Branching process inspired numerical approaches to the Neutron Transport Equation

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Neutron Transport Equation (NTE)

$$\frac{\partial}{\partial t}\psi_t(r,\upsilon) = (\mathrm{T}+\mathrm{S}+\mathrm{F})\psi_t(r,\upsilon), \quad r \in D, \upsilon \in V,$$

$$\psi_t(r,\upsilon) = 0, \quad r \in \partial D, \upsilon \cdot \mathbf{n}_r > 0.$$

where

- $\psi_t(r,\upsilon) =$ neutron flux at time t emitted from the initial config. (r,υ).
- Transport:

$$\mathrm{T}\psi_t(r,\upsilon) = \upsilon \cdot \nabla\psi_t(r,\upsilon).$$

- Scattering:

$$\mathrm{S}\psi_t(r,\upsilon) = \sigma_{\mathrm{s}}(r,\upsilon)\int_V \psi_t(r,\upsilon')\pi_{\mathrm{s}}(r,\upsilon,\upsilon')d\upsilon' - \sigma_{\mathrm{s}}(r,\upsilon)\psi_t(r,\upsilon).$$

- Fission:

$$\mathrm{F}\psi_t(r,\upsilon) = \sigma_{\mathrm{f}}(r,\upsilon)\int_V \psi_t(r,\upsilon')\pi_{\mathrm{f}}(r,\upsilon,\upsilon')d\upsilon' - \sigma_{\mathrm{f}}(r,\upsilon)\psi_t(r,\upsilon).$$

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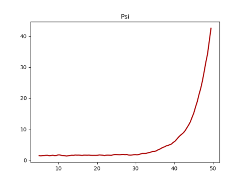
Spectral properties of the NTE

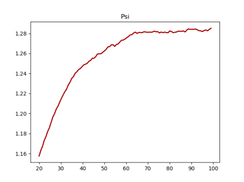
- Let $\psi_t = \psi_t[g]$ solve the NTE with the initial condition

$$\psi_0(r, \upsilon) = g(r, \upsilon), \quad r \in D, \upsilon \in V.$$

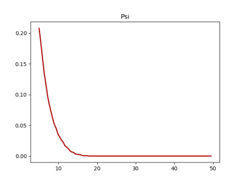
- $\psi_t \asymp e^{\lambda_* t}$, where $\lambda_* =$ lead eigenvalue.



$\lambda_* > 0$ **(Supercritical)**



$\lambda_* = 0$ **(Critical)**



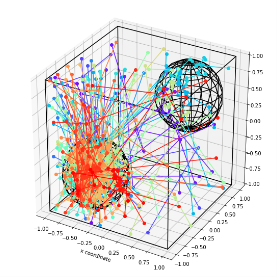
$\lambda_* < 0$ **(Subcritical)**

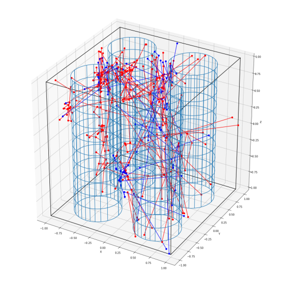
- **Aim:** Estimate the value of λ_*.

Overview

- Three Monte-Carlo algorithms:
    - Neutron branching process (NBP)
    - Basic Neutron random walk (NRW)
    - *h*-neutron random walk (*h*-NRW)
- Analysis on
    - accuracy
    - complexity

  of each algorithm.





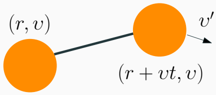
Neutron branching process (NBP)

Start with one particle at configuration (r, υ), which moves along the trajectory $r + \upsilon t$ until one of the following things happens:

- The particle leaves D and is killed.
- At rate $\sigma_{\mathrm{s}}(r, \upsilon)$, the particle picks a new velocity υ' with probability $\pi_{\mathrm{s}}(r, \upsilon, \upsilon')d\upsilon'$ at (r, υ).
- Independently, at rate $\sigma_{\mathrm{f}}(r, \upsilon)$, the particle is replaced by N new particles at (r, υ_1), $(r, \upsilon_2), \ldots, (r, \upsilon_N)$ satisfying

$$\mathcal{E}_{(r,\upsilon)}\Big[\sum_{i=1}^{N} f(\upsilon_i)\Big] = \int_V \pi_{\mathrm{f}}(r, \upsilon, \upsilon')f(\upsilon')d\upsilon', \ \forall f \geq 0.$$

Each new particle evolves independently in the same way as the old particle.



