

CONNECTING STOCHASTIC OPTIMIZATION WITH SCHRÖDINGER EVOLUTION WITH RESPECT TO NON HERMITIAN HAMILTONIANS

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1 - INTRODUCTION

- Our goal is to study systems whose evolution is given by the following stochastic differential equation:

$$\dot{\mathbf{x}}_t = \mathbf{f}(\mathbf{x}_t, \mathbf{t}) + \mathbf{G}(\mathbf{x}_t) (\mathbf{u}_t + \boldsymbol{\xi}_t)$$

where $\mathbf{x}_t \in \mathbb{R}^n$ is the state of the system, $\mathbf{f}(\mathbf{x}_t, \mathbf{t}) \in \mathbb{R}^n$ describes the passive dynamics, $\mathbf{G}(\mathbf{x}_t) \in \mathbb{R}^{n \times p}$ is the control matrix, $\mathbf{u}_t \in \mathbb{R}^p$ are the control variables and $\boldsymbol{\xi}_t \in \mathbb{R}^p$ is the Gaussian white noise with variance matrix Σ_{ξ} .

- To this equation we have an associated cost function which we want to minimize:

$$R(T_i) = \phi_{t_N} + \int_{t_i}^{t_N} r_t dt$$

where the first term represents the final cost and the second one the integration of a instantaneous cost specified below.

- Our **objective** is to **draw a connection between this stochastic model and the Schrödinger evolution of a non-Hermitian Hamiltonian**. Specifically we studied this connection for 1D quadratic Hamiltonians.

2 - THE HJB EQUATION

- Following [1], define the value function as:

$$V(\mathbf{x}_{t_i}) = V_{t_i} = \min_{\mathbf{u}_{t_i:t_N}} E_{T_i} [R(T_i)]$$

which depends on the initial state \mathbf{x}_{t_i} and on the time interval T_i . This function satisfies:

$$-\partial_t V = \min_{\mathbf{u}} \left[r_t + (\partial_{\mathbf{x}} V)^T \mathbf{F}_t + \frac{1}{2} \text{Tr} \left((\partial_{\mathbf{x}\mathbf{x}}^2 V) (\mathbf{G}_t \Sigma_t \mathbf{G}_t^T) \right) \right]$$

- Considering an instantaneous cost of the form:

$$r_t = \mathbf{q}(\mathbf{x}_t, t) + \frac{1}{2} \mathbf{u}_t^T \mathbf{R} \mathbf{u}_t$$

one obtains the following equation [1]:

$$-\partial_t V = q_t - \frac{1}{2} (\partial_{\mathbf{x}} V)^T \mathbf{G}_t \mathbf{R}^{-1} \mathbf{G}_t^T (\partial_{\mathbf{x}} V) + (\partial_{\mathbf{x}} V)^T \mathbf{f}_t + \frac{1}{2} \text{Tr} \left((\partial_{\mathbf{x}\mathbf{x}}^2 V) (\mathbf{G}_t \Sigma_t \mathbf{G}_t^T) \right)$$

3 - SCHRÖDINGER

- By making a change of variables [1] of the form $V_t = -\hbar \log \psi_{-t}$ and assuming $\hbar \mathbf{R}^{-1} = \boldsymbol{\Sigma}$ we can convert the above equation to a linear equation of the Schrödinger form:

$$\hat{\mathcal{H}} \psi_t = \frac{i}{2} \hbar^2 \text{Tr} \left(\partial_{\mathbf{x}\mathbf{x}}^2 (\psi_t) \mathbf{G}_t \mathbf{R}^{-1} \mathbf{G}_t^T \right) + i \mathbf{f}_t^T \hbar (\partial_{\mathbf{x}} \psi_t) - i q_t \psi_t$$

- The symbol of $\hat{\mathcal{H}}$ is given by the Hamiltonian function $\mathcal{H}(x, p)$ which is used to study the semiclassical dynamics of the system.

