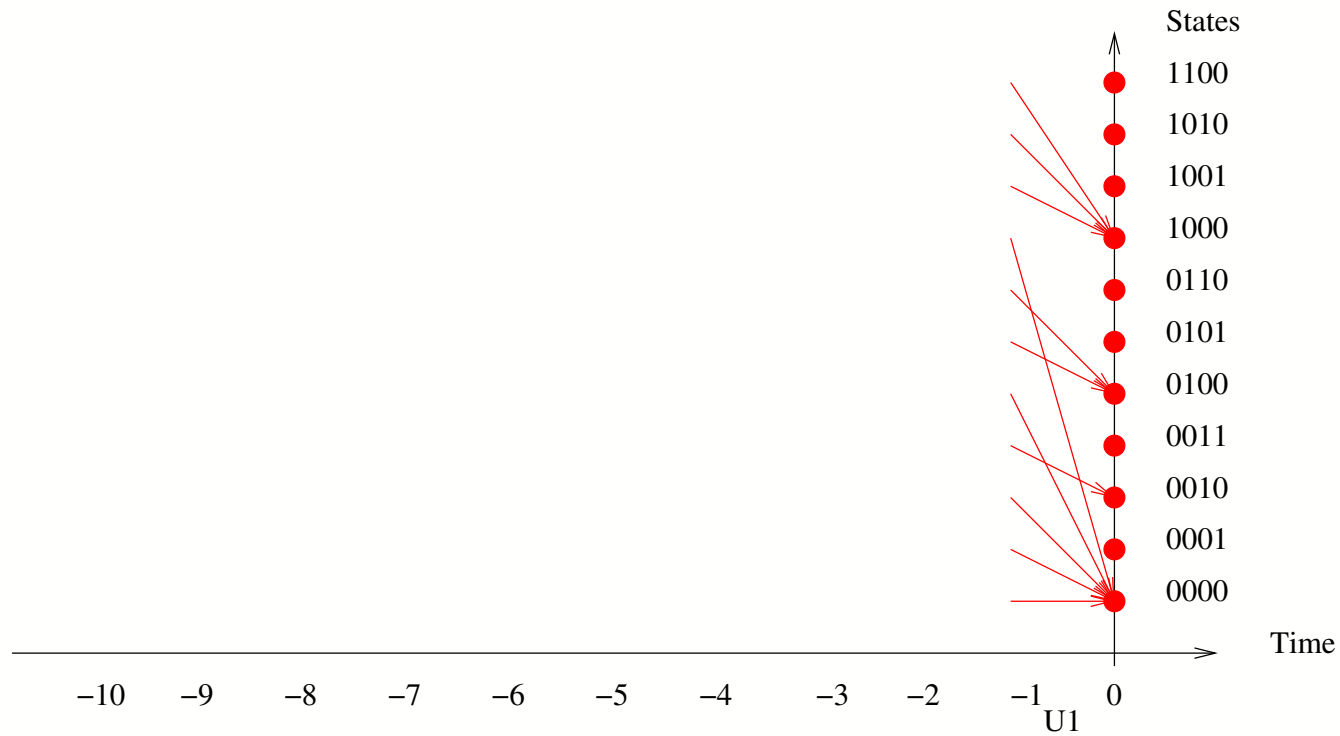
Backward simulation example



$$Z_0 = \mathcal{X}$$



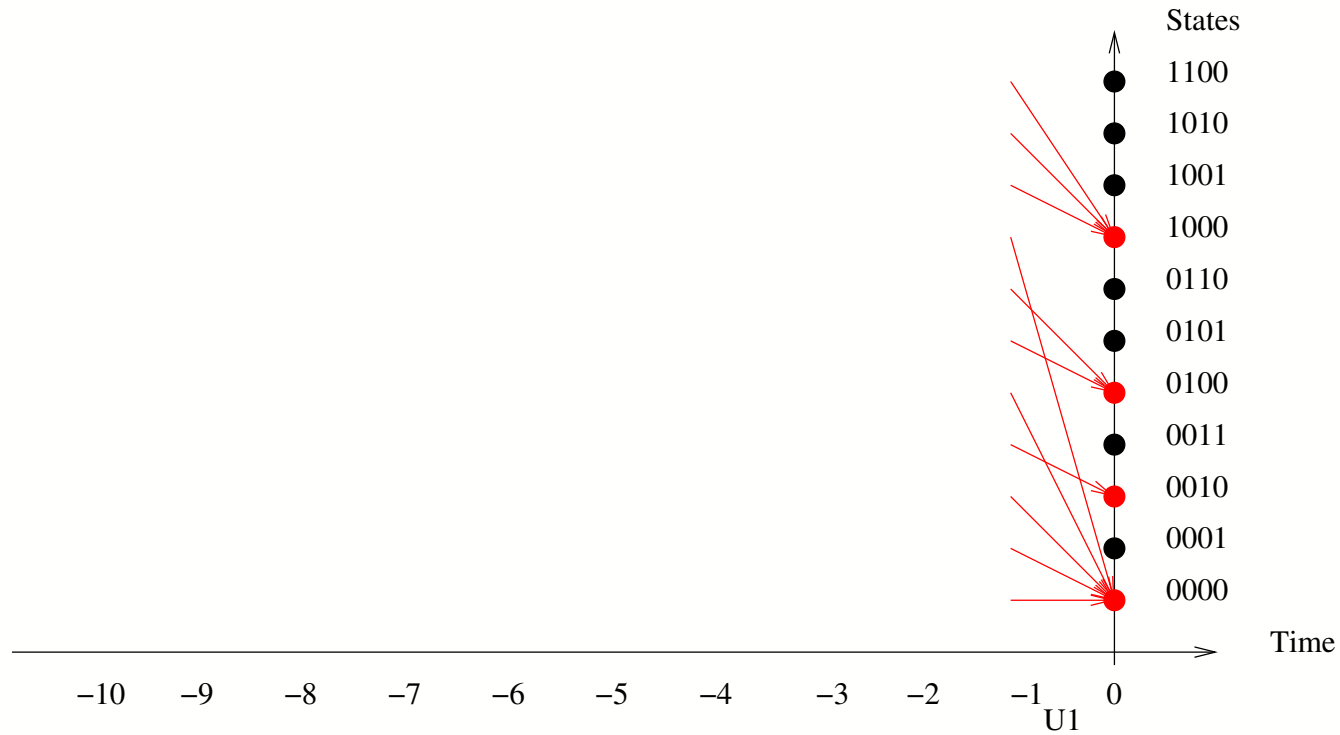
Backward simulation example



$$Z_0 = \mathcal{X}$$



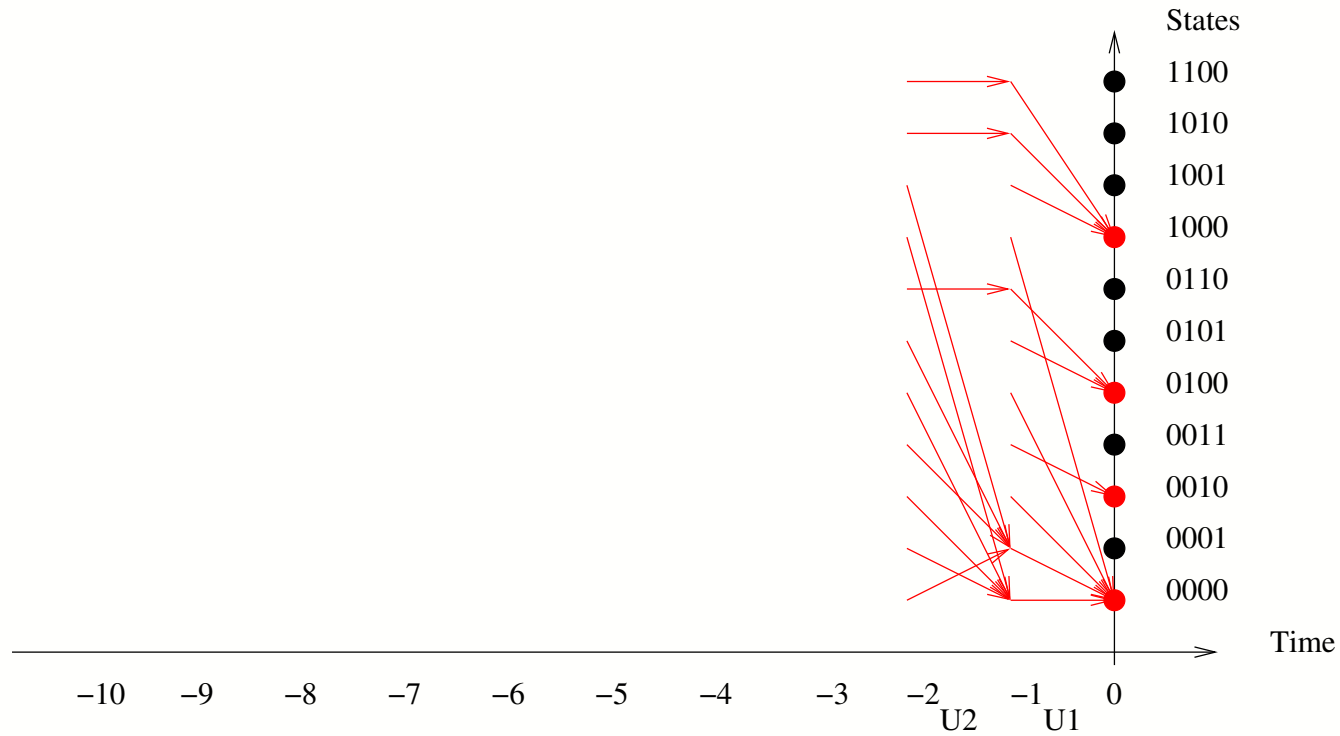
Backward simulation example



$$\mathcal{Z}_0 = \mathcal{X}$$

$$\mathcal{Z}_1 = \{0000, 0010, 0100, 1000\}$$

Backward simulation example

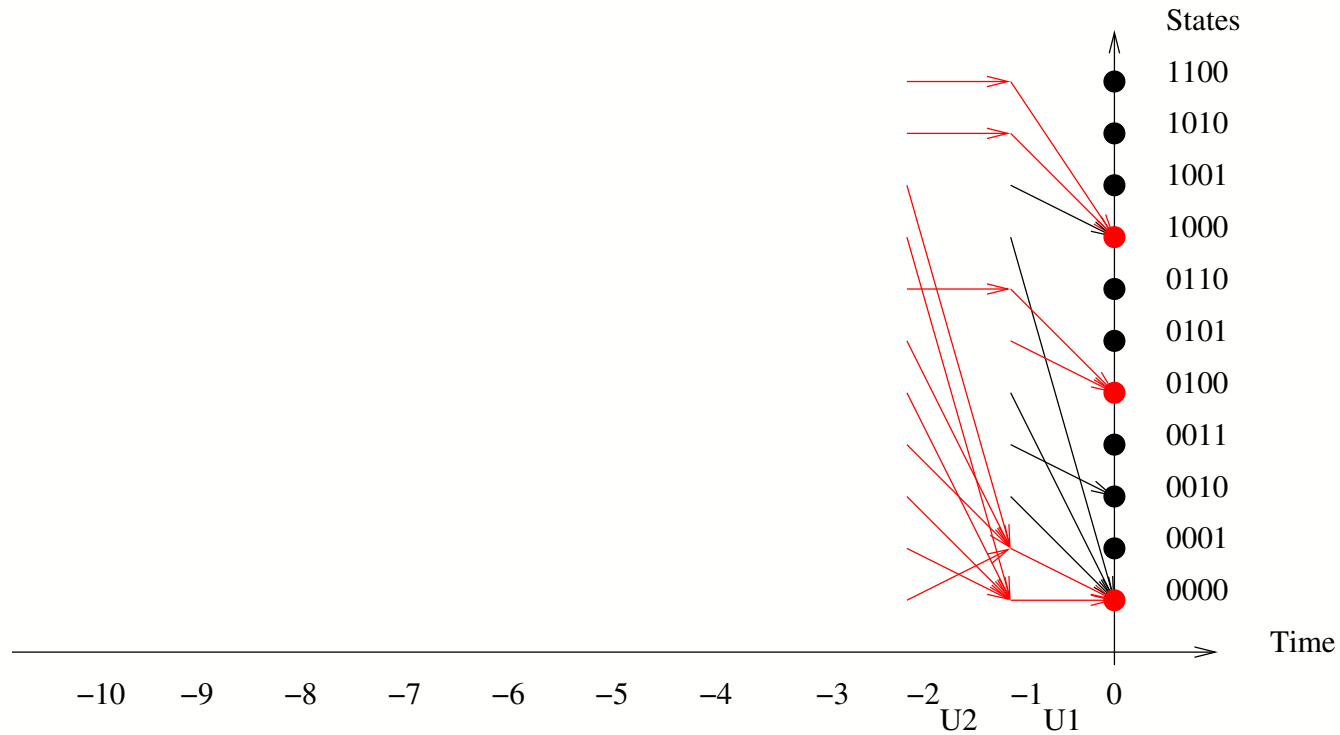


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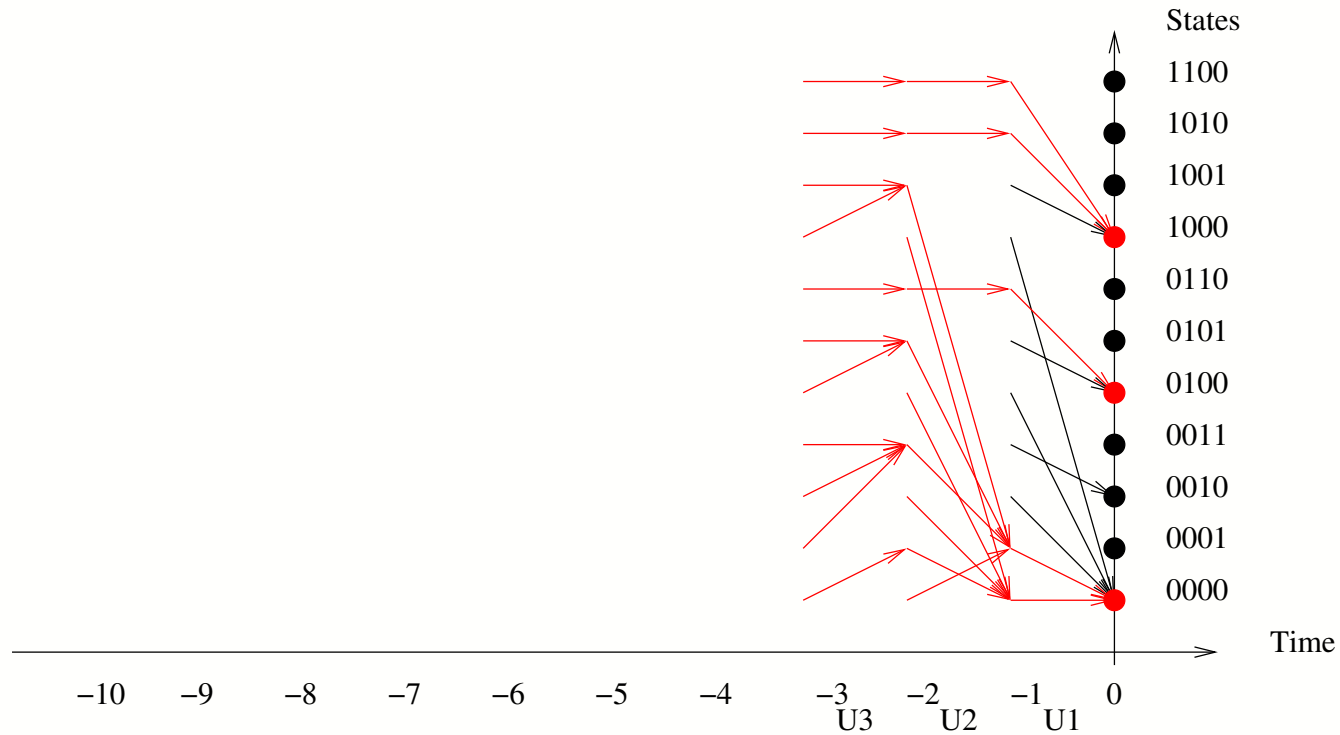


$$\mathcal{Z}_0 = \mathcal{X}$$

$$\mathcal{Z}_1 = \{0000, 0010, 0100, 1000\}$$

$$\mathcal{Z}_2 = \{0000, 0100, 1000\}$$

