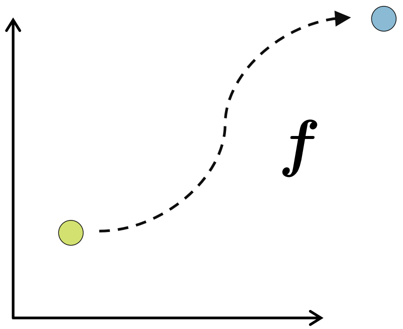
Learning Neural Observables for Koopman Operators

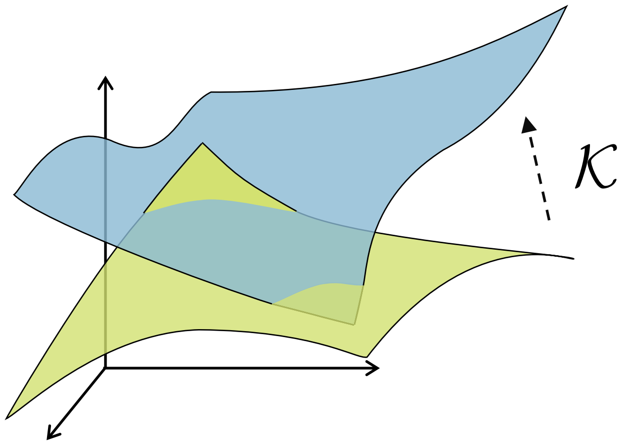
Naoya Takeishi (UTokyo)

Workshop on Koopman Operators in Robotics, RSS 2024
2024-07-15

Koopman operators



$$\boldsymbol{x}_{t+1} = \boldsymbol{f}(\boldsymbol{x}_t)$$



$$g(\boldsymbol{f}(\boldsymbol{x})) = \mathcal{K} g(\boldsymbol{x})$$

- Linear (but infinite-dimensional) representation
  - Useful for spectral analysis, long-range prediction, control, …
  - Does it make sense to call something "Koopman" simply because it is linear? 🤔

Observables

$$g(\boldsymbol{f}(\boldsymbol{x})) = \mathcal{K}g(\boldsymbol{x}), \quad g \in \mathcal{G}$$

- We want a finite-dimensional function space $\mathcal{D} \subset \mathcal{G}$ invariant to $\mathcal{K}$'s action
  - or something close, in some sense, to invariant

$$\dim \mathcal{D} = d < \infty \quad \text{and} \quad \forall g \in \mathcal{D},\ \mathcal{K}g \in \mathcal{D}$$

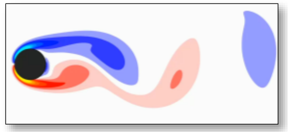
- with which we have a matrix representation of $\mathcal{K}$

$$g = \sum_{i=1}^{d} a_i e_{\mathcal{D},i} \in \mathcal{D}, \quad \mathcal{K}g = \sum_{i=1}^{d} b_i e_{\mathcal{D},i} \in \mathcal{D}, \quad \begin{bmatrix} b_1 \\ \vdots \\ b_d \end{bmatrix} = \boldsymbol{K} \begin{bmatrix} a_1 \\ \vdots \\ a_d \end{bmatrix}$$

Designing observables

- Identity function

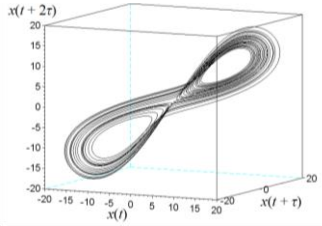
$$\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{x}$$



  - ➢ Practically works well especially when x is high-dimensional

- Time delay embedding

$$\boldsymbol{g}_t = \begin{bmatrix} \boldsymbol{x}_t^\top & \boldsymbol{x}_{t-1}^\top & \cdots & \boldsymbol{x}_{t-k+1}^\top \end{bmatrix}^\top$$



  - ➢ cf. Taken's embedding theorem
  - ➢ Popularly used in DMD / Koopman too (Hankel DMD)
    [Brunton+ 17; Das & Giannakis 19; Kamb+ 20; etc]

Designing observables

- Predefined basis functions

$$\boldsymbol{g}(\boldsymbol{x}) = \left[g_1(\boldsymbol{x}), \dots, g_d(\boldsymbol{x})\right]^\top, \quad \forall i \; g_i \in \mathcal{D}$$

  - ➢ extended DMD [Williams+ 15]
    - dictionary $\mathcal{D}$ as a set of polynomials, RBFs centered on datapoints, etc.

