Monte-Carlo Methods for transport problems and kinetic equations

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Introduction

Principle of the classical MC method for transport problems. + (Probabilist Interpretation)

Limit of the method (transport problem in collisonal media)

Symbolic Monte-Carlo Method

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1 Introduction

$$\text{Evaluation of } I = \int f(x)p(x)dx$$

According to the law of large numbers

$$I = \mathbf{E}(f(X)) \simeq \frac{1}{N} \sum_{j=1,N} f(X_j)$$

X_i are realizations of the r. v. X whose law is p.

Particle technique

Representation of a function $u(t,x)$ by particles

$$u(t,x)dx \simeq \sum_j w_j \delta_{X_j(t)}(dx)$$

Toy problem .

let g probability density and $u = u(t,z)$ verifying

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial z}.(\overrightarrow{B} u) = 0, \qquad u(0,.) \ = \ g, \qquad +\text{boundary cond } u = 0, (\overrightarrow{B}(z).\overrightarrow{n}_z > 0) \tag{1}$$

$$\text{Evaluation of } M = \int \phi(z) u(t,z) dz \qquad \text{for } \phi \text{ indicatrix f.}$$

define the flow Z_t^z

$$\frac{d}{dt} Z_t^z = \overrightarrow{B}(Z_t^z), \qquad Z_{t=0}^z = z$$

Denote $\mathcal{Z}_t$ the r.p. $\frac{d}{dt}\mathcal{Z}_t = \overrightarrow{B}(\mathcal{Z}_t)$, whose law $\mathcal{Z}_{t=0}$ is $g(.)dz$

Proposition. (proba. interpretation) For T positive :

$$\int \phi(z) u(T,z) dz = \int g(z) \phi(Z_T^z) dz = \mathbf{E}_g \left(\phi(\mathcal{Z}_T) \right)$$

Proof. Let φ verifying :

$$-\frac{\partial \varphi}{\partial t} - \overrightarrow{B}.\frac{\partial \varphi}{\partial z} = 0, \qquad \varphi(T) = \phi, \qquad \text{then : } \frac{\partial}{\partial t}\left(\varphi(t, Z_t^z)\right) = 0. \qquad \text{But } \frac{\partial}{\partial t}(\int \varphi(t) u(t)) = 0$$

2 Principle of the classical MC method: Proba. Interpretation

■Evolution transport equations

$$\frac{\partial u}{\partial t} + v.\frac{\partial u}{\partial x} + ru - Ku = 0, \quad (2)$$
$$u(0,.) = G$$
$$u|_{\partial\mathcal{D}}(x,v) = h(x,v), \qquad v \in Z_x^+ = \{v.n_x > 0\} \quad (3)$$

where K is conservative (collision operator)

$$Ku(x,v) = \int_{\mathcal{V}} \sigma_x(v')\, k_x(v',v)\, u(x,v')\ dv' \ - \sigma_x(v)\, u(x,v)$$

such that $\int k(v',v)dv = 1$.

Set of velocity $\mathcal{V}$ provided with dv s.t. $\int_{\mathcal{V}} dv = 1$

■ Stationary transport equations .

Let $u = u(x, v)$ be solution of

$$\begin{aligned} v.\nabla u + ru - Ku &= f \\ u|_{\partial \mathcal{D}}(x, v) &= h(x, v), \qquad \forall v \in Z_x^+ \end{aligned}$$

■Evolution equations (2)

$$u \longmapsto (v.\frac{\partial}{\partial x} - K)u \qquad \text{is associated to the processus } X(t),\ V(t)$$

characterized by:

•Between the jump of V :

$$\frac{\partial}{\partial t}X(t) = V(t), \qquad V \text{ constant}$$

• The stopping time η is such that

$$P\left(\eta \in [t, t+dt]\right) = \mathrm{e}^{-\sigma(X,V)t}\sigma(X,V)\, dt$$

