A Monte Carlo method to compute principal eigenelements of some linear operators

Organization of the talk

1. Introduction

2. homogeneous neutron transport operators

3. Inhomogeneous operators

4. Laplace operator

5. Variance reduction + eigenfunction

The Monte Carlo method

Numerical computation of $A = E(X)$

X random variable, X_i samples of X

Monte Carlo method: law of large numbers

$$A \simeq \frac{1}{N} \sum_{i=1}^{N} X_i$$

Central-limit theorem: confidence interval

$$\frac{1}{N} \sum_{i=1}^{N} X_i - a\frac{\sigma_X}{\sqrt{N}} \leq E(X) \leq \frac{1}{N} \sum_{i=1}^{N} X_i + a\frac{\sigma_X}{\sqrt{N}}$$

Speed of convergence: $\frac{\sigma_X}{\sqrt{N}}$

Cauchy problem in a domain D

$$\frac{\partial u}{\partial t} = Lu$$

Neutron transport: sign of the principal eigenvalue α_1 determins whether the system is subcritical or supercritical.

Diffusions operators : speed of convergence towards the steady state.

Numerical computation of α_1 by deterministic methods: discretization of L in many dimensions + power method.

Spectral expansion in $L^1(D)$

$$u(x,v,t) = D_0 e^{\alpha_1 t} + D_1 e^{\alpha_2 t} + ... + D_k e^{\alpha_k t} + o(e^{\alpha_k t})$$

α_0 real and simple, D_0 independent of t

Neutron transport: Mika (1968), Vidav (1971)

Leading terms $E \subset D$

$$\frac{1}{t} \log(\int_E u(x,v,t) dxdv) \simeq \frac{1}{t} \log(C_0 e^{\alpha_1 t} + C_1 e^{\alpha_2 t})$$

Stochastic representation

$$\lim_{t\to\infty} \frac{1}{t} \log(\int_E u(x,v,t) dxdv) = \alpha_1$$

Approximation model

$$\frac{1}{t} \log(\int_E u(x,v,t) dxdv) \simeq \alpha_1 + \frac{\log(C_0)}{t} + \frac{C_1}{C_0} \frac{e^{(\alpha_2 - \alpha_1)t}}{t}.$$

Monte Carlo estimators of α_1

Approximation model

$$\frac{1}{t}\log\left(\int_E u(x,t)dx\right) \simeq \alpha_1 + \frac{\log(C_0)}{t} + \frac{C_1}{C_0}\frac{e^{(\alpha_2-\alpha_1)t}}{t}$$

Interpolation method

$$\alpha_1(t_1,t_2) = \frac{\log(\int_E u(x,t_2)dx) - \log(\int_E u(x,t_1)dx)}{t_2 - t_1}$$

Linear least square problem

$$\sum_{i=p}^{q}\left(\alpha_1 + \frac{\beta}{t_i} - \frac{1}{t_i}\log\left(\int_E u(x,v,t_i)dx\right)\right)^2$$

Optimization and variance reduction tools

Maire, Talay IMAJNA(06), Lejay, Maire MCS(07)

Neutron transport equations

Cauchy problem in $A \times V \subset \Re^3 \times \Re^3$

$$\frac{\partial u}{\partial t}(x, v, t) = Tu(x, v, t)$$

Neutron transport operator T

$$Tu(x, v, t) = -v\nabla_x u(x, v, t) - \Sigma(x, v)u(x, v, t) + \int_V f(x, z, v)u(x, z, t)dz + s(x, v, t)$$

$u(x, v, t)$ density of neutrons

Initial condition $u(x, v, 0) = u_0(x, v)$

Boundary conditions

Heterogeneous problem in dimension 7

Criticality problem

Sources come from fission

$$T_\lambda u(x,v,t) = -v\nabla_x u(x,v,t) - \Sigma(x,v)u(x,v,t) + \int_V f_r(x,z,v)u(x,z,t)dz + \frac{1}{\lambda}\int_V f_f(x,z,v)u(x,z,t)dz$$

$v.\nabla u$: loss of neutrons by transport

Σu : loss of neutrons by collisions

$\int_V f_r u dz$: sources from slowing

$\frac{1}{\lambda}\int_V f_f u dz$: source from fission

Criticality : find λ such that the principal eigenvalue α_λ of the operator T_λ is zero

Neutron transport operators

Cauchy problem in $A \times V$

$$\frac{\partial u\,(x,y,t)}{\partial t} = b\,(x,y)\,\nabla_x u\,(x,y,t) + c\,(x,y)\,u\,(x,y,t) + \gamma\,(x,y)\left[\int_V u\,(x,z,t)\,\Pi^{x,y}\,(dz) - u\,(x,y,t)\right]$$