- Observables in RKHS

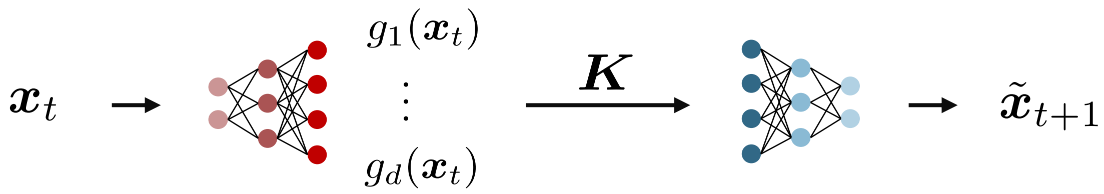
$$\forall g \in \mathcal{G},\ \exists k(\boldsymbol{x}, \cdot) \in \mathcal{G} \quad \text{s.t.} \quad \langle g, k(\boldsymbol{x}, \cdot)\rangle_{\mathcal{G}} = g(\boldsymbol{x})$$

  - ➢ kernel DMD [Williams+ 16; Kawahara 16; etc.]
  - ➢ analysis of the Koopman operator on RKHS
  - ➢ cf. observables as Gaussian process [Lian & Jones 19; — 22; Kawashima & Hino 23]

Designing observables

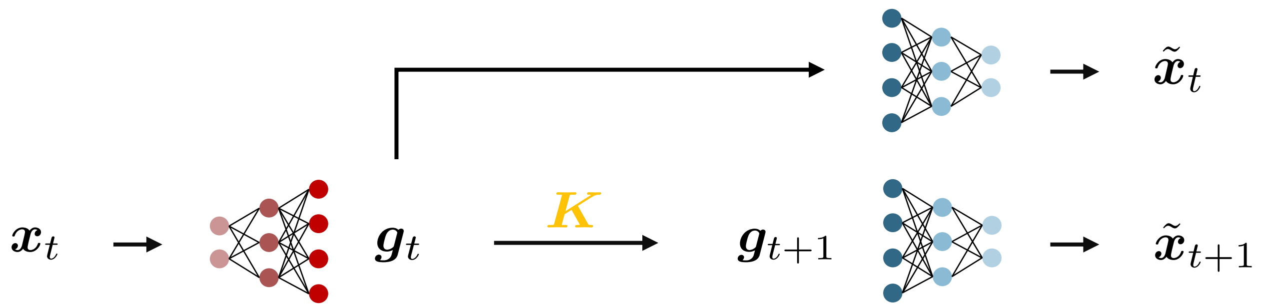
- Neural networks

$$\boldsymbol{g}(\boldsymbol{x}) = \left[g_1(\boldsymbol{x}), \ldots, g_d(\boldsymbol{x})\right]^\top = \mathrm{NN}(\boldsymbol{x}; \theta)$$



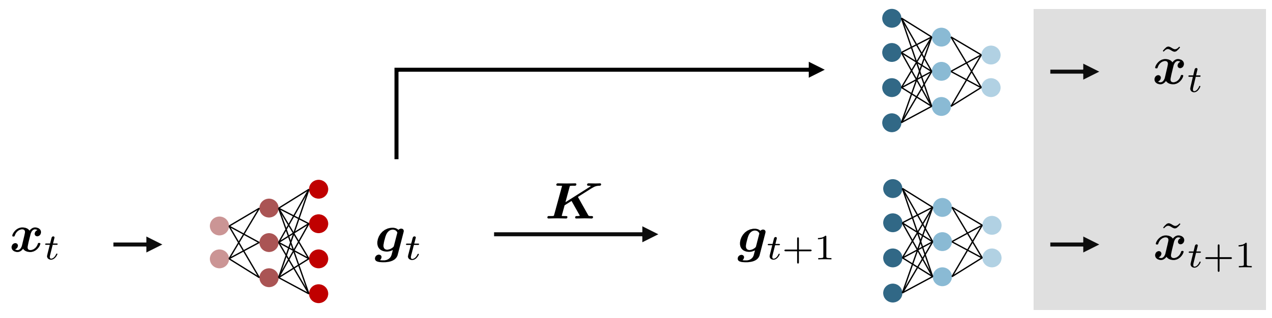
- ➢ Learn a neural net spanning a Koopman invariant subspace
- ➢ $\boldsymbol{g}(\boldsymbol{x})$ must retain the information of x
- ➢ Active research in these 8 years; what networks / loss / … were used there?

Basic architecture



- Encoder maps $\boldsymbol{x}$ to $\boldsymbol{g}$
- Decoder should reconstruct $\boldsymbol{x}$ given $\boldsymbol{g}$
- $\boldsymbol{g}$'s temporal transition should be linear, represented by a matrix $\boldsymbol{K}$

