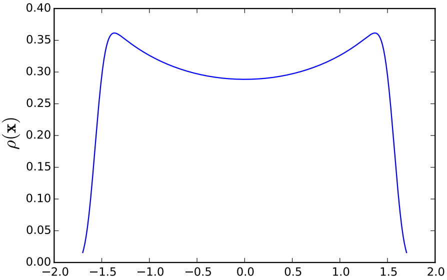
Pieter Van Nuffel

- 2006-2011: Master in Physics and Astronomy (UGent)
  - **Master thesis**: Simulation of Information Entropy in Financial Markets with Molecular Dynamics.
- 2012-2015: Teaching assistent (KU Leuven KULAK)
- 2015-current: PhD student
  - **Promotor**: Giovanni Samaey
  - **Research topics and interests**: Coarse Bifurcation Analysis of Stochastic Agent-based Network Models, Uncertainty Quantification, Multiscale Methods

Fokker-Planck equation

$$\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial (a(x)\rho(x,t))}{\partial x} = D\frac{\partial^2 \rho(x,t)}{\partial x^2}$$



Simulate an ensemble of N particles evolving according to the corresponding SDE

$$\mathrm{d}x = a(x)\mathrm{d}t + \sqrt{2D}\cdot \mathrm{d}W_t.$$

Coarse time stepper

$$\boldsymbol{\rho}(t+n\Delta t) = \boldsymbol{\Phi}_T(\boldsymbol{\rho}) = (\mathcal{R} \circ \mathcal{E}(n\Delta t, \omega) \circ \mathcal{L}(\omega))(\boldsymbol{\rho}(t))$$

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- Lifting $\mathcal{L} : \boldsymbol{\rho} \to \mathbf{x}$

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- Lifting $\mathcal{L} : \boldsymbol{\rho} \to \mathbf{x}$
- Evolution $\mathcal{E}$:
  Simulation of the SDE for N particles over n timesteps.

$$\mathbf{x}^{n+1} = \mathbf{x}^n + a(\mathbf{x}^n)\Delta t + \sqrt{2D\Delta t} \cdot \boldsymbol{\xi}^n$$

with

$$\xi^n(\omega) \sim \mathcal{N}(0, 1)$$

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  with

$$\xi^n(\omega)\sim\mathcal{N}(0,1)$$

- Restriction $\mathcal{R}:\mathbf{x}\to\boldsymbol{\rho}$

$$\frac{1}{N}\sum_{i=1}^{N}w_i\cdot\chi_{\Delta_j}(x_i)=\rho_j$$

Evaluating Jacobian-vector products

$$\boldsymbol{\rho}_* - \mathbf{\Phi}_T(\boldsymbol{\rho}_*) = 0$$

$$\mathbf{Jv} = D(\mathbf{\Phi}_T) \cdot \mathbf{v} \approx \frac{\mathbf{\Phi}_T(\boldsymbol{\rho} + \varepsilon \mathbf{v}, \boldsymbol{\omega}_\mathbf{1}) - \mathbf{\Phi}_T(\boldsymbol{\rho}, \boldsymbol{\omega}_\mathbf{2})}{\varepsilon}$$

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Problem: numerical noise for $\varepsilon \ll 1$

Repeating $\boldsymbol{\Phi}_T$ with two sets of random numbers $\boldsymbol{\omega}_\mathbf{1}, \boldsymbol{\omega}_\mathbf{2}$ will give different results $\rightarrow \mathcal{O}(1/(\varepsilon^2 N))$ variance.

Variance reduction of Jacobian-vector products

$$
\begin{aligned}
\mathbf{J}\mathbf{v} = D(\boldsymbol{\Phi}_T) \cdot \mathbf{v} \quad &\approx \quad \frac{\boldsymbol{\Phi}_T(\boldsymbol{\rho} + \varepsilon \mathbf{v}, \boldsymbol{\omega}_1) - \boldsymbol{\Phi}_T(\boldsymbol{\rho}, \boldsymbol{\omega}_2)}{\varepsilon} \\
&\approx \quad \frac{\boldsymbol{\Phi}_T(\boldsymbol{\rho}, \boldsymbol{\omega}_1) + \varepsilon D(\boldsymbol{\Phi}_T)(\boldsymbol{\rho}, \boldsymbol{\omega}_1) \cdot \mathbf{v} - \boldsymbol{\Phi}_T(\boldsymbol{\rho}, \boldsymbol{\omega}_2)}{\varepsilon}
\end{aligned}
$$