Backward simulation example

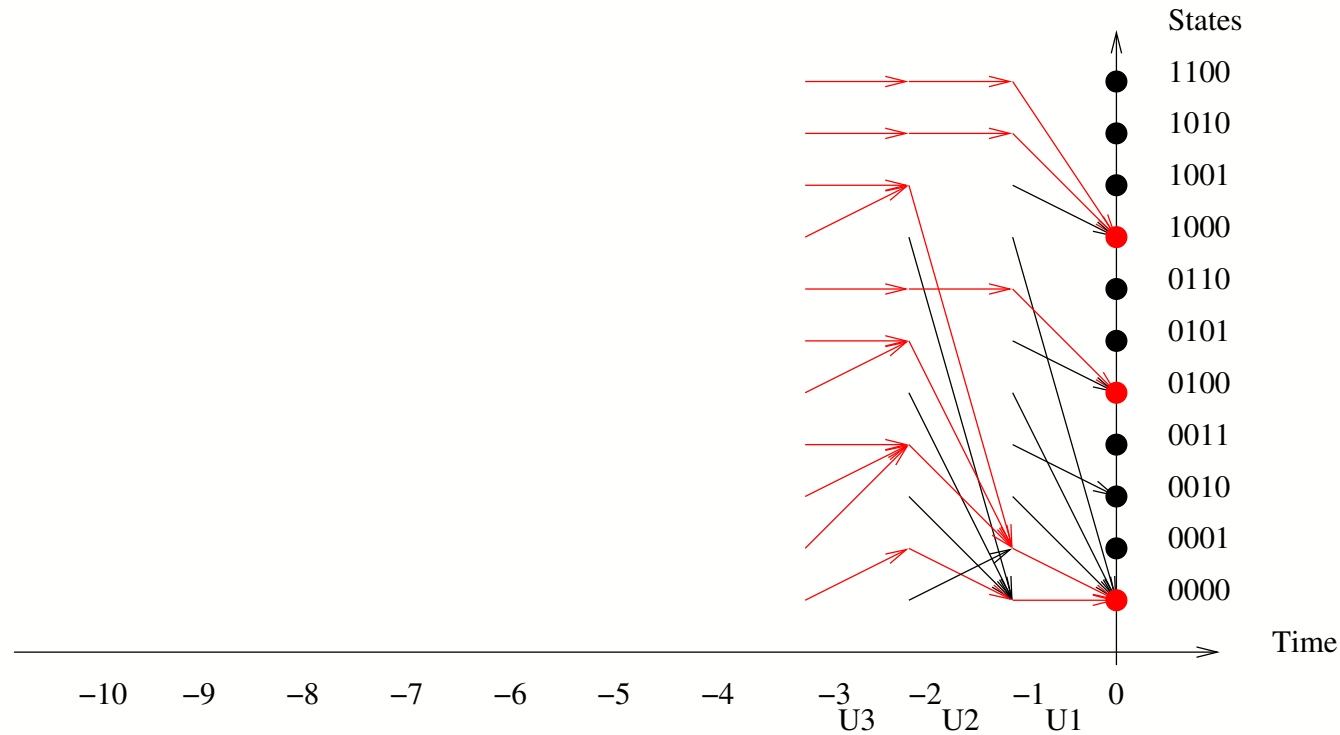


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$$\mathcal{Z}_1 = \{0000, 0010, 0100, 1000\}$$

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Backward simulation example



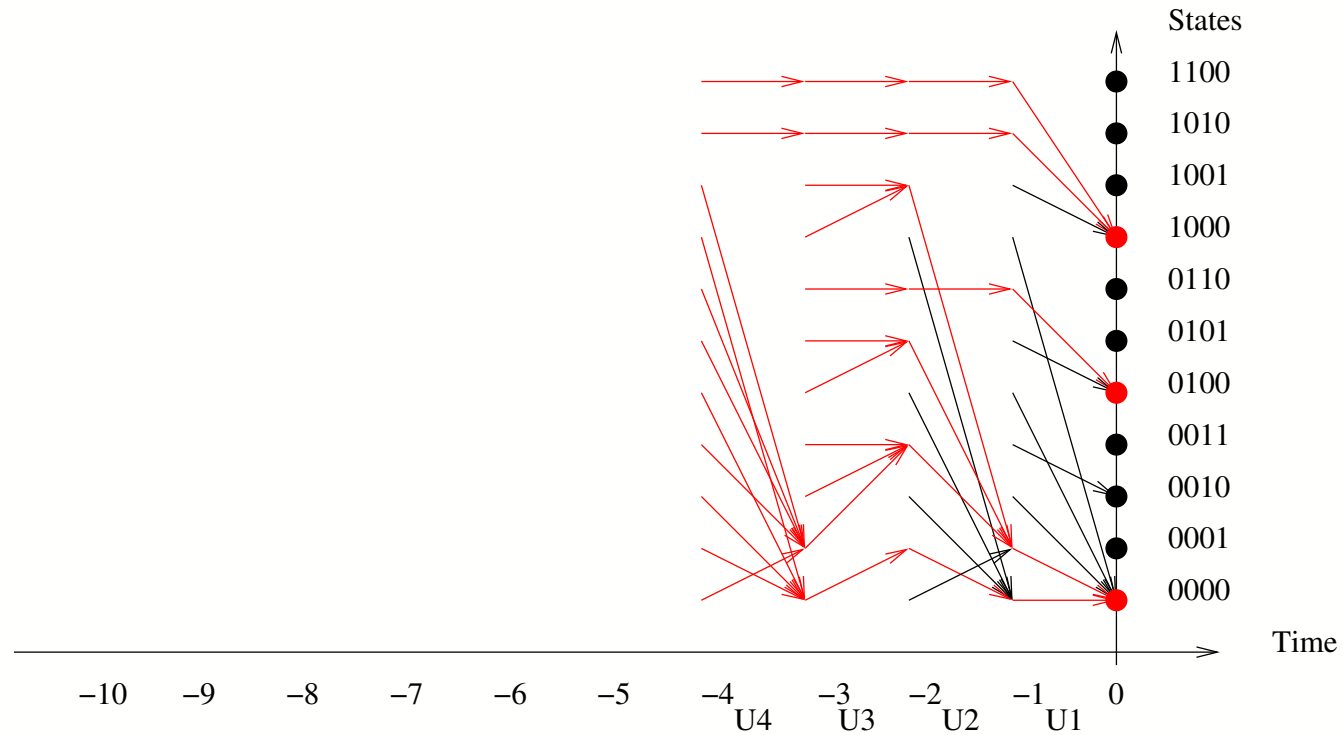
$$\mathcal{Z}_0 = \mathcal{X}$$

$$\mathcal{Z}_1 = \{0000, 0010, 0100, 1000\}$$

$$\mathcal{Z}_2 = \{0000, 0100, 1000\}$$

$$\mathcal{Z}_3 = \{0000, 0100, 1000\}$$

Backward simulation example



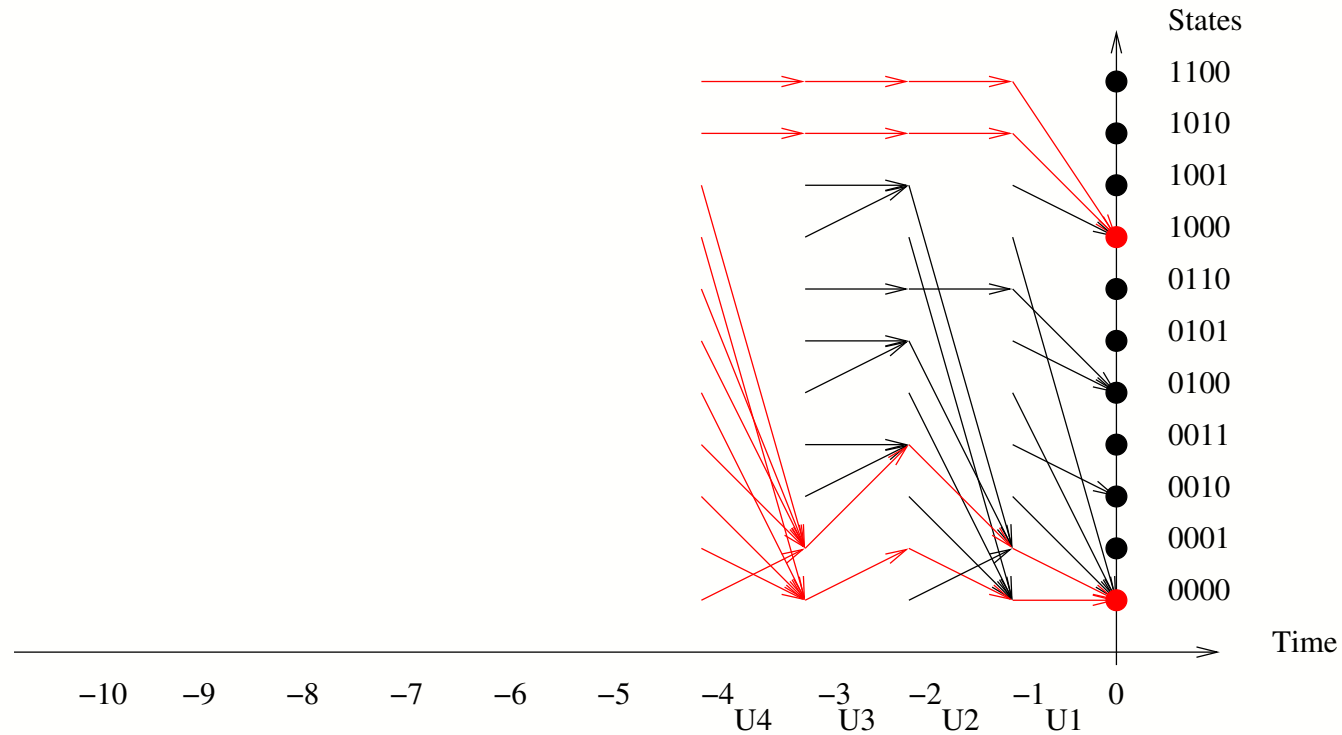
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Backward simulation example