Feynman-Kac representation of $u(x,y,t)$

$$E_{x,y}\left[1_{\tau_A^{x,y}>t}\,u_0\,(X_t,Y_t)\exp\left(\int_0^t c\,(X_s,Y_s)\,ds\right)\right]$$

$\tau_A^{x,y}$ exit time from A

Y_t jump process on V

X_t is solution of $\frac{dX_t}{dt} = b(X_t,Y_t)$

Exact simulation schemes

The model of Lehner and Wing

$$\frac{\partial u}{\partial t} = -v\frac{\partial u}{\partial x} + c\left\{\frac{1}{2}\int_{-1}^{1} u(x,v',t)dv' - u(x,v,t)\right\} + (c-1)\,u(x,v,t)$$

Stochastic representation of $u(x,v,t)$

$$E_{x,v}\left[u_0\left(X_t, Y_t\right)\exp\left(\int_0^t (c-1)\,ds\right)1_{t<\sigma_D^{x,v}}\right]$$

$\sigma_D^{x,v}$: exit time from $D = [0, A]$

$\frac{dX_t}{dt} = -Y_t$; $X_0 = x$ and $Y_0 = v$.

Velocity at collision uniform law on $[-1, 1]$.

Time between two collisions

$$F^{x,v}(t) = 1 - \exp\left[-\int_0^t cds\right] = 1 - \exp\left(-ct\right)$$

Choice of u_0 : $u_0(x, v) \equiv 1$

$$u(x, v, t) = P_{x,v}(\sigma_D^{x,v} > t) \exp(c - 1)t$$

$$\int_E u(x, v, t)dxdv = \exp(c-1)t \int_E P_{x,v}(\sigma_D^{x,v} > t)dxdv$$

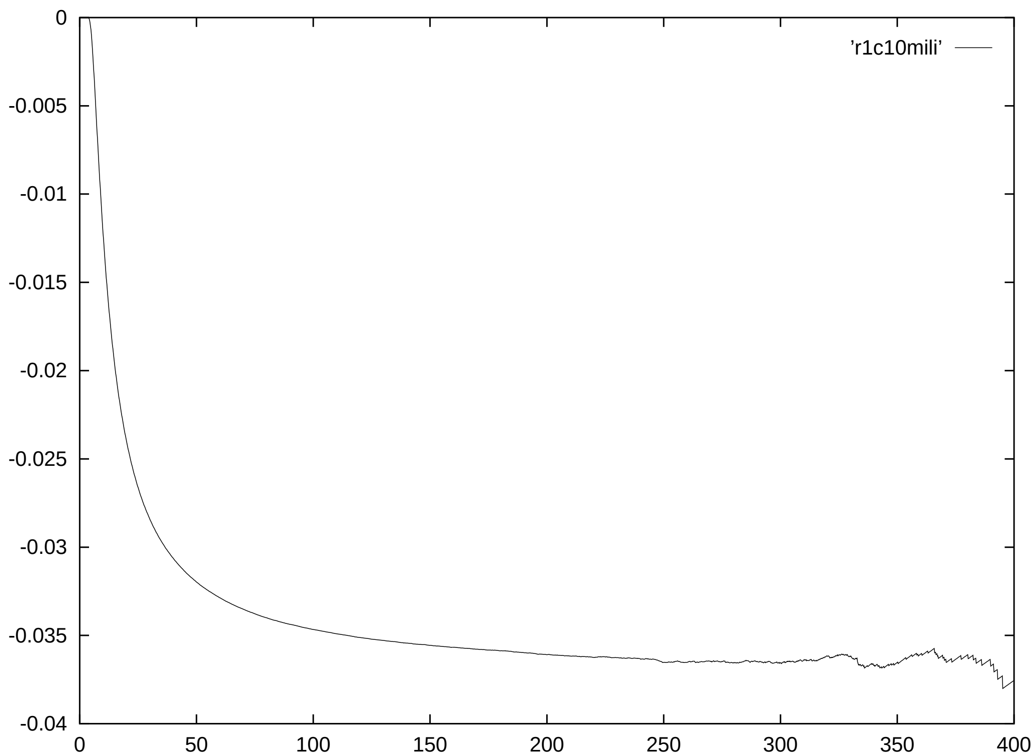
Monte-Carlo Approximation

$$\int_E P_{x,v}(\sigma_D^{x,v} > t)dxdv \simeq \frac{vol(E)N(t)}{N}$$

$N(t)$ number of trajectories still alive at time t among N starting from a random uniform point in E.

$$\frac{1}{t} \log(\int_E u(x, v, t)dxdv) \approx c - 1 + \frac{1}{t} \log(\frac{N(t)}{N})$$

Naive approximation of α_0



$\frac{1}{t}\log(\frac{N(t)}{N})$ as a function of time t.