• At this stopping time η, the velocity jump from $V(\eta-)$ to $V(\eta)$

according to prob. law $\quad k(X(\eta), V(\eta_{-}), w)\, dw$

Remark :

$$\sigma^{-1} \qquad \text{m. f. time,} \qquad v\sigma^{-1} \qquad \text{m. f. p.}$$

Proposition (probabilist interpretation).

$$\text{Assume that } g \geq 0, \qquad \int_D \int_{\mathcal{V}} g(x,v) dx dv = 1$$

For any test fonction $\varphi \in C_b(\mathcal{D} \times \mathcal{V})$,

$$\begin{aligned} \ll \; & u(t,.)\varphi \gg = \int \int_{\mathcal{D}\mathcal{V}} u(t,x,v)\varphi(x,v)\, dx\, dv = \\ = \; & E_g \left[\varphi(X(t), V(t)) \ \mathrm{exp}(- \int_0^t r(X,V)\, d\zeta) \right] \end{aligned}$$

$E_g =$ expectation knowing the law of $(X(0), V(0))$ is $g(,)dxdv$.

2.1 Principle of the method

■Pb without boundary conditions

* Generation of N processes, ind. equid. : $(X_p, V_p), p = 1, ..., N$.

knowing that

$$\frac{\partial}{\partial t} X_p = V_p, \quad V_p \text{ jump process}$$

$$\text{at time } t = 0, \qquad (X_p, V_p) \text{ distribu a. to } g$$

* Initialization of the weights w_p^0 s.t. in D

$$\sum_{p=1}^{N} w_p^0 = 1, \qquad \sup |w_p^0| \to 0$$

* Each weight solves

$$\frac{\partial}{\partial t} w_p + w_p r(X_p, V_p) = 0.$$

■ **Corollary**. $N \to \infty$, we get

$$\Phi^N(t) = \sum_{p=1,..N} w_p(t) \quad \delta_{X_p(t)}(dx) \quad \delta_{V_p(t)}(dv)$$

$$\ll \Phi^N(t)\varphi \gg \quad \to \quad \ll u(t,.)\varphi \gg$$

2.2 Implentation of the method.

* Discretization into sub-domains D' such that the coef. are constant

* In each sub-domain D' , initialize the weights w_p^0 s.t.

$$\sum_{p/X_p \in D'} w_p^0 = \int_{D'} \int_{\mathcal{V}} g(x,v)dxdv$$

$$X_p(0), V_p(0) \text{ generated a. to } \qquad g(.,.)|_{D'}$$

* Tracking of the particles.

$$\begin{aligned} \frac{\partial}{\partial t} X_p &= V_p, \\ & V_p \text{ jump process} \end{aligned}$$

* Compute the outgoing time τ_p out of D' and the collision time η_p.

If $\eta_p < \tau_p$, velocity jumps a. to the law k.

* The weight varies a. to

$$\frac{\partial}{\partial t} w_p + w_p r(X_p, V_p) = 0.$$

* Tally of the weights of the particles and evaluate at final time

$$w_p(t)\varphi(X_p(t), V_p(t))$$

.Boundary condition.

Assume V with spherical symmetry

Consider transport equation with h independent of v.

Particles are generated on each face Γ of the boundary in the half-sphere

$$Z^{+} = v \qquad / \; v.n_{\Gamma} > 0$$

s. t. the prob. law of $\Omega = v/|v|$ is :

$$\frac{1}{\int_{Z^{+}} \Omega'.n_{\Gamma} d\Omega'} \Omega.n_{\Gamma} d\Omega$$

i.e. for $\mu = \Omega.n_{\Gamma}$ on $[0, 1]$, the prob. law is (Lambert law)

$$2\mu d\mu.$$

the azymutal angle is equidistributed.

For a general function $h(\mu)$, the proba. law is $\mu h(\mu)$ for each particle.

