

Problem: $\text{Var}(\hat{\mathbf{J}}\mathbf{v}) \sim \mathcal{O}(1/(\varepsilon^2 N)) \Rightarrow$ Numerical noise for $\varepsilon \ll 1$

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 assistant (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

$$dx = a(x)dt + \sqrt{2D} \cdot dW_t.$$

Coarse time stepper

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

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- ▶ Evolution \mathcal{E} :
Simulation of the SDE for N particles over n timesteps.

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

with

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

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- ▶ Restriction $\mathcal{R} : \mathbf{x} \rightarrow \rho$

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

Evaluating Jacobian-vector products

$$\rho_* - \Phi_T(\rho_*) = 0$$

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

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

Repeating Φ_T with two sets of random numbers ω_1, ω_2 will give different results $\rightarrow \mathcal{O}(1/(\varepsilon^2 N))$ variance.

Variance reduction of Jacobian-vector products

$$\begin{aligned} \mathbf{J}\mathbf{v} = D(\Phi_T) \cdot \mathbf{v} &\approx \frac{\Phi_T(\rho + \varepsilon\mathbf{v}, \omega_1) - \Phi_T(\rho, \omega_2)}{\varepsilon} \\ &\approx \frac{\Phi_T(\rho, \omega_1) + \varepsilon D(\Phi_T)(\rho, \omega_1) \cdot \mathbf{v} - \Phi_T(\rho, \omega_2)}{\varepsilon} \end{aligned}$$

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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 perturbed 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 .

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Solution:

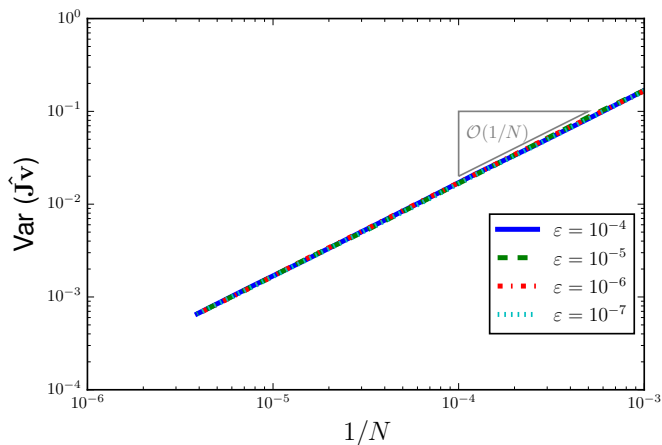
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Variance reduction of Jacobian-vector products

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



Evaluating the bias on Jacobian-vector products

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

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

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and ρ calculated by explicitly solving

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

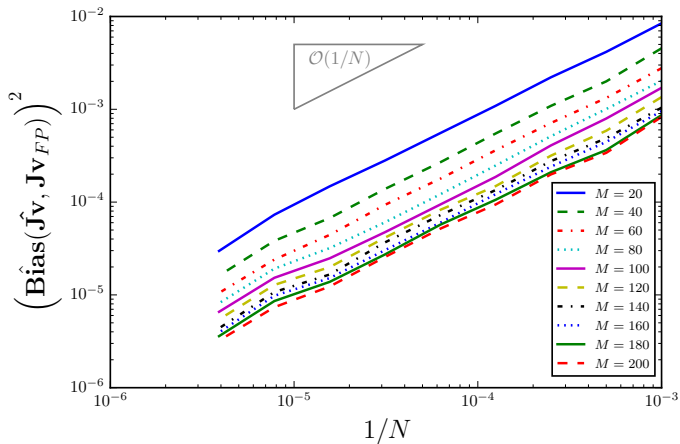
using

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

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

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