4 - SEMICLASSICAL EVOLUTION

- Using the **Wigner function formalism**, a given wave function is transformed into a real valued function that lives in phase space.
- By considering gaussian wavepackets the corresponding Wigner function will also be gaussian, of the form:

$$W(z) = \alpha(t) (\pi \hbar)^{-n} \exp \left[-\frac{1}{\hbar} (z - Z) \cdot G (z - Z) \right],$$

$$z = (p, q), \quad Z = (P, Q)$$

- The Schrödinger semiclassical evolution of the Wigner function under $\mathcal{H} = H - i\Gamma$ is governed by the following system for the centers and intrinsic geometry of the state [2]:

$$\dot{Z} = \Omega \nabla H(Z) - G^{-1} \nabla \Gamma(Z)$$

$$\dot{G} = H''(Z) \Omega G - G \Omega H''(Z) + \Gamma''(Z) - G \Gamma''_{\Omega}(Z) G$$

$$\frac{\dot{\alpha}}{\alpha} = -\frac{2}{\hbar} \Gamma(Z) - \frac{1}{2} \text{Tr} [\Gamma''_{\Omega}(Z) G]$$

where Ω is the usual symplectic form.

5 - QUADRATIC EXAMPLE

- As a simple example, consider the 1D equation $\dot{x} = -\alpha x + (u_t + \eta)$ with a cost function of the form $r_t = \frac{\beta}{2} x^2 + \frac{1}{2} \frac{\hbar}{\delta} u^2$.
- The complex Hamiltonian $\mathcal{H} = H - i\Gamma$ is then:

$$H = \alpha x p \quad \text{and} \quad \Gamma = \frac{\delta p^2}{2} + \frac{\beta x^2}{2} - \frac{\alpha \hbar}{2}$$

- From this Hamiltonian we obtain the time evolution of the center of the gaussian, its associated metric and of the multiplicative factor of the initial wave function, as seen on the figures on the right.

- For most quadratic Hamiltonians the underlying metric of the phase space tends to a finite value, whereas both the multiplicative factor and the center's position tend to zero.