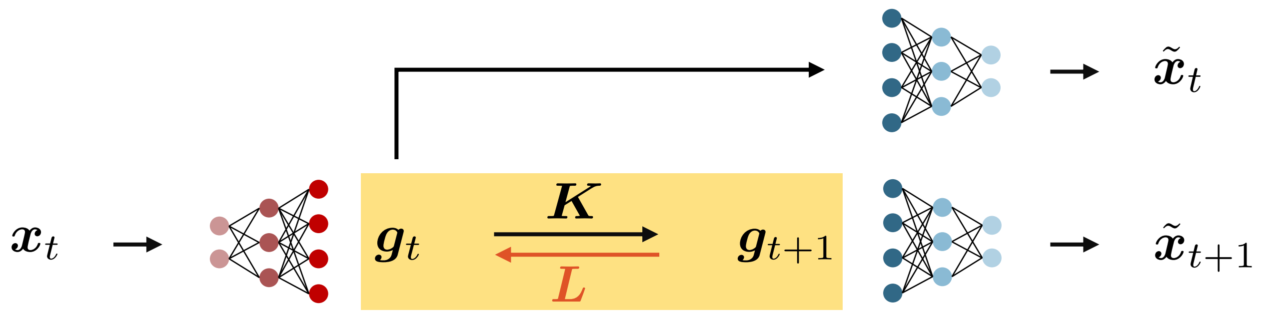
Loss functions



- For reconstruction, simply:

$$\text{minimize} \quad \|\tilde{\boldsymbol{x}}_t - \boldsymbol{x}\|^2$$

Loss functions



- For Koopman invariantness:
  - Residual of linear prediction [Takeishi+ 17; Li+ 17; Lusch+ 18; Morton+ 18; Yeung+ 19; Otto & Rowley 19; etc.]

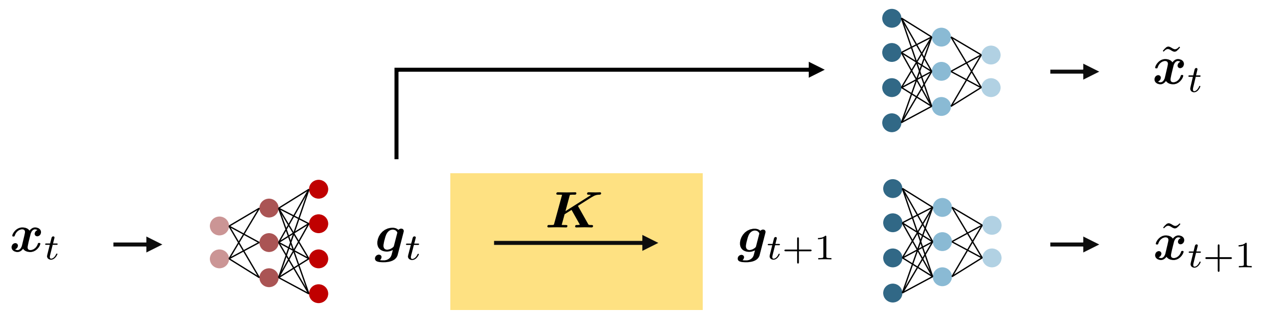
$$\text{minimize} \ \ \|\boldsymbol{g}_{t+1} - \boldsymbol{K}\boldsymbol{g}_t\|^2$$

  - Forward-backward consistency [Morton+ 19; Azencot+ 20; Tayal+ 23; Haseli & Cortés 23]

$$\text{minimize} \ \ \|\boldsymbol{I} - \boldsymbol{K}\boldsymbol{L}\|^2$$

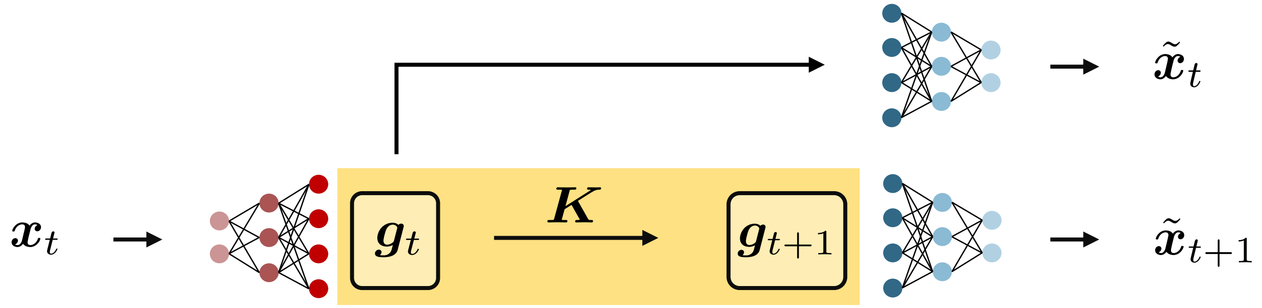
  - CCA-like formulation [Mardt+ 18; Wu & Noé 20; etc.]

Architectures: K's parametrization



- K as a trainable linear layer [Li+ 17; Lusch+ 18; Yeung+ 19; Azencot+ 20; etc.]
  - ➢ Practically simple and works stably
  - ➢ Miller+ 22 pointed out that the initialization methods used for NNs result in inappropriate eigenvalues of K

Architectures: K's parametrization

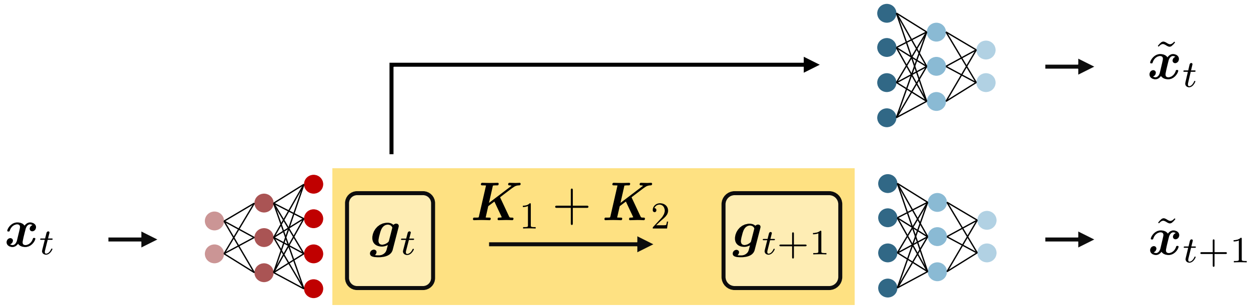


- $\boldsymbol{K}$ computed by least squares [Takeishi+ 17; Morton+ 18; Otto & Rowley 19; etc.]

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{g}_{t_1} & \cdots & \boldsymbol{g}_{t_{n-1}} \end{bmatrix} \begin{bmatrix} \boldsymbol{g}_{t_2} & \cdots & \boldsymbol{g}_{t_n} \end{bmatrix}^{\dagger}$$

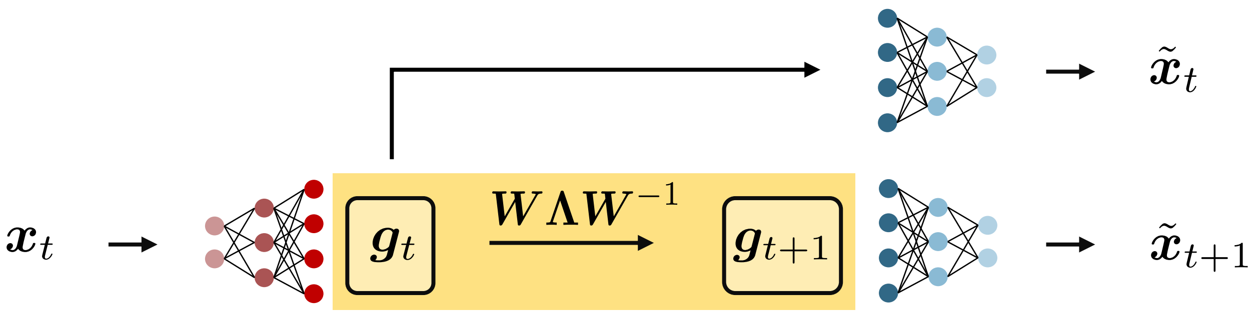
  - ➢ Theoretically simpler but mini-batching becomes a little tricky

Architectures: K's parametrization



- Combination of the two [Lin+ 23]
  - K_1 as a trainable layer
    - works as time-invariant component
  - K_2 computed locally by least squares
    - works as time-variant component

Architectures: K's parametrization



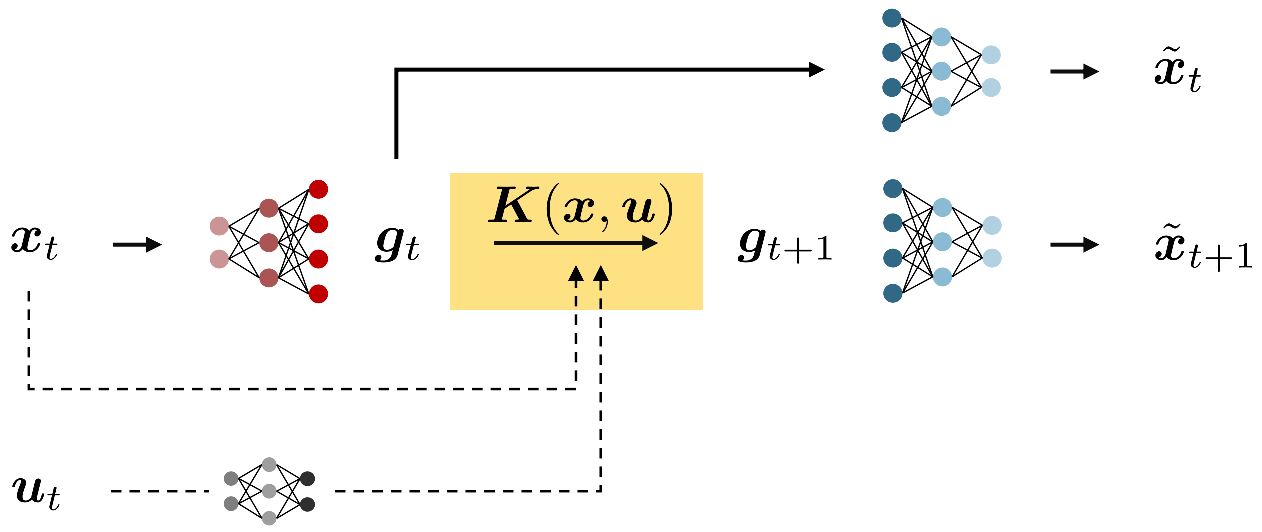
- Eigendecomposed $\boldsymbol{K}$ [Li+ 21; Alford-Lago+ 22; Iwata & Kawahara 23]

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{g}_{t_1} & \cdots & \boldsymbol{g}_{t_{n-1}} \end{bmatrix} \begin{bmatrix} \boldsymbol{g}_{t_2} & \cdots & \boldsymbol{g}_{t_n} \end{bmatrix}^{\dagger}$$

$$\boldsymbol{\Lambda}, \boldsymbol{W} = \mathrm{eig}(\boldsymbol{K})$$

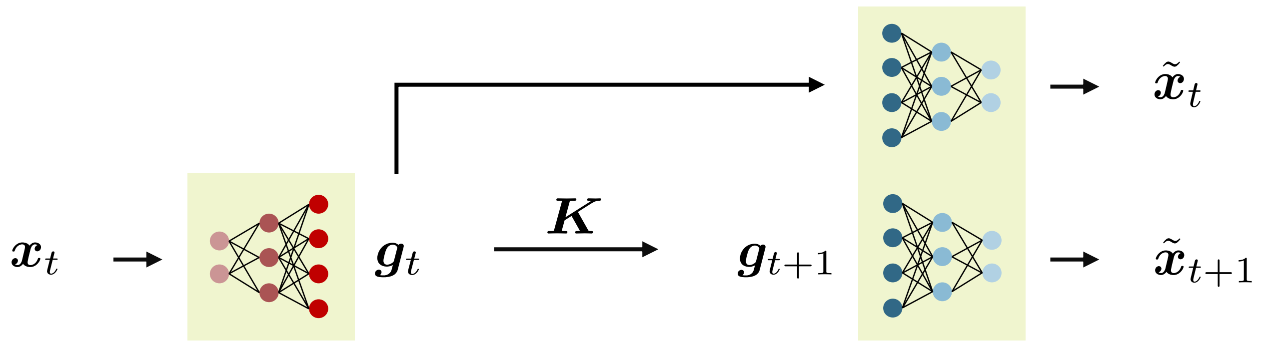
  - ➢ Can impose low-rank structure
  - ➢ Can use inductive bias on eigenvalues
  - ➢ Advantageous in computing multi-step prediction loss

Architectures: K's parametrization



- Parametrized $\boldsymbol{K}$ [Lusch+ 18; Guo+ 23; etc.]
  - i.e., locally linear model
  - State-dependent eigenvalues for chaotic systems [Lusch+ 18]
  - Input-dependent $\boldsymbol{K}$ for taking control inputs into account [Guo+ 23]

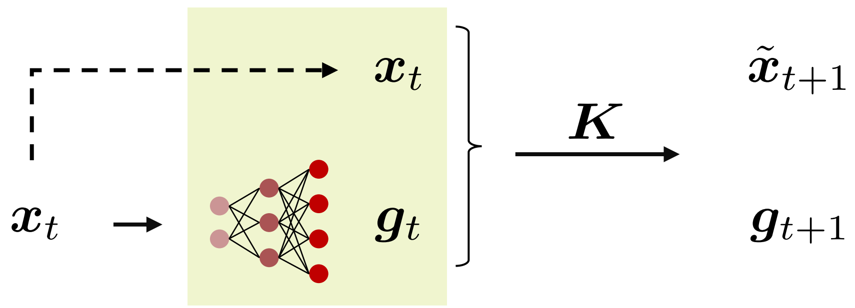
Architecture: Observable networks



- A standard choice is networks w/ fully-connected layers (MLPs)
- Arbitrary networks can be used in principle
  - ➢ Depending on the type of inputs, e.g., CNN for images
  - ➢ Use of graph neural nets [Xie+ 19; Li+ 20; etc.]

- Auto-encoding inevitably causes reconstruction errors 🙁

Architecture: Observable networks

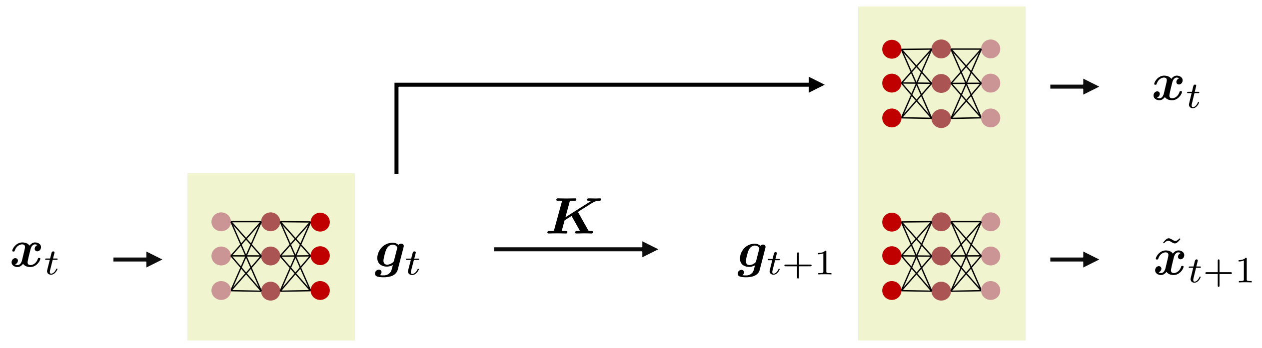


- State-inclusive form [Brunton+ 16; — 22; Fan+ 22; Johnson+ 22; etc.]

$$\boldsymbol{x} \mapsto \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{g}(\boldsymbol{x}) \end{bmatrix}$$

  - ➢ No need for reconstruction
  - ➢ May have limited expressivity
    - A space topologically conjugate to the space of x cannot have general attractors like multiple fixed points [Brunton+ 16]

Architecture: Observable networks

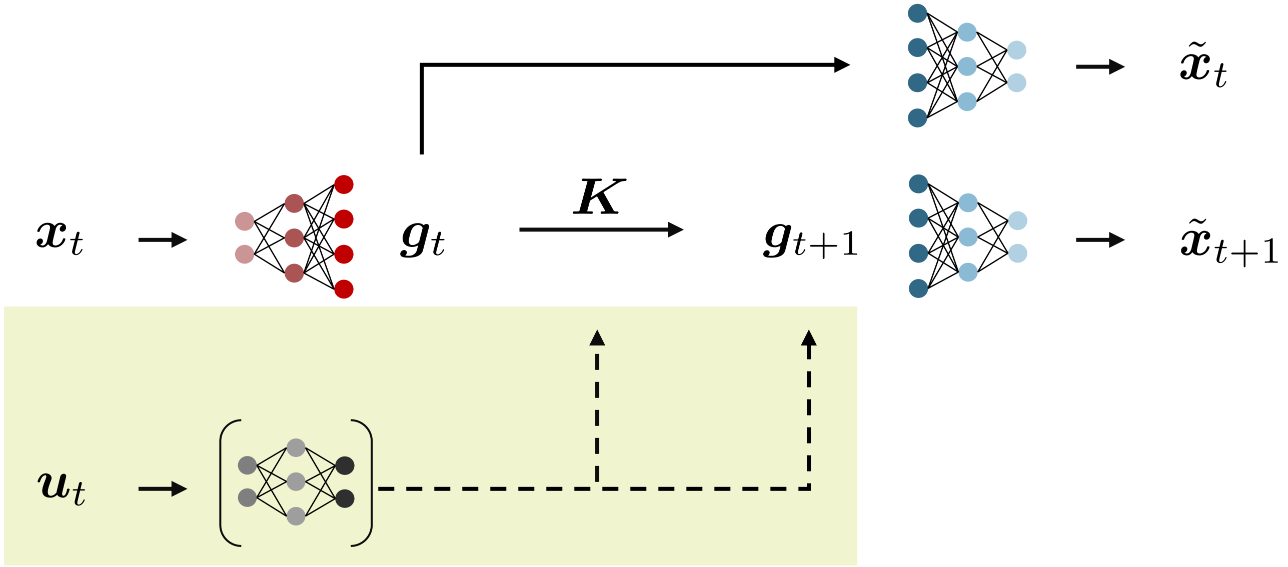


- Invertible neural nets [Jin+ 23; Meng+ 24]

$$\boldsymbol{g} : \boldsymbol{x} \mapsto \boldsymbol{g}(\boldsymbol{x}) \quad \text{s.t.} \quad \boldsymbol{g}^{-1} \text{ exists and can be easily computed}$$

  - No need to learn reconstruction
  - Homeomorphism would face difficulty similar to the state-inclusive form, though

Architecture: Non-observable networks



- With control inputs

  [Morton+ 18; Bonnert & Konigorski 20; Han+ 22; Guo+ 23; Uchida & Duraisamy 23; Wang+ 24]

$$\boldsymbol{g}_{t+1} = \boldsymbol{K}\boldsymbol{g}_t + \boldsymbol{h}(\boldsymbol{u}_t)$$

  - ➢ slight variants: $\boldsymbol{h}$ linear or nonlinear, $\boldsymbol{K}$ parametrized by $\boldsymbol{u}$ or not, etc.

Summary

- Koopman operator + neural networks
  - Active studies in the past 8 years
  - Many variants
    - loss function
    - K's parametrization
    - observable network
  - Highly dependent on problem settings

- Remaining challenges
  - Global / switching observables for systems with contacts;
  - Uncertainty quantification;
  - Controllability; Online training; etc.

Slides available at https://ntake.jp/

References 1/3

[Alford-Lago+ 22] D. J. Alford-Lago, C. W. Curtis, A. T. Ihler, O. Issan: Deep learning enhanced dynamic mode decomposition, Chaos: An Interdisciplinary Journal of Nonlinear Science, vol. 32, no. 3, p. 033116, 2022.

[Azencot+ 20] O. Azencot, N. B. Erichson, V. Lin, M. W. Mahoney: Forecasting sequential data using consistent Koopman autoencoders, Proceedings of the 37th International Conference on Machine Learning, 2020, pp. 475–485.

[Balkrishnan & Upadhyay 21] K. Balakrishnan, D. Upadhyay: Stochastic adversarial Koopman model for dynamical systems. arXiv:2109.05095.

[Bonnert & Konigorski 20] M. Bonnert, U. Konigorski: Estimating Koopman invariant subspaces of excited systems using artificial neural networks, IFAC-PapersOnLine, vol. 53, no. 2, pp. 1156–1162, 2020.

[Brunton+ 16] S. L. Brunton, B. W. Brunton, J. L. Proctor, J. N. Kutz: Koopman invariant subspaces and finite linear representations of nonlinear dynamical systems for control, PLOS ONE, vol. 11, no. 2, p. e0150171, 2016.

[Brunton+ 17] S. L. Brunton, B. W. Brunton, J. L. Proctor, E. Kaiser, J. N. Kutz: Chaos as an intermittently forced linear system, Nature Communications, vol. 8, no. 1, p. 19, 2017.

[Brunton+ 22] S. L. Brunton, M. Budišić, E. Kaiser, J. N. Kutz: Modern Koopman theory for dynamical systems, SIAM Review, vol. 64, no. 2, pp. 229–340, 2022.

[Das & Giannakis 19] S. Das, D. Giannakis: Delay-coordinate maps and the spectra of Koopman operators, Journal of Statistical Physics, vol. 175, no. 6, pp. 1107–1145, 2019.

[Fan+ 22] F. Fan, B. Yi, D. Rye, G. Shi, I. R. Manchester: Learning stable Koopman embeddings, Proceedings of the 2022 American Control Conference, 2022, pp. 2742–2747.

[Gin+ 21] C. Gin, B. Lusch, S. L. Brunton, J. N. Kutz: Deep learning models for global coordinate transformations that linearise PDEs, European Journal of Applied Mathematics, vol. 32, no. 3, pp. 515–539, 2021.

[Guo+ 23] Y. Guo, M. Korda, I. G. Kevrekidis, Q. Li: Learning parametric Koopman decompositions for prediction and control. arXiv:2310.01124.

[Gupta+ 23] P. Gupta, P. J. Schmid, D. Sipp, T. Sayadi, G. Rigas: Mori-Zwanzig latent space Koopman closure for nonlinear autoencoder. arXiv:2310.10745.

[Han+ 22] M. Han, J. Euler-Rolle, R. K. Katzschmann: DeSKO: Stability-assured robust control with a deep stochastic Koopman operator, Proceedings of the 10th International Conference on Learning Representations, 2022.

[Haseli & Cortés 23] M. Haseli, J. Cortés: Temporal forward-backward consistency, not residual error, measures the prediction accuracy of extended dynamic mode decomposition, IEEE Control Systems Letters, vol. 7, pp. 649–654, 2023.

References 2/3

[Iwata & Kawahara 23] T. Iwata, Y. Kawahara: Neural dynamic mode decomposition for end-to-end modeling of nonlinear dynamics, Journal of Computational Dynamics, vol. 10, no. 2, pp. 268–280, 2023.

[Johnson+ 18] C. A. Johnson, E. Yeung: A class of logistic functions for approximating state-inclusive Koopman operators, Proceedings of the 2018 Annual American Control Conference, 2018, pp. 4803–4810.

[Johnson+ 22] C. A. Johnson, S. Balakrishnan, E. Yeung: Learning invariant subspaces of Koopman operators--Part 1: A methodology for demonstrating a dictionary's approximate subspace invariance. arXiv:2212.07358.

[Kamb+ 20] M. Kamb, E. Kaiser, S. L. Brunton, J. N. Kutz: Time-delay observables for Koopman: Theory and applications, SIAM Journal on Applied Dynamical Systems, vol. 19, no. 2, pp. 886–917, 2020.

[Kawahara 16] Y. Kawahara: Dynamic mode decomposition with reproducing kernels for Koopman spectral analysis, Advances in Neural Information Processing Systems 29, 2016, pp. 911–919.

[Kawashima & Hino 23] T. Kawashima, H. Hino: Gaussian process Koopman mode decomposition, Neural Computation, vol. 35, no. 1, pp. 82–103, 2023.

[Li & Jiang 21] M. Li, L. Jiang: Deep learning nonlinear multiscale dynamic problems using Koopman operator, Journal of Computational Physics, vol. 446, p. 110660, 2021.

[Li+ 17] Q. Li, F. Dietrich, E. M. Bollt, I. G. Kevrekidis: Extended dynamic mode decomposition with dictionary learning: A data-driven adaptive spectral decomposition of the Koopman operator, Chaos: An Interdisciplinary Journal of Nonlinear Science, vol. 27, no. 10, p. 103111, 2017.

[Li+ 20] Y. Li, H. He, J. Wu, D. Katabi, A. Torralba: Learning compositional Koopman operators for model-based control, Proceedings of the 8th International Conference on Learning Representations, 2020.

[Lian & Jones 19] Y. Lian, C. N. Jones: Learning feature maps of the Koopman operator: A subspace viewpoint, Proceedings of the IEEE 58th Conference on Decision and Control, 2019, pp. 860–866.

[Liand & Jones 20] Y. Lian, C. N. Jones: On Gaussian process based Koopman operators, IFAC-PapersOnLine, vol. 53, no. 2, pp. 449–455, 2020.

[Liu+ 23] Y. Liu, C. Li, J. Wang, M. Long: Koopa: Learning non-stationary time series dynamics with Koopman predictors, Advances in Neural Information Processing Systems 36, 2023, pp. 12271–12290.

[Lusch+ 18] B. Lusch, J. N. Kutz, S. L. Brunton: Deep learning for universal linear embeddings of nonlinear dynamics, Nature Communications, vol. 9, no. 1, p. 4950, 2018.

[Mardt+ 18] A. Mardt, L. Pasquali, H. Wu, F. Noé: VAMPnets for deep learning of molecular kinetics, Nature Communications, vol. 9, no. 1, p. 5, 2018.

References 3/3

[Meng+ 24] Y. Meng, J. Huang, Y. Qiu: Koopman operator learning using invertible neural networks, Journal of Computational Physics, vol. 501, p. 112795, 2024.

[Miler+ 22] J. W. Miller, C. O'Neill, N. C. Constantinou, O. Azencot: Eigenvalue initialisation and regularisation for Koopman autoencoders. arXiv:2212.12086.

[Morton+ 18] J. Morton, A. Jameson, M. J. Kochenderfer, F. Witherden: Deep dynamical modeling and control of unsteady fluid flows, Advances in Neural Information Processing Systems 31, 2018, pp. 9258–9268.

[Morton+ 19] J. Morton, F. D. Witherden, M. J. Kochenderfer: Deep variational Koopman models: Inferring Koopman observations for uncertainty-aware dynamics modeling and control, Proceedings of the 28th International Joint Conference on Artificial Intelligence, 2019, pp. 3173–3179.

[Otto & Rowley 19] S. E. Otto, C. W. Rowley: Linearly recurrent autoencoder networks for learning dynamics, SIAM Journal on Applied Dynamical Systems, vol. 18, no. 1, pp. 558–593, 2019.

[Takeishi+ 17] N. Takeishi, Y. Kawahara, T. Yairi: Learning Koopman invariant subspaces for dynamic mode decomposition, Advances in Neural Information Processing Systems 30, 2017, pp. 1130–1140.

[Tayal 23] K. Tayal, A. Renganathan, R. Ghosh, X. Jia, V. Kumar: Koopman invertible autoencoder: Leveraging forward and backward dynamics for temporal modeling, Proceedings of the 2023 IEEE International Conference on Data Mining, 2023, pp. 588–597.

[Uchida & Duraisamy 23] D. Uchida, K. Duraisamy: Extracting Koopman operators for prediction and control of non-linear dynamics using two-stage learning and oblique projections. arXiv:2308.13051.

[Wang+ 24] M. Wang, X. Lou, B. Cui: Deep bilinear Koopman realization for dynamics modeling and predictive control, International Journal of Machine Learning and Cybernetics, 2024.

[Williams+ 15] M. O. Williams, I. G. Kevrekidis, C. W. Rowley: A data-driven approximation of the Koopman operator: Extending dynamic mode decomposition, Journal of Nonlinear Science, vol. 25, no. 6, pp. 1307–1346, 2015.

[Willaims+ 16] M. O. Williams, C. W. Rowley, I. G. Kevrekidis: A kernel-based method for data-driven Koopman spectral analysis, Journal of Computational Dynamics, vol. 2, no. 2, pp. 247–265, 2016.

[Wu & Noé 20] H. Wu, F. Noé: Variational approach for learning Markov processes from time series data, Journal of Nonlinear Science, vol. 30, no. 1, pp. 23–66, 2020.

[Xie+ 19] T. Xie, A. France-Lanord, Y. Wang, Y. Shao-Horn, J. C. Grossman: Graph dynamical networks for unsupervised learning of atomic scale dynamics in materials, Nature Communications, vol. 10, no. 1, p. 2667, 2019.

[Yeung+ 19] E. Yeung, S. Kundu, N. Hodas: Learning deep neural network representations for Koopman operators of nonlinear dynamical systems, Proceedings of the 2019 American Control Conference, 2019, pp. 4832–4839.