Markov Chain

Markov Chains and Computer Science A not so Short Introduction

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Grenoble











- Approaches
- Pormalisation
- 3 Long run behavior
- Cache modeling
- Synthesis



History (Andreï Markov)

This study investigates a text excerpt containing 20,000 Russian letters of the alphabet, excluding **b** and **b**,² from Pushkin's novel *Engene Onegin* – the entire first chapter and sixteen starzas of the second.

This sequence provides us with 20,000 connected trials, which are either a vowel or a consonant.

Accordingly, we assume the existence of an unknown constant probability *p* that the observed letter is a vowel. We determine the approximate value of *p* by observation, by counting all the vowels and consonants. Apart from *p*, we shall find – also through observation – the approximate values of two numbers p_1 and p_0 , and four numbers $p_{1,1}$, $p_{1,0}$, $p_{0,1}$, and $p_{0,0}$. They represent the following probabilities: $p_1 - a$ vowel follows a consonant; $p_{1,1} - a$ vowel follows two vowels: $p_{10} - a$ vowel follows a consonant that is preceded by a vowel; $p_{0,1} - a$ vowel follows two consonants.

The indices follow the same system that I introduced in my paper "On a Case of Samples Connected in Complex Chain" [Markov 1911b]; with reference to my other paper, "Investigation of a Remarkable Case of Dependent Samples" [Markov 1907a], however, $p_0 = p_2$. We denote the opposite probabilities for consonants with q and indices that follow the same pattern.

If we seek the value of p, we first find 200 approximate values from which we can determine the arithmetic mean. To be precise, we divide the entire sequence of 20,000 letters into 200 separate sequences of 100 letters, and count how many vowels there are in each 100: we obtain 200 numbers, which, when divided by 100, yield 200 approximate values of p.

An example of statistical investigation in the text of "Eugene Onegin" illustrating coupling of "tests" in chains. (1913) In Proceedings of Academic Scientific St. Petersburg, VI, pages 153-162.



1856-1922



Graphs and Paths



Random Walks

Path in a graph: X_n *n*-th visited node path : i_0, i_1, \dots, i_n normalized weight : arc $(i, j) \longrightarrow p_{i,j}$

concatenation : . $\longrightarrow \times$ $\mathcal{P}(i_0, i_1, \cdots, i_n) = p_{i_0, i_1} p_{i_1, i_2} \cdots p_{i_{n-1}, i_n}$

disjoint union : $\cup \longrightarrow +$ $\mathcal{P}(i_0 \rightsquigarrow i_n) = \sum_{i_1, \cdots, i_{n-1}} p_{i_0, i_1} p_{i_1, i_2} \cdots p_{i_{n-1}, i_n}$

automaton : state/transitions randomized (language)



Dynamical Systems

Figure 3. A fern drawn by a Markov chain



Diaconis-Freedman 99

Evolution Operator

Initial value : X_0 Recurrence equation : $X_{n+1} = \Phi(X_n, \xi_{n+1})$

Innovation at step n + 1: ξ_{n+1} Finite set of innovations: { $\phi_1, \phi_2, \cdots, \phi_K$ }

Random function (chosen with a given probability)

Randomized Iterated Systems



Measure Approach



Ehrenfest's Urn (1907)



Paul Ehrenfest (1880-1933)

Distribution of *K* **particles**

Initial State $X_0 = 0$ State = nb of particles in 0 Dynamic : uniform choice of a particle and jump to the other side

$$\pi_n(i) = \mathbb{P}(X_n = i | X_0 = 0)$$

= $\pi_{n-1}(i-1) \cdot \frac{K-i+1}{K}$
 $+\pi_{n-1}(i+1) \cdot \frac{i+1}{K}$

 $\pi_n = \pi_{n-1}.P$

Iterated product of matrices



Algorithmic Interpretation

int minimum (T,K) min= $+\infty$ cpt=0; for (k=0; k < K; k++) do if (T[i]< min) then min = T[k]; process(min); cpt++; end if end for return(cpt) Worst case K; Best case 1; on average ?