$$\mathcal{Z}_0 = \mathcal{X}$$

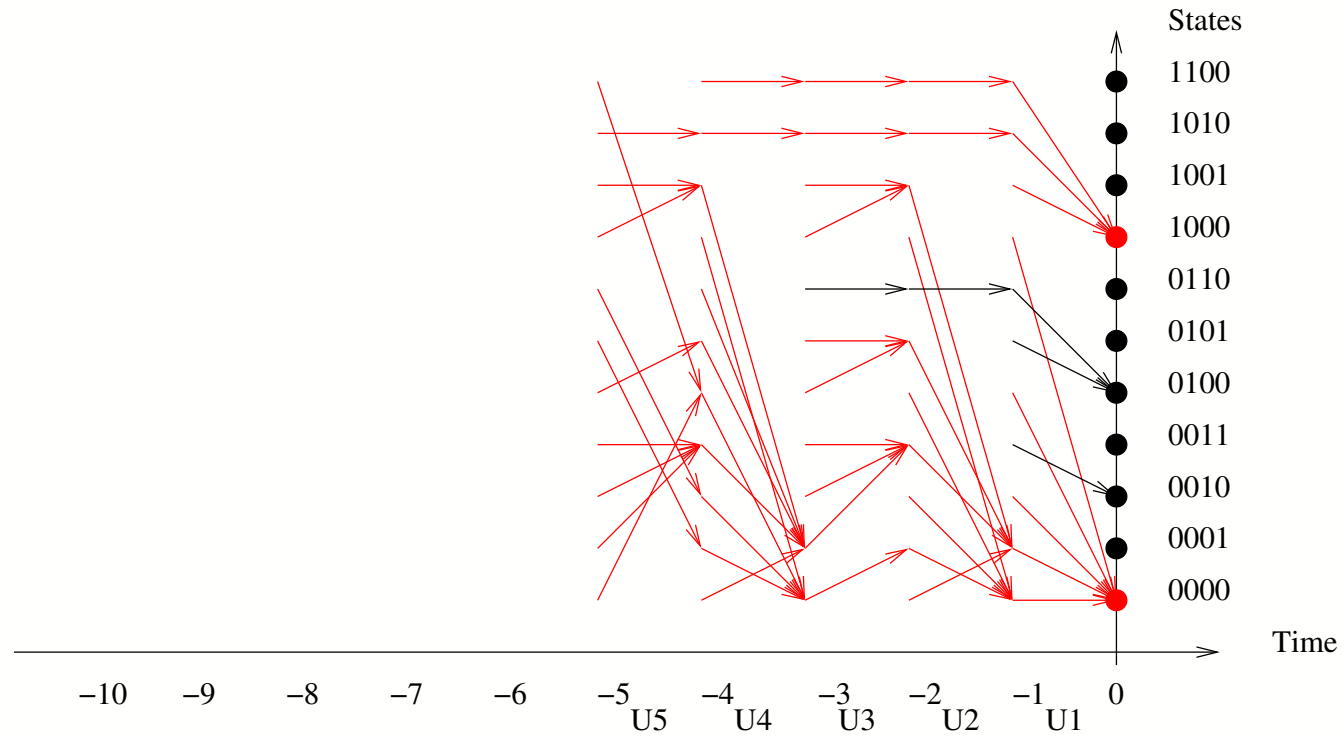
$$\mathcal{Z}_3 = \{0000, 0100, 1000\}$$

$$\mathcal{Z}_1 = \{0000, 0010, 0100, 1000\}$$

$$\mathcal{Z}_4 = \{0000, 1000\}$$

$$\mathcal{Z}_2 = \{0000, 0100, 1000\}$$

Backward simulation example



$$\mathcal{Z}_0 = \mathcal{X}$$

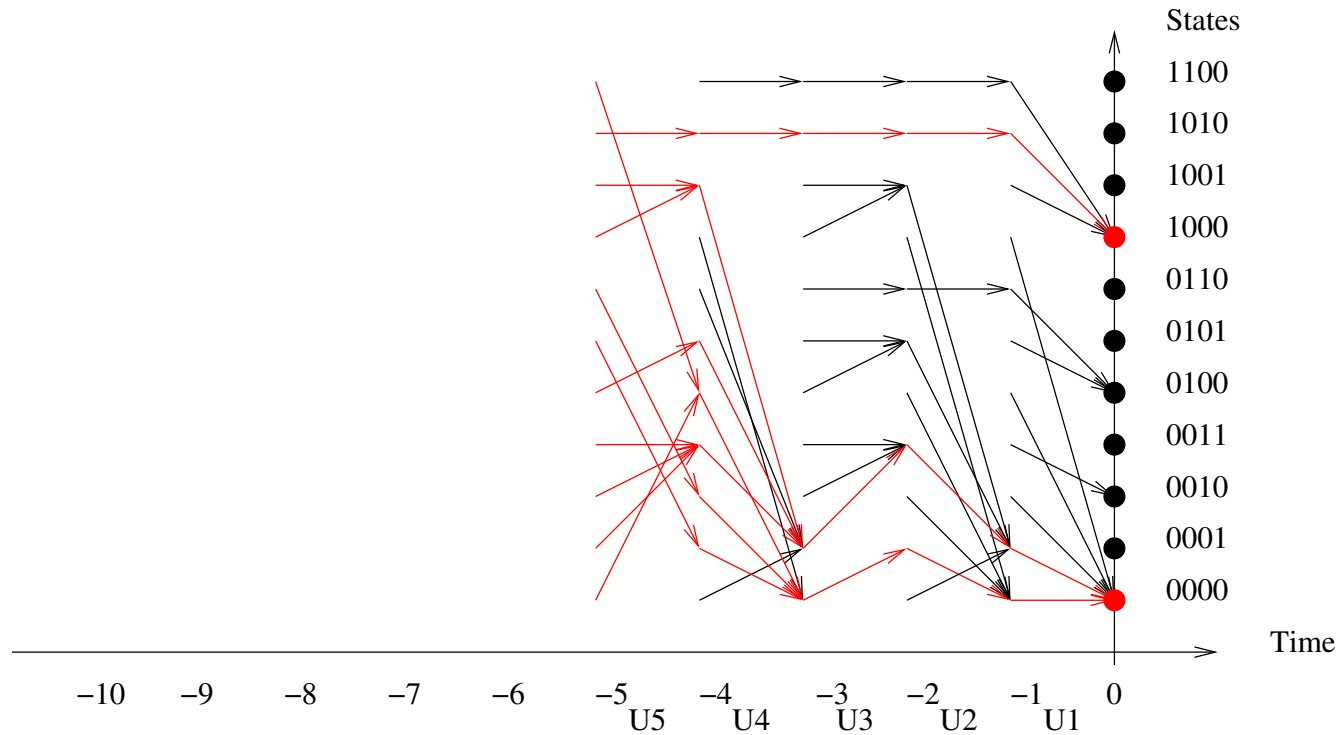
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Backward simulation example



$$\mathcal{Z}_0 = \mathcal{X}$$

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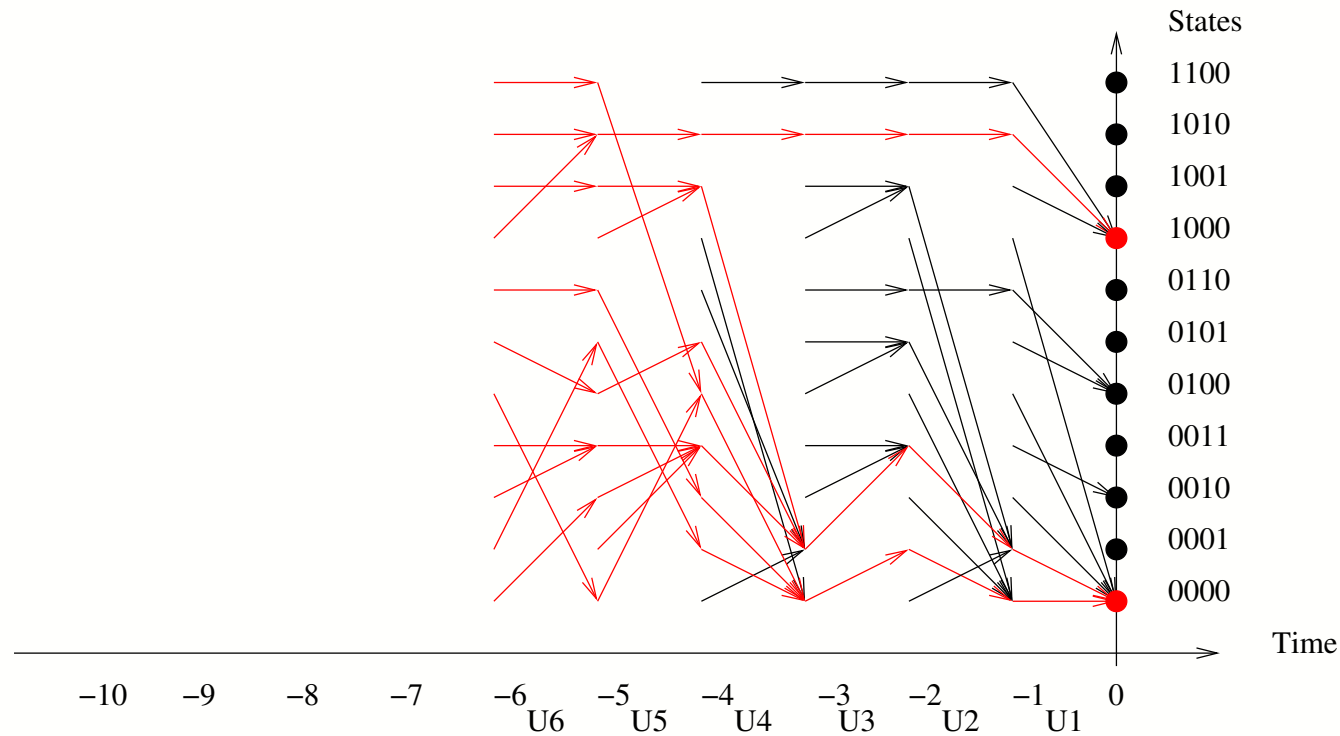
$$\mathcal{Z}_2 = \{0000, 0100, 1000\}$$

$$\mathcal{Z}_3 = \{0000, 0100, 1000\}$$

$$\mathcal{Z}_4 = \{0000, 1000\}$$

$$\mathcal{Z}_5 = \{0000, 1000\}$$

Backward simulation example



$$\mathcal{Z}_0 = \mathcal{X}$$

$$\mathcal{Z}_1 = \{0000, 0010, 0100, 1000\}$$

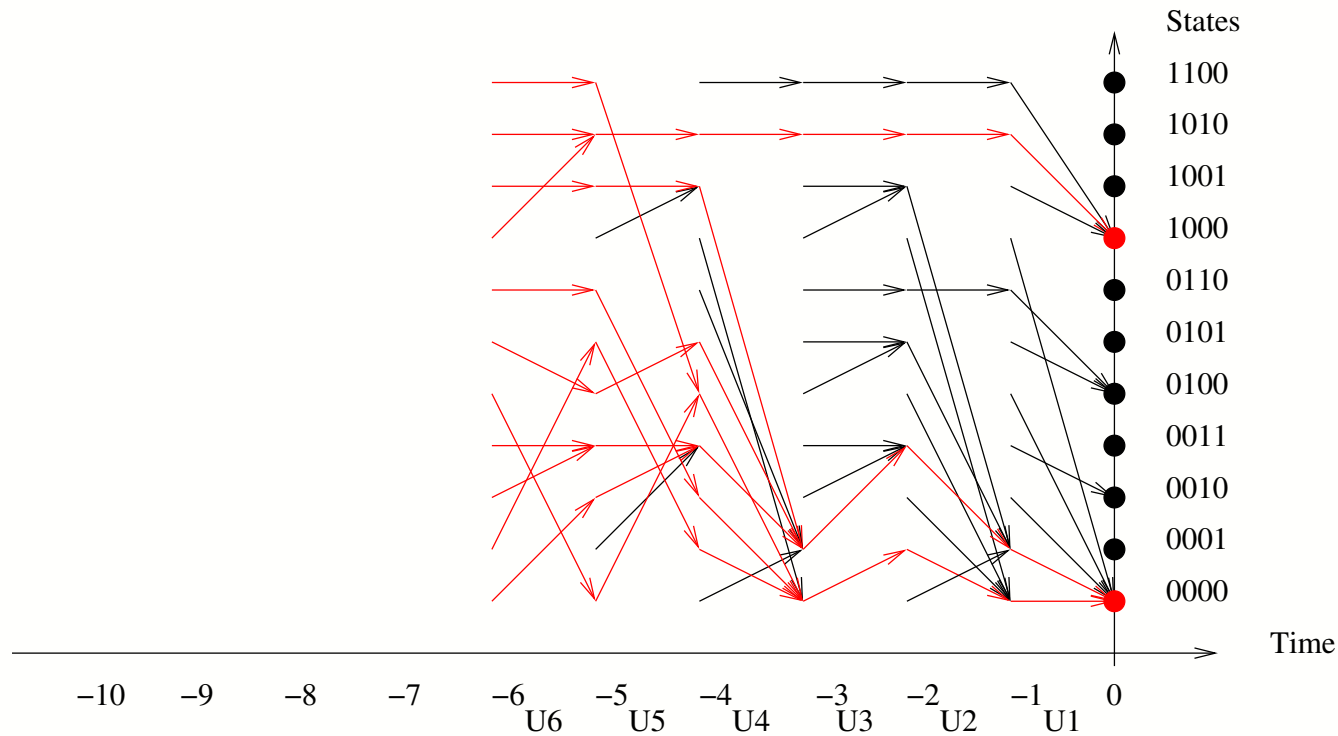
$$\mathcal{Z}_2 = \{0000, 0100, 1000\}$$

