Foundations of Differentiable Programming in Probabilistic Models

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Differentiable Programming

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- (over-)parameterized models trained in an end-to-end fashion to minimize a loss function
- Models are differentiable. Training is through gradient-based optimization.

Why Differentiable Programming?

Mnih et al. 13; Jumper et al. 21; Dosovitskiy et al. 20

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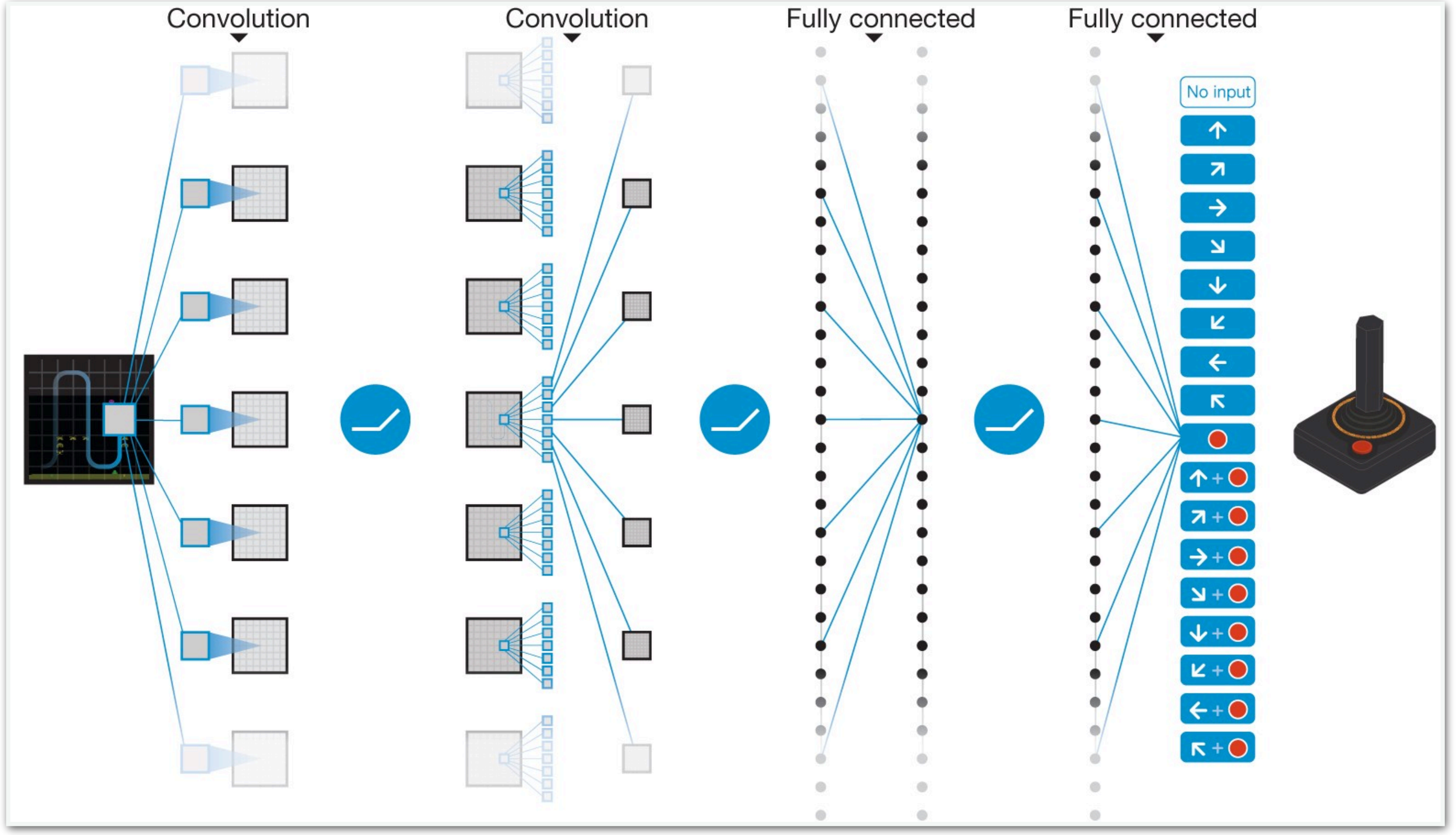

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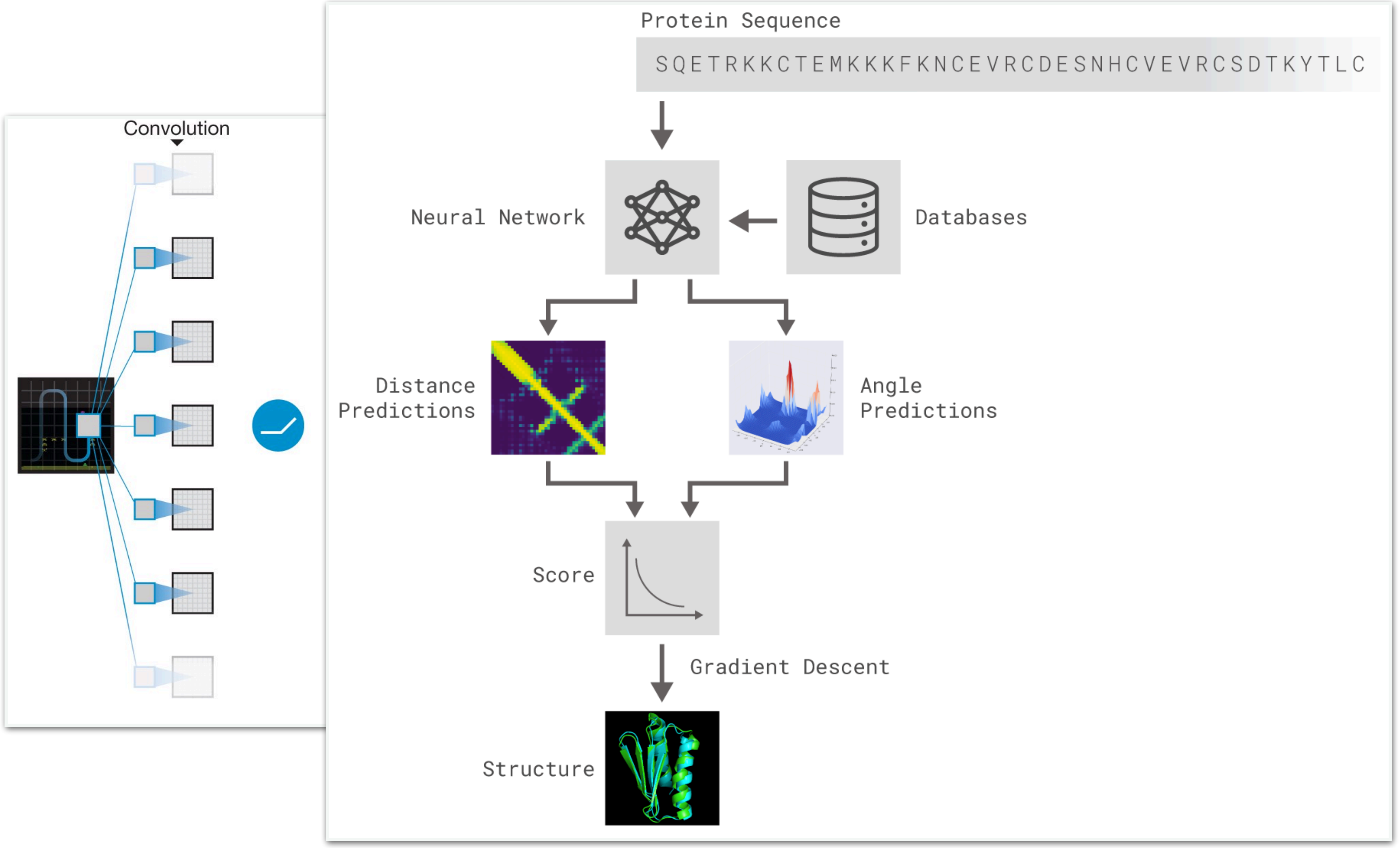

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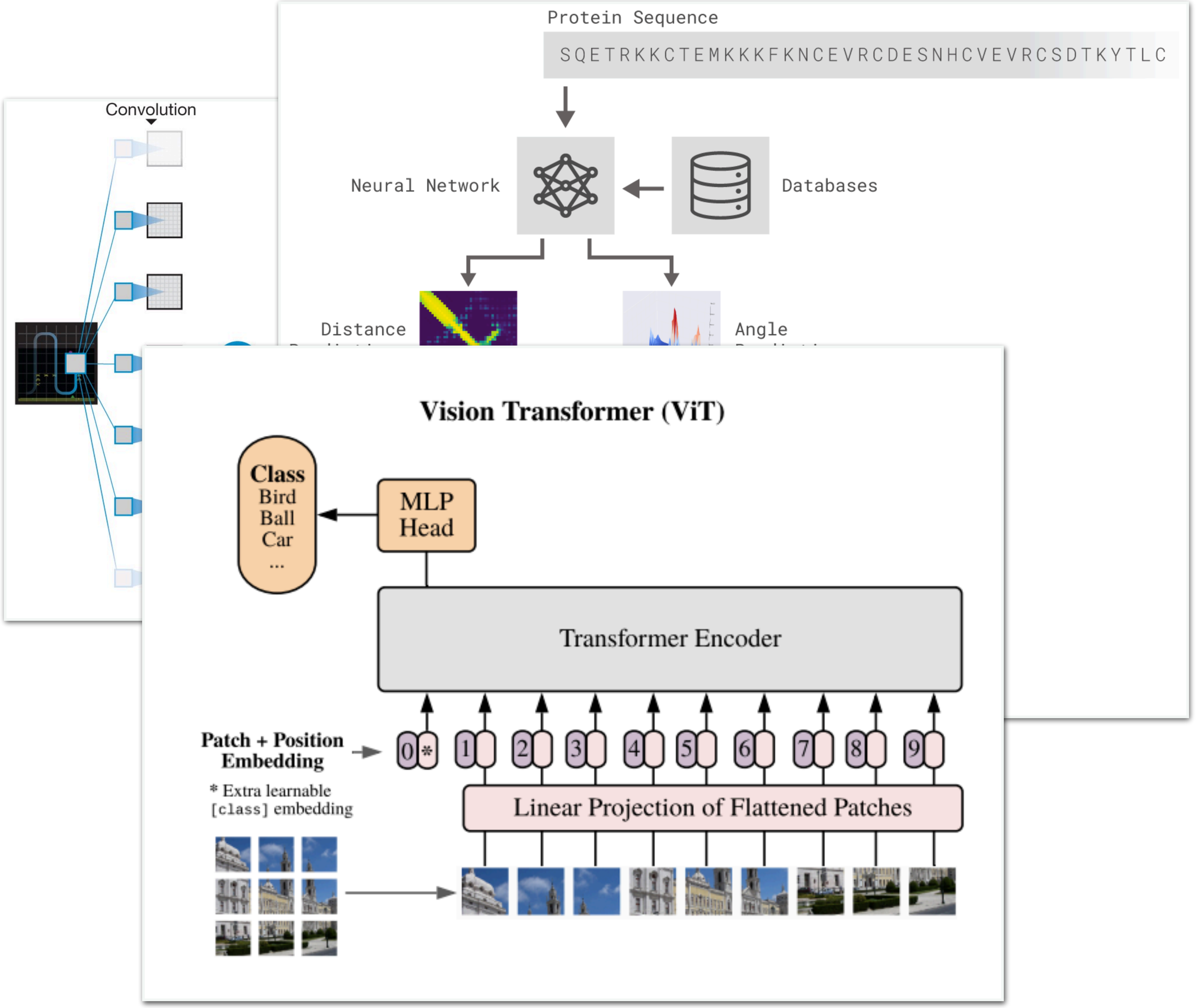

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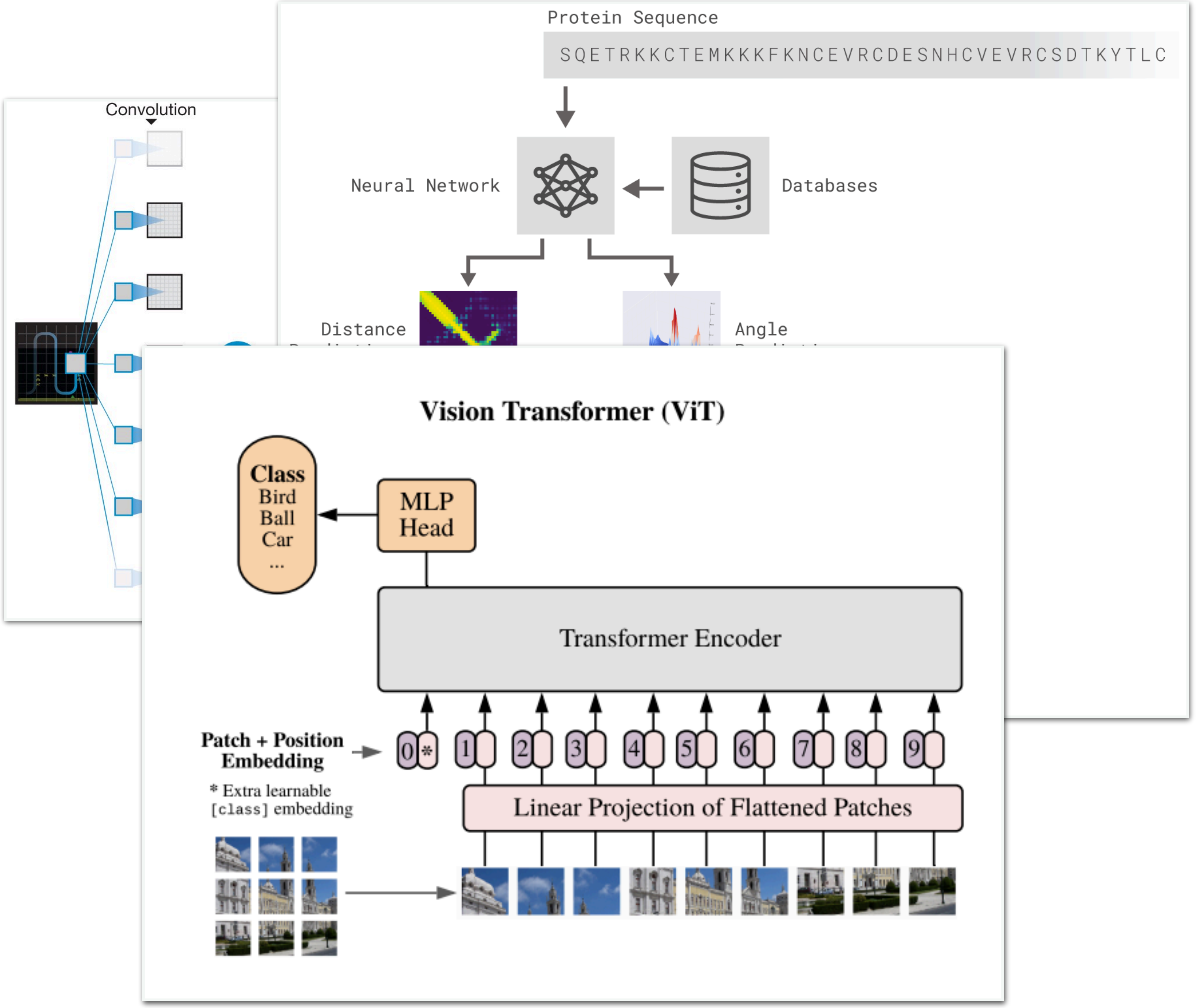
Why Differentiable Programming?

- Expressiveness



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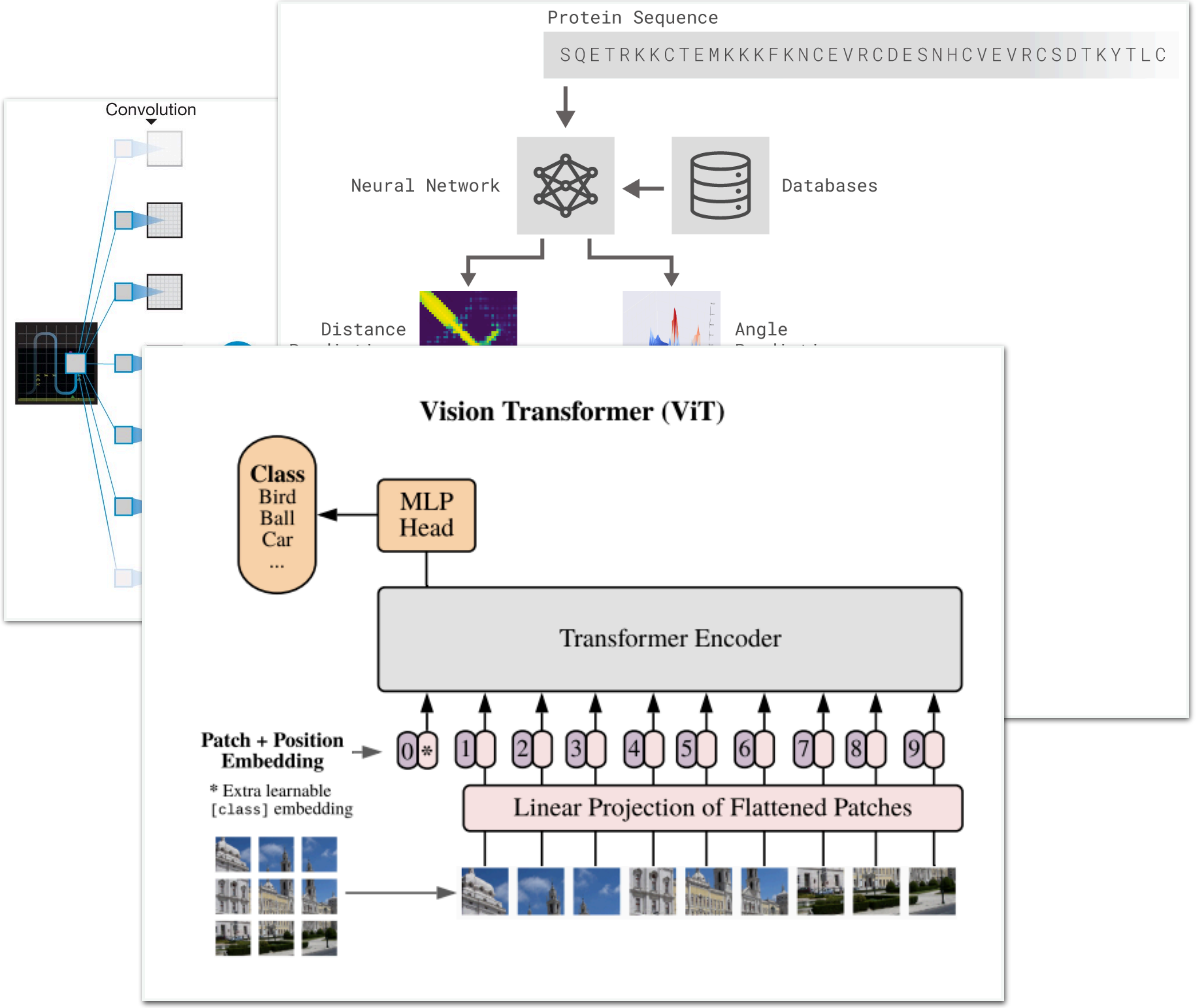

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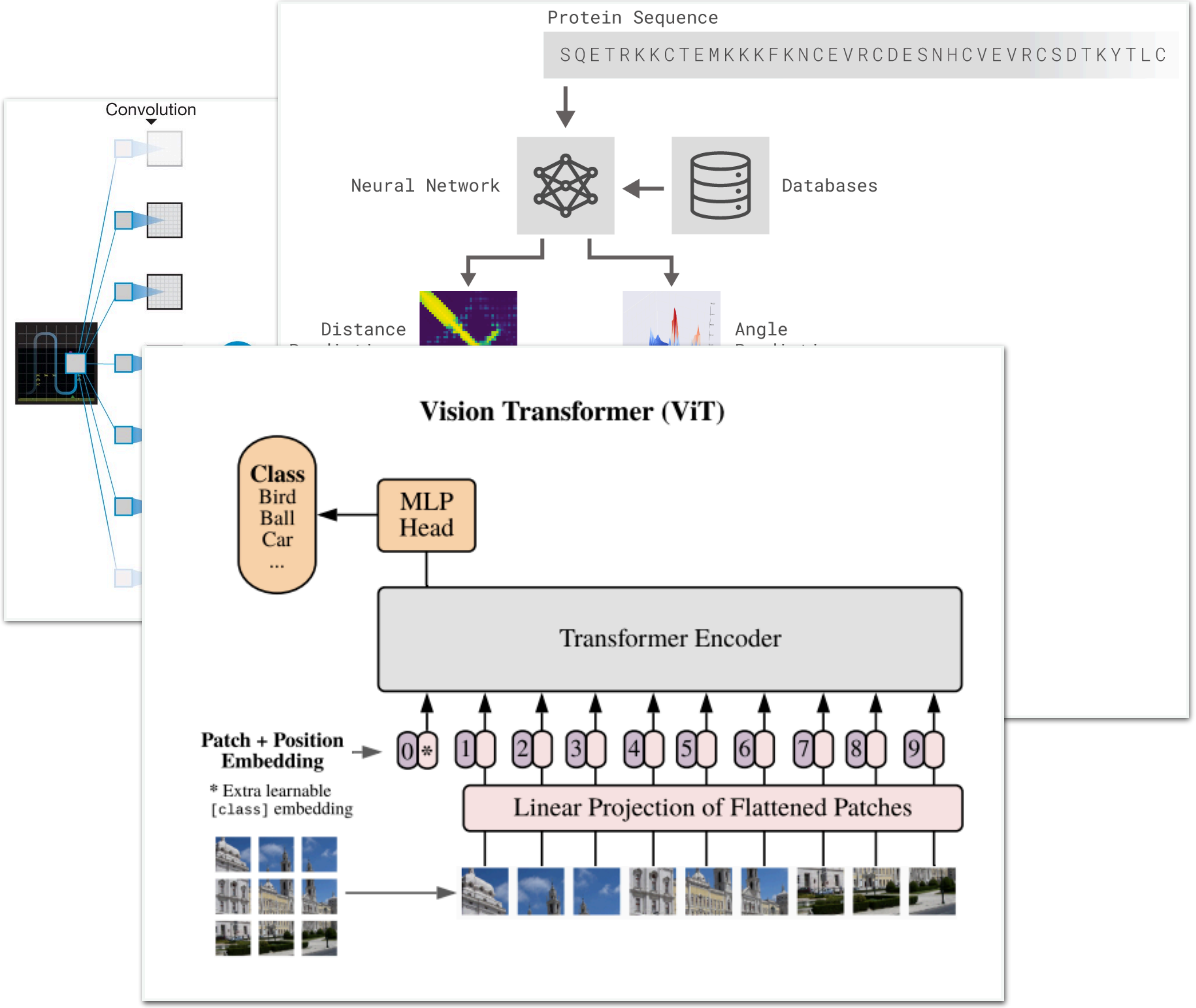

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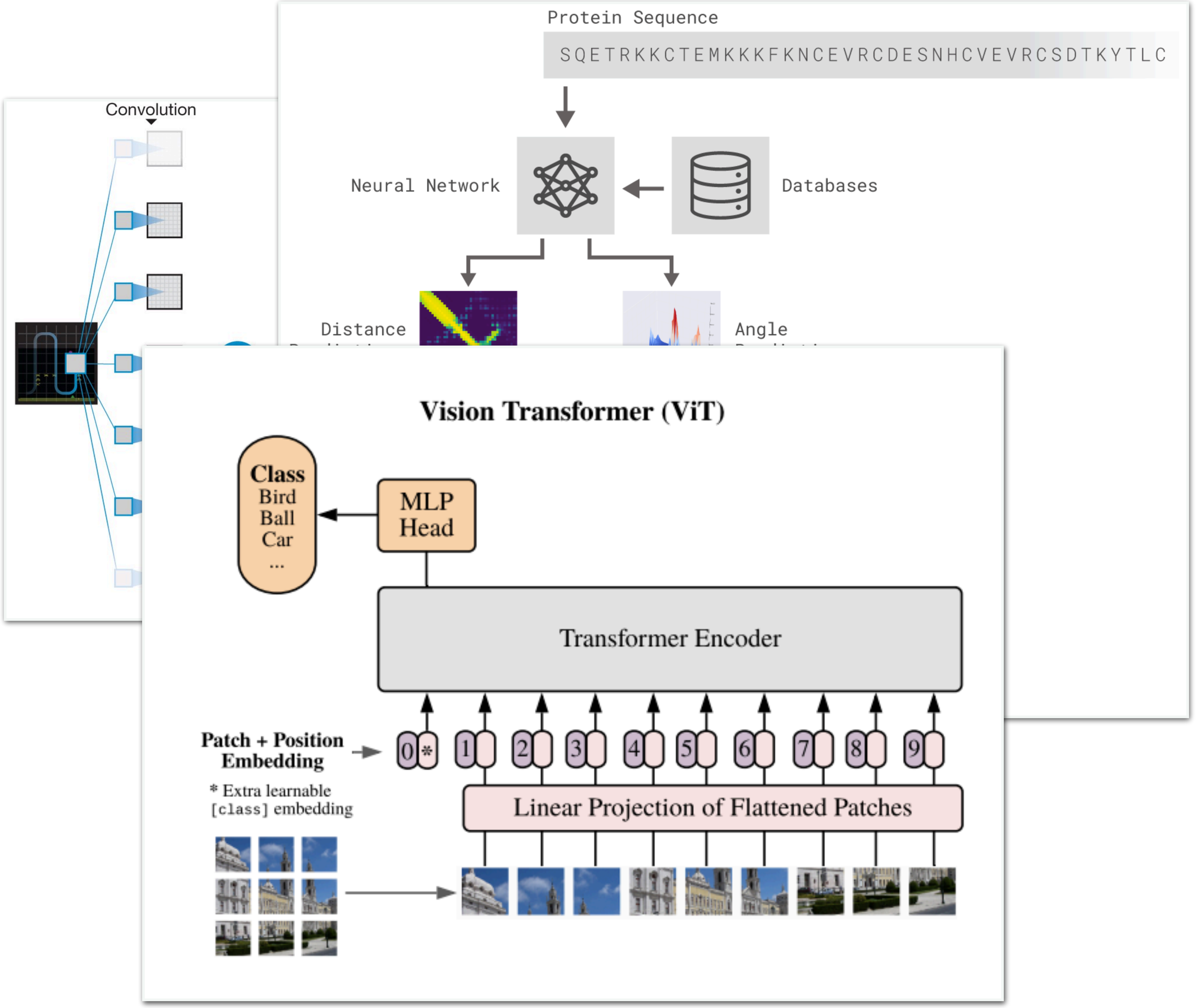

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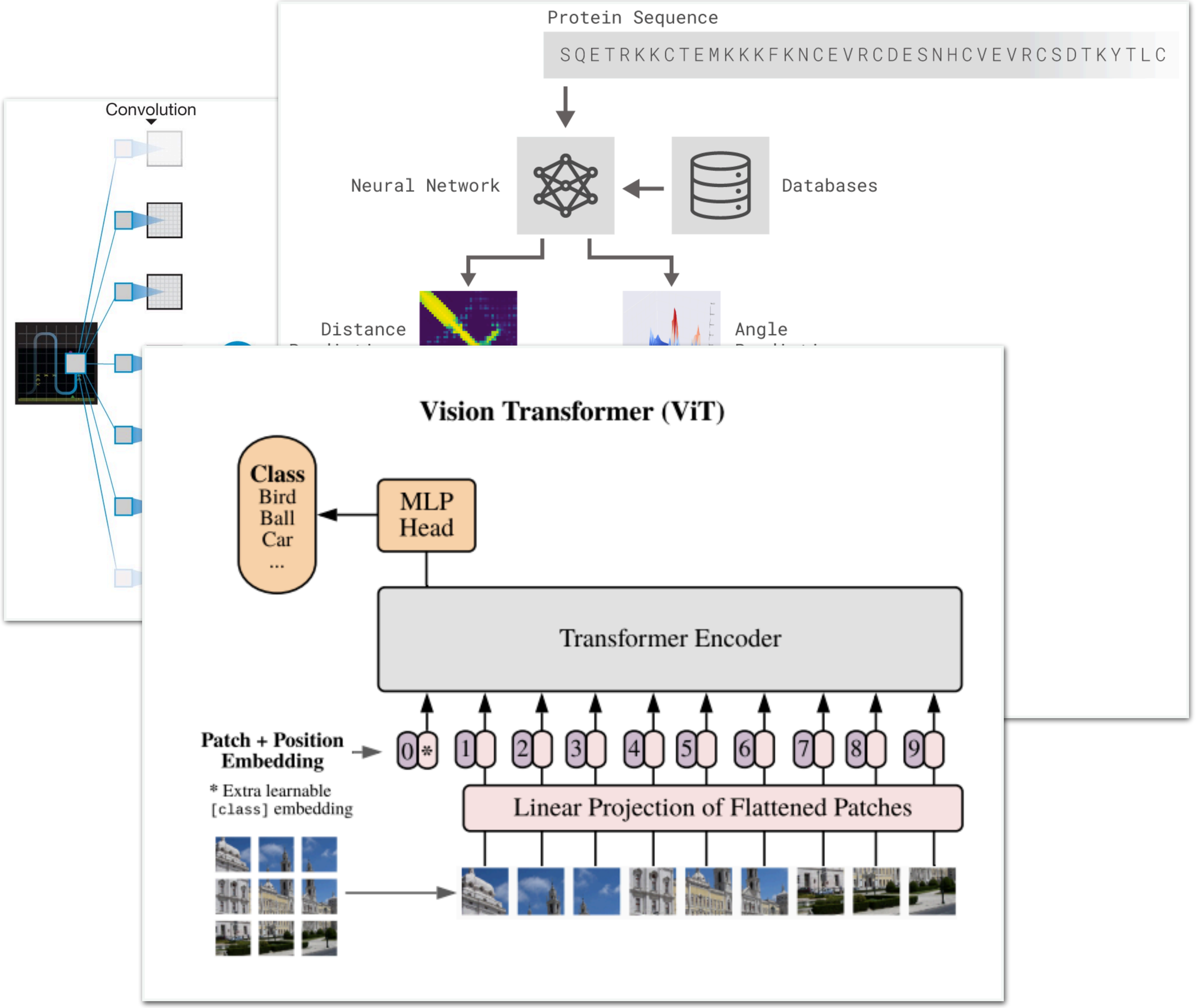

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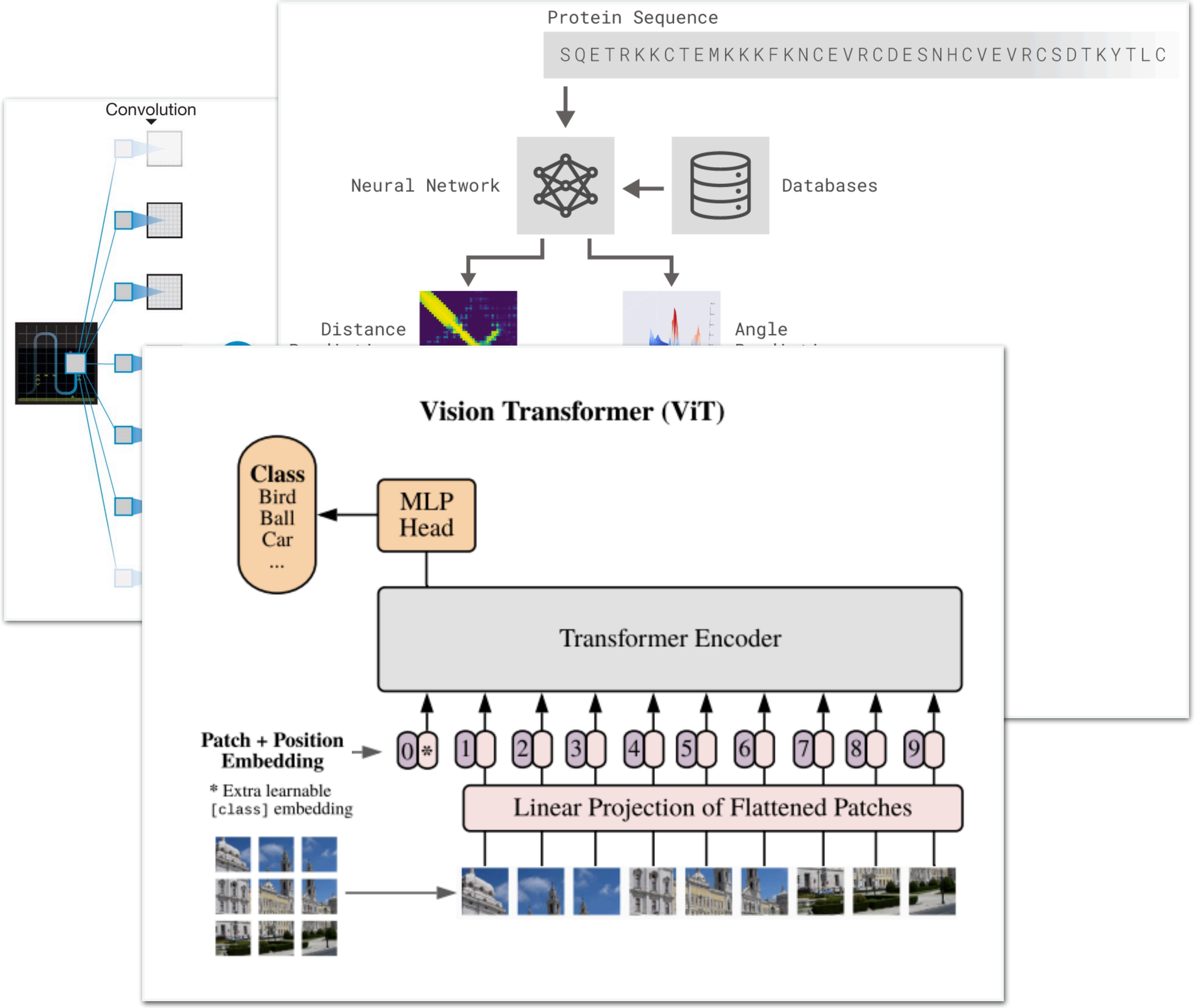
scales to high-dimensional inputs and huge datasets on modern hardware



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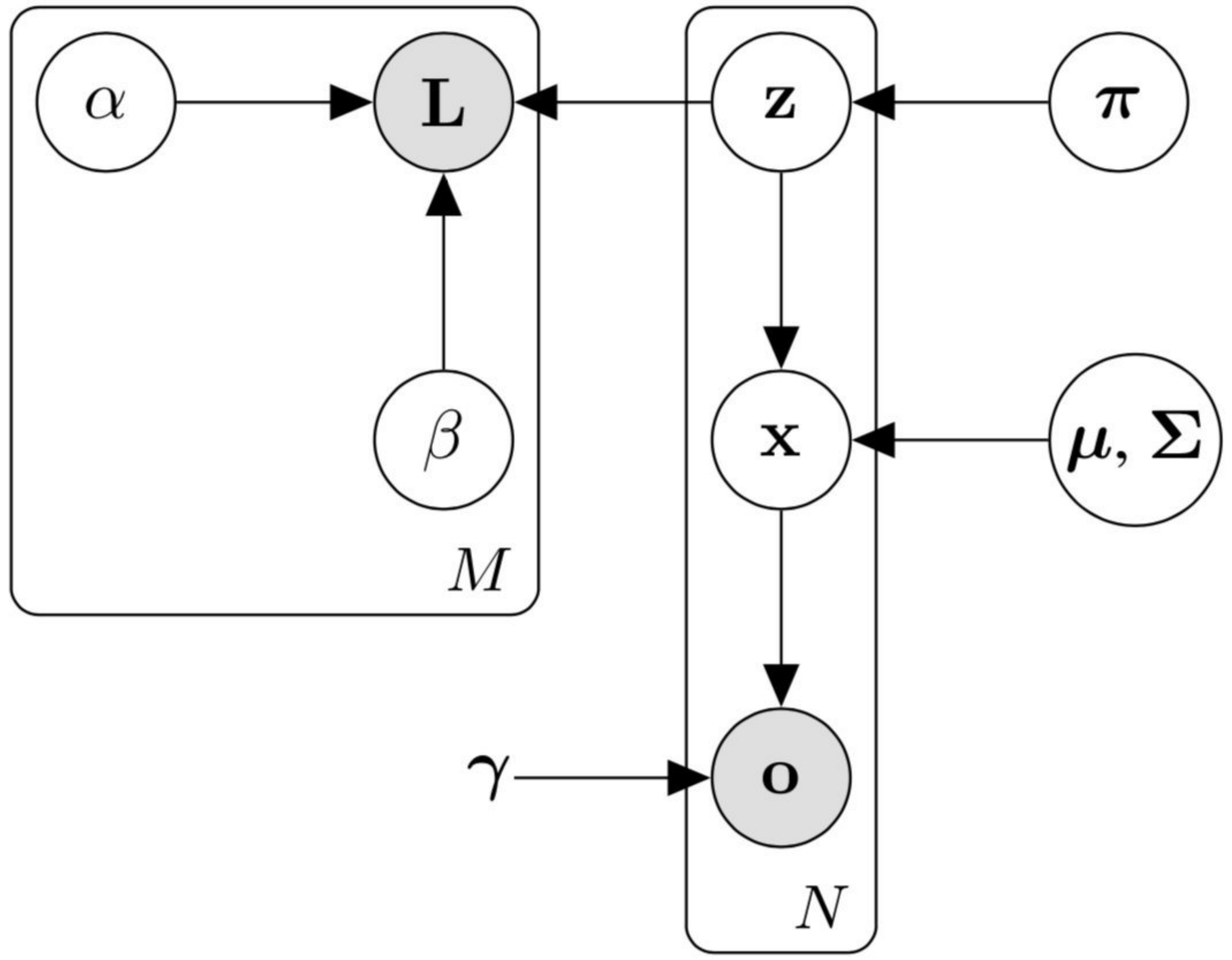
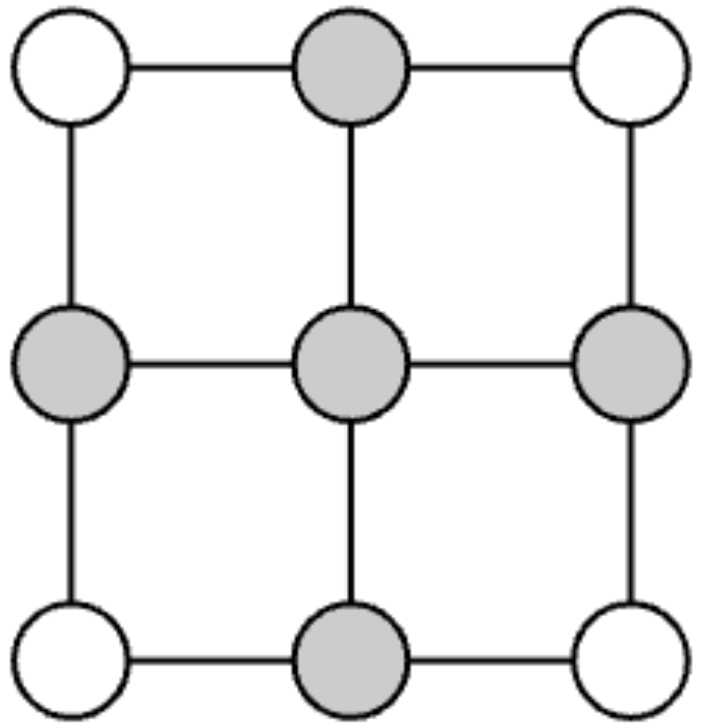
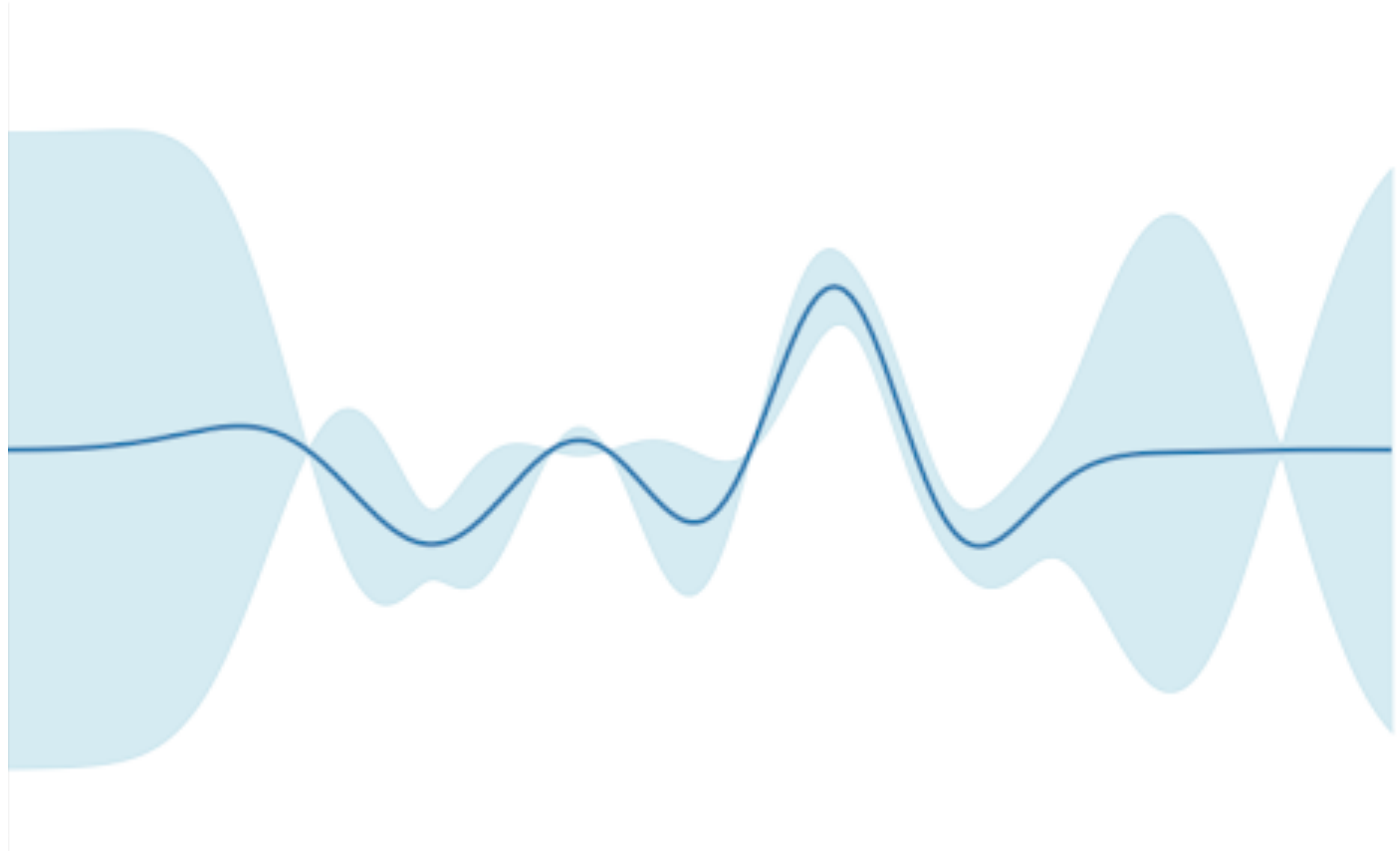
Probabilistic Modeling







Luo, Tian, **Shi,** Zhu & Zhang (NeurIPS'18)
Zhuo, Liu, **Shi**, Chen, Zhu & Zhang (ICML'18)
Shi, Titsias & Mnih (AISTATS'20)

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Statistical Science
2001, Vol. 16, No. 3, 199–231

Statistical Modeling: The Two Cultures

Leo Breiman

Abstract. There are two cultures in the use of statistical modeling to reach conclusions from data. One assumes that the data are generated by a given stochastic data model. The other uses algorithmic models and treats the data mechanism as unknown. The statistical community has

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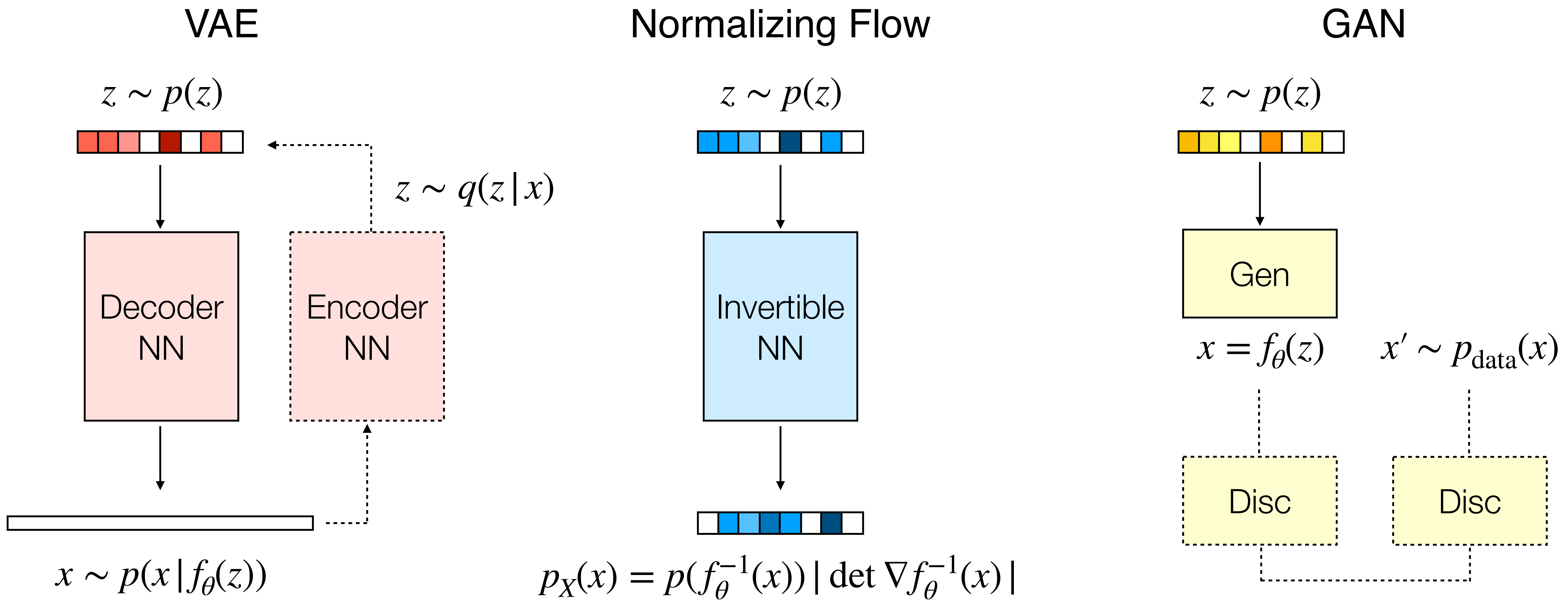
- Use differentiable programming ideas to improve the situation?

Existing Attempts are Highly Model-Specific



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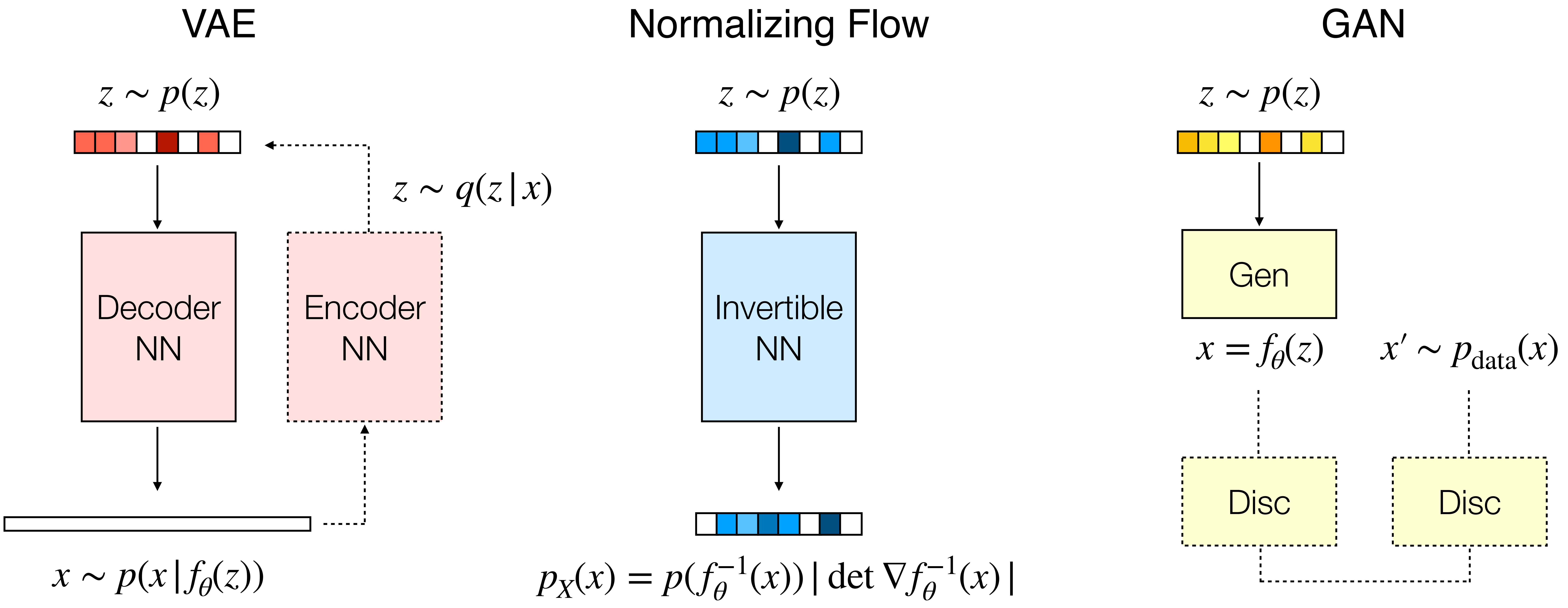

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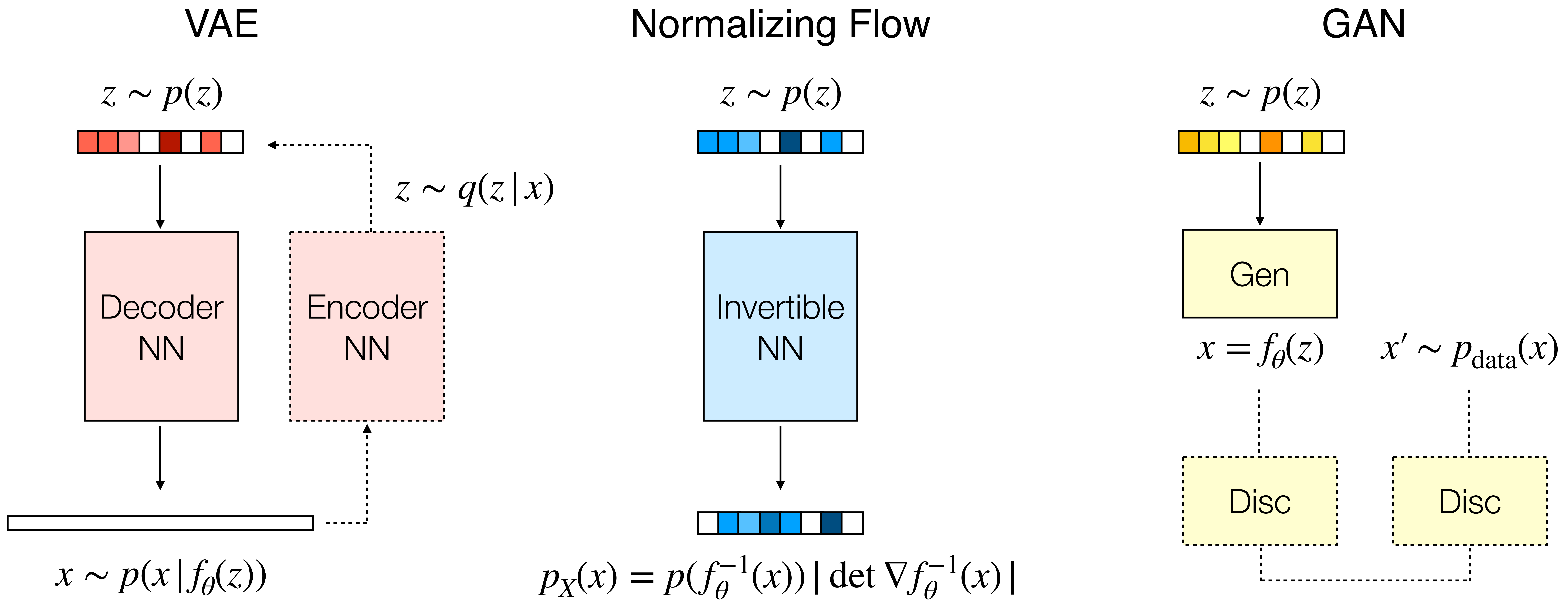

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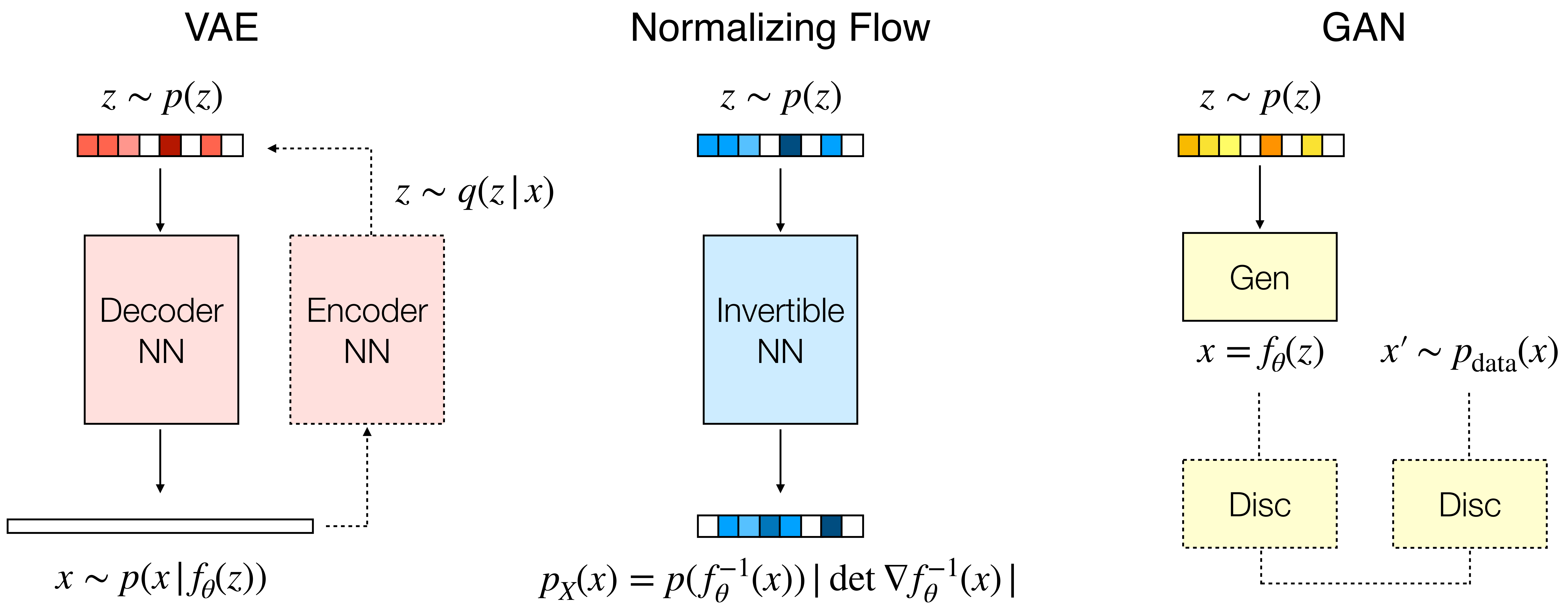

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- Intractable expectation (sum/integration)
- Intractable density functions: L could depend on $p_Y(y)$.

Today's Talk

Gradient estimation for differentiable programming in probabilistic models

- Gradient Estimation for Discrete Expectations
  - Titsias & **Shi**. (AISTATS'22)
  - **Shi**, Zhou, Hwang, Titsias & Mackey. (In Submission)
- Gradient Estimation for Intractable Densities
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X : d-dim binary vector => 2^d terms to sum

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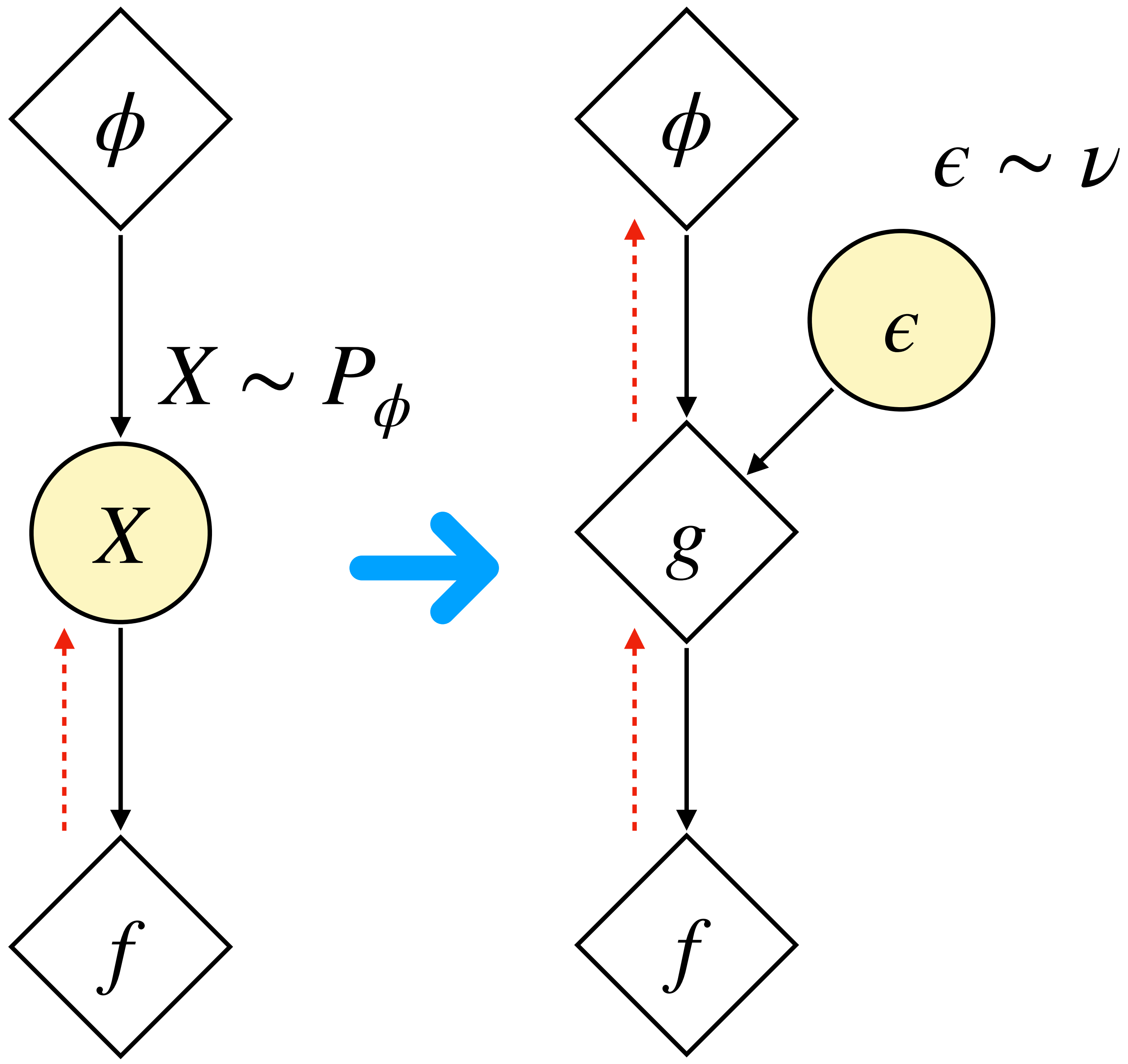

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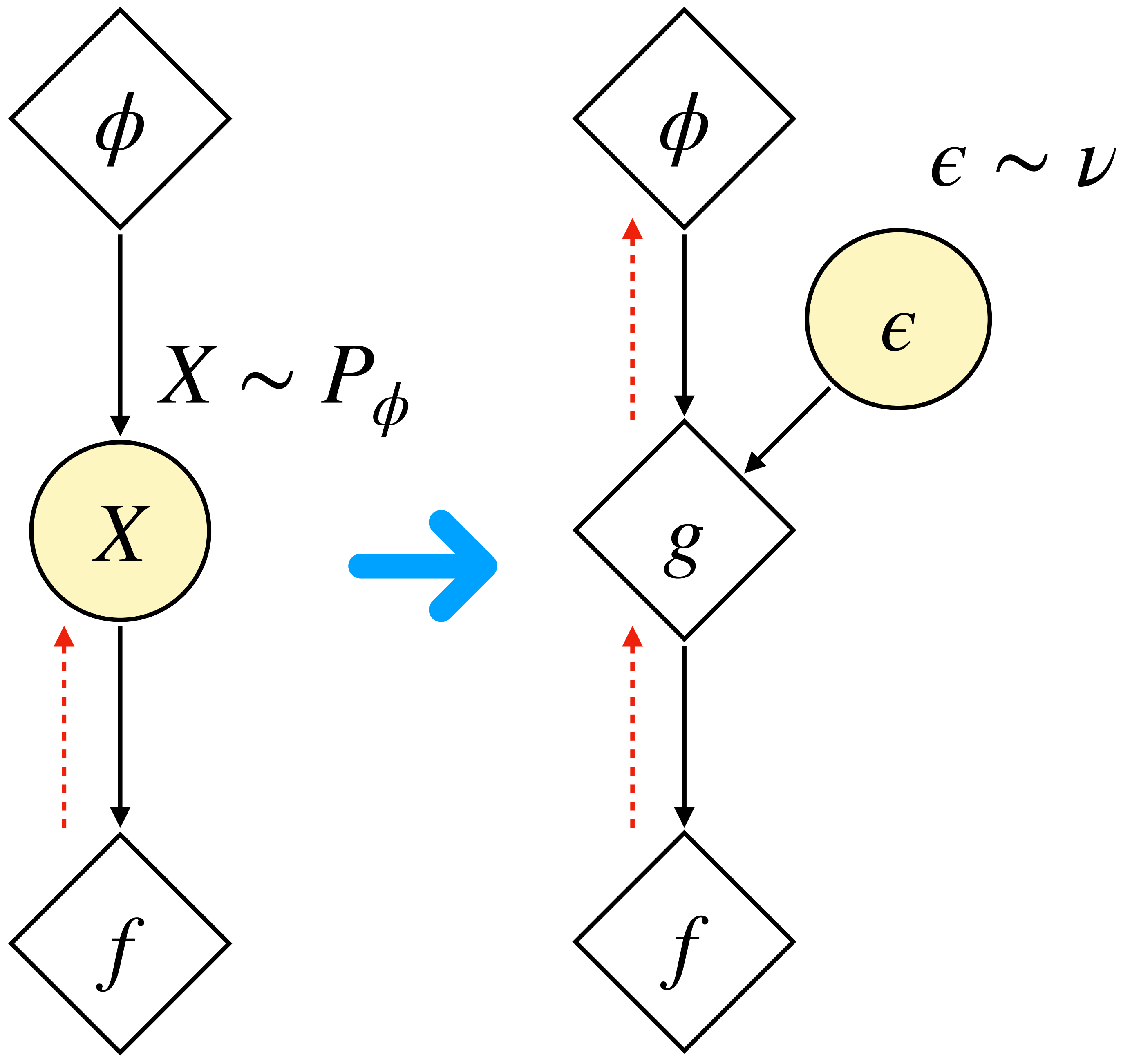

only works for continuous distributions

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very high variance

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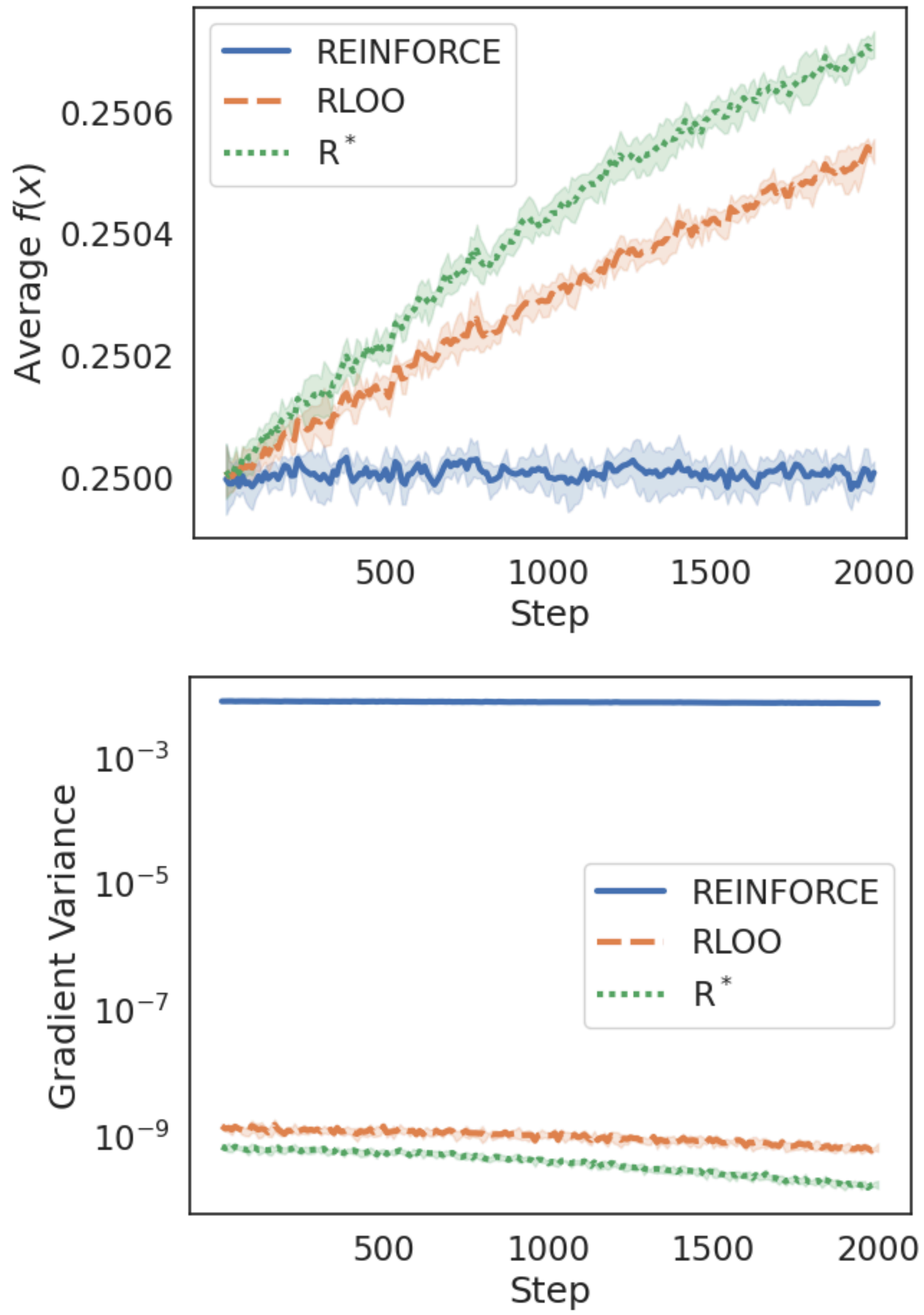

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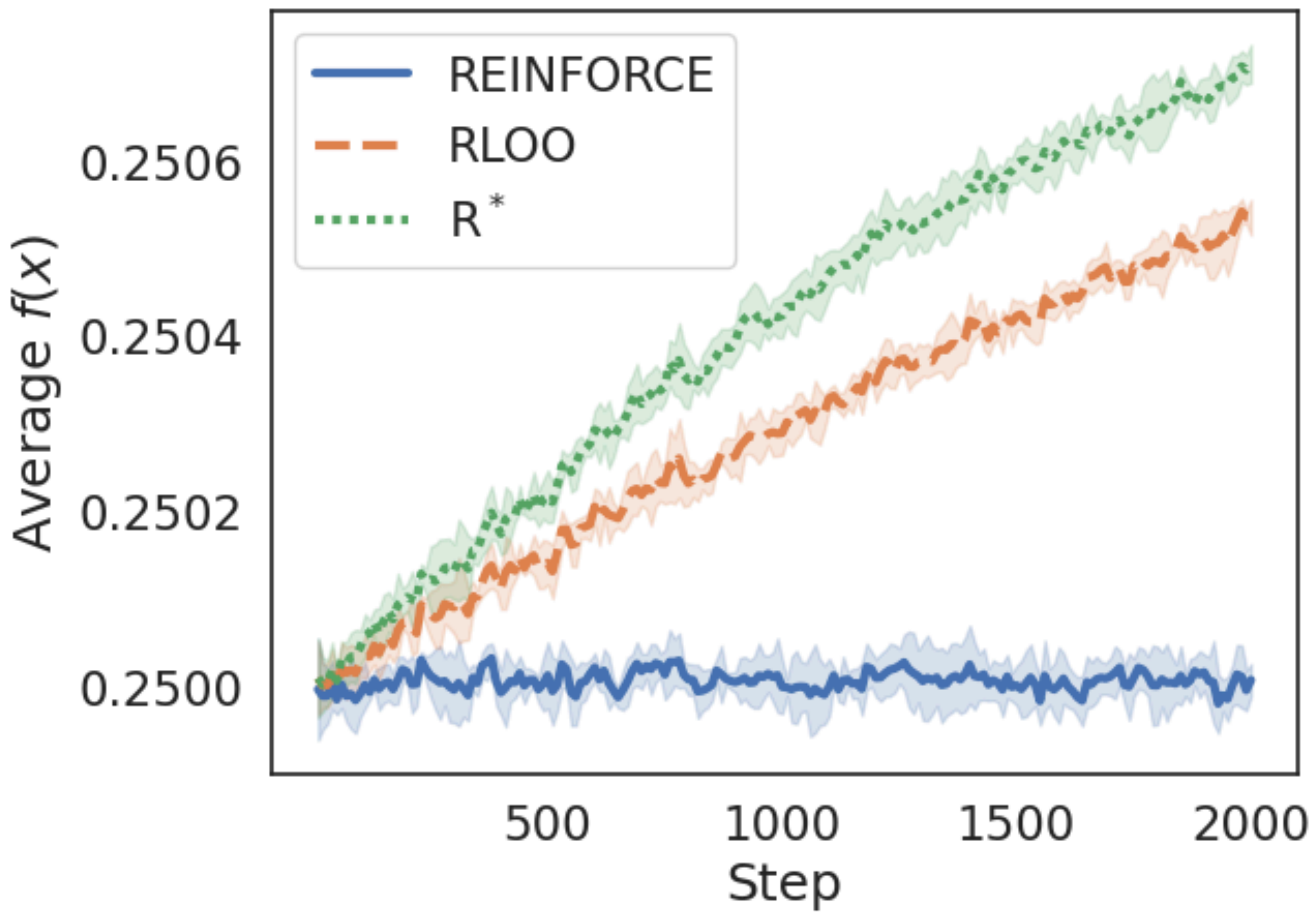

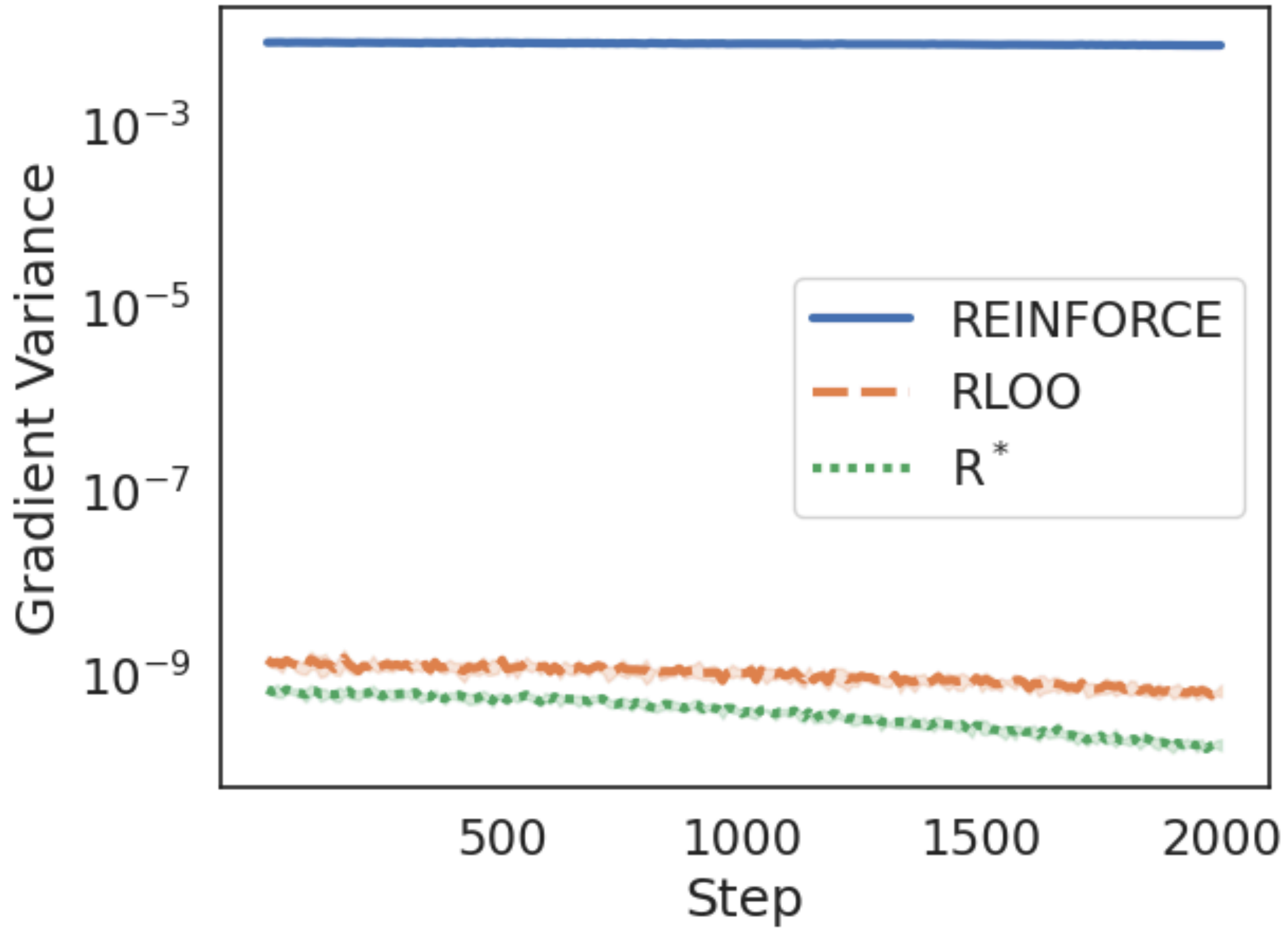

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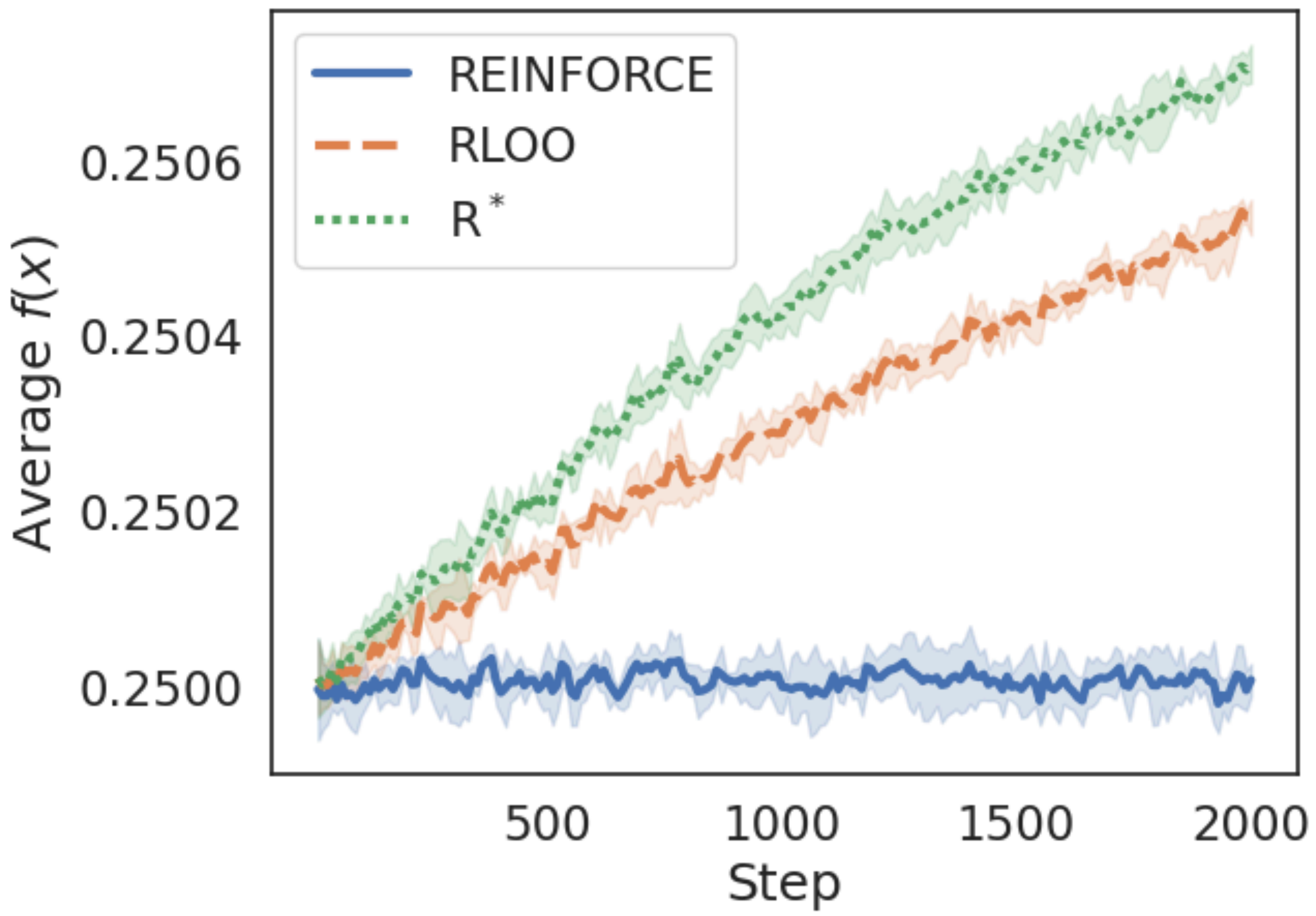

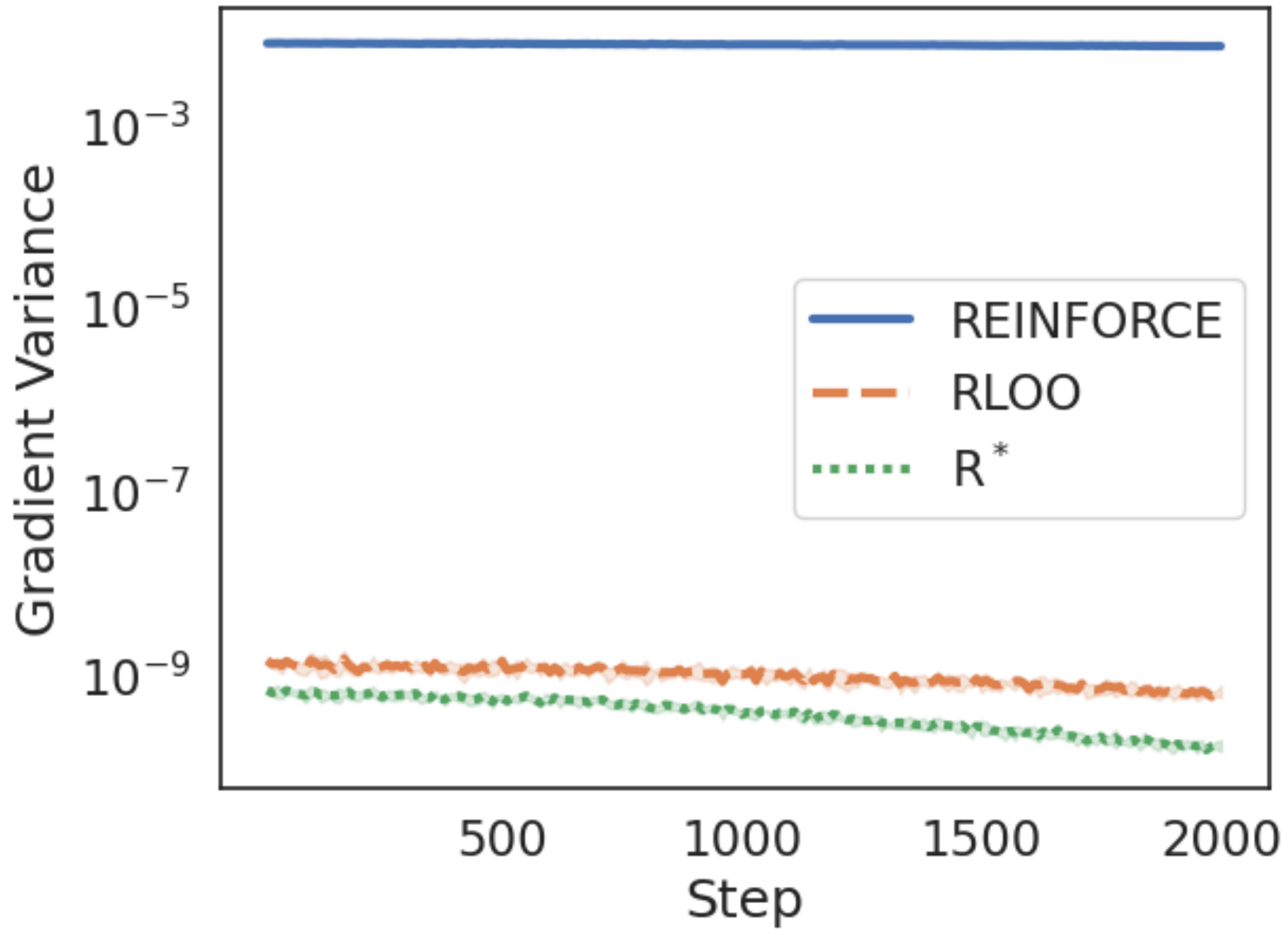

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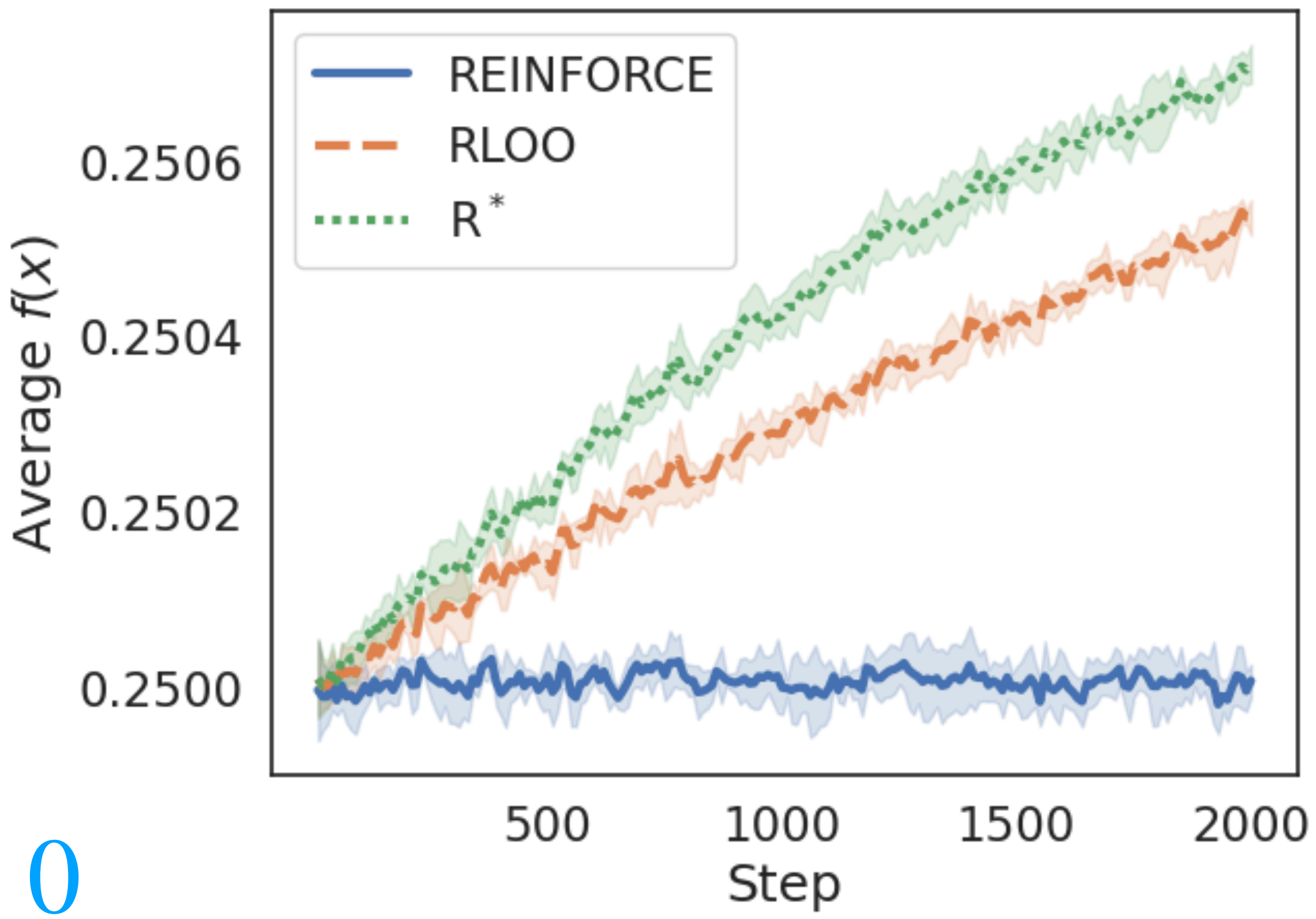

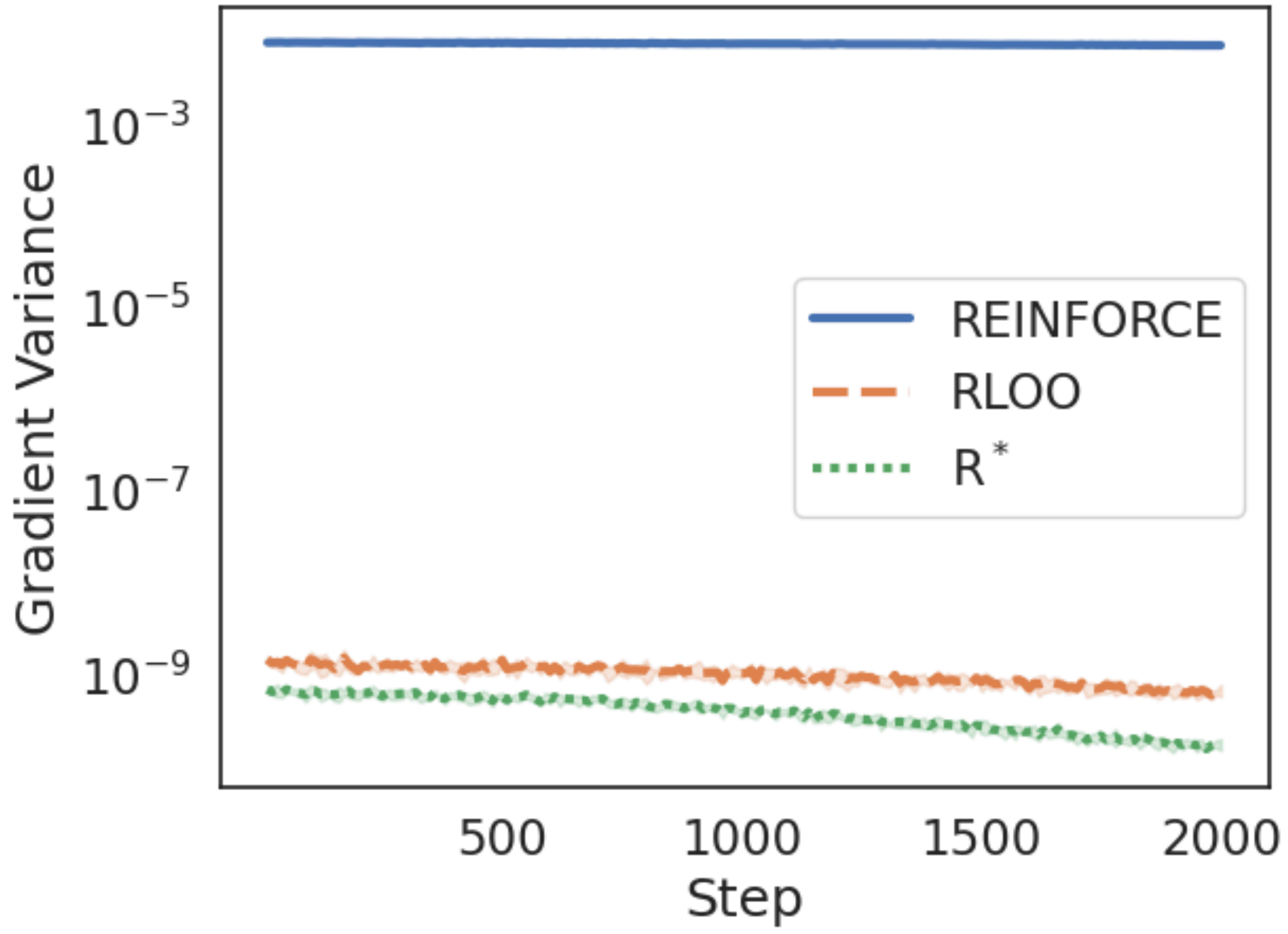

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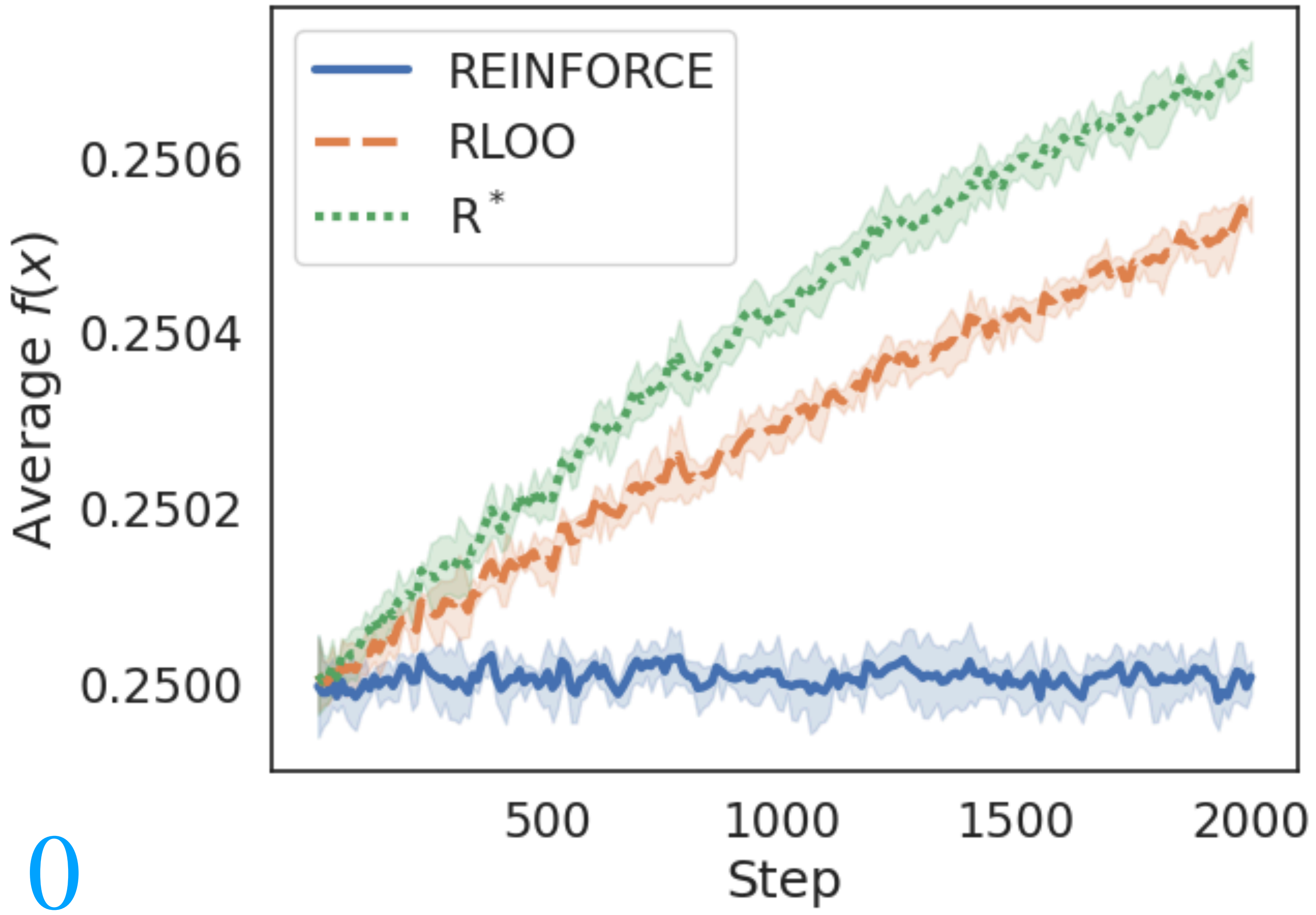

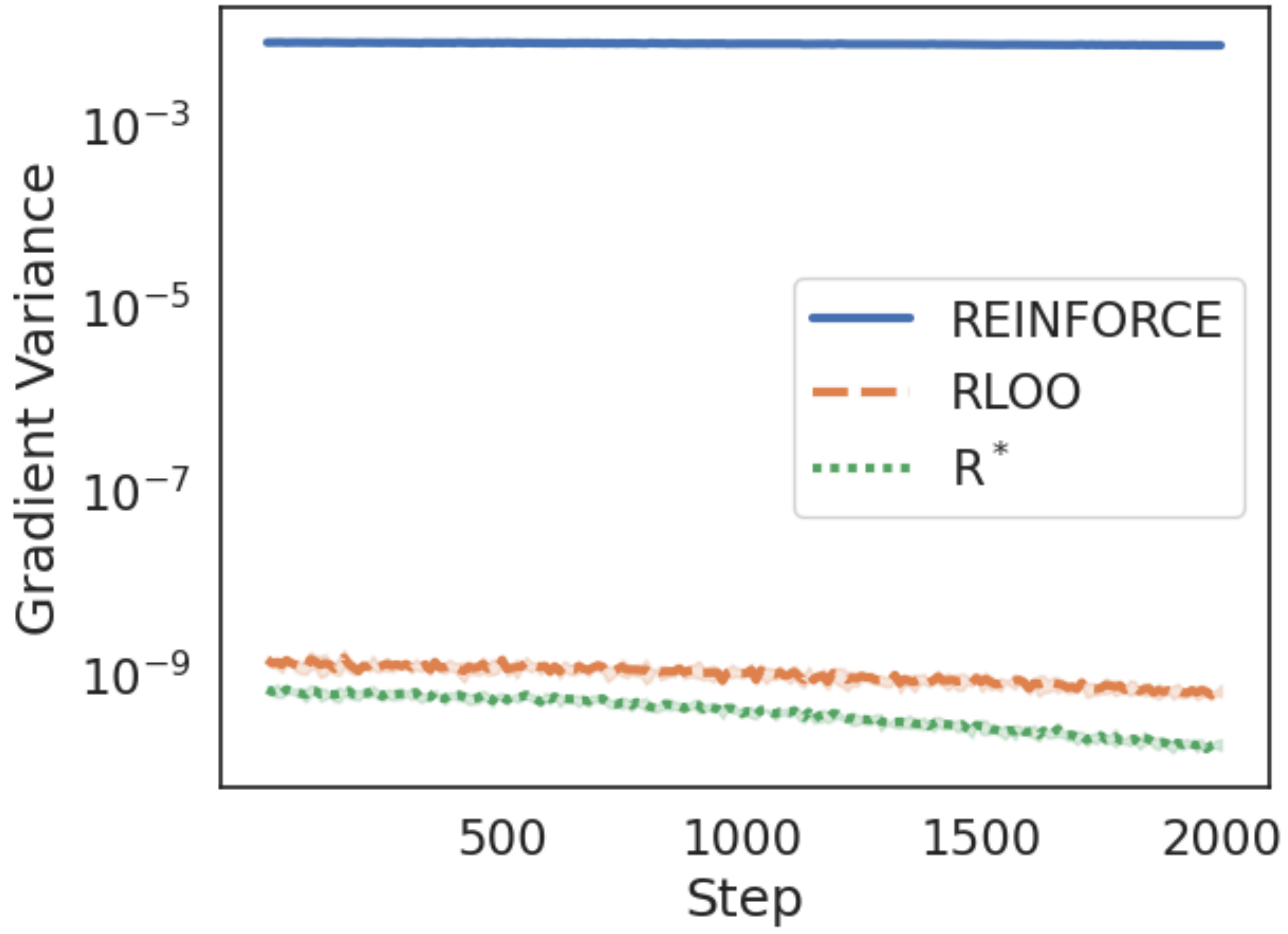

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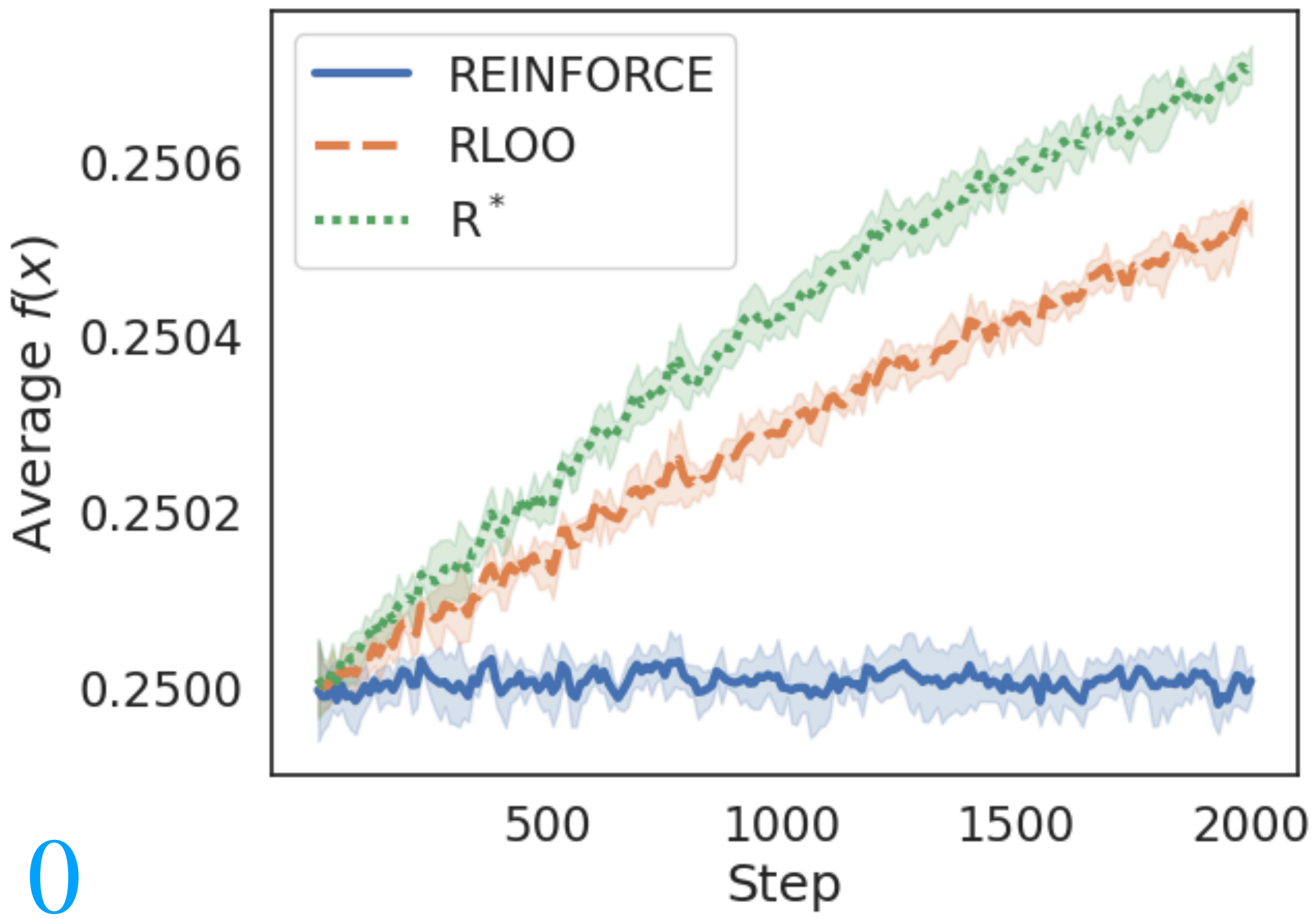

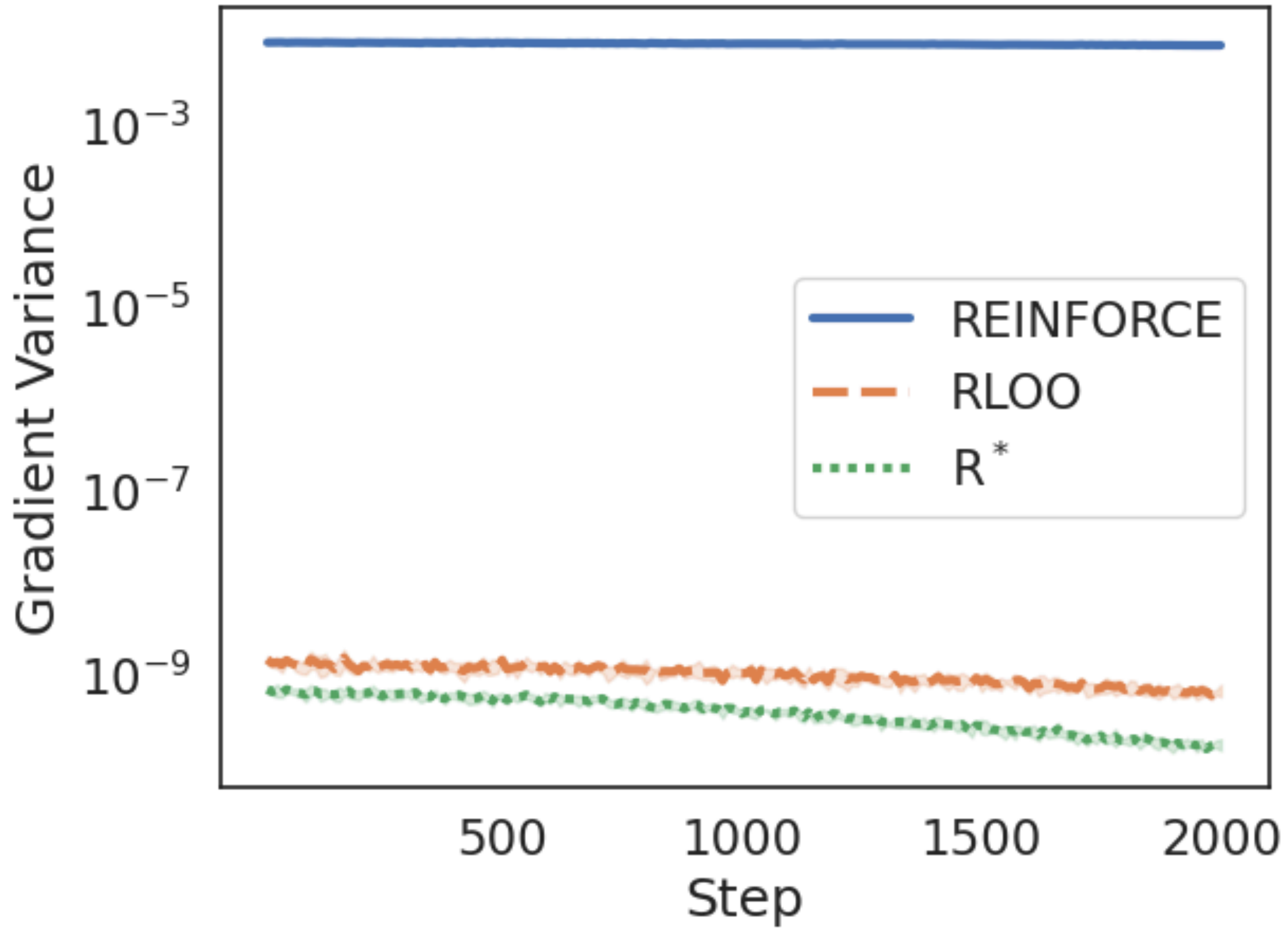

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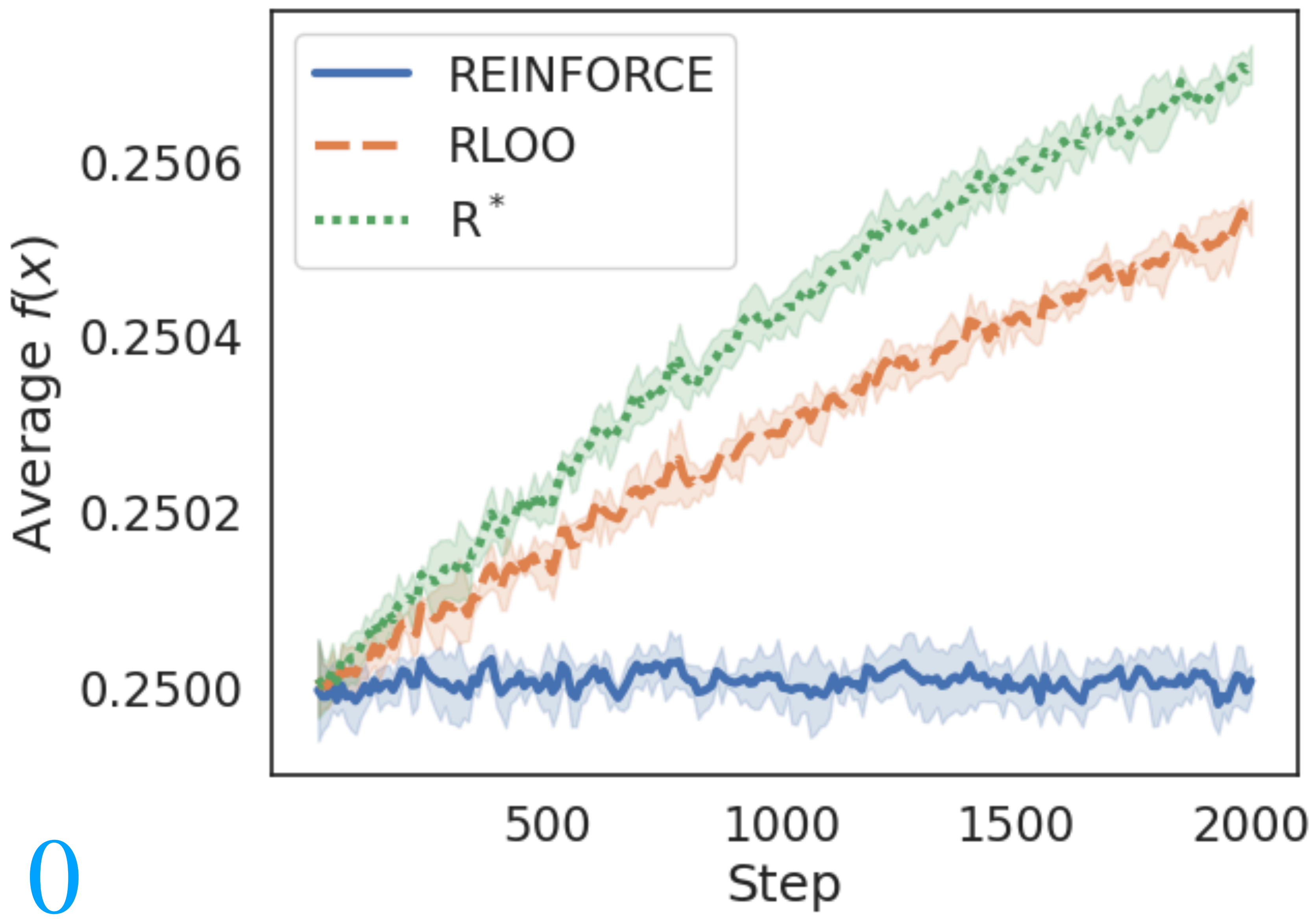
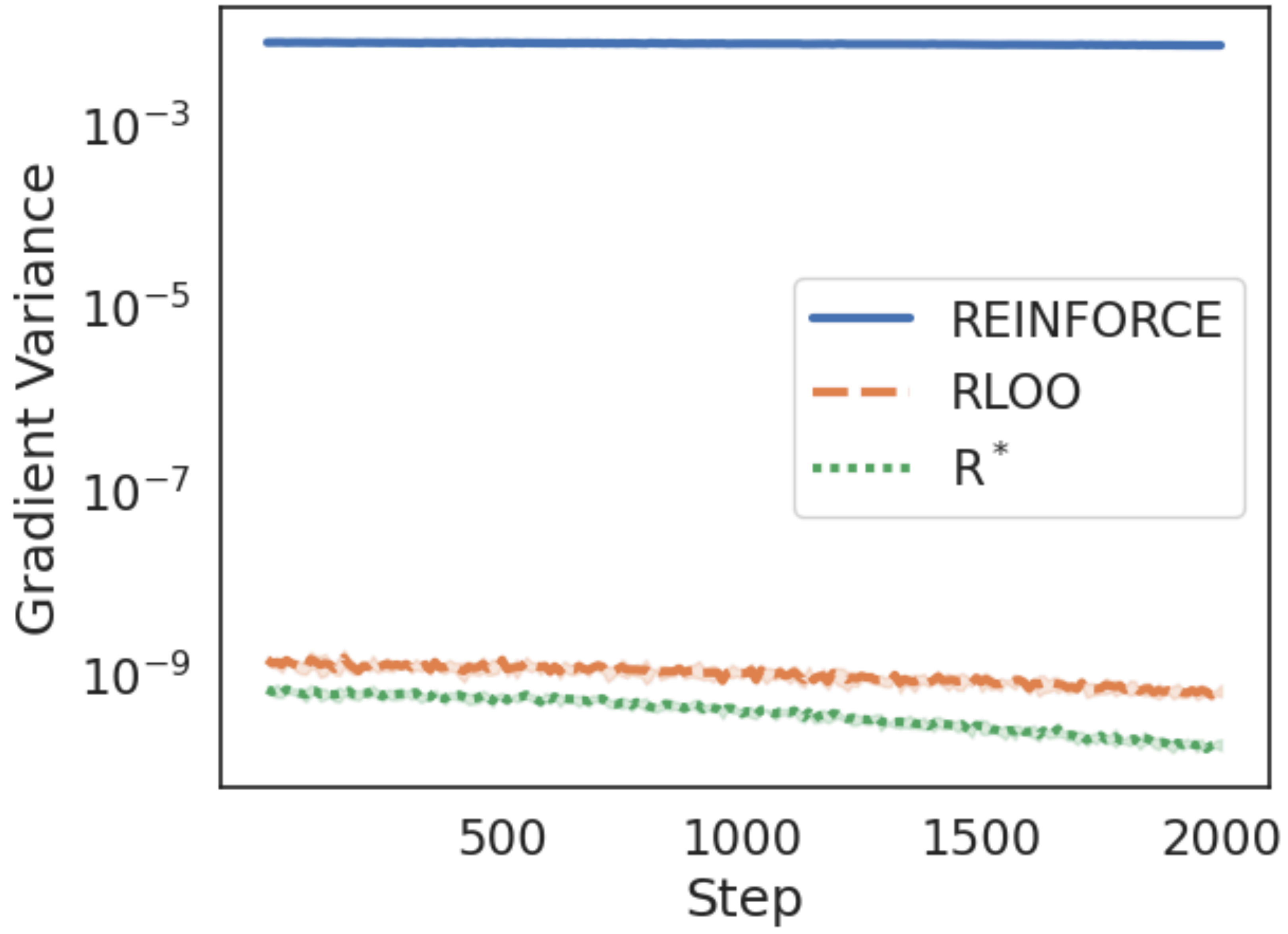
- REINFORCE Leave-One-Out: $b = \frac{1}{K-1}\sum_{j \neq k} f(x_j)$





Proposition Define the two gradient estimators:

$$\text{RLOO: } \frac{1}{K}\sum_{k=1}^{K}\left(f(x_k) - \frac{1}{K-1}\sum_{j\neq k} f(x_j)\right)\nabla_\phi \log p_\phi(x_k)$$

$$\text{R*: } \frac{1}{K}\sum_{k=1}^{K}\left(f(x_k) - \mathbb{E}_{X\sim P_\phi}[f(X)]\right)\nabla_\phi \log p_\phi(x_k)$$

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There is room for improving the state-of-the-art REINFORCE estimators

- potential direction: variance reduction for the leave-one-out baseline?

Gradient Estimation for Discrete Expectations

Roadmap

Double Control Variates

A new framework for variance reduction in REINFORCE-type estimators

Discrete Stein Operators

A general recipe for building flexible control variates for discrete distributions

Titsias & **Shi**. Double Control Variates for Gradient Estimation in Discrete Latent-Variable Models. AISTATS 2022
Shi, et al. Gradient Estimation with Discrete Stein Operators. In Submission.

Double Control Variates

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α is a regression coefficient adapted online by minimizing variance.

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	RLOO	Double CV
Time (sec/step)	0.0035	0.0036

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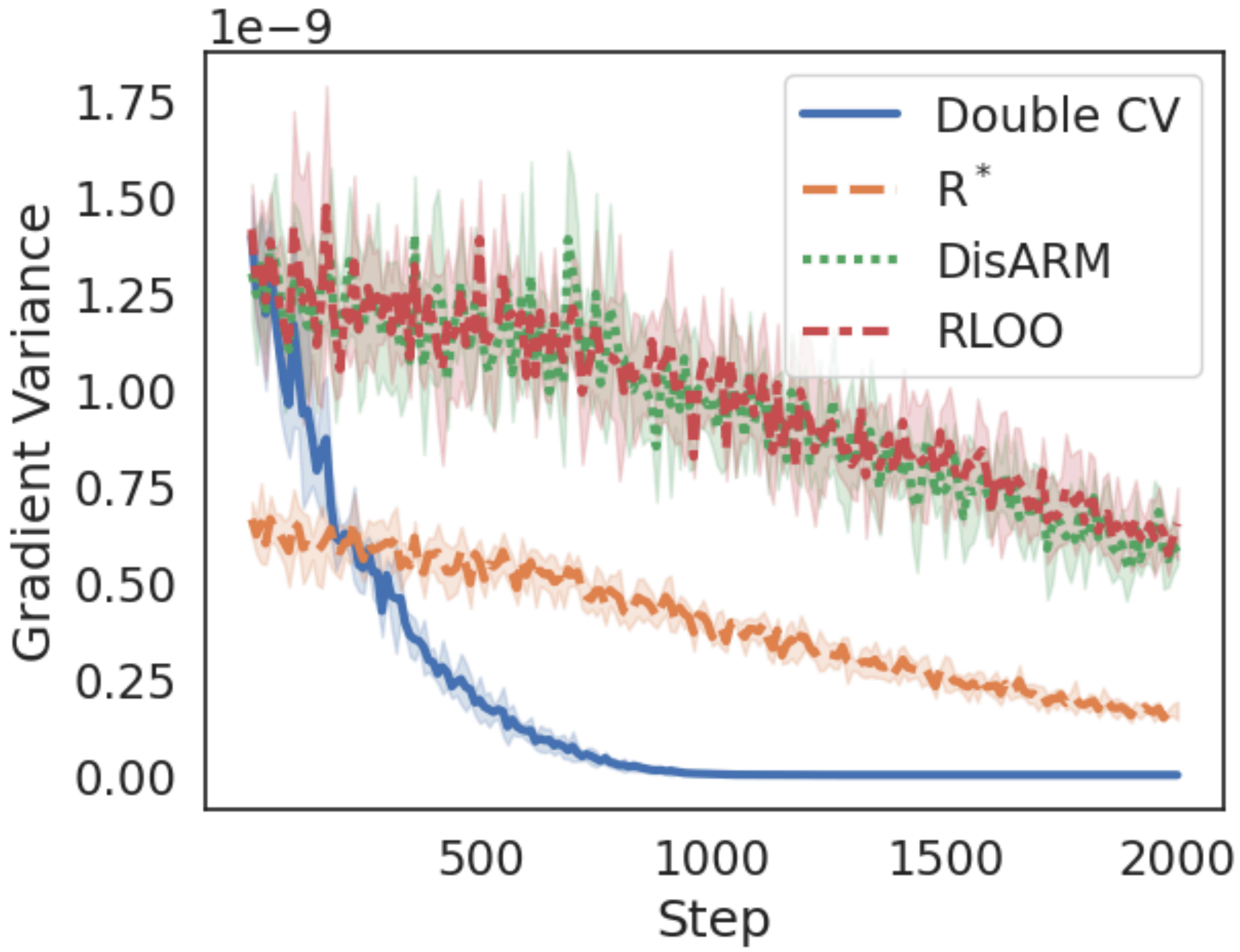
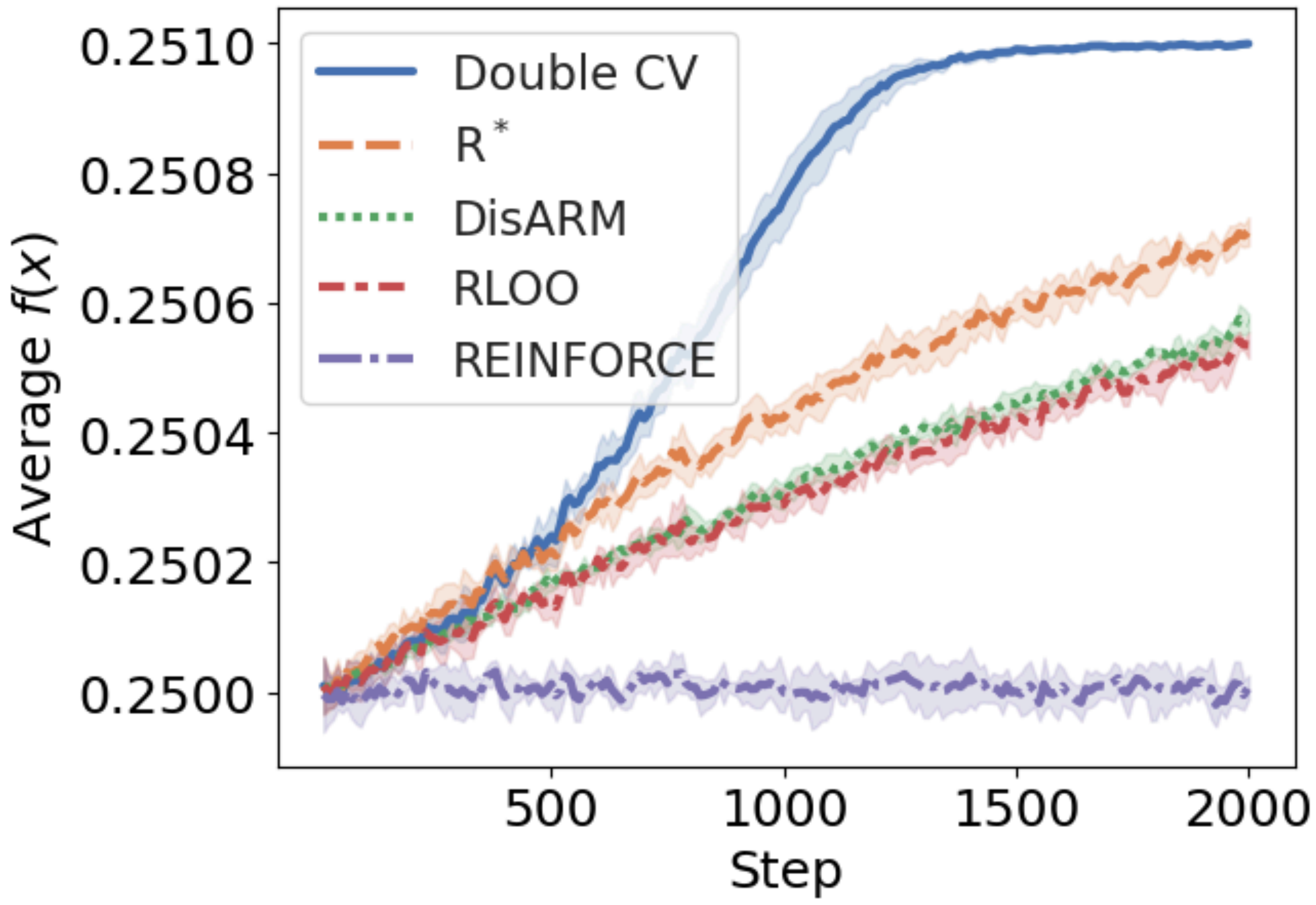
Quadratic Loss Example

$$\max_{\eta} \mathbb{E}_{X \sim P_\eta} \left[\frac{1}{d} \sum_{i=1}^{d} (X_i - 0.499)^2 \right], \text{ where } p_\eta(x) = \prod_{i=1}^{d} \sigma(\eta_i)^{x_i} (1 - \sigma(\eta_i))^{1-x_i}$$





The Quest for More Flexible Control Variates

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- Control variates are effective only when they are strongly correlated with the original statistic
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- Ideally, would like a very flexible control variate that can be adapted online to minimize the variance
- Still, they need to have analytic expectations

Stein Operators

Computable functionals that generate zero-mean functions

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- introduced by Stein (1972) for characterizing distributional convergence.

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$$(Ah)(x) = h'(x) - xh(x)$$

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- see paper for generalization to continuous-time chains

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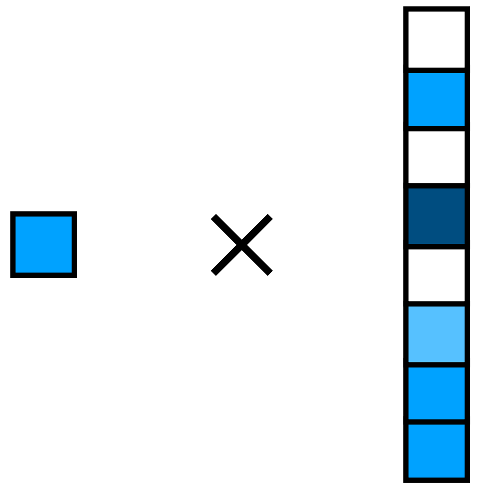

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$\mathcal{X} \to \mathbb{R}^d$

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