Number of processing min

State : X_n = rank of the n^{th} processing

$$\mathbb{P}(X_{n+1} = j | X_n = i, X_{n-1} = i_{k-1}, \cdots, X_0 = i_0) = \mathbb{P}(X_{n+1} = j | X_n = i)$$

$$\mathbb{P}(X_{n+1} = j | X_n = i) = \begin{cases} \frac{1}{K - i + 1} & \text{si } j < i; \\ 0 & \text{sinon.} \end{cases}$$

All the information of for the step n + 1 is contained in the state at step n

 $\tau = \min\{n; X_n = 1\}$

Correlation of length 1





Markov Chain

Pormalisation

- States and transitions
- Applications

3 Long run behavior

Cache modeling

5 Synthesis



Formal definition

Let $\{X_n\}_{n\in\mathbb{N}}$ a random sequence of variables in a discrete state-space \mathcal{X}

 $\{X_n\}_{n \in \mathbb{N}}$ is a Markov chain with initial law $\pi(0)$ iff

- $X_0 \sim \pi(0)$ and
- for all $n \in \mathbb{N}$ and for all $(j, i, i_{n-1}, \cdots, i_0) \in \mathcal{X}^{n+2}$

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 $\{X_n\}_{n\in\mathbb{N}}$ is a **homogeneous** Markov chain iff

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 $\mathbb{P}(X_{n+1}=j|X_n=i)=\mathbb{P}(X_1=j|X_0=i)\stackrel{\text{def}}{=}p_{i,j}.$

(invariance during time of probability transition)



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Algebraic representation

- $P = ((p_{i,j}))$ is the **transition matrix** of the chain
 - P is a stochastic matrix

$$p_{i,j} \ge 0; \quad \sum_j p_{i,j} = 1.$$

Linear recurrence equation $\pi_i(n) = \mathbb{P}(X_n = i)$

$$\pi_n = \pi_{n-1} P.$$

• Equation of Chapman-Kolmogorov (homogeneous): $P^n = ((p_{i,j}^{(n)}))$

$$p_{i,j}^{(n)} = \mathbb{P}(X_n = j | X_0 = i); \quad P^{n+m} = P^n.P^m;$$

$$\mathbb{P}(X_{n+m} = j | X_0 = i) = \sum_{k} \mathbb{P}(X_{n+m} = j | X_m = k) \mathbb{P}(X_m = k | X_0 = i);$$

=
$$\sum_{k} \mathbb{P}(X_n = j | X_0 = k) \mathbb{P}(X_m = k | X_0 = i).$$

Interpretation: decomposition of the set of paths with length n + m from *i* to *j*.



Problems

Finite horizon

- Estimation of $\pi(n)$
- Estimation of stopping times

 $\tau_A = \inf\{n \ge 0; X_n \in A\}$

- . . .

Infinite horizon

- Convergence properties
- Estimation of the asymptotics
- Estimation speed of convergence

- . . .



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Applications in computer science

Applications in most of scientific domains ... In computer science :

Markov chain : an algorithmic tool

- Numerical methods (Monte-Carlo methods)
- Randomized algorithms (ex: TCP, searching, pageRank...)
- Learning machines (hidden Markov chains)
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Markov chains : a modeling tool

- Performance evaluation (quantification and dimensionning)
- Stochastic control
- Program verification
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Markov Chain

Cache modeling

Synthesis

Nicholas Metropolis (1915-1999)



Nick Metropolis

Metropolis contributed several original ideas to mathematics and physics. Perhaps the most widely known is the Monte Carlo method. Also, in 1953 Metropolis co-authored the first paper on a technique that was central to the method known now as simulated annealing. He also developed an algorithm (the Metropolis algorithm or Metropolis-Hastings algorithm) for generating samples from the Boltzmann distribution, later generatized by W.K. Hastings.