$$\mathcal{Z}_3 = \{0000, 0100, 1000\}$$

$$\mathcal{Z}_4 = \{0000, 1000\}$$

$$\mathcal{Z}_5 = \{0000, 1000\}$$

Backward simulation example



$$\mathcal{Z}_0 = \mathcal{X}$$

$$\mathcal{Z}_1 = \{0000, 0010, 0100, 1000\}$$

$$\mathcal{Z}_2 = \{0000, 0100, 1000\}$$

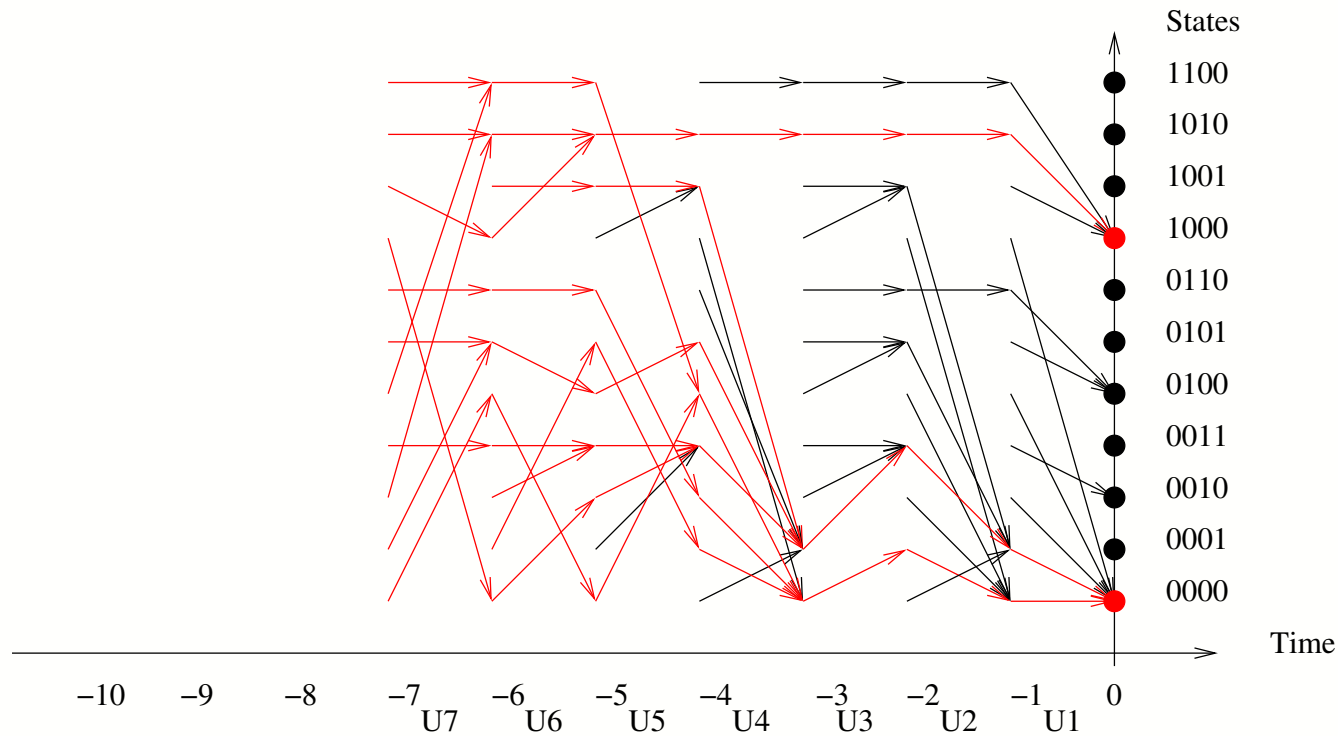
$$\mathcal{Z}_3 = \{0000, 0100, 1000\}$$

$$\mathcal{Z}_4 = \{0000, 1000\}$$

$$\mathcal{Z}_5 = \{0000, 1000\}$$

$$\mathcal{Z}_6 = \{0000, 1000\}$$

Backward simulation example



$$\mathcal{Z}_0 = \mathcal{X}$$

$$\mathcal{Z}_1 = \{0000, 0010, 0100, 1000\}$$

$$\mathcal{Z}_2 = \{0000, 0100, 1000\}$$

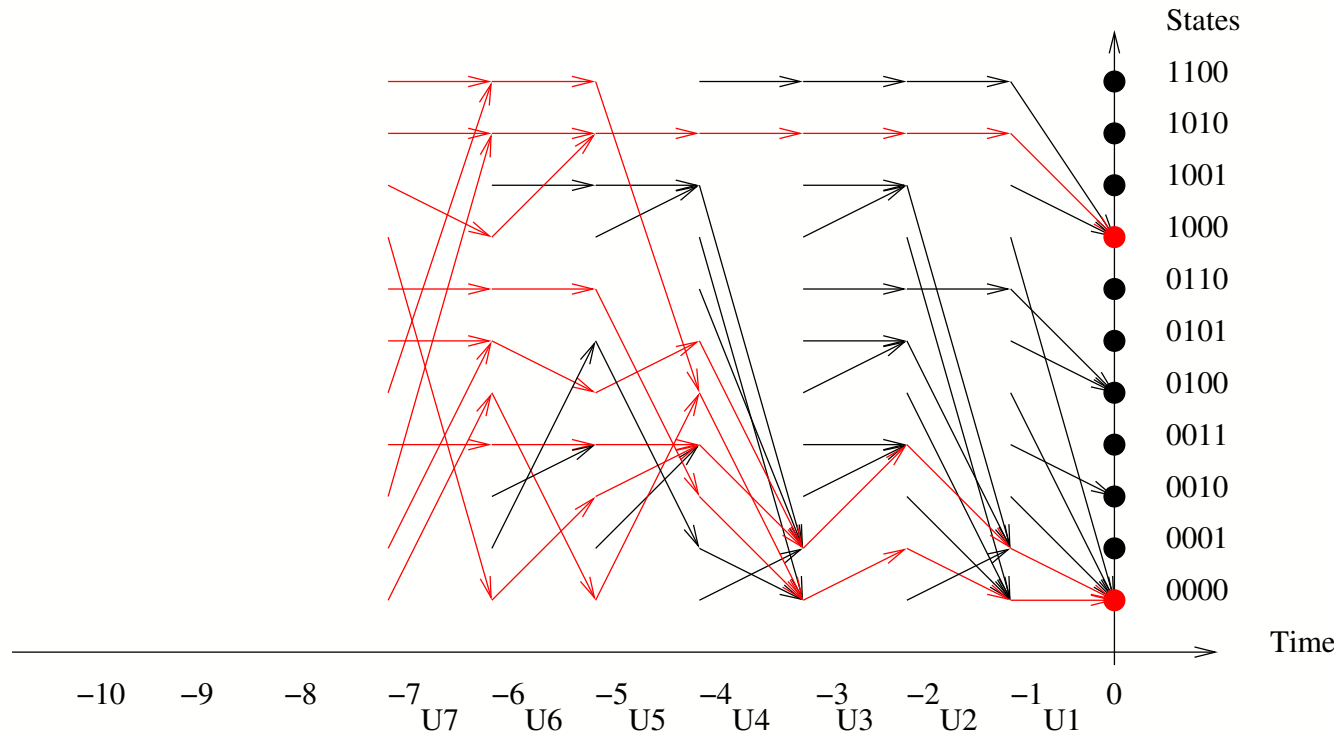
$$\mathcal{Z}_3 = \{0000, 0100, 1000\}$$

$$\mathcal{Z}_4 = \{0000, 1000\}$$

$$\mathcal{Z}_5 = \{0000, 1000\}$$

$$\mathcal{Z}_6 = \{0000, 1000\}$$

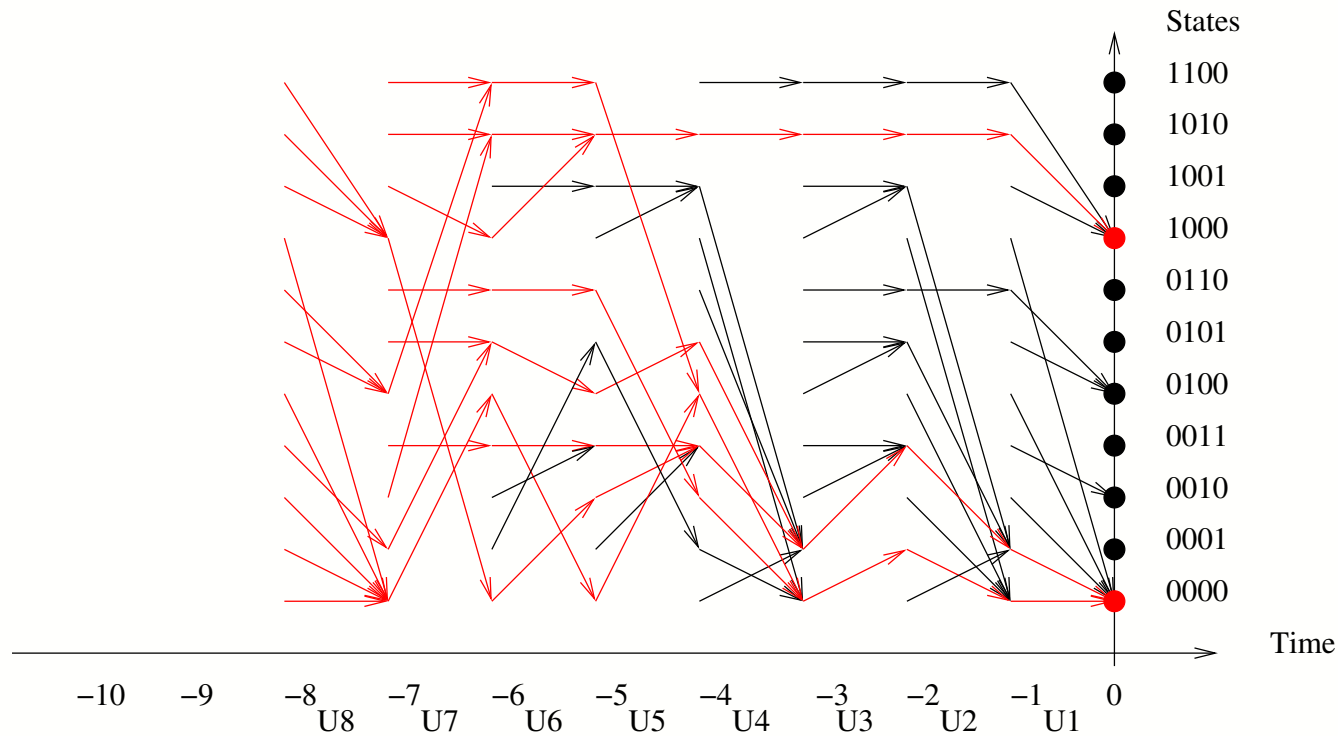
Backward simulation example



- | | | |
|--|--|----------------------------------|
| $\mathcal{Z}_0 = \mathcal{X}$ | $\mathcal{Z}_3 = \{0000, 0100, 1000\}$ | $\mathcal{Z}_6 = \{0000, 1000\}$ |
| $\mathcal{Z}_1 = \{0000, 0010, 0100, 1000\}$ | $\mathcal{Z}_4 = \{0000, 1000\}$ | $\mathcal{Z}_7 = \{0000, 1000\}$ |
| $\mathcal{Z}_2 = \{0000, 0100, 1000\}$ | $\mathcal{Z}_5 = \{0000, 1000\}$ | |