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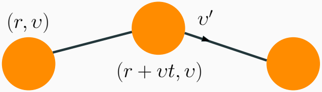

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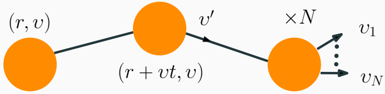


Neutron Branching Process & NTE

Mean behaviour of the neutron branching process verifies NTE:

Denote by N_t the number of particles alive at time t and by (r_i, υ_i) their configurations. Write

$$X_t = \sum_{i=1}^{N_t} \delta_{(r_i, \upsilon_i)}$$

Then

$$\psi_t[g](r,\upsilon) := \mathbb{E}[\langle g, X_t\rangle \,|\, X_0 = \delta_{(r,\upsilon)}] = \mathbb{E}\Big[\sum_{i=1}^{N_t} g(r_i,\upsilon_i)\,\Big|\, X_0 = \delta_{(r,\upsilon)}\Big]$$

solves the (NTE) for all g sufficiently smooth.

Neutron Branching Process: Algorithm

- Simulate a neutron branching process starting from a single particle at (r, υ).

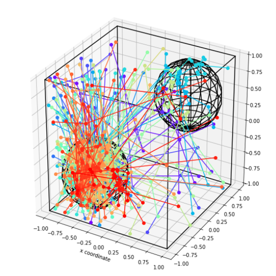
  X_t = empirical measure of the process at t.

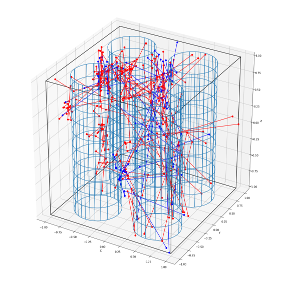
- Repeat the simulations for k times.

  X_t^i = output from the i-th simulation.

- $\psi_t[g](r, \upsilon) \approx \frac{1}{k} \sum_{i=1}^{k} \langle g, X_t^i \rangle$ for k large.
  Then, the NBP-estimator for e^{λ_*} is given by

$$\Psi_{\mathrm{NBP}}(t, k) = \Big(\frac{1}{k} \sum_{i=1}^{k} \langle g, X_t^i \rangle \Big)^{\frac{1}{t}}$$



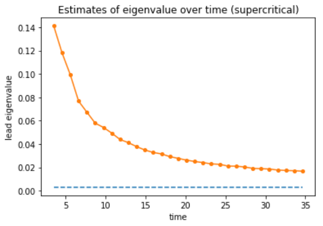


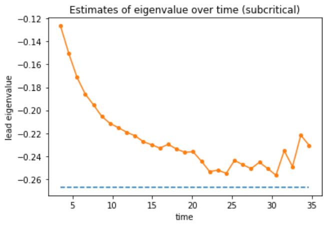
Neutron Branching Process: Convergence rate

Theorem (CHKW. 20+)

As $t, k \to \infty$, we have

- for $\lambda_* > 0$: $\mathbb{E}[(\Psi_{\mathrm{NBP}}(t,k) - e^{\lambda_*})^2] = \mathcal{O}(\frac{1}{k} + \frac{1}{t^2})$;
- for $\lambda_* = 0$: $\mathbb{E}[(\Psi_{\mathrm{NBP}}(t,k) - e^{\lambda_*})^2] = \mathcal{O}(\frac{t}{k} + \frac{1}{t^2})$;
- for $\lambda_* < 0$: $\mathbb{E}[(\Psi_{\mathrm{NBP}}(t,k) - e^{\lambda_*})^2] = \mathcal{O}(\frac{e^{-\lambda_* t}}{k} + \frac{1}{t^2})$;





Sketch of proof

$$\mathbb{E}[(\Psi_{\mathrm{NBP}}(t,k)-e^{\lambda_*})^2] \leq 2\mathbb{E}[(\Psi_{\mathrm{NBP}}(t,k)-\psi_t(r,\upsilon)^{\frac{1}{t}})^2]+2(\psi_t(r,\upsilon)^{\frac{1}{t}}-e^{\lambda_*})^2.$$