Simulated annealing

Convergence to a global minimum by a stochastic gradient scheme.

$$X_{n+1} = X_n - grad \Phi(X_n) \Delta_n(Random).$$

 $\Delta_n(random) \stackrel{n \to \infty}{\longrightarrow} 0$





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Complex system



Basic model assumptions

System :

- automaton (discrete state space)
- discrete or continuous time
- Environment : non deterministic
- time homogeneous
- stochastically regular

Problem

- steady-state estimation
- ergodic simulation
- state space exploring techniques





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Cache modeling

Synthesis





Formalisation

3 Long run behavior

- Convergence
- Solving
- Simulation

Cache modeling

Synthesis



States classification

Graph analysis



Irreducible class

Strongly connected components *i* and *j* are in the same component if there exist a path from *i* to *j* and a path from *j* to *i* with a positive probability Leaves of the tree of strongly connected components are **irreducible** classes States in irreducible classes are called **recurrent**

Other states are called transient

Periodicity

An irreducible class is **aperiodic** if the gcd of length of all cycles is 1

A Markov chain is **irreducible** if there is only one class. Each state is reachable from any other state with a positive probability path.



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States classification : matrix form



LIG

Synthesis

Automaton Flip-flop

ON-OFF system

Two states model :

- communication line
- processor activity

- ...



Parameters :

- proportion of transitions : p, a
- mean sojourn time in state 1 :
- mean sojourn time in state 2 : 🖞

Problem

Estimation of π_n : state prevision, resource utilization



Trajectory

 X_n state of the automaton at time n.

Transient distribution

$$\pi_n(1) = \mathbb{P}(X_n = 1);$$

$$\pi_n(2) = \mathbb{P}(X_n = 2)$$
Automaton Flip-flop

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Long run behavior

Automaton Flip-flop

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Mathematical model

Transition probabilities

$$P = \begin{bmatrix} 1-p & p \\ q & 1-q \end{bmatrix}$$
$$\mathbb{P}(X_{n+1} = 1 | X_n = 1) = 1-p;$$
$$\mathbb{P}(X_{n+1} = 2 | X_n = 1) = p;$$
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 $\pi_{n+1}(1) = \pi_n(1)(1-p) + \pi_n(2)q;$ $\pi_{n+1}(2) = \pi_n(1)p + \pi_n(2)(1-q);$

 $\pi_{n+1} = \pi_n P$ Linear iterations Spectrum of *P* (eigenvalues) $Sp = \{1, 1 - p - q\}$

System resolution

1 - p - q| < 1 Non pathologic case

$$\begin{cases} \pi_{n}(1) = \frac{q}{p+q} + \left(\pi_{0}(1) - \frac{q}{p+q}\right)(1-p-q)^{n}; \\ \pi_{n}(2) = \frac{p}{p+q} + \left(\pi_{0}(2) - \frac{p}{p+q}\right)(1-p-q)^{n}; \end{cases}$$

1 - p - q = 1 p = q = 0 Reducible behavior

1 - p - q = -1 p = q = 1 Periodic behavio



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Linear iterations
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G

Recurrent behavior



Steady state behavior

$$\left(\begin{array}{c} \pi_{\infty}(1) = \frac{q}{p+q}; \\ \pi_{\infty}(2) = \frac{p}{p+q}. \end{array}\right)$$

π_∞ unique probability vector solution

 $\pi_{\infty}=\pi_{\infty}\boldsymbol{P}.$

If $\pi_0 = \pi_\infty$ then $\pi_n = \pi_\infty$ for all *n* stationary behavior



Recurrent behavior



Steady state behavior

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Convergence In Law

Let $\{X_n\}_{n\in\mathbb{N}}$ a homogeneous, irreducible and aperiodic Markov chain taking values in a discrete state \mathcal{X} then

• The following limits exist (and do not depend on *i*)

$$\lim_{n\to+\infty}\mathbb{P}(X_n=j|X_0=i)=\pi_j;$$

• π is the unique probability vector invariant by *P*

$$\pi P = \pi;$$

• The convergence is rapid (geometric); there is C > 0 and $0 < \alpha < 1$ such that

$$||\mathbb{P}(X_n = j | X_0 = i) - \pi_j|| \leq C . \alpha^n$$

Denote

$$X_n \xrightarrow{\mathcal{L}} X_\infty;$$

with X_{∞} with law π π is the **steady-state probability** associated to the chain



Interpretation

Equilibrium equation



Probability to enter *j* =probability to exit *j* balance equation

$$\sum_{i \neq j} \pi_i p_{i,j} = \sum_{k \neq j} \pi_j p_{j,k} = \pi_j \sum_{k \neq j} p_{j,k} = \pi_j (1 - p_{j,j})$$