Backward simulation example



$$\mathcal{Z}_0 = \mathcal{X}$$

$$\mathcal{Z}_1 = \{0000, 0010, 0100, 1000\}$$

$$\mathcal{Z}_2 = \{0000, 0100, 1000\}$$

$$\mathcal{Z}_3 = \{0000, 0100, 1000\}$$

$$\mathcal{Z}_4 = \{0000, 1000\}$$

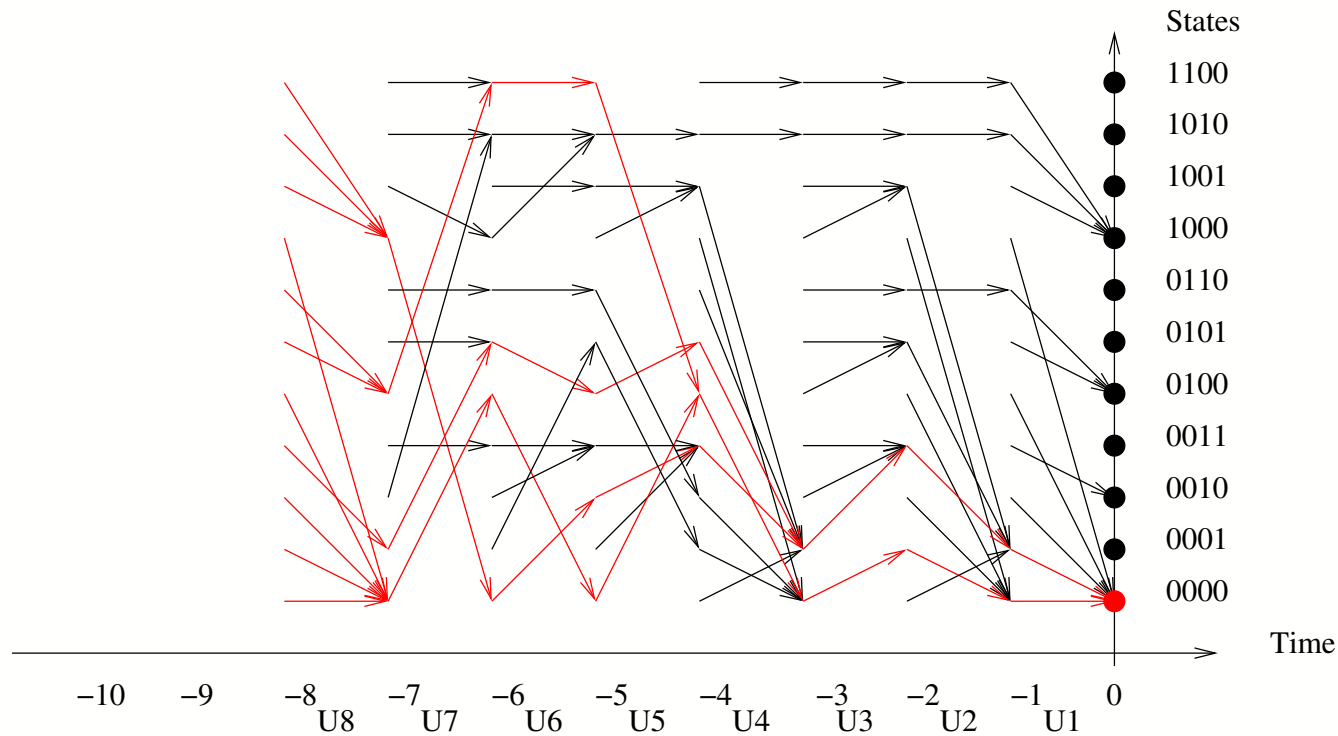
$$\mathcal{Z}_5 = \{0000, 1000\}$$

$$\mathcal{Z}_6 = \{0000, 1000\}$$

$$\mathcal{Z}_7 = \{0000, 1000\}$$



Backward simulation example



$$\mathcal{Z}_0 = \mathcal{X}$$

$$\mathcal{Z}_1 = \{0000, 0010, 0100, 1000\}$$

$$\mathcal{Z}_2 = \{0000, 0100, 1000\}$$

$$\mathcal{Z}_3 = \{0000, 0100, 1000\}$$

$$\mathcal{Z}_4 = \{0000, 1000\}$$

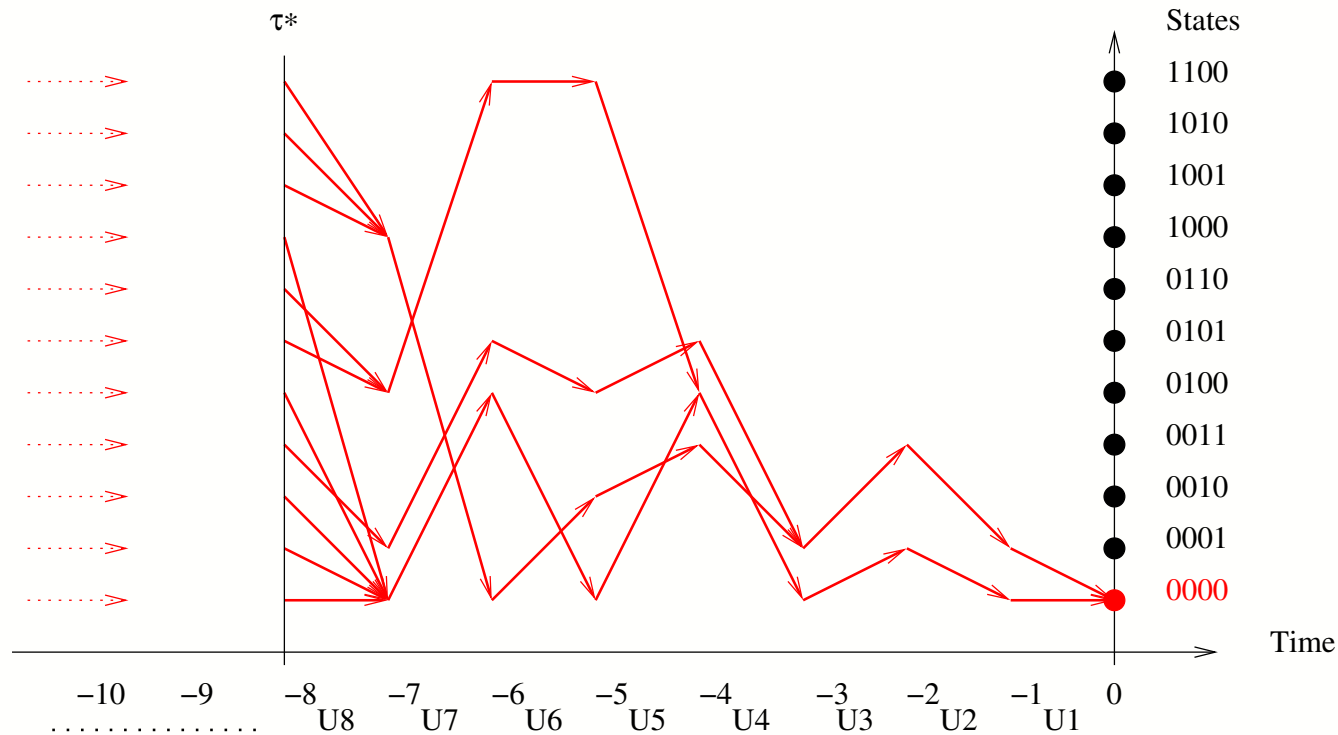
$$\mathcal{Z}_5 = \{0000, 1000\}$$

$$\mathcal{Z}_6 = \{0000, 1000\}$$

$$\mathcal{Z}_7 = \{0000, 1000\}$$

$$\mathcal{Z}_8 = \{0000\}$$

Backward simulation example



Process stops when $|\mathcal{Z}_n| = 1$

Stopping time $\tau^* = 8$

Number of computation of Φ (complexity) : $n \cdot \tau^*$

Backward coupling simulation

Proposition 1 (Propp & Wilson) *If $\tau^* < +\infty$ a.s. then the returned value is stationary distributed.*

Proof :

$\{Z_n\}_{n \in \mathbb{N}}$ is non-increasing and constant for n sufficiently large

$$\Phi(\Phi(\dots(\Phi(\mathcal{X}, U_{-n+1}), \dots), U_{-1}), U_0) \stackrel{\mathcal{L}}{\sim} \Phi(\Phi(\dots(\Phi(\mathcal{X}, U_1), \dots), U_{n-1}), U_n)$$

Remarks :

Stopping times τ and τ^* have the same law,

τ depends on Φ coding (not only on the transition matrix !)

\Rightarrow optimization problem



Functional backward coupling

Idea:

- Directly compute the cost function C
- Same backward scheme
- wait for coupling
- stopping time τ_C^*

$$\tau_C^* \leq \tau^* \text{ a.s.}$$

⇒ speedup

$$\mathcal{Z}_n^C = C(\Phi(\Phi(\cdots(\Phi(\mathcal{X}, U_{-n+1}), \cdots), U_{-1}), U_0)).$$

potential set of reachable costs at step n

```
for all  $x \in \mathcal{X}$  do  
     $y(x) \leftarrow C(x)$   
end for  
repeat  
     $u \leftarrow \text{Random};$   
    for all  $x \in \mathcal{X}$  do  
         $y(x) \leftarrow y(\Phi(x, u));$   
    end for  
until All  $y(x)$  are equal  
return  $y(x)$ 
```

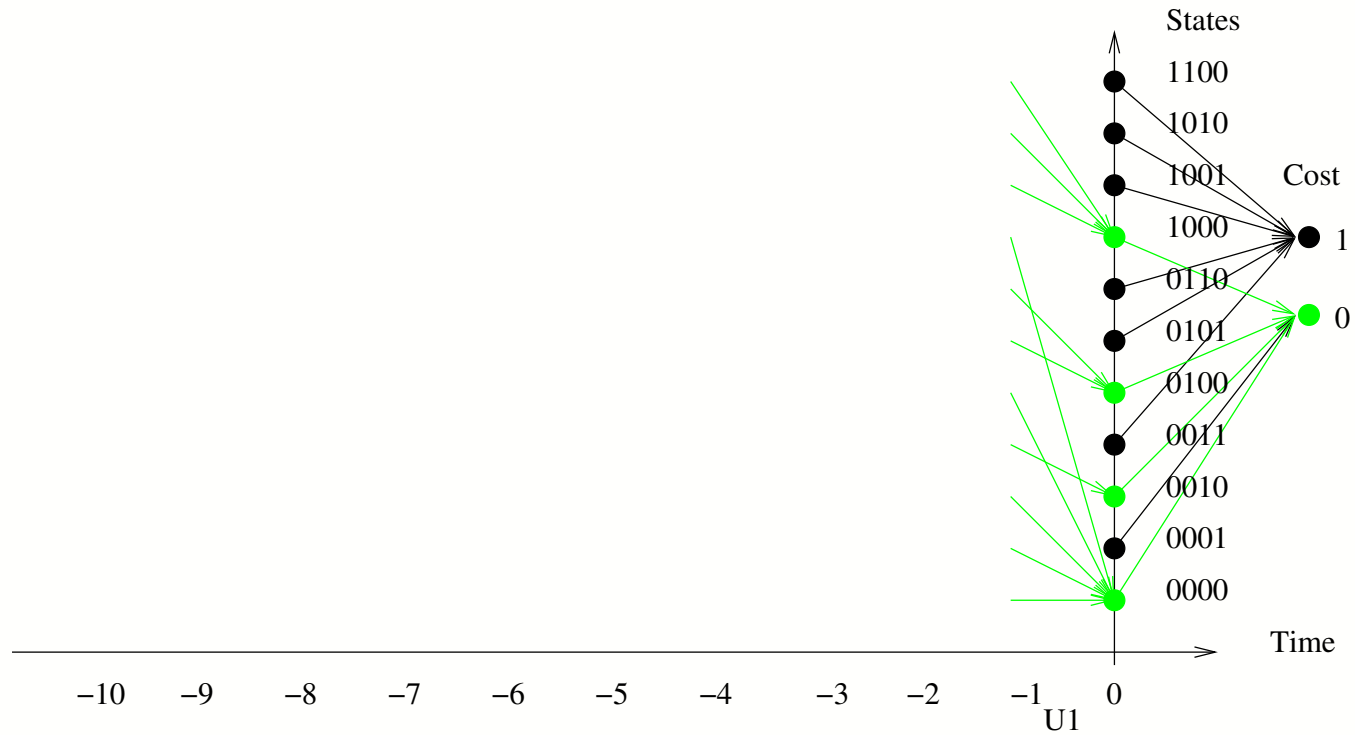


Backward functional simulation



$$Z_0^C = \{0, 1\}$$

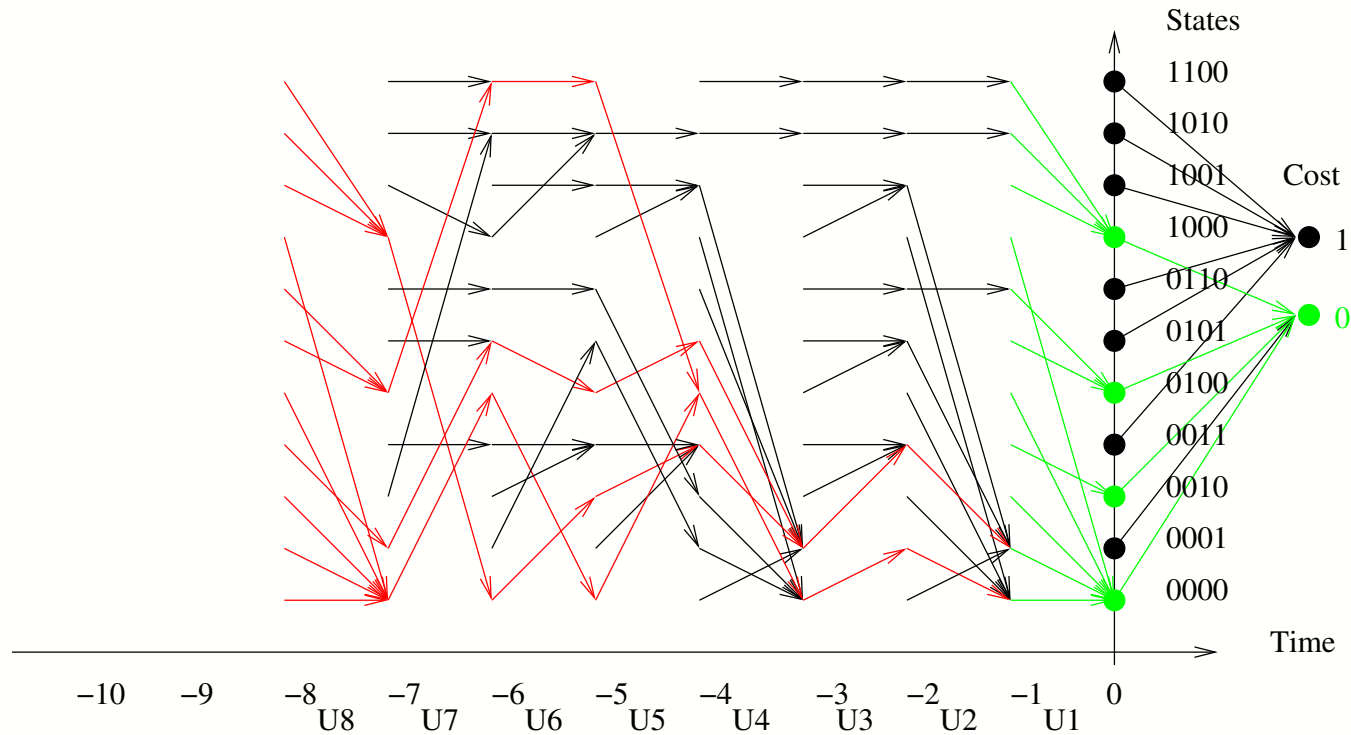
Backward functional simulation



$$\mathcal{Z}_0^C = \{0, 1\}$$

$$\mathcal{Z}_1^C = \{0\}$$

Backward functional simulation



$$\mathcal{Z}_0^C = \{0, 1\}$$

$$\mathcal{Z}_1^C = \{0\}$$

$$\tau^* = 8 \quad \tau_C^* = 1$$

Is the coupling time reduction significant ?

