Operator Algebras for Closure of Dynamical Systems

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Motivation

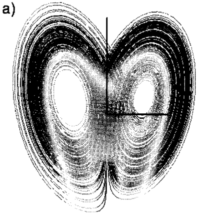
Original system

$$x_{n+1} = \phi(x_n, Z(y_n))$$
$$y_{n+1} = \psi(x_n, y_n)$$

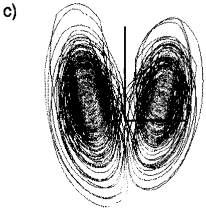
Parameterized system

$$x_{n+1} = \tilde{\phi}(x_n, \tilde{Z}(\tilde{y}_n))$$
$$\tilde{y}_{n+1} = \tilde{\psi}(x_n, \tilde{y}_n)$$

Lorenz 63 system



Stochastic closure



Palmer (2001), QJRMS.

Axioms of quantum mechanics

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3. Measurement expectation and probability:

$$\mathbb{E}_\rho A = \operatorname{tr}(\rho A), \quad \mathbb{P}_\rho(\Omega) = \mathbb{E}_\rho(E(\Omega)), \quad A = \int_{\mathbb{R}} a \, dE(a).$$

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5. State conditioning by quantum effects:

$$\rho|_e = \frac{\sqrt{e}\rho\sqrt{e}}{\operatorname{tr}(\sqrt{e}\rho\sqrt{e})}, \quad 0 < e \leq I.$$

Embedding into a quantum mechanical system

Classical statistical $\mathcal{P}(M) \xrightarrow{P} \mathcal{P}(M)$

- $\Phi : M \to M$: Dynamical flow with invariant measure μ.
- $\mathcal{P}(\mu)$: Probability densities in $L^1(\mu)$.
- $P : \mathcal{P}(\mu) \to P(\mu)$: Transfer operator, $Pp = p \circ \Phi^{-1}$.
- $L^\infty(\mu)$: Algebra of classical observables.
- $U : H \to H$: Koopman operator on $H = L^2(\mu)$, $Uf = f \circ \Phi$.

Embedding into a quantum mechanical system

$$
\begin{array}{lccc}
\text{Classical statistical} & \mathcal{P}(M) & \xrightarrow{P} & \mathcal{P}(M) \\
 & \Gamma \big\downarrow & & \big\downarrow \Gamma \\
\text{Quantum mechanical} & \mathcal{Q}(H) & \xrightarrow{\mathcal{P}} & \mathcal{Q}(H)
\end{array}
$$

- Embedding of probability densities into quantum states on H:

$$\Gamma : \mathcal{P}(M) \to \mathcal{Q}(H), \quad \Gamma(\nu) = \rho := \langle \nu^{1/2}, \cdot \rangle \nu^{1/2}.$$

- Embedding of observables: $\pi : L^\infty(\mu) \to B(H)$, $(\pi f)g = fg$.
- Unitary evolution: $\mathcal{P}\rho = U^* \rho U$.
- Quantum–classical consistency:

$$\mathbb{E}_{Pp} f = \mathbb{E}_{\mathcal{P}(\Gamma p)}(\pi f) \equiv \mathrm{tr}((\mathcal{P}(\Gamma p))(\pi f)).$$

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 & \mathbf{\Pi}'_L \big\downarrow & & \vdots\downarrow \mathbf{\Pi}'_L \\
\text{Matrix mechanical} & \mathcal{Q}(H_L) & \xrightarrow{\mathcal{P}_L} & \mathcal{Q}(H_L)
\end{array}
$$

- $H_L \subset H$: Finite-dimensional approximation space, $\Pi_L = \text{proj}_{H_L}$.
- Projection of quantum states:

$$\mathbf{\Pi}'_L(\rho) = \rho_L := \frac{\Pi_L \rho \Pi_L}{\text{tr}(\Pi_L \rho \Pi_L)}$$

- Projection of evolution operators:

$$\mathcal{P}_L \rho_L = \frac{U_L^* \rho_L U_L}{\text{tr}(U_L^* \rho_L U_L)}, \quad U_L = \Pi_L U \Pi_L.$$

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Structure preservation

- Unlike a projection $\Pi_L \nu$ of a classical probability density, a projected quantum state $\Pi_L \rho \Pi_L$ is a positive operator.
- Embedding into the infinite-dimensional quantum system on H, and *then* projecting to finite dimensions, allows us to construct positivity-preserving approximation schemes in ways which are not possible in abelian spaces.

State conditioning by effect-valued feature maps

$$\rho|_{\mathcal{F}(x)} = \frac{\sqrt{\mathcal{F}(x)}\rho\sqrt{\mathcal{F}(x)}}{\operatorname{tr}(\sqrt{\mathcal{F}(x)}\rho\sqrt{\mathcal{F}(x)})}$$

- Observation map: $Z : M \to \mathcal{X}$.
- Kernel on observation space: $k : \mathcal{X} \times \mathcal{X} \to [0, 1]$.
- Feature map: $F : \mathcal{X} \to L^\infty(\mu)$, $F(y) = k(y, Z(\cdot))$.
- Operator-valued feature map: $\mathcal{F} : \mathcal{X} \to B(H)$, $\mathcal{F} = \pi \circ F$.
- Projected feature map: $\mathcal{F}_L : \mathcal{X} \to B(H_L)$, $\mathcal{F}_L(x) = \Pi_L \mathcal{F}(x) \Pi_L$.

Quantum mechanical closure

Original system	Parameterized system
$x_{n+1} = \phi(x_n, Z(y_n))$	$x_{n+1} = \tilde{\phi}(x_n, \tilde{Z}(\rho_n))$
$y_{n+1} = \psi(x_n, y_n)$	$\rho_{n+1} = \tilde{\psi}(x_n, \rho_n)$

- Resolved variables: $x_n \in \mathcal{X}$.
- Unresolved variables: $y_n \in \mathcal{Y}$.
- Fluxes from unresolved variables: $Z : \mathcal{Y} \to \mathbb{R}^d$, $Z = (Z_1, \ldots, Z_d)$.
- Surrogate unresolved variables (quantum states): $\rho_n \in \mathcal{Q}(H_L)$.
- Parameterized fluxes: $\tilde{Z} : \mathcal{Q}(H_L) \to \mathbb{R}^d$, $\tilde{Z} = (\tilde{Z}_1, \ldots, \tilde{Z}_d)$,

$$\tilde{Z}_k(\rho_n) = \operatorname{tr}(\rho_n(\pi Z_k)).$$

- Evolution map for quantum states: $\tilde{\psi} : \mathcal{X} \times \mathcal{Q}(H_L) \to \mathcal{Q}(H_L)$,

$$\tilde{\psi}(x_n, \rho_n) = \tilde{\rho}_{n+1}|_{\mathcal{F}(x_{n+1})}, \quad \tilde{\rho}_{n+1} = \mathcal{P}_L \rho_n, \quad x_{n+1} = \tilde{\phi}(x_n, \tilde{Z}(\rho_n)).$$

Quantum mechanical closure

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$x_{n+1} = \phi(x_n, Z(y_n))$	$x_{n+1} = \tilde\phi(x_n, \tilde Z(\rho_n))$
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Given: Samples $x_0, \dots, x_{N-1} \in \mathcal{X}$, $z_0, \dots, z_{N-1} \in \mathbb{R}^d$ with $z_n = Z(y_n)$, along dynamical trajectory of the original system.

- Build data-driven basis $\{\phi_0, \dots, \phi_{L-1}\}$ of H_L.
- Compute $L \times L$ transfer operator matrix $\boldsymbol{P} = [P_{ij}]$,

$$P_{ij} = \langle \phi_i, P\phi_j \rangle.$$

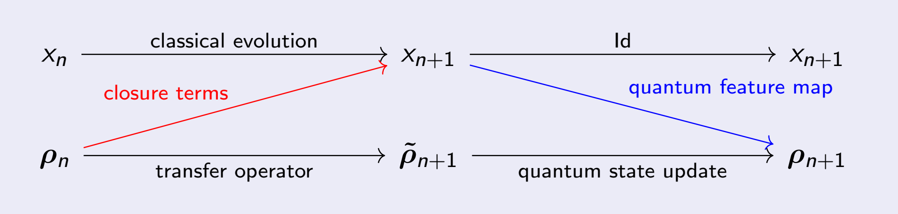
- Compute $L \times L$ multiplication operator matrices $\tilde{\boldsymbol{Z}}_1, \dots, \tilde{\boldsymbol{Z}}_d$,

$$\tilde{\boldsymbol{Z}}_k = [Z_{k,ij}], \quad Z_{k,ij} = \langle \phi_i, (\pi Z_k)\phi_j \rangle.$$

- Construct matrix-valued feature map, $\boldsymbol{F} : \mathcal{X} \to \mathbb{R}^{L\times L}$,

$$\boldsymbol{F}(x) = [F_{ij}(x)], \quad F_{ij}(x) = \langle \phi_i, \mathcal{F}_L(x)\phi_j \rangle.$$

Quantum mechanical closure



Closure algorithm

1. Compute parameterized fluxes: $\tilde{z}_n = (\tilde{z}_{n,1}, \dots, \tilde{z}_{n,d})$, $z_{n,k} = \operatorname{tr}(\boldsymbol{\rho}_n \tilde{\boldsymbol{Z}}_k)$.
2. Update resolved variables: $x_{n+1} = \tilde{\phi}(x_n, z_n)$.
3. Compute prior quantum state: $\tilde{\boldsymbol{\rho}}_{n+1} = \boldsymbol{P} \tilde{\boldsymbol{\rho}}_n$.
4. Compute conditional state: $\boldsymbol{\rho}_{n+1} = \tilde{\boldsymbol{\rho}}_{n+1}|_{\boldsymbol{F}(x_{n+1})}$.

Lorenz 63 (after Palmer 2001)

$$\dot{a}_1 = 2.3\, a_1 - 6.2\, a_3 - 0.49\, a_1 a_2 - 0.57\, a_2 a_3$$
$$\dot{a}_2 = -62 - 2.7\, a_2 + 0.49\, a_1^2 - 0.49\, a_3^2 + 0.14\, a_1 a_3$$
$$\dot{a}_3 = -0.63\, a_1 - 13\, a_3 + 0.43\, a_1 a_2 + 0.49\, a_2 a_3$$

- (a_1, a_2, a_3): PCA coordinates.
- Resolved variables: $(a_1, a_2) = x \in \mathcal{X} \equiv \mathbb{R}^2$.
- Unresolved variables: $a_3 = y \in \mathcal{Y} \equiv \mathbb{R}$.
- Flux terms: $Z : \mathcal{Y} \to \mathbb{R}$, $Z(a_3) = a_3$.

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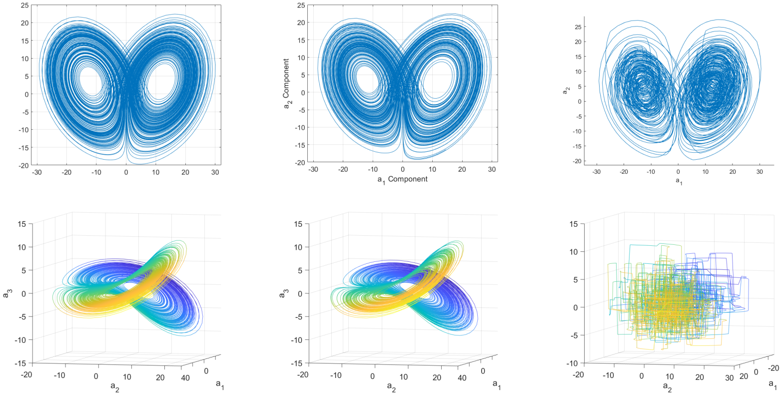
L63 system | **QM closure** | **Gaussian closure**



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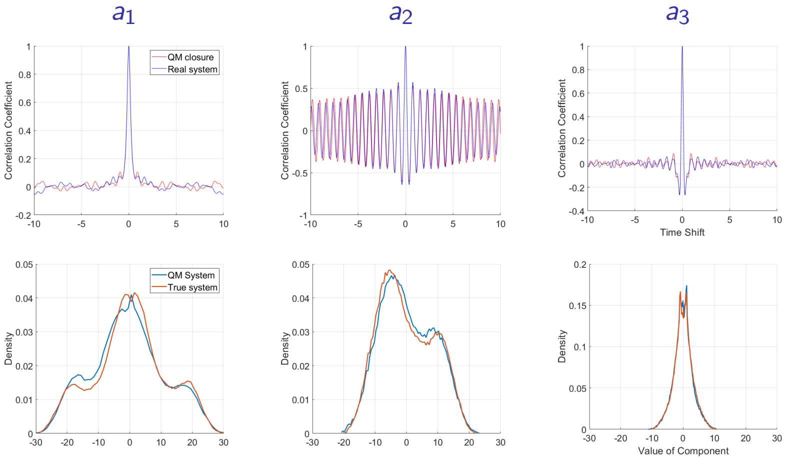

Lorenz 96 multiscale (after Fatkullin & Vanden-Eijnden 2004)

$$\dot{x}_k = -x_{k-1}(x_{k-2} - x_{k+1}) - x_k + F + \frac{h_x}{J}\sum_{j=1}^{J} y_{j,k}$$

$$\dot{y}_{j,k} = \frac{1}{\varepsilon}\left(-y_{j+1,k}(y_{j+2,k} - y_{j-1,k}) - y_{j,k} + h_y x_k\right)$$

- Resolved variables: $(x_k)_{k=1}^{J} = x \in \mathcal{X} \equiv \mathbb{R}^K$.
- Unresolved variables: $(y_{j,k})_{j,k=1}^{J,K} = y \in \mathcal{Y} \equiv \mathbb{R}^{JK}$.
- Flux terms: $Z : \mathcal{Y} \to \mathbb{R}^K$, $Z_k(y) = h_x \sum_{j=1}^{J} y_{j,k}/J$.
- Chaotic regime: $K = 9$, $J = 8$, $h_x = -0.8$, $h_y = 1.0$.

Lorenz 96 multiscale

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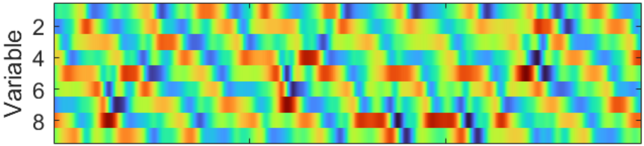
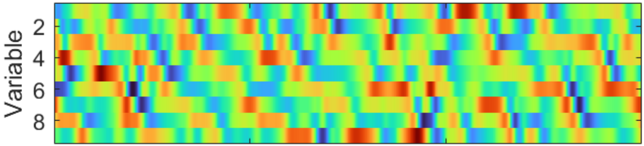


QM closure



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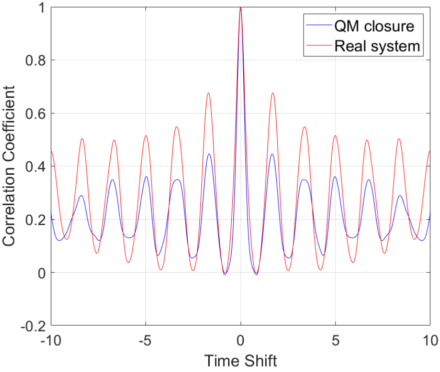

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