10 millions of simulations, $A = 8$

Variance increases as t increases

Rare events simulations

Approximation of α_0 using interpolation

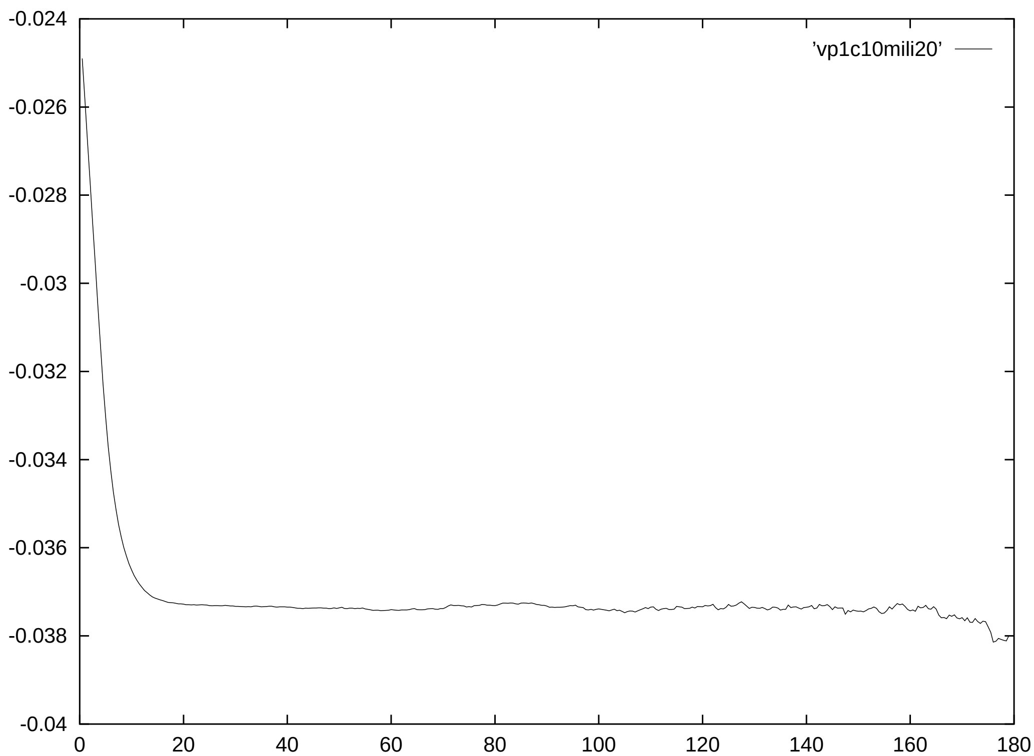
$$c - 1 + \frac{1}{t_1} \log(\frac{N(t_1)}{N}) \simeq \alpha_0 + \frac{\log(K_0)}{t_1}$$

$$c - 1 + \frac{1}{t_2} \log(\frac{N(t_2)}{N}) \simeq \alpha_0 + \frac{\log(K_0)}{t_2}$$

$$\alpha_0(t_1, t_2) = c - 1 + \frac{\log(\frac{N(t_2)}{N}) - \log(\frac{N(t_1)}{N})}{t_2 - t_1}.$$

Confidence interval for $\alpha_0(t_1, t_2)$

Approximation using interpolation



$\alpha_0(t_1, t_1 + 20) - c + 1$ as a function of t_1.

10 millions of simulations

Approximation stable and accurate

Criticality computation

$c = 1.036$

t_1	binf	$\alpha_0 min(t_1, t_2)$	bsup
50	-4.28 10^{-4}	-4.12*10^{-4}	-3.94 10^{-4}
55	-4.28 10^{-4}	-4.13*10^{-4}	-3.94 10^{-4}
60	-4.28 10^{-4}	-4.16*10^{-4}	-3.96 10^{-4}

$c = 1.037$

t_1	binf	$\alpha_0 max(t_1, t_2)$	bsup
50	6.05 10^{-4}	6.22 10^{-4}	6.38 10^{-4}
55	6.02 10^{-4}	6.21 10^{-4}	6.39 10^{-4}
60	5.9 10^{-4}	6.19 10^{-4}	6.4 10^{-4}

Secant method gives c_c

$$c_c = cmin - \alpha min \frac{cmax - cmin}{\alpha max - \alpha min} = 1.036399$$

Error : 10^{-5} on c_c. Dahl-Sjostrand (1978).