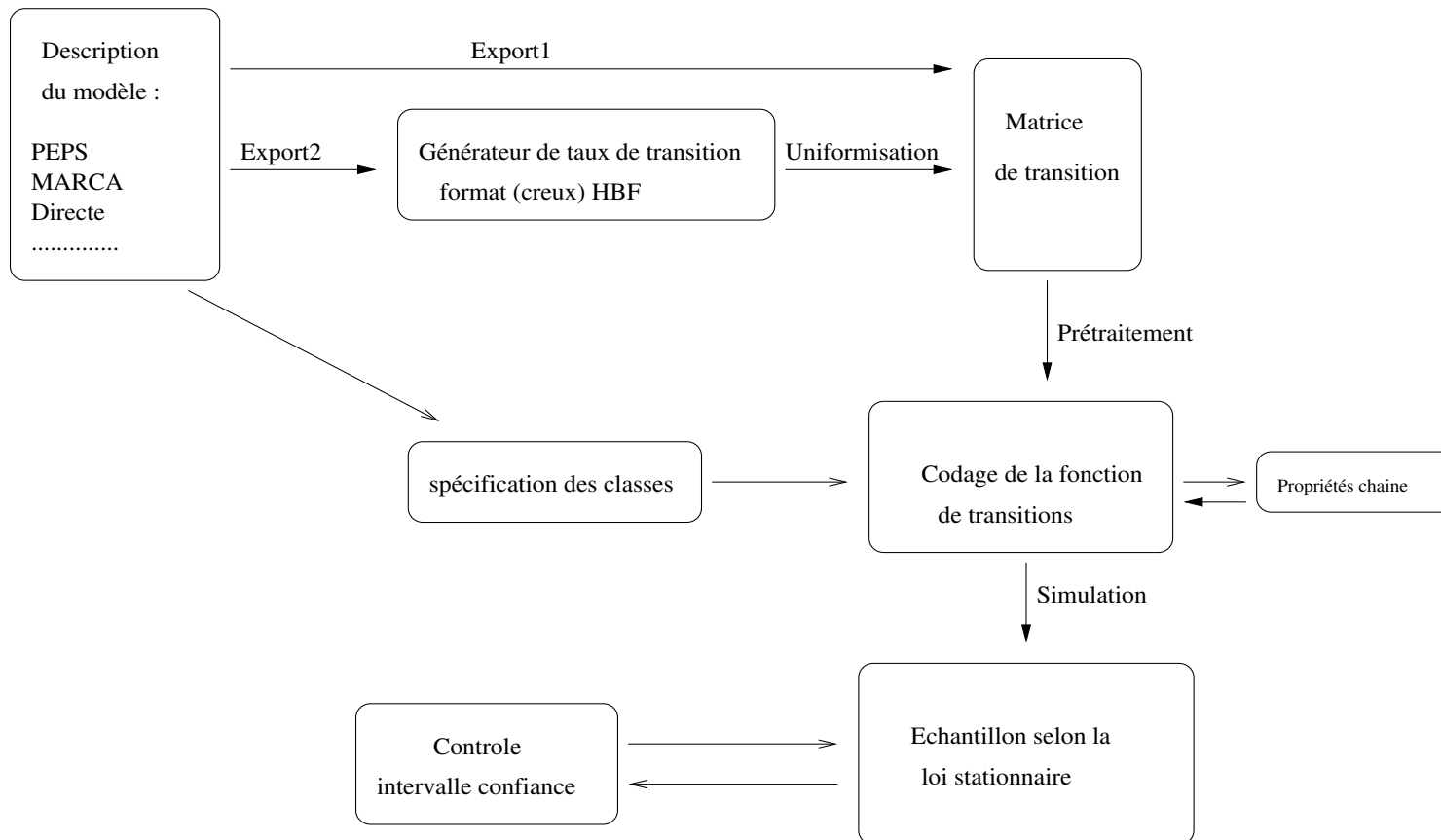
Implementation considerations

Φ coding : choice of a representation

- Sparse description of Markov generators (m non negative elements)
- Discretization (Uniformization)
- Aliasing table
- Coupling condition



General architecture of Ψ



Aliasing technique

- * *Walker* (1974) algorithm \Rightarrow discrete distribution simulation.
- * Pre-computation : alias tables : threshold and alias value .

Algorithm :

$u \leftarrow \text{Random};$

$v \leftarrow \text{Random};$

$ind \leftarrow (int)N * u;$

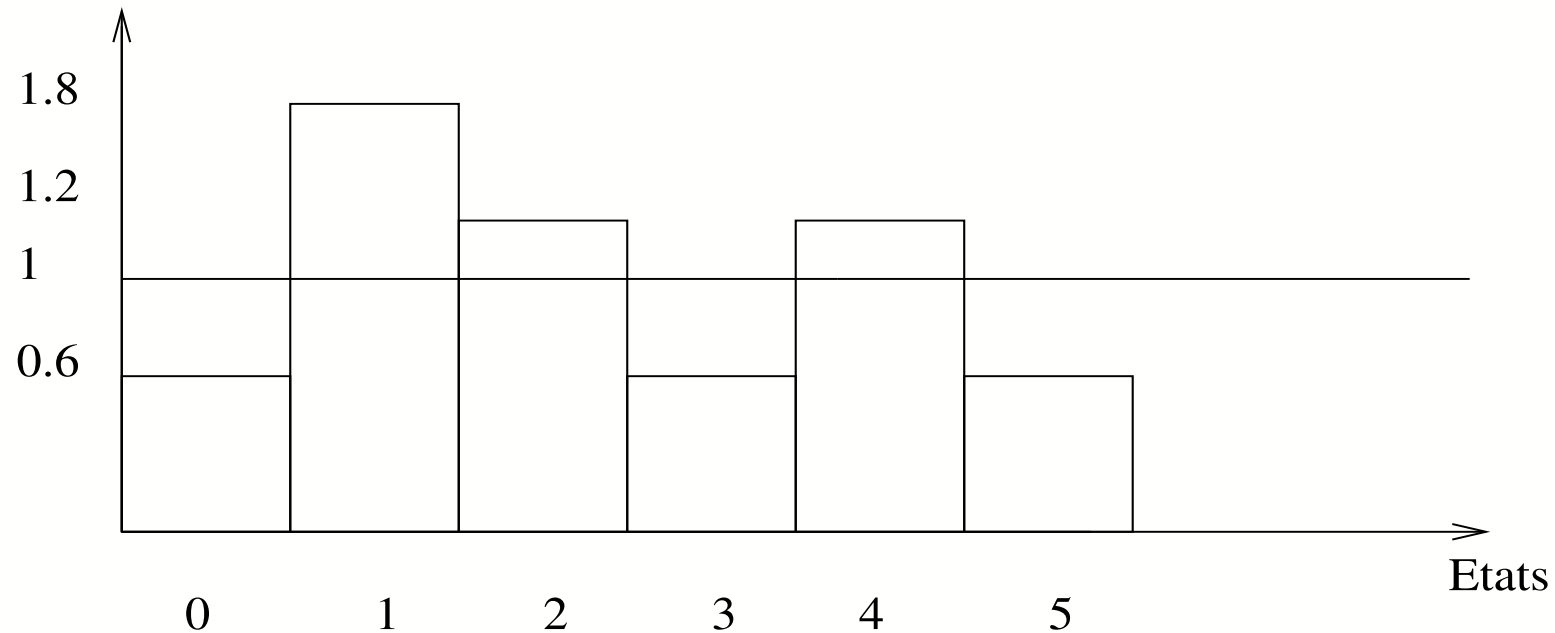
If ($v \leq \text{Seuil}[ind]$) **then** return ind ; *{standard value.}*

else return $\text{Alias}[ind]$; *{alias value.}*

endif;



Aliasing technique



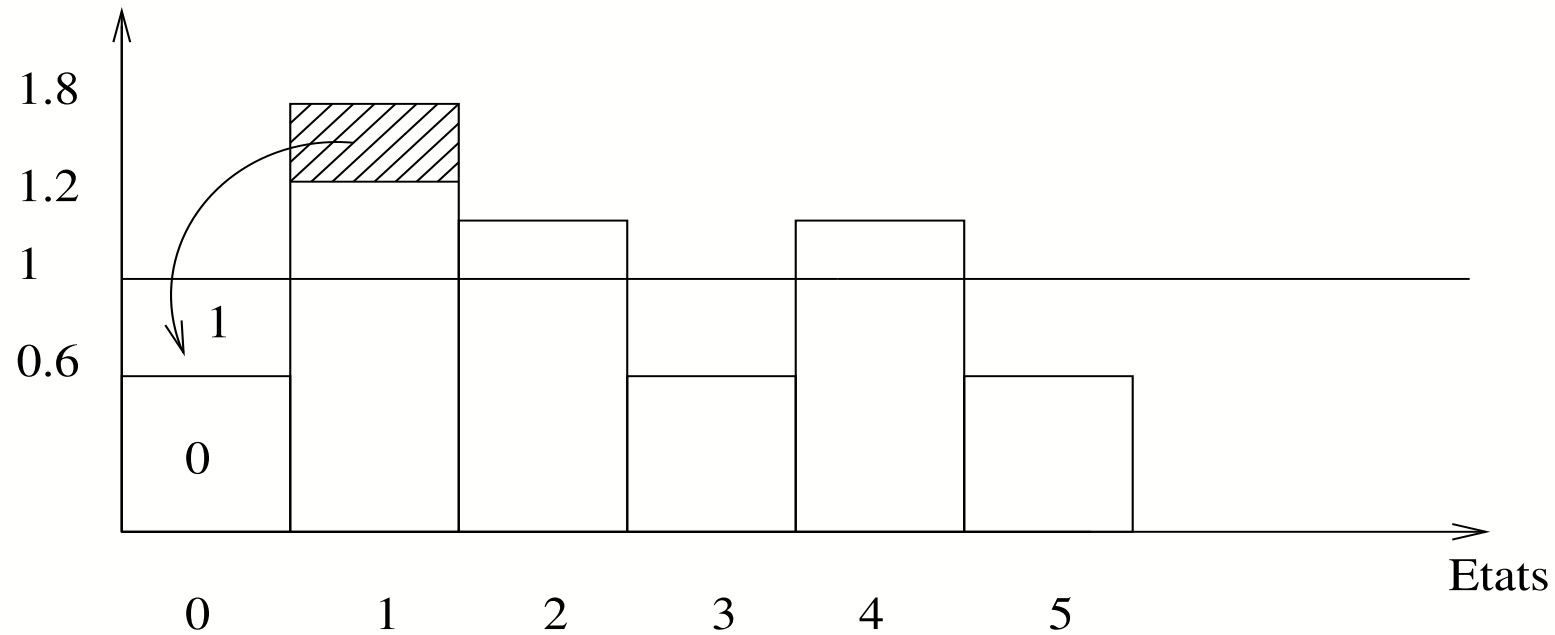
X r.v. defined on $\{0, \dots, 5\}$ by :

$$\mathbb{P}(X = 0) = \mathbb{P}(X = 3) = \mathbb{P}(X = 5) = 0.1$$

$$\mathbb{P}(X = 2) = \mathbb{P}(X = 4) = 0.2, \quad \mathbb{P}(X = 1) = 0.3$$



Aliasing technique



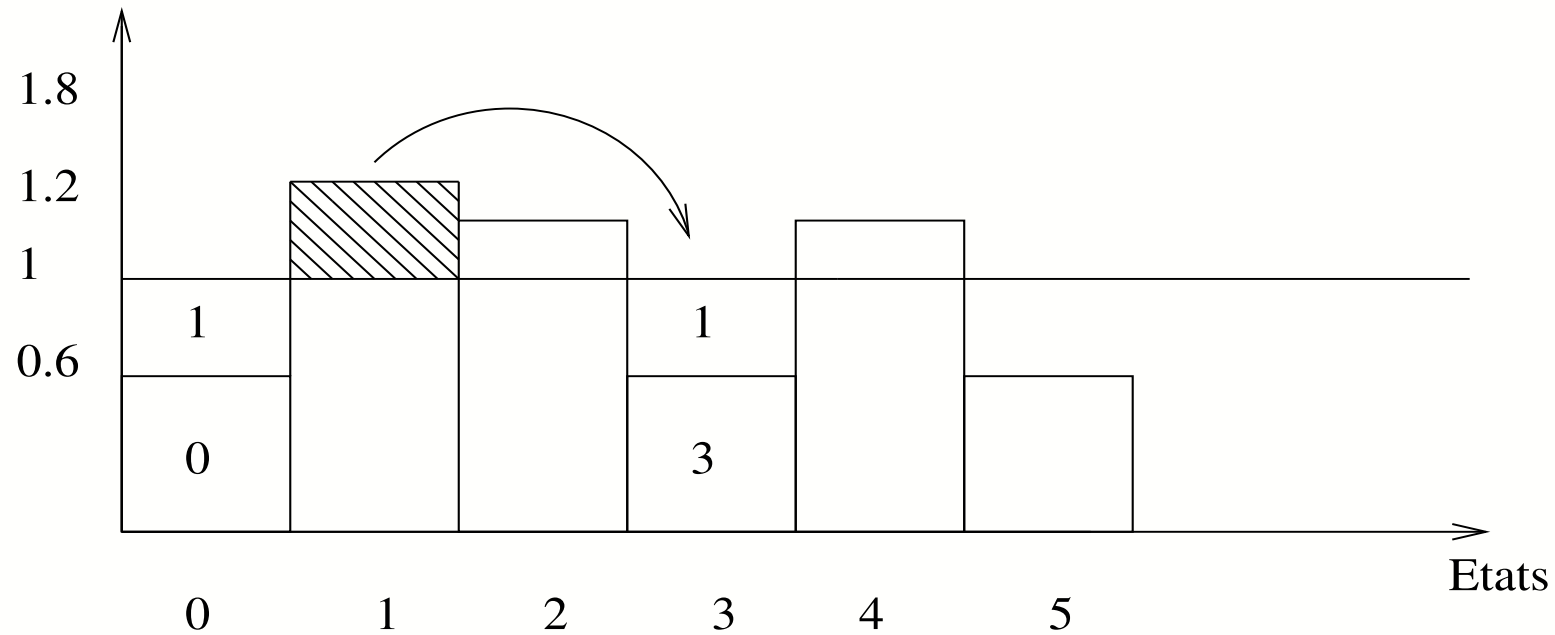
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Aliasing technique