3 Limit of the method

Monte-Carlo algorithms are non efficient if

$$\lambda = \frac{\overline{|v|}}{\overline{\sigma}} \ll L_{char}, \qquad L_{char} \text{ char. length}, \qquad \overline{\sigma} \text{ char. value}$$

The Monte-Carlo method becomes prohibitive (to much jumps in each cell)

Then diffusion approximation is necessary

Hypothesis: k is symmetric, V spherical symmetry and

$$\varepsilon = \lambda / L_{char}, \qquad r \ll \sigma, \quad r = \varepsilon r_0,$$

$$Ku = \sigma(x) Mu, \qquad \sigma = \frac{\sigma_0}{\varepsilon} \qquad Mu(v) = \int_{\mathcal{V}} k(v', v) u(v') dv' - u(v)$$

$$\widetilde{\bullet} = \int_{\mathcal{V}} \bullet(v) dv$$

Let u_ε be the solution of

$$\begin{aligned} v.\nabla u_\varepsilon + \varepsilon r_0 u_\varepsilon - \frac{\sigma_0}{\varepsilon} M u_\varepsilon &= \varepsilon f_0 \\ u_\varepsilon|_{\partial\mathcal{D}}(x,v) &= h_x(v), \qquad \forall v \in Z_x \end{aligned}$$

Theorem (classical result ~1960)

If $h(x,.)$ independent of v ; when $\varepsilon \to 0$, we get $u_\varepsilon(x,v) \to U(x)$ where

$$r_0 U - \nabla.(\frac{1}{3\sigma_0}\nabla U) = \widetilde{f_0}\ , \qquad \text{with boundary cond. } U(x)|_\Gamma = h_x$$

So the behavior of the solution of (2) is like a diffusion one.

Remark. If $h(x,.)$ depends on v, there exists boundary layers (Chandrasekhar)

Transport problem in a zoom region near a boundary point x_b. (V is the sphere, $\mu = v.n_{x_b}$).

$$\text{Set } \ y = \frac{x - x_b}{\varepsilon}.n_{x_b} \text{ and } \ u_\varepsilon(x) = U_0(x) + \phi_{x_b}(\frac{x-x_b}{\varepsilon}.n_{x_b}, \mu) + \varepsilon u_1 + \varepsilon^2 u_2 + ...$$

ϕ is a boundary layer, solution to a transport equation.

Theorem (G. Papanicolaou ~1975, R.S. 1981).

The solution u_ε satisfies $u_\varepsilon(x,v) \simeq U(x)$

$$r_0 U - \nabla.(\frac{1}{3\sigma_0}\nabla U) = \widetilde{f}_0 \ , \qquad \text{with boundary cond. } U(x)|_\Gamma = C(h_x)$$

where the operator C is defined by the way. Let $\psi(y,\mu)$ be the unique bounded solution of

$$\begin{aligned} \mu\frac{\partial}{\partial y}\psi - M\psi &= 0 \qquad \text{with } y \in [0,+\infty] \\ \psi(0,\mu) &= g(\mu), \text{ on } Z^+ \end{aligned} \tag{4}$$

then there exists a fonction H (Chandrasekhar) such that

$$\lim_{y\to\infty} \psi(y,\mu) = C(g) = \int_0^1 g(\mu)H(\mu)\mu\frac{d\mu}{2}. \ \blacksquare$$

4 The symbolic Monte-Carlo method

Stationary problem with $r > 0$. ($q = \sigma + r$)

$$\begin{aligned} \Omega.\nabla u + qu &= \sigma \widetilde{u} \\ u(x,\Omega) &= h, \text{ on } Z^+. \end{aligned}$$

Denote now $v = v(x,\Omega)$, the solution

$$\begin{aligned} \Omega.\nabla v + qv &= 0 \\ v(x,\Omega) &= h, \text{ on } Z^+ \end{aligned}$$

For each cell C_j, denote ζ_j the solutions

$$\begin{aligned} \Omega.\nabla \zeta_j + q\zeta_j &= q\mathbf{1}_{C_j} \\ \zeta_j &= 0 \text{ on } Z^+ \end{aligned} \tag{5}$$

We introduce the coefficients M_{kj},

$$M_{kj} = \int_{C_k} \sigma_k \widetilde{\zeta}_j(x) \frac{dx}{|C_k|}$$

and the data

$$V_k = \int_{C_k} \widetilde{v}(x) \frac{dx}{|C_k|}$$

We can check that

$$\boldsymbol{\Sigma}_j M_{kj} \leq \sigma_k \tag{6}$$

Proposition.