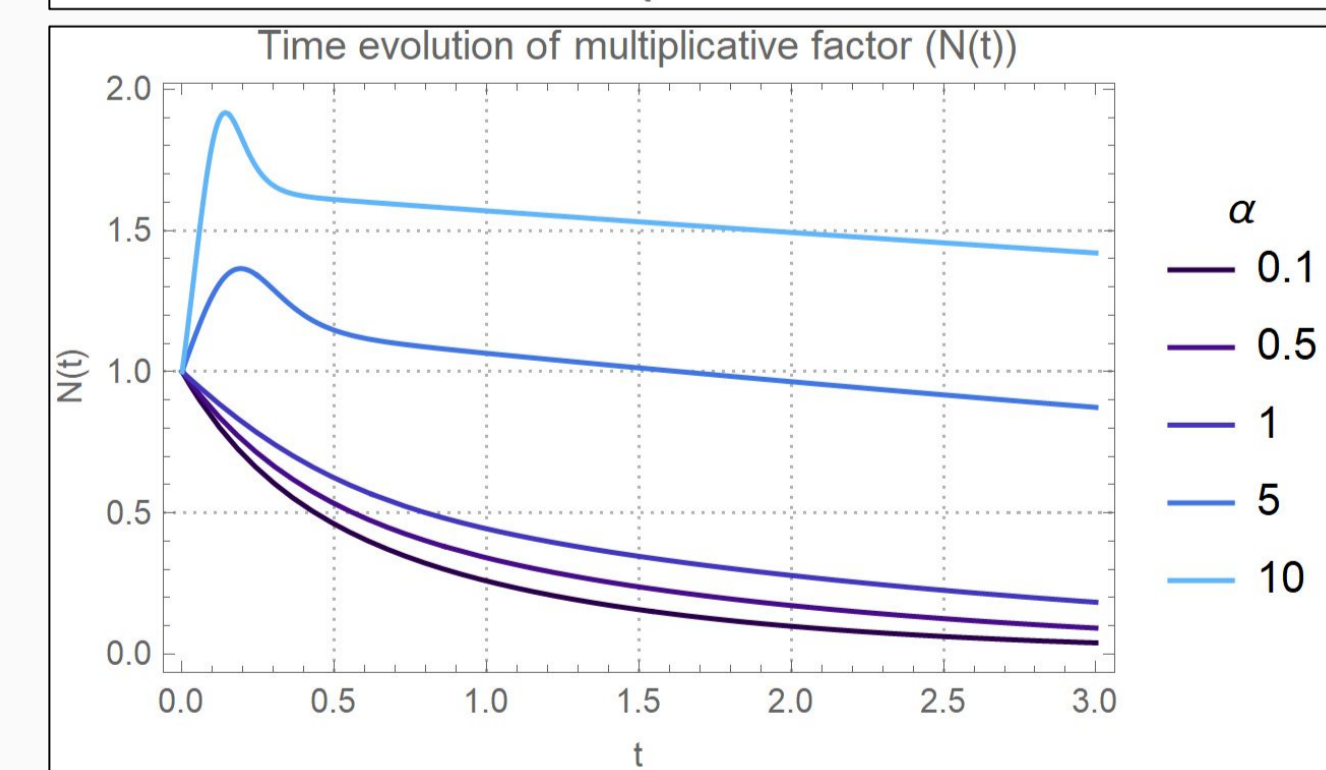
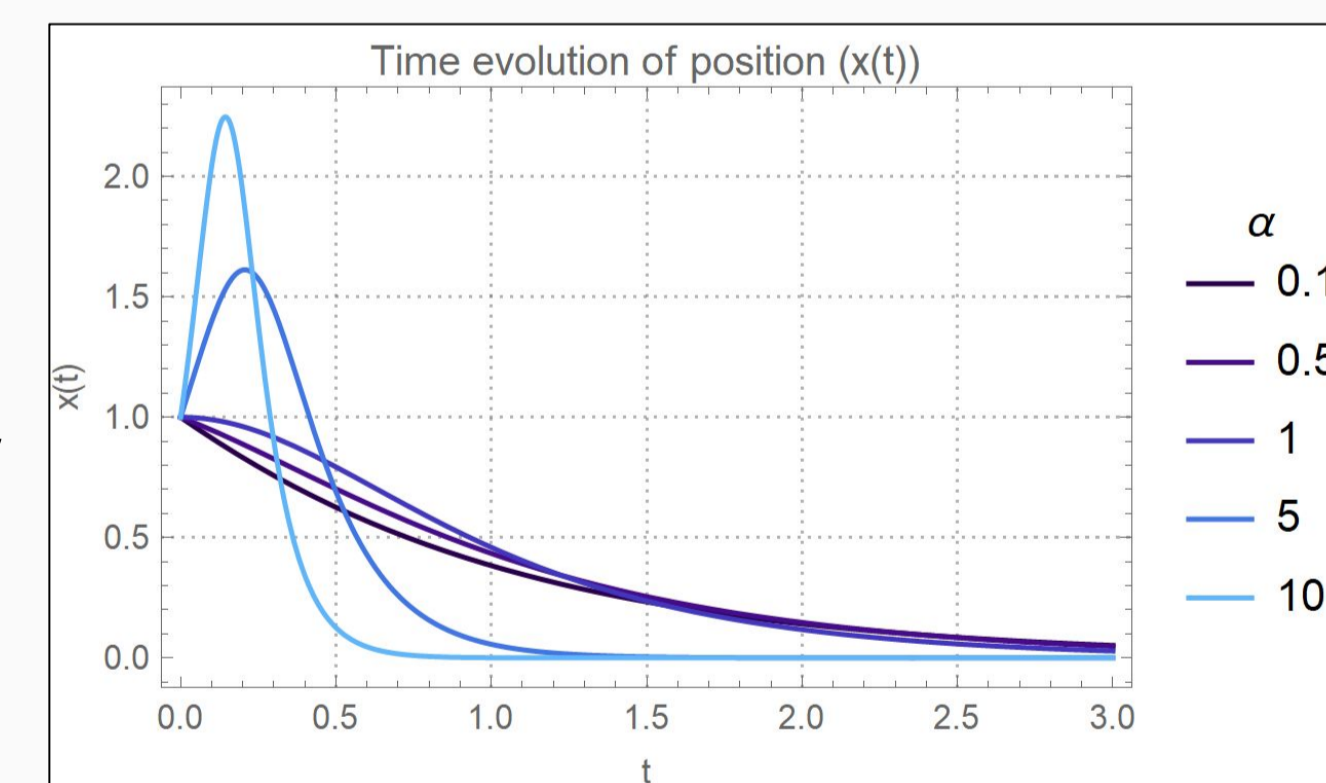


Figure: Time evolution of the position of wave packet's center and on the multiplicative factor for a gaussian wave function, in terms of α .

References:

[1] - Evangelos Theodorou, Jonas Buchli, and Stefan Schaal. "A Generalized Path Integral Control Approach to Reinforcement Learning". In: *J. Mach. Learn. Res.* 11 (Jan 2010).
[2] - E.-M. Graefe and R. Schubert. "Wave-packet evolution in non-Hermitian quantum systems". In: *Physical Review A* 83.6 (June 2011).

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