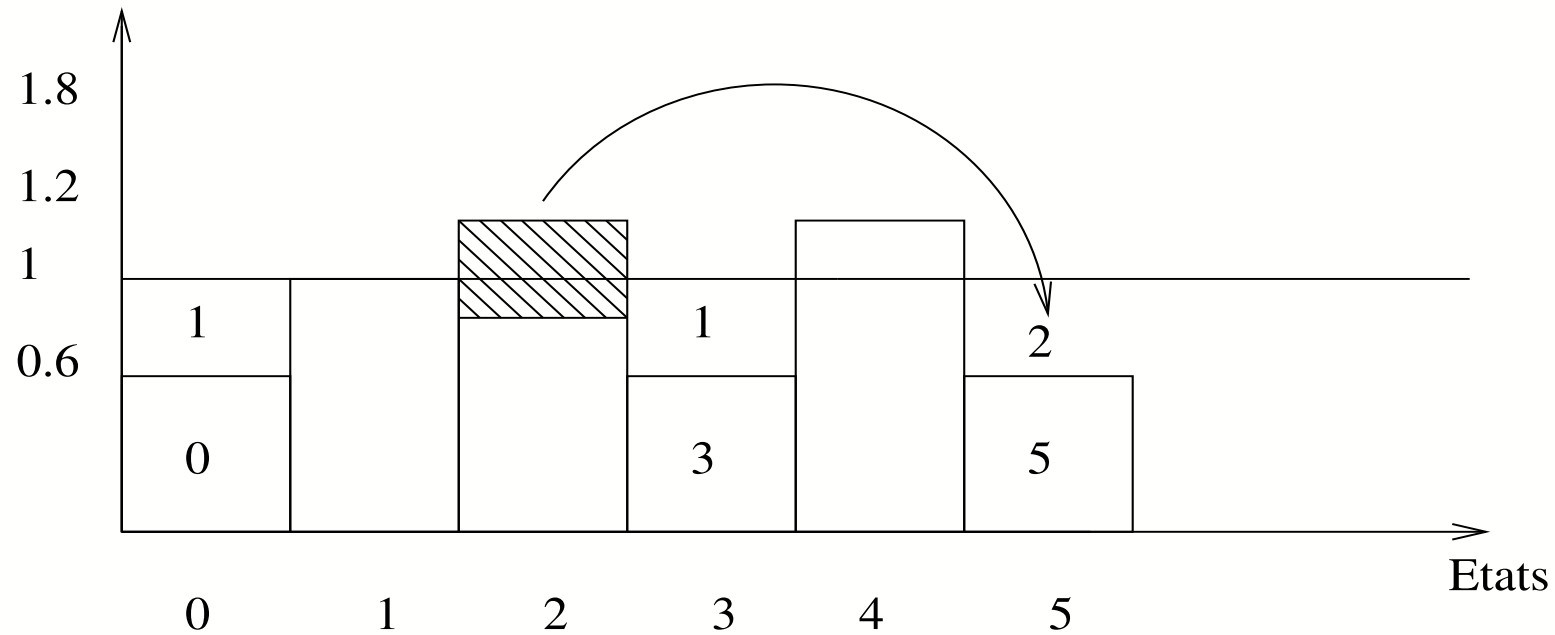
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Aliasing technique

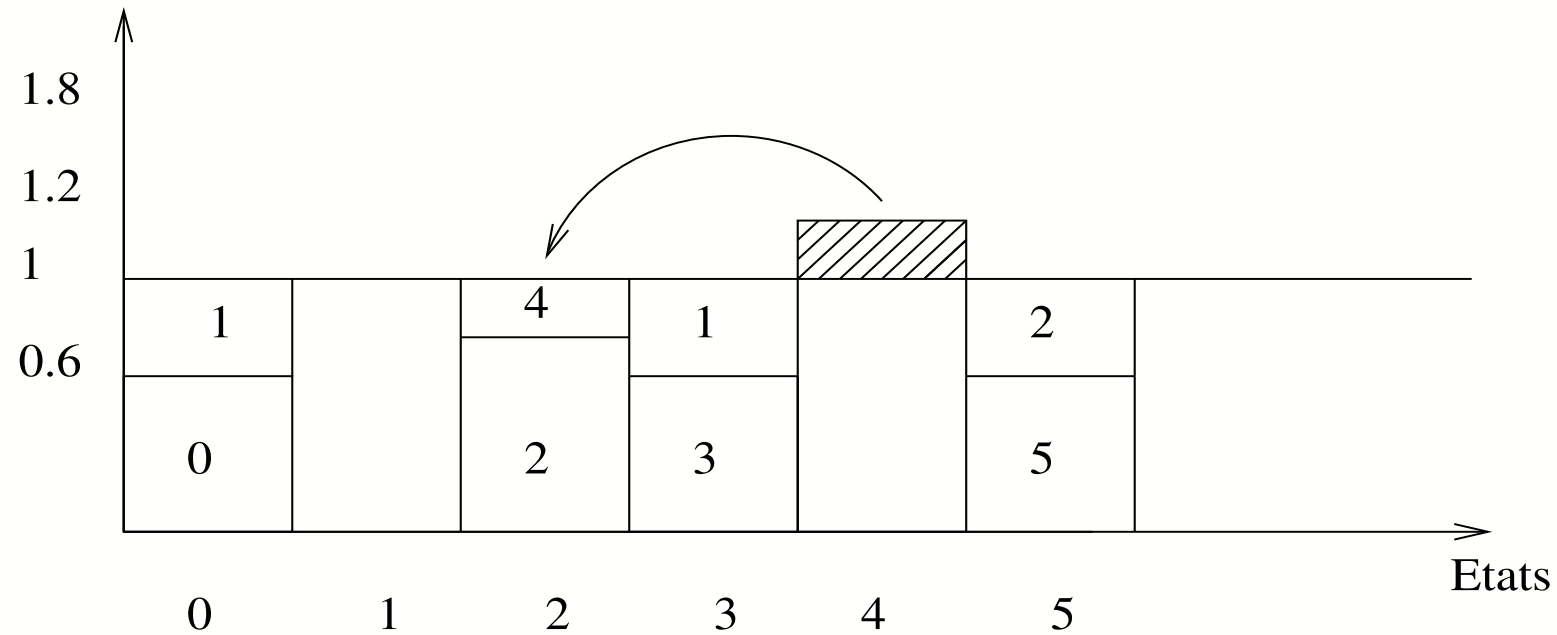


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Aliasing technique

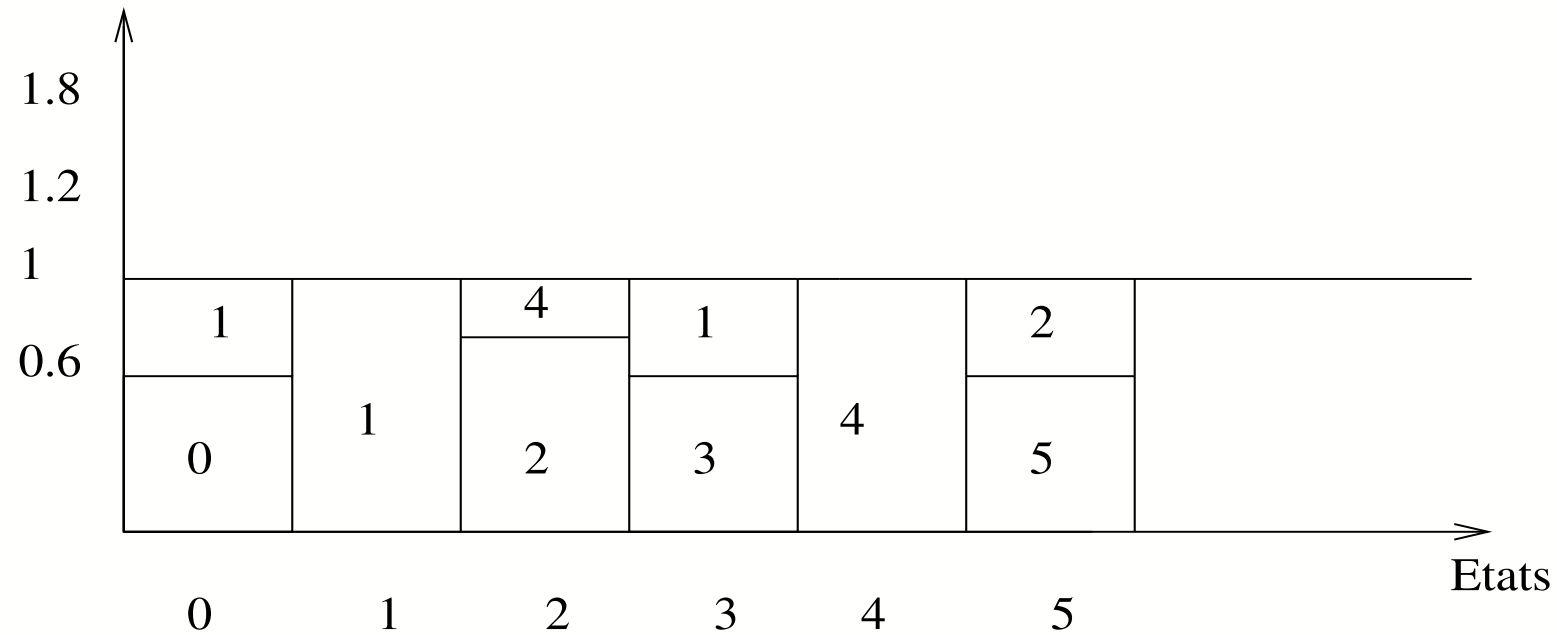


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Aliasing technique



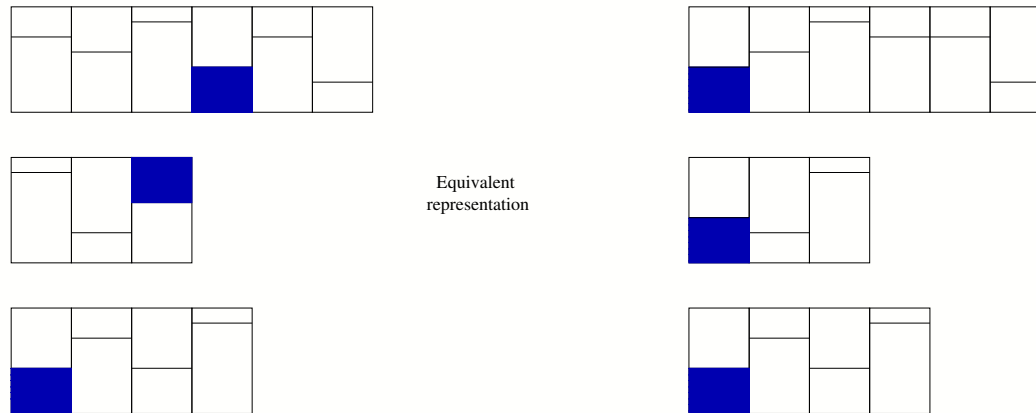
X r.v. defined on $\{0, \dots, 5\}$ by :

$$\mathbb{P}(X = 0) = \mathbb{P}(X = 3) = \mathbb{P}(X = 5) = 0.1$$

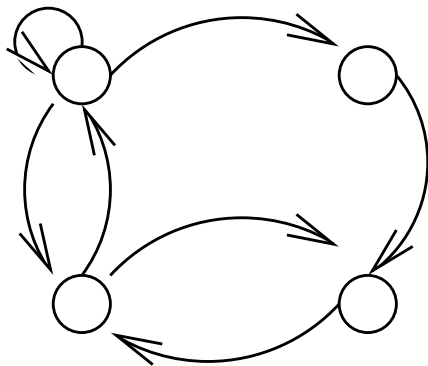
$$\mathbb{P}(X = 2) = \mathbb{P}(X = 4) = 0.2, \quad \mathbb{P}(X = 1) = 0.3$$

Coupling property

Exchange of columns or thresholds give an equivalent representative

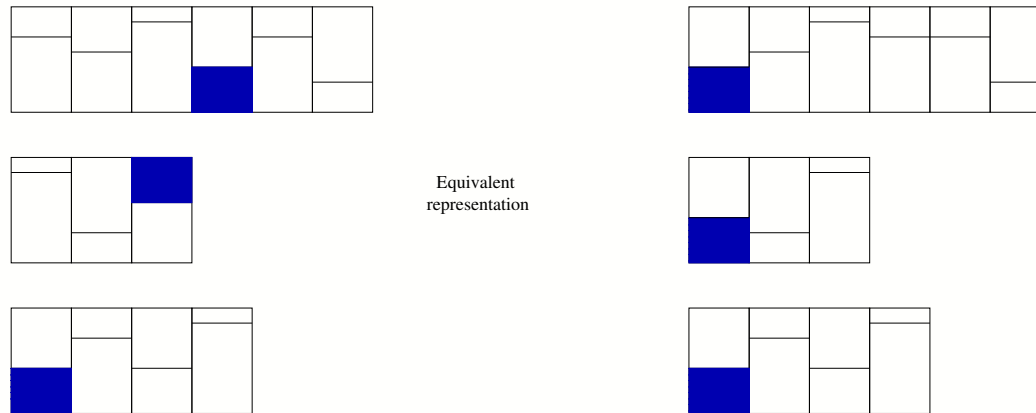


Irreducibility \implies there exists a spanning tree conducting to a single state where coupling occurs.