Variance reduction of Jacobian-vector products

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$$\approx \frac{\boldsymbol{\Phi}_T(\boldsymbol{\rho}, \boldsymbol{\omega}_1) + \varepsilon D(\boldsymbol{\Phi}_T)(\boldsymbol{\rho}, \boldsymbol{\omega}_1) \cdot \mathbf{v} - \boldsymbol{\Phi}_T(\boldsymbol{\rho}, \boldsymbol{\omega}_2)}{\varepsilon}$$

Solution:
Perturbations on the density $\rightarrow$ perturbations in the weights

$$\frac{1}{N}\sum_{i=1}^{N} w_i \cdot \chi_{\Delta_j}(x_i) = \rho_j$$

$$\frac{1}{N}\sum_{i=1}^{N} w_\varepsilon^i \cdot \chi_{\Delta_j}(x^i) = \rho_j + \varepsilon v_j.$$

For the perturbated density: compute the weight per bin as $w_\varepsilon^j = 1 + \frac{\varepsilon v_j}{\rho_j}$ and assign this value to each particle in Δ_j.

Variance reduction of Jacobian-vector products

$$\mathbf{J}\mathbf{v} = D(\mathbf{\Phi}_T)\cdot\mathbf{v} \approx \frac{\mathbf{\Phi}_T(\boldsymbol{\rho}+\varepsilon\mathbf{v},\boldsymbol{\omega}_1) - \mathbf{\Phi}_T(\boldsymbol{\rho},\boldsymbol{\omega}_2)}{\varepsilon}$$

$$\approx \frac{\cancel{\mathbf{\Phi}_T(\boldsymbol{\rho},\boldsymbol{\omega}_1)} + \varepsilon D(\mathbf{\Phi}_T)(\boldsymbol{\rho},\boldsymbol{\omega}_1)\cdot\mathbf{v} - \cancel{\mathbf{\Phi}_T(\boldsymbol{\rho},\boldsymbol{\omega}_1)}}{\varepsilon}$$

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$$\mathbf{J}\mathbf{v} = D(\boldsymbol{\Phi}_T) \cdot \mathbf{v} \approx \frac{\boldsymbol{\Phi}_T(\boldsymbol{\rho} + \varepsilon \mathbf{v}, \boldsymbol{\omega_1}) - \boldsymbol{\Phi}_T(\boldsymbol{\rho}, \boldsymbol{\omega_2})}{\varepsilon}$$

$$\approx \frac{\cancel{\boldsymbol{\Phi}_T(\boldsymbol{\rho}, \boldsymbol{\omega_1})} + \varepsilon D(\boldsymbol{\Phi}_T)(\boldsymbol{\rho}, \boldsymbol{\omega_1}) \cdot \mathbf{v} - \cancel{\boldsymbol{\Phi}_T(\boldsymbol{\rho}, \boldsymbol{\omega_1})}}{\varepsilon}$$

Solution:
Perturbations on the density $\rightarrow$ perturbations in the weights

$$\begin{aligned} \frac{1}{N} \sum_{i=1}^{N} w_i \cdot \chi_{\Delta_j}(x_i) &= \rho_j \\ \frac{1}{N} \sum_{i=1}^{N} w_\varepsilon^i \cdot \chi_{\Delta_j}(x^i) &= \rho_j + \varepsilon v_j. \end{aligned}$$

For the perturbated density: compute the weight per bin as $w_\varepsilon^j = 1 + \frac{\varepsilon v_j}{\rho_j}$ and assign this value to each particle in Δ_j.

Variance reduction of Jacobian-vector products

$$\mathbf{J}\mathbf{v} = D(\mathbf{\Phi}_T) \cdot \mathbf{v} \approx \frac{\mathbf{\Phi}_T(\boldsymbol{\rho} + \varepsilon \mathbf{v}, \boldsymbol{\omega}_1) - \mathbf{\Phi}_T(\boldsymbol{\rho}, \boldsymbol{\omega}_2)}{\varepsilon}$$

$$\approx \frac{\cancel{\mathbf{\Phi}_T(\boldsymbol{\rho}, \boldsymbol{\omega}_1)} + \cancel{\varepsilon} D(\mathbf{\Phi}_T)(\boldsymbol{\rho}, \boldsymbol{\omega}_1) \cdot \mathbf{v} - \cancel{\mathbf{\Phi}_T(\boldsymbol{\rho}, \boldsymbol{\omega}_1)}}{\cancel{\varepsilon}}$$