The first term is estimated using the many-to-two:

$$\mathbb{E}\big[\langle f, X_t\rangle\langle g, X_t\rangle\big] = \psi_t[fg] + \int_0^t \psi_s\Big[\eta[\psi_{t-s}[f], \psi_{t-s}[g]]\Big]ds$$

where $\eta[f,g] = \sigma_{\mathrm{f}} \cdot \mathcal{E}\Big[\sum_{i\neq j}^N f(\upsilon_i)g(\upsilon_j)\Big]$. It follows that

$$\mathrm{Var}[\langle g, X_t\rangle] \asymp \begin{cases} e^{2\lambda_* t}, & \lambda_* > 0, \\ t, & \lambda_* = 0, \\ e^{\lambda_* t}, & \lambda_* < 0. \end{cases}$$

Neutron Branching Process: Cost estimates

- Roughly speaking, the cost of simulating a NBP consists of
  - memory cost: storing the trajectory of each particle
  - CPU time: sampling scattering and fission events
- We need a counter for the above events: for $f, g \in L^+_\infty(D \times V)$, let

$$\mathrm{Cost}_t[f,g] = \sum_u g\left(r^u_{b_u}, \upsilon^u_{b_u}\right)\mathbf{1}_{\{b_u \le t\}} + \sum_u \sum_i f\left(r^u_{s^u_i}, \upsilon^u_{s^u_i}\right)\mathbf{1}_{\{s^u_i \le t\}},$$

  where $\sum_u$ is over all the particles u, b_u is the birth time of u, (r^u_t, υ^u_t) its trajectory, and (s^u_i) the sequence of its scattering times.
- In particular, $\mathrm{Cost}_t[\mathbf{0}, \mathbf{1}] \asymp$ memory cost, while $\mathrm{Cost}_t[\mathbf{1}, \mathbf{1}] \asymp$ CPU-time.

Neutron Branching Process: Cost estimates

Using standard tools on point processes, we can show that

Theorem (CHKW. 20+)

As $t \to \infty$, we have

- for $\lambda_* > 0$: $\mathbb{E}\big[\mathrm{Cost}_t[f, g]\big] = \mathcal{O}(e^{\lambda_* t})$;
- for $\lambda_* = 0$: $\mathbb{E}\big[\mathrm{Cost}_t[f, g]\big] = \mathcal{O}(t)$;
- for $\lambda_* < 0$: $\mathbb{E}\big[\mathrm{Cost}_t[f, g]\big] = \mathcal{O}(1)$.

Applications: Combining this with the previous estimates, we can determine the "optimal" choice of k, t to minimise total computational cost for a given level of accuracy.

Neutron Random Walk via Many-to-one

Recall (NTE): $\partial_t \psi_t = (\mathrm{T} + \mathrm{S} + \mathrm{F})\psi_t$. We can scrap fission using many-to-one.

- Set $\beta(\cdot) = \sigma_\mathrm{f}(\cdot)\big(\int_V \pi_\mathrm{f}(\cdot, \upsilon')d\upsilon' - 1\big)$.
- Let (r_t, υ_t), $t \geq 0$, be the path of the following particle: starting at (r, υ), it moves along the trajectory $r + \upsilon t$ until
  - either the particle leaves D and is killed;
  - or at rate $\alpha(\cdot) = \sigma_\mathrm{s}(\cdot) + \sigma_\mathrm{f}(\cdot)\int_V \pi_\mathrm{f}(\cdot, \upsilon')d\upsilon'$, the particle picks a new velocity υ' with probability $\pi(\cdot, \upsilon')d\upsilon'$, where $\pi = (\sigma_\mathrm{s}\pi_\mathrm{s} + \sigma_\mathrm{f}\pi_\mathrm{f})/\alpha$.
- Then
$$\widetilde{\psi}_t[g](r, \upsilon) := \mathbb{E}\Big[e^{\int_0^t \beta(r_s, \upsilon_s)ds} g(r_t, \upsilon_t)\mathbf{1}_{\{\text{alive at } t\}}\Big]$$
solves the (NTE).