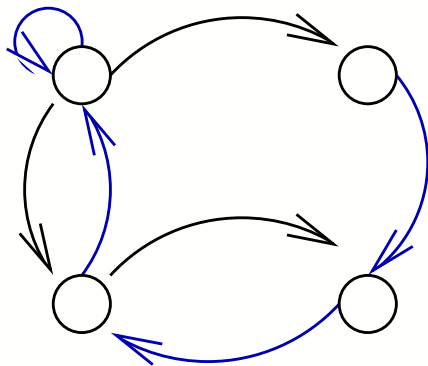


Coupling property

Exchange of columns or thresholds give an equivalent representative



Irreducibility \implies there exists a spanning tree conducting to a single state where coupling occurs.



$$\mathbb{P}(\tau^* < +\infty) = 1.$$

τ is geometrically bounded, so τ^* and τ_C^* .

Examples

- Functionality tests : "random transition matrices"
- Resource sharing model : statistical verification
- Overflow model : sparsity and gain



Example 1

Random transition coefficients:

Number of states	10	100	500	1000	3000
Mean coupling time	3.1	4.5	5.3	5.7	6.1
Mean execution time μs	3	17	170	360	1100

Pentium III 700MHz and 256Mb memory. Sample size 10000.

Remarks:

- **very small coupling time**
- Coefficients : same order of magnitude, aliasing enforces coupling

Comparison with birth and death process :

Number of states	10	100	500	1000	3000
Mean coupling time	41	557	2850	5680	17000
Mean execution time μs	28	1800	88177	366000	3.5s

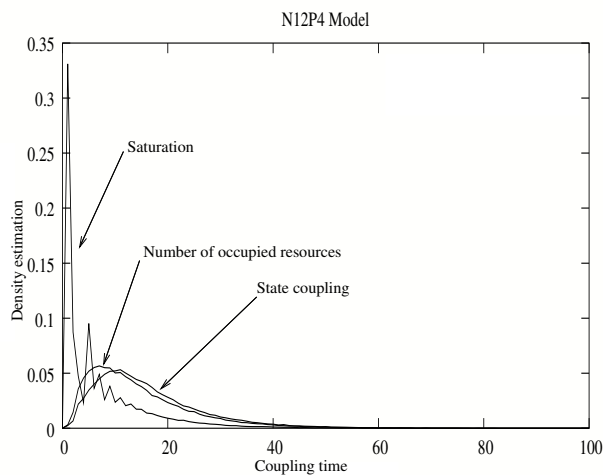
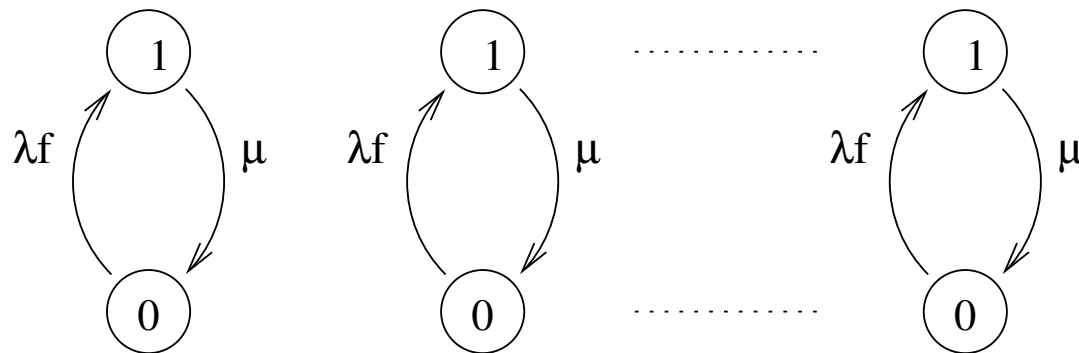
Remarks:

- **large coupling time**
- sparse matrix, large graph diameter



Resource sharing model

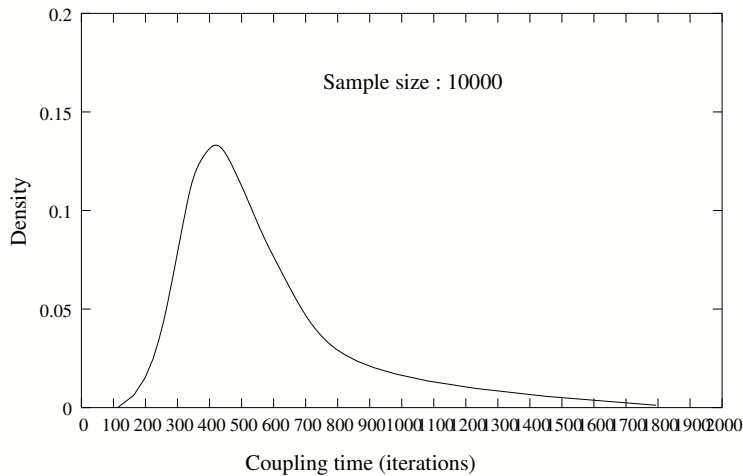
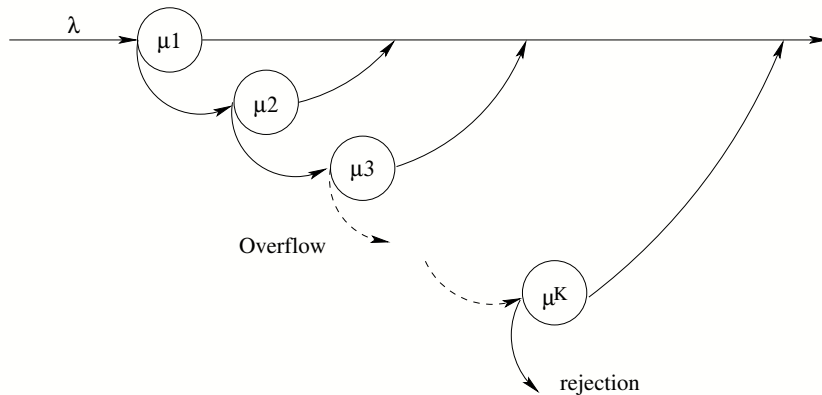
P resources N users; state $= (x_1, \dots, x_N)$; access constraint $f = (\sum x_i < P)$
 product form solution \Rightarrow statistical validation



- state coupling
- functional coupling :
- number of occupied resources :
- $\sum_i x_i,$
- saturation : $(\sum_i x_i = P),$

High reduction of the functional coupling time

Overflow model



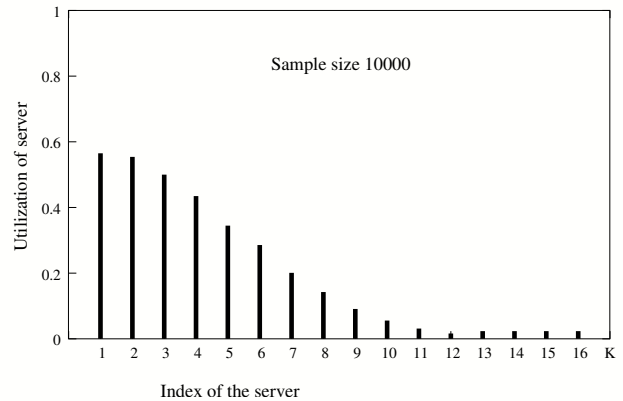
K servers,
priority on overflows
input rate λ ,
different service rate
state (x_1, \dots, x_K) , $x_i \in \{0, 1\}$,
size ~ 130000
low diameter
non product-form structure,

Parameter	Value
minimum	113
maximum	1794
median	465
mean	498
Std	180

exponential tail, low mean value

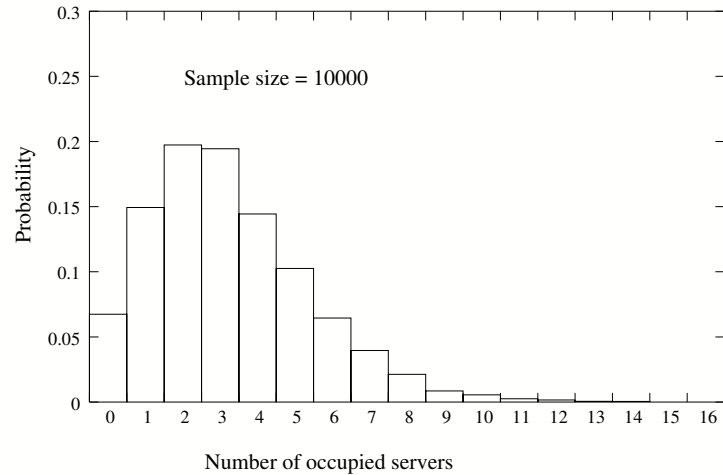


Overflow model (2)



Marginal probabilities estimation

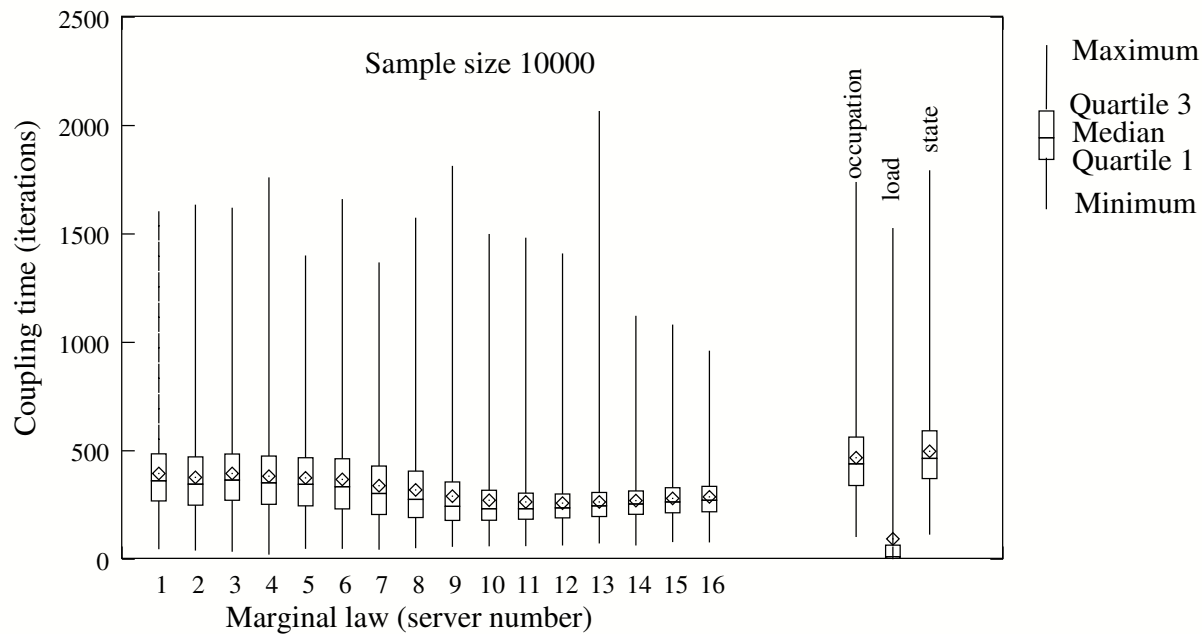
$$\mathbb{P}(X_i = 1)$$



Marginal distribution of the occupied servers



Overflow model (3)



Functional coupling time

- gain 20% for the first marginals
- utilization : best reduction

Conclusion (1)

- Theoretical results :
 - reverse scheme + contracting operator
 - coupling condition
 - functional reduction
- Algorithmic results:
 - general coding of a chain
 - guaranteed coupling algorithm
 - compact representation
- Experimental results
 - complexity reduction
 - significant results (depending on the diameter and the coding of the chain)



Conclusion (2)

Software tool: **PSI : Perfect Simulator**

<http://www-id.imag.fr/Software/PSI/>

Two versions : unix command / with a simple interface

```
psi_alias -i example.marca -o example
```

generates alias tables (`example.simu`)

```
psi_sample -i example.simu -d sample-size -c example.cost -o  
example
```

`example.cost` associates to each state its cost

generates samples of costs stationary distributed (`example.sample`)



Future works

- Theoretical improvements:
 - deeper understanding of Φ properties and the spectrum of the transition matrix
 - evaluation or bounds on the coupling time
- Algorithmic perspectives:
 - building of alias table,
 - transform of alias table,
 - parallelization
- Model based approach :
 - structuration of the matrix : adapted strategies (QN, SAN, GSPN, PA,...)
 - model properties : monotonicity, reversibility,...
- Experimental results
 - find limit models : (ex Birth and death)
 - significant results (depending on the diameter and the coding of the chain)
 - huge models (size 2^{22})