Solution:
Perturbations on the density $\rightarrow$ perturbations in the weights

$$\frac{1}{N} \sum_{i=1}^{N} w_i \cdot \chi_{\Delta_j}(x_i) = \rho_j$$

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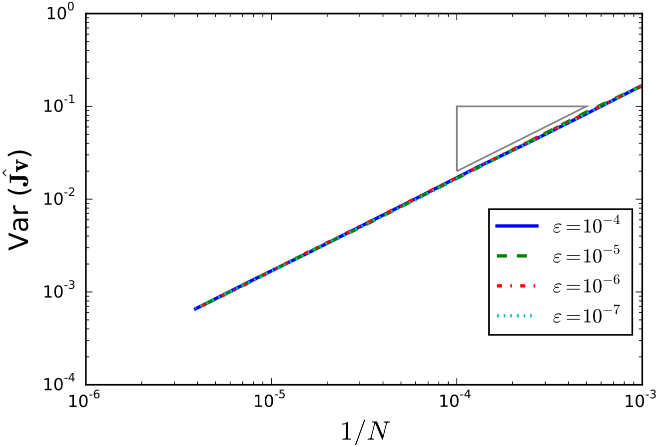
For the perturbated density: compute the weight per bin as $w_\varepsilon^j = 1 + \frac{\varepsilon v_j}{\rho_j}$ and assign this value to each particle in Δ_j.

Variance reduction of Jacobian-vector products

$$\mathtt{Var}(\hat{\mathbf{J}}\mathbf{v}) = \hat{\mathbb{E}}\left[\left(\hat{\mathbf{J}}\mathbf{v} - \hat{\mathbb{E}}[\hat{\mathbf{J}}\mathbf{v}]\right)^2\right] \sim \mathcal{O}(1/N)$$



Evaluating the bias on Jacobian-vector products

$$\mathbf{Bias}(\hat{\mathbf{J}}\mathbf{v}, \mathbf{J}\mathbf{v}_{FP}) = \hat{\mathbb{E}}[\hat{\mathbf{J}}\mathbf{v}] - \mathbf{J}\mathbf{v}_{FP}$$

Evaluating the bias on Jacobian-vector products

$$\mathbf{Bias}(\hat{\mathbf{J}}\mathbf{v}, \mathbf{J}\mathbf{v}_{FP}) = \hat{\mathbb{E}}[\hat{\mathbf{J}}\mathbf{v}] - \mathbf{J}\mathbf{v}_{FP}$$

with

$$\mathbf{J}\mathbf{v}_{FP} \approx \frac{\rho^{\varepsilon}(t + n\Delta t) - \rho(t + n\Delta t)}{\varepsilon}$$

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with

$$\mathbf{J}\mathbf{v}_{FP} \approx \frac{\boldsymbol{\rho}^{\varepsilon}(t + n\Delta t) - \boldsymbol{\rho}(t + n\Delta t)}{\varepsilon}$$

and $\boldsymbol{\rho}$ calculated by explicitly solving

$$\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial (a(x)\rho(x,t))}{\partial x} = D\frac{\partial^2 \rho(x,t)}{\partial x^2}$$

using

$$\rho_i^{n+1} = \rho_i^n + \Delta t \left(\frac{D}{\Delta x^2} \left(\rho_{i+1}^n - 2\rho_i^n + \rho_{i-1}^n\right) - \frac{a(x)}{\Delta x}(\rho_i^n - \rho_{i-1}^n) \right)$$

for the value of ρ at position $x = i\Delta x$ and time $t = (n+1)\Delta t$

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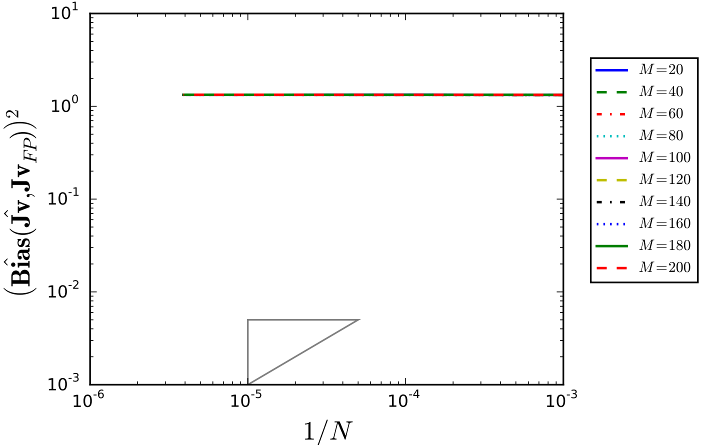

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