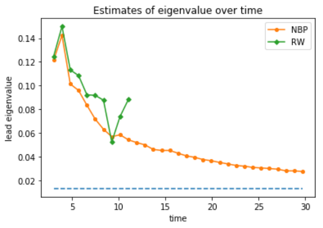
Neutron Random Walk: Algorithm

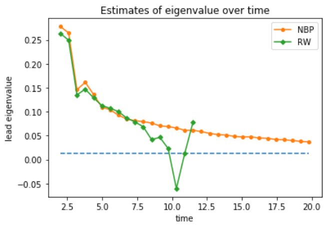
- The following is an estimator of e^{λ_*}:

$$\Psi_{\mathrm{NRW}}(t,k) = \left(\frac{1}{k}\sum_{i=1}^{k} e^{\int_0^t \beta(r_s^i, \upsilon_s^i)ds}\, g(r_t^i, \upsilon_t^i)\mathbf{1}_{\{\text{alive at } t\}}\right)^{\frac{1}{t}},$$

where (r_s^i, υ_s^i), $1 \le i \le k$, are independent (α, π)-neutron random walks.

- **Problem:** large variance due to exponentially small chance of survival.





Dooh h-transform for Neutron Random Walk

- Write L for the infinitesimal generator of the (α, π)-neutron random walk, i.e.

$$\mathrm{L}h(r, \upsilon) = \upsilon \cdot \nabla h(r, \upsilon) + \alpha(r, \upsilon) \int_V (h(r, \upsilon') - h(r, \upsilon))\pi(r, \upsilon, \upsilon')d\upsilon'.$$

- Let $h \in L^+_\infty(D \times V)$ and define

$$\frac{d\mathbf{P}^h_{(r,\upsilon)}}{d\mathbb{P}_{(r,\upsilon)}} = \exp\left(-\int_0^t \frac{\mathrm{L}h(r_s, \upsilon_s)}{h(r_s, \upsilon_s)} ds \right) \frac{h(r_t, \upsilon_t)}{h(r, \upsilon)} \mathbf{1}_{\{\text{alive at } t\}}.$$

Then under $\mathbf{P}^h$, $(r_t, \upsilon_t)_{t \geq 0}$ is distributed as a neutron random walk with scattering rates

$$\alpha^h(r, \upsilon) = \frac{\alpha(r, \upsilon)}{h(r, \upsilon)} \int_V h(r, \upsilon')\pi(r, \upsilon, \upsilon')d\upsilon'$$

- In particular, if $h \to 0+$ at ∂D, then the scattering rate $\alpha^h \to \infty$ at ∂D; the particle will never leave D under $\mathbf{P}^h$.

h-Neutron Random Walk: Implementation

The following is an estimator of e^{λ_*}:

$$\Psi_{h\text{-RW}}(t,k) = \left\{ \frac{1}{k} \sum_{i=1}^{k} \exp\left(\int_0^t \frac{\mathrm{L}h(r_s^i, \upsilon_s^i)}{h(r_s^i, \upsilon_s^i)} + \beta(r_s^i, \upsilon_s^i) ds \right) \frac{g(r_t^i, \upsilon_t^i)}{h(r_t^i, \upsilon_t^i)} \right\}^{\frac{1}{t}},$$

where (r_s^i, υ_s^i), $1 \le i \le k$, are independent (α^h, π^h)-neutron random walks.

Theorem (CHKW. 20+)

As $k, t \to \infty$, we have

$$\mathbf{E}^h[(\Psi_{h\text{-RW}}(t,k) - e^{\lambda_*})^2] = \mathcal{O}\left(\tfrac{e^{2(\lambda_h - \lambda_*)t}}{k} + \tfrac{1}{t^2}\right),$$

and

$$\mathbf{E}^h[\mathrm{Cost}_t] = \mathcal{O}(e^{(\lambda_* - \lambda_h')t}),$$

where $\lambda_h \ge \lambda_* \ge \lambda_h'$.

h-Neutron Random Walk: Choice of h

- The "optimal" choice of h is given by the lead eigenfunction φ, i.e.

$$(\mathrm{L}+\beta)\varphi = (\mathrm{T}+\mathrm{S}+\mathrm{F})\varphi = \lambda_*\varphi.$$