The linear system

$$q_k \phi_k - \sum_j M_{kj} \phi_j = \sigma_k V_k$$

has a unique solution (ϕ_j). If we set

$$\eta(x, \Omega) = \sum_k \zeta_k(x, \Omega)\phi_k$$

then $v + \eta$ is a good approximation of u, when δx tends to 0.

Sketch of the proof

The matrix of the linear system is diagonal dominent.

Since the V_j are positive, the solution (ϕ_j) exits, is positive.

. η is solution to

$$\begin{aligned} \mathbf{\Omega}.\nabla\eta + q\eta &= \sum_k \mathbf{1}_{C_k} q\phi_k \\ \eta &= 0 \text{ on } Z^+ \end{aligned}$$

According to the definition of $\phi_.$, we get

$$\sum_k \mathbf{1}_{C_k} q\phi_k = \sum_k \mathbf{1}_{C_k}\sigma_k V_k + \sum_k\sum_j \mathbf{1}_{C_k}\sigma_k \int_{C_k} \widetilde{\zeta}_j(x)\frac{dx}{|C_k|}\phi_j = \sum_k \mathbf{1}_{C_k}\sigma_k \int_{C_k} (\widetilde{v}+\widetilde{\eta})(x)\frac{dx}{|C_k|}$$

Thus $\qquad (\mathbf{\Omega}.\nabla + q)(v+\eta) = \sum_k \mathbf{1}_{C_k}\sigma_k \int_{C_k} (\widetilde{v+\eta})(x)\frac{dx}{|C_k|}. \qquad \Box$

Remark : $\displaystyle\int_{\partial C_k} \widetilde{\zeta_j\mathbf{\Omega}}.\mathbf{n}d\gamma(x) = q_k \int_{C_k} \widetilde{\zeta}_j dx, \qquad \Rightarrow M_{kj}|C_k| = \frac{\sigma_k}{q_k}\int_{\partial C_k} \widetilde{\zeta_j\mathbf{\Omega}}.\mathbf{n}d\gamma(x)$

this corresponds to the particles born in C_j , absorbed in cell C_k.

Numerical method .

1. Free fly. We first generate particles on the boundary

Track them according to a free fly technique (without coll.)

2. Evaluation of the coefficients $M_{..}$

For each C_j, generate particles (X_p, Ω_p) such that their weights w_p^0

$$\sum_p w_p^0 = |C_j| q_j$$

Track these particles according to free fly without collisions

Estimation of M_{kj} by using the flux on the boundary of C_k

$$M_{kj}|C_k| = \frac{\sigma_k}{q_k} \sum_{p,\text{born in } j} \left(w_{p,C_k}^{in} - w_{p,C_k}^{out} \right) \tag{7}$$

w_{p,C_k}^{in} and w_{p,C_k}^{out} = weights of p when it goes in and out C_k. Thus (6) holds.

3. Finaly, we solve the linear system

$$q_k \phi_k - \sum_j M_{kj} \phi_j = \sigma_k V_k$$

The method is very adaptable. Example of generalization

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\begin{aligned}
\Omega.\nabla u + ru + \sigma(u - \widetilde{u}) + \tau u &= \tau\theta \\
u(x, \Omega) &= h, \text{ on } Z^+. \\
\frac{\partial}{\partial t}\theta + \tau\theta - \tau\widetilde{u} - \nabla(\lambda\nabla\theta) &= 0. \\
& \quad +B.C \text{ for } \theta
\end{aligned}
$$

5 Conclusion

The Monte Carlo method are very adaptable, powerfull

but are prohibitive in collisional domain.

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The Symbolic MC method for stationary problems is a variant of a well known method in neutronics :

the collision probability method.

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The mathematical analysis allows to adapt this method to other situations for example to radiative transfer problems

and to perform coupling with other methods.