 $\pi \stackrel{\text{der}}{=} \text{steady-state.}$ If $\pi_0 = \pi$ the process is stationary ($\pi_n = \pi$



Interpretation

Equilibrium equation



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Proof 1 : Finite state space algebraic approach

Positive matrix P > 0

contraction max_i $p_{i,j}^{(n)}$ – min_i $p_{i,j}^{(n)}$

Perron-Froebenius *P* > 0

P is positive and stochastic then the spectral radius $\rho = 1$ is an eigenvalue with multiplicity 1, the corresponding eigenvector is positive and the other eigenvalues have module < 1.

Case $P \ge 0$

Aperiodique and irreducible \Rightarrow there is *k* such that $P^k > 0$ and apply the above result.



Proof 1 : details P > 0

Soit x et
$$y = Px$$
, $\omega = \min_{i,j} p_{i,j}$
 $\overline{x} = \max_{i} x_i, \ \underline{x} = \min_{i} x_i.$
 $y_i = \sum_{j} p_{i,j} x_j$

Property of centroid :

$$(1 - \omega)\underline{x} + \omega \overline{x} \leq y_i \leq (1 - \omega)\overline{x} + \omega \underline{x}$$
$$0 \leq \overline{y} - \underline{y} \leq (1 - 2\omega)(\overline{x} - \underline{x})$$
$$P^n x \longrightarrow s(x)(1, 1, \dots, 1)^t$$

Then P^n converges to a matrix where all lines are identical.



Cache modeling

Synthesis

Proof 2 : Return time

$$\tau_i^+ = \inf\{n \ge 1; \ X_n = i | X_0 = i\}.$$

then $\frac{1}{\mathbb{E}\tau_{i}^{+}}$ is an invariant probability (Kac's lemma)



1914-1984

Proof :



Study on a regeneration interval (Strong Markov property)

Oniqueness by harmonic functions



Proof 3 : Coupling

Let $\{X_n\}_{n\in\mathbb{N}}$ a homogeneous aperiodic and irreducible Markov chain with initial law $\pi(0)$ and steady-state probability π . Let $\{\tilde{X}_n\}_{n\in\mathbb{N}}$ another Markov chain $\tilde{\pi}(0)$ with the same transition matrix as $\{X_n\}$ $\{X_n\}$ et $\{\tilde{X}_n\}$ independent $Z_n = (X_n, \tilde{X}_n)$ is a homogeneous Markov chain - if $\{X_n\}$ is aperiodic and irreducible, so it is for Z_n Let τ be the hitting time of the diagonal, $\tau < \infty$ P-a.s. then

$$|\mathbb{P}(X_n = i) - \mathbb{P}(\tilde{X}_n = i)| < 2\mathbb{P}(\tau > n)$$

 $|\mathbb{P}(X_n = i) - \pi(i)| < 2\mathbb{P}(\tau > n) \longrightarrow 0.$



Ergodic Theorem

Let $\{X_n\}_{n \in \mathbb{N}}$ a homogeneous aperiodic and irreducible Markov chain on \mathcal{X} with steady-state probability π then

- for all function f satisfying $\mathbb{E}_{\pi}|f| < +\infty$

$$\frac{1}{N}\sum_{n=1}^{N}f(X_n)\stackrel{P-\rho.s.}{\longrightarrow}\mathbb{E}_{\pi}f.$$

generalization of the strong law of large numbers

- If $\mathbb{E}_{\pi} f = 0$ then there exist σ such that

$$\frac{1}{\sigma\sqrt{N}}\sum_{n=1}^{N}f(X_n)\overset{\mathcal{L}}{\longrightarrow}\mathcal{N}(0,1).$$

generalization of the central limit theorem



Cache modeling

Synthesis

Fundamental question

Given a function f (cost, reward, performance,...) estimate $\mathbb{E}_{\pi}f$ and give the quality of this estimation.