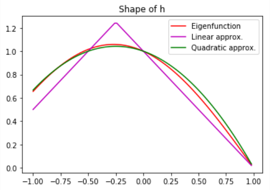
In that case, we have

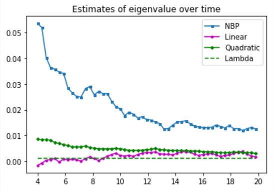
$$\mathbf{E}^{\varphi}[(\Psi_{\varphi\text{-RW}}(t,k) - e^{\lambda_*})^2] = \mathcal{O}(\tfrac{1}{k} + \tfrac{1}{t^2}) \ \text{ and } \ \mathbf{E}^{h}[\mathrm{Cost}_t]] = \mathcal{O}(1).$$

- In practice, one starts with a guess of φ. Since

$$e^{-\lambda_* t}\psi_t[g](r,\upsilon) \overset{t\to\infty}{\to} C_g\varphi(r,\upsilon),$$

estimates from the first simulations will provide better choice of h.





Summary

Borrowing tools from branching particle systems, we have

- presented some Monte-Carlo algorithms (NBP, h-NRW),
- estimated their convergence rates and complexity.

Thank You

Abstract Cauchy Problem: Existence and uniqueness

[CHHK19] Suppose that

- D is a bounded and convex domain of $\mathbb{R}^3$ with smooth boundary and $V \subset \mathbb{R}^3_+$ is bounded;
- $\sigma_{\rm s}, \sigma_{\rm f}, \pi_{\rm s}$ and $\pi_{\rm f}$ are uniformly bounded;
- $\inf_{(r,\upsilon,\upsilon')} \sigma_{\rm s}\pi_{\rm s} + \sigma_{\rm f}\pi_{\rm f} > 0$.

Then for $g \in L^+_\infty(D \times V)$ (resp. $g \in L^+_2(D \times V)$), there is a unique solution in $L^+_\infty(D \times V)$ (resp. in $L^+_2(D \times V)$) to the mild equation

$$\psi_t[g] = \mathrm{U}_t[g] + \int_0^t \mathrm{U}_s[(\mathrm{S} + \mathrm{F})\psi_{t-s}[g]]ds, \ \ t \geq 0,$$

where

$$\mathrm{U}_t[g](r, \upsilon) = g(r + \upsilon t, \upsilon)\mathbf{1}_{\{\kappa_{r,\upsilon} > t\}} \text{ with } \kappa_{r,\upsilon} = \inf\{t : r + \upsilon t \notin D\}.$$

Perron-Frobenius

[HKV20] Under the previous assumptions, for the solution (ψ_t) to the mild equation, there exists a $\lambda_* \in \mathbb{R}$, a positive right eigenfunction $\varphi \in L^+_\infty(D \times V)$ and a left eigenmeasure which is absolutely continuous with respect to Lebesgue measure on $D \times V$ with density $\tilde{\varphi} \in L^+_\infty(D \times V)$, both having associated eigenvalue $e^{\lambda_* t}$ and such that φ (resp. $\tilde{\varphi}$) is uniformly (resp. a.e. uniformly) bounded away from zero on each compactly embedded subset of $D \times V$. In particular, for all $g \in L^+_\infty(D \times V)$,

$$\langle \tilde{\varphi}, \psi_t[g] \rangle = e^{\lambda_* t} \langle \tilde{\varphi}, g \rangle \quad \text{and} \quad \psi_t[\varphi] = e^{\lambda_* t} \varphi, \ t \geq 0.$$

Moreover, there exists $\epsilon > 0$ such that

$$\sup_{\|g\|_\infty \leq 1} \|e^{-\lambda_* t} \varphi^{-1} \psi_t[g] - \langle \tilde{\varphi}, g \rangle\|_\infty = O(e^{-\epsilon t}), \ t \to \infty.$$

References

[CHHK19] Multi-species neutron transport equation. Alexander M.G. Cox, Simon C. Harris, Emma Horton and Andreas E. Kyprianou. Journal of Statistical Physics (2019), 176(2), 425-455.

[HKV20] Stochastic Methods for the Neutron Transport Equation I: Linear Semigroup asymptotics. Emma Horton, Andreas E. Kyprianou and Denis Villemonais. Annals of Applied Probability (2020) Vol. 30, No. 6, 2815–2845.

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