Least square approximation

Find α_0 and $\beta = \log(K_0)$ minimizing

$$\sum_{i=p}^{q} (\alpha_0 + \frac{\beta}{t_i} - \frac{1}{t_i} \log(\int_E u(x, v, t_i) dx dv))^2.$$

Linear least square problem

Improvement of the accuracy

Other inhomogeneous problems

Anisotropic problem

$$\frac{\partial t}{\partial u} = -v\frac{\partial u}{\partial x} + (c-1)u + \frac{c}{2}\int_V (1+3\mu v v')u(x,v',t)dv'.$$

$\Rightarrow$ Change the law of the velocity

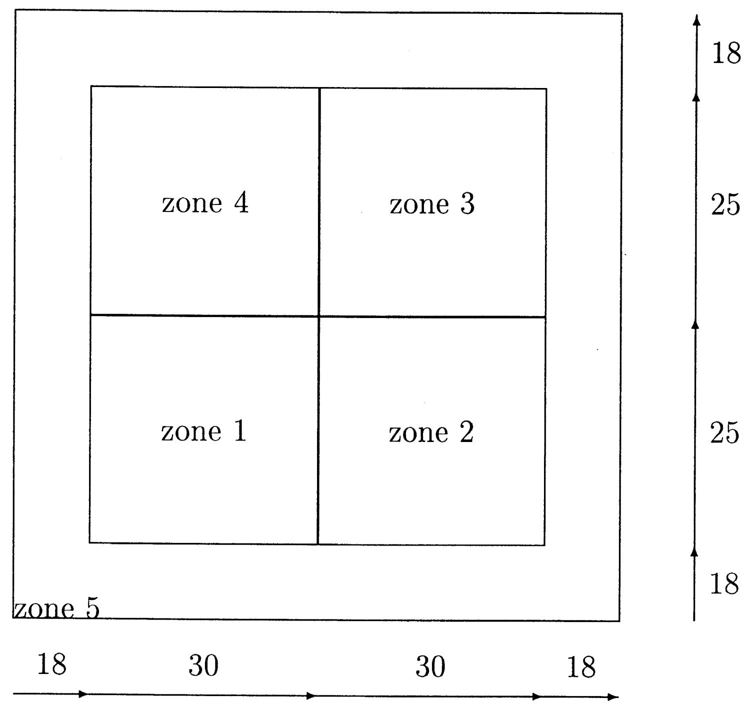
$$f(v') = \left(\frac{1+3\mu v v'}{2}\right)$$

Dimension 3 : Case of a sphere

$$\frac{\partial u(x,v,t)}{\partial t} = -v\nabla_x u(x,v,t) + (c-1)u(x,v,t) + \\ c\left(\frac{1}{4\pi}\int_{S_2} u(x,z_1,t)dz_1 - u(x,z,t)\right)$$

Same accuracy

Inhomogeneous cases



Zone 1 and 3 : splitting zones

Zone 2 and 4 : very absorbing zones

Zone 5 : absorbing zone

Additional difficulties

$$u(x,y,t) = E_{x,y}\left[1_{\sigma_A^{x,y}>t} u_0\left(X_t, Y_t\right) \exp\left(\int_0^t c\left(X_s, Y_s\right) ds\right)\right]$$

1. Following the motion precisely

2. Computation of u at differents times

3. Handle change of zones

4. Initial condition u_0 chosen using another numerical method

5. Computation of u on the most splitting zone

Laplace operator with Dirichlet conditions

Cauchy problem in D

$$\frac{\partial u\,(x,t)}{\partial t} = \frac{1}{2}\triangle u$$

Feynman-Kac representation of $u(x,t)$

$$E_x\left[1_{\tau_D > t} u_0\,(B_t)\right]$$

If $u_0(x) \equiv 1$ then

$$u(x,t) = P_x(\tau_D > t)$$

τ_D^x : exit time from D of B_t

Simulation schemes: Euler Scheme with or without boundary correction, walk on spheres or rectangles

Homogeneous transport or Laplace operator

Branching method to compute $P_x(\tau_D > T)$

Cutting time to reach into slices

Markov property

$$P_x\,(\tau_D > T) = P_x\,(\tau_D > T_1)\,P_{\pi_{T_1}}\,(\tau_D > T - T_1)$$

Particular approximation of π_{T_1}

Law of X_t assuming that $\tau_D > t$

$$E_x[u_0(X_t)/\tau_D > t] = \frac{E_x[u_0(X_t);\tau_D > t]}{E_x[1;\tau_D > t]} \longrightarrow \frac{< u_0, \varphi_1^* >}{< 1, \varphi_1^* >}$$

for t large , we obtain $\frac{\varphi_1^*}{<1,\varphi_1^*>}$

Variance reduction + eigenfunction

Conclusion

Good accuracy on the principal eigenvalue on many test-cases.

Method well adapted to high dimensions

Sensitive to the simulation schemes

Approximation of the principal eigenfunction in the case of the Laplace operator

Stochastic representation of the principal eigenvalue for some homogeneous transport operator.

Computation of the second leading eigenvalue?