Solving methods

Solving $\pi = \pi P$

- Analytical/approximation methods
- Formal methods N ≤ 50 Maple, Sage,...
- Direct numerical methods N ≤ 1000 Mathematica, Scilab,...
- Iterative methods with preconditioning $N \leq 100,000$ Marca,...
- Adapted methods (structured Markov chains) $N \leq 1,000,000$ PEPS,...
- Monte-Carlo simulation $N \ge 10^7$

Postprocessing of the stationary distribution

Computation of rewards (expected stationary functions) Utilization, response time,...



Synthesis

Ergodic Sampling(1)

Ergodic sampling algorithm

Representation : transition fonction

$$X_{n+1} = \Phi(X_n, e_{n+1}).$$

```
x \leftarrow x_0
{choice of the initial state at time =0}
n = 0;
repeat
n \leftarrow n + 1;
e \leftarrow Random\_event();
x \leftarrow \Phi(x, e);
Store x
{computation of the next state X_{n+1}}
until some empirical criteria
return the trajectory
```

Problem : Stopping criteria



Ergodic Sampling(2)

Start-up

Convergence to stationary behavior

 $\lim_{n\to+\infty}\mathbb{P}(X_n=x)=\pi_x.$

Warm-up period : Avoid initial state dependence Estimation error :

 $||\mathbb{P}(X_n = x) - \pi_x|| \leq C\lambda_2^n.$

 λ_2 second greatest eigenvalue of the transition matrix

- bounds on C and λ_2 (spectral gap)
- cut-off phenomena

 λ_2 and *C* non reachable in practice (complexity equivalent to the computation of π) some known results (Birth and Death processes)



Ergodic Sampling(3)

Estimation quality

Ergodic theorem :

$$\lim_{n\to+\infty}\frac{1}{n}\sum_{i=1}^n f(X_i)=\mathbb{E}_{\pi}f.$$

Length of the sampling : Error control (CLT theorem)

Complexity

Complexity of the transition function evaluation (computation of $\Phi(x, .)$) Related to the stabilization period + Estimation time



Ergodic sampling(4)



Synthesis

Replication Method



Sample of independent states Drawback : length of the replication period (dependence from initial state)



Regeneration Method



Sample of independent trajectories Drawback : length of the regeneration period (choice of the regenerative state)





Synthesis





- Pormalisation
- 3 Long run behavior
- Cache modeling
- 5 Synthesis



Cache modelling

Virtual memory

Paging in OS



Move-to-front strategy

Least		used	(\mathbf{R})
	Coontry		

Move-ahead strategy

Ranking algorithm

State of the system : Page position

data caches (databases)
 proxy-web (internet)
 routing tables (networking)

Huge number of pages, small memory capacity

Problem

Performance : mean response time (memory access << disk access Choose the strategy that achieves the best long-term performance



Cache modelling

Virtual memory

Paging in OS



Move-to-front strategy

Least recently used (LRU)

		Virtual memory									
		Memory	y	Disque							
Adress	1	2	3	4	5	6	7	8	State		
Pages	P ₃	P7	P2	P ₆	P5	P ₁	P ₈	P_4	Е		
Pages	P ₅	P3	P ₇	P ₂	P_6	P ₁	P ₈	P_4	E ₁		

Move-ahead strategy

- cache hierarchy (processor)

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State of the system

N = number of pages State = permutation of $\{1, \dots, N\}$ Size of the state space = N! \implies numerically untractable

Example : Linux system

- Size of page = 4kb

```
    Memory size = 1 Gb
```

```
- Swap disk size = 1 Gb
```

Size of the state space = 500000! exercise : compute the orde of magnitude

Flow modelling

Requests are random Request have the same probability distributions Requests are stochastically independent $\{R_n\}_{n \in \mathbb{N}}$ random sequence of i.i.d. requests

State space reduction

 P_A = More frequent page All other pages have the same frequency

$$a = \mathbb{P}(R_n = P_A), \ b = \mathbb{P}(R_n = P_i),$$

a > b, a + (N - 1)b = 1.

 ${X_n}_{n \in \mathbb{N}}$ position of page P_A at time n. State space = $\{1, \dots, N\}$ (size reduction) Markov chain (state dependent policy)



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1 1 6
Move to front analysis

Markov chain graph



I G

Move to front analysis

Markov chain graph



Tran	sitio	on matri	x	Example			
	a 	(N - 1)b b 0 0	0 (N - 2)b 2b 	 (N - 3)b 	 	0	N = 8, a = 0.3 and b = 0.1 $\pi = \begin{bmatrix} 0.30 \\ 0.23 \\ 0.18 \\ 0.12 \\ 0.08 \\ 0.05 \\ 0.03 \\ 0.01 \end{bmatrix}.$

LIG

Move to front analysis

Markov chain graph



$\begin{bmatrix} a & (N-1)b & 0 & \ddots \\ a & b & (N-2)b & \ddots \\ \vdots & 0 & 2b & (N-2)b & 0 \\ \vdots & \vdots & \ddots & 0 \\ \vdots & \vdots & \ddots & 0 \end{bmatrix}$		0 1
: : ·	- 3)b · · · · · · · · · · · · · · · · · · ·	$ {}^{\circ} N = 8, a = 0.3 \text{ and } b = 0.1 $
 	$ (N-2)b \\ 0 (N)$	b - 1)b

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Move ahead analysis





Move ahead analysis



Τ	Transition matrix								
ſ	a + (N - 2)b	b	0			0	1		
	а	(N - 2)b	b	·.		:			
	0	а	(N - 2)b	b	·.	÷			
	÷	·.	·.	·.	·.	0			
	0	0	·. 	·. 0	(N — 2)b a	b (N - 1)b			

Example V = 8, a = 0.3 and b = 0.1 $\pi = \begin{bmatrix} 0.67 \\ 0.22 \\ 0.07 \\ 0.02 \\ 0.01 \\ 0.01 \end{bmatrix}.$



Move ahead analysis



Transition r	matrix						
	The contract of the contract o						Example
$\begin{bmatrix} a+(N-2)b \end{bmatrix}$	b	0			[٥		N = 8, $a = 0.3$ and $b = 0.1$
а	(N - 2)b	b	·.		:		г 0.67 т
0	а	(N – 2)b	b	·	:		0.22 0.07
÷	·.	·.	·.	·.	0	ĺ	$\pi = \begin{bmatrix} 0.02 \\ 0.01 \\ 0.01 \end{bmatrix} .$
:	:	·.	•.	(N – 2)b	b		
L O	0		0	а	(N – 1)b]		



Performances

Steady state

$$MF = \begin{bmatrix} 0.30 \\ 0.23 \\ 0.18 \\ 0.08 \\ 0.05 \\ 0.03 \\ 0.01 \end{bmatrix} MA = \begin{bmatrix} 0.67 \\ 0.22 \\ 0.07 \\ 0.02 \\ 0.01 \\ 0.00 \\ 0.00 \\ 0.00 \end{bmatrix}.$$

Move to front

$$\pi(i) = \frac{(N-1-i)\cdots(N-2)(N-1)b^{i-1}}{(a+(N-i)b)\cdots(a+(N-2)b)(a+(N-1)b)}\pi_1.$$

Move ahead

$$\pi_i = (\frac{b}{a})^{i-1} \frac{1 - \frac{b}{a}}{1 - (\frac{b}{a})^N}$$

Comments

Self-ordering protocol : decreasing probability Convergence speed to steady state : Move to front : 0.7" Move ahead : 0.92" Tradeoff between "stabilization" and long term performance Depends on the input flow of requests

Cache miss



Performances

Steady state



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0	1.00	1.00
1	0.70	0.33
2	0.47	0.11
3	0.28	0.04
4	0.17	0.02
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Performances

Steady state



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Synthesis

Outline



- Pormalisation
- **3** Long run behavior
- Cache modeling





Synthesis : Modelling and Performance

Methodology

- Identify states of the system
- ② Estimate transition parameters, build the Markov chain (verify properties)
- Specify performances as a function of steady-state
- Compute steady-state distribution and steady-state performance
- Analyse performances as a function of input parameters

Classical methods to compute the steady state

- Analytical formulae : structure of the Markov chain (closed form)
- 2 Formal computation (N < 50)
- I Direct numerical computation (classical linear algebra kernels) (N < 1000)
- Iterative numerical computation (classical linear algebra kernels) (N < 100.000)
- Model adapted numerical computation (N < 10.000.000)</p>
- Simulation of random trajectories (sampling)



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