# Performance guarantees for deep Koopman autoencoders

Rachel Morris, Jason Bramburger, Simone Brugiapaglia

Université Concordia University Montréal

CRM Centre de Recherches Mathématiques

## Introduction

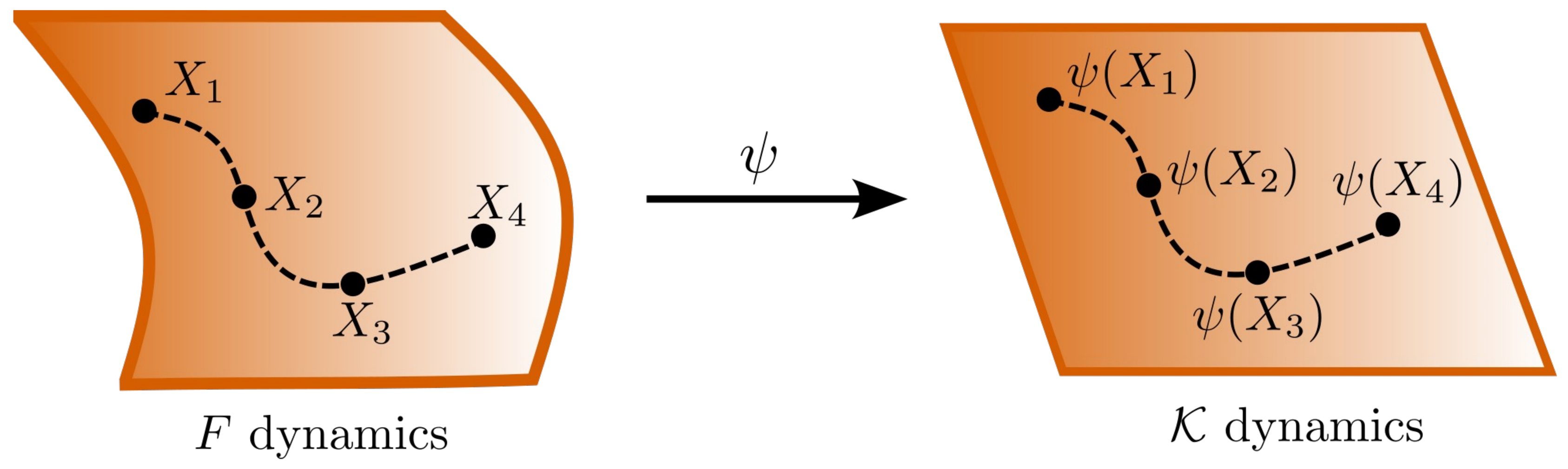
Any dynamical system (DS), $X_{j+1} = F(X_j)$, can be transformed into linear evolution via the appropriate coordinates.

$$\mathcal{K}[\mathrm{g}](X_j) = \psi\left(F(X_j)\right) = \psi(X_{j+1})$$

$\mathcal{K}$: Koopman operator $\quad$ $\mathrm{g} \in L^2$: observable function

$\mathcal{U}$: state space $\quad$ $\mathrm{F}: \mathcal{U} \to \mathcal{U}$ $\quad$ $\mathrm{g}: \mathcal{U} \to \mathbb{R}$

$\mathcal{K}$ defines an *$\infty$-dimensional* but *linear* DS on observables.




## Approximating the Koopman Spectrum

Koopman eigenfunctions provide *global geometric information* about the DS (ex. invariant manifolds as level sets of Koopman eigenfunctions).

$$\mathcal{K}[\phi_i](X_j) = \lambda_i \phi_i(X_j) = \phi_i(X_{j+1})$$

$\phi_i$: Koopman eigenfunction with eigenvalue $\lambda_i$

**Goal:** Approximate Koopman eigenfunctions from data to understand global dynamics

## Extended Dynamic Mode Decomposition[1] (EDMD)

Fix dictionary $\mathbf{\Psi}$, approximate eigenfunctions $\phi_i$ from data $\mathbf{X}, \mathbf{Y}$ by

| | | |
|---|---|---|
| In: $\mathbf{X} = \{X_1, \ldots, X_m\}$<br>$\mathbf{Y} = \{F(X_1), \ldots, F(X_m)\}$<br>Dictionary: $\mathbf{\Psi} = \{\psi_1, \ldots, \psi_\ell\}$ | Solve $\min_{\mathbf{Z} \in \mathbb{R}^{\ell \times \ell}} \lVert \mathbf{\Psi}(\mathbf{Y}) - \mathbf{\Psi}(\mathbf{X})\mathbf{Z} \rVert_F^2$<br>$\mathbf{\Psi}(\mathbf{X}) = (\psi_i(X_j))_{i,j=1}^{\ell,m}$<br>$\mathbf{\Psi}(\mathbf{Y}) = (\psi_i(X_{j+1}))_{i,j=1}^{\ell,m}$ | Out: $\phi_i(x) \approx \sum v_i \psi_i(x)$<br>$\mathbf{v}$ left eigenvector of $\mathbf{Z}$<br>$\phi_i, \mathbf{v}$ share eigenvalue $\lambda_i$ |

- EDMD converges[2] in the infinite data and infinite size limits.
- Finite EDMD approximation quality depends on $\mathbf{\Psi}$

**Idea: Use deep neural network (DNN) autoencoders to simultaneously step data forward in time and learn optimal dictionary[3].**

## Function Approximation and Neural Networks

**Universal Approximation Theorem (UAT)**: There *exists* a DNN that can accurately approximate a *continuous* function.

**Practical Existence Theorem**[4]: *Specifies* DNN architecture, training problem, and number of samples required to accurately approximate *analytic* functions.

**Koopman Autoencoder:**

DNN trained to satisfy $F \approx \mathcal{E} \circ \mathcal{T} \circ \mathcal{D}$

$\mathcal{E}$: encoder $\quad$ $\mathcal{T}$: (linear) time step

$\mathcal{D}$: decoder $\quad$ **Note:** $\mathcal{E} \circ \mathcal{D} \approx Id$

$$\begin{tikzcd}
\mathcal{U} \arrow[r, "F"] \arrow[d, shift right, "\mathcal{E}"'] & \mathcal{U} \arrow[d, shift right, "\mathcal{E}"'] \\
\mathcal{V} \arrow[r, "\mathcal{T}"'] \arrow[u, shift right, "\mathcal{D}"'] & \mathcal{V} \arrow[u, shift right, "\mathcal{D}"']
\end{tikzcd}$$

## Theorem: Koopman Autoencoder Guarantees[5]

For $m$ $\rho$-i.i.d. samples $\{X_j\}_{j=1}^m \subset [-1,1]^d$ of a DS, there exist

- class of ReLU DNNs $\mathcal{N}$, size scaling polynomially in $\tilde{m} = cm/(\log^3(m)\log(d))$ and
- regularization function $\mathcal{J}$ and parameter $\lambda > 0$

such that with high probability:

For all $\mathcal{K}[\mathbf{\Psi}]$ analytic in a suitable region with noisy evaluations $d_{ij} = \mathcal{K}[\psi_i](X_j) + \eta_{ij}$, the DNN approximation $\mathcal{K}_\Phi[\mathbf{\Psi}]$ trained according to

$$\min_{\Phi \in \mathcal{N}} \frac{1}{m} \sum_{i=1}^{\ell} \sum_{j=1}^{m} \left| \mathcal{K}_\Phi[\psi_i](X_j) - d_{ij} \right|^2 + \lambda \mathcal{J}(\Phi) \qquad (1)$$

is guaranteed to satisfy ($C_1, C_2$ universal constants)

$$\mathcal{L}_{\text{auto}} \le C_1(E_1 + E_2) \text{ and } \mathcal{L}_{\text{gen}} \le C_2(E_1 + E_2).$$

$$\mathcal{L}_{\text{auto}} = \frac{1}{m} \sum_{j=1}^{m} \lVert \mathcal{D}(\mathcal{E}(X_j)) - X_j \rVert_2^2 + \lVert \mathcal{D}(\mathcal{T}\mathcal{E}(X_j)) - \mathrm{F}(X_j) \rVert_2^2 + \lVert \mathcal{T}\mathcal{E}(X_j) - \mathcal{E}(\mathrm{F}(X_j)) \rVert_2^2$$

$$\mathcal{L}_{\text{gen}} = \lVert \mathcal{K}_\Phi[\mathbf{\Psi}] - \mathcal{K}[\mathbf{\Psi}] \rVert_{L_\rho^2(\mathcal{U})}$$

$E_1 = \ell \exp(-\gamma \tilde{m}^{1/(2d)}/\sqrt{2})$ **(Approximation error)**

$E_2 = \sum_{i=1}^{\ell} \lVert \mathbf{e}_i \rVert_2$ **(Measurement error)**

$\gamma > 0$ is a smoothness parameter and $\mathbf{e}_i = (\eta_{ij})_{j=1}^m$

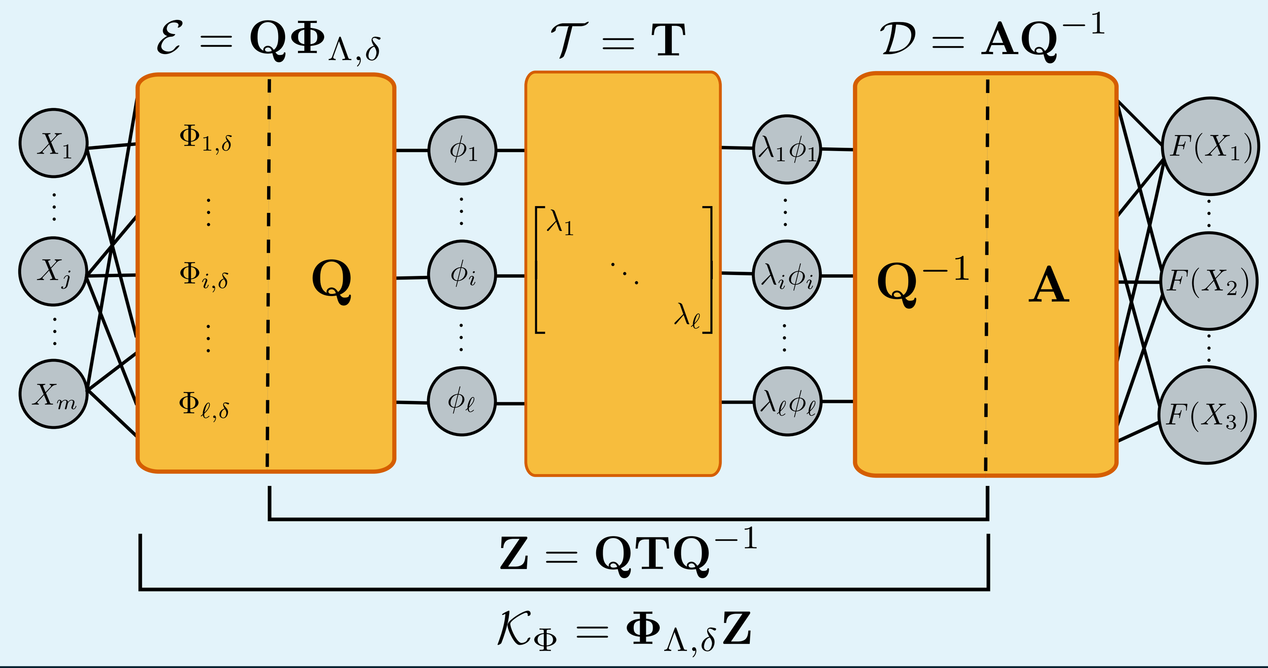
## Our Koopman Autoencoder

$\Phi_{\Lambda,\delta}$: Emulated polynomial basis of $\mathcal{V}$ up to $\delta$ accuracy

**Z**: Trainable weight matrix of $\Phi$, diagonalized $\mathbf{Z} = \mathbf{QTQ}^{-1}$

**A**: Projection matrix from latent space to $\mathcal{U}$

$\mathbf{\Phi}$:




## Conclusion

First theoretical result ensuring accuracy of DNN Koopman approximations.

- (1) corresponds to a new, *weighted-sparse EDMD* problem

$$\min_{\mathbf{Z} \in \mathbf{R}^{\ell \times \ell}} \lVert \mathbf{\Psi}(\mathbf{Y}) - \mathbf{\Psi}(\mathbf{X})\mathbf{Z} \rVert_2^2 + \lambda \lVert \mathbf{Z} \rVert_{F,1,\mathbf{w}}$$

with $\lVert \cdot \rVert_{F,1,\mathbf{w}} = \sum w_i |z_{ij}|$, $\mathbf{w} \in \mathbb{R}^\ell$.

- Novel *matrix LASSO setting* for practical existence theory

References

[1]Williams et al. **A Data-Driven Approximation of the Koopman Operator: Extending Dynamic Mode Decomposition** (2017).

[2]Korda and Mezić **On Convergence of Extended Dynamic Mode Decomposition to the Koopman Operator** (2017).

[3]Li et al. **Extended dynamic mode decomposition with dictionary learning: a data-driven adaptive spectral decomposition of the Koopman operator** (2017).

[4]Adcock et al.**Learning smooth functions in high dimensions** (2024).

[5]Morris et al. **Performance Guarantees and Training Strategies for Koopman Neural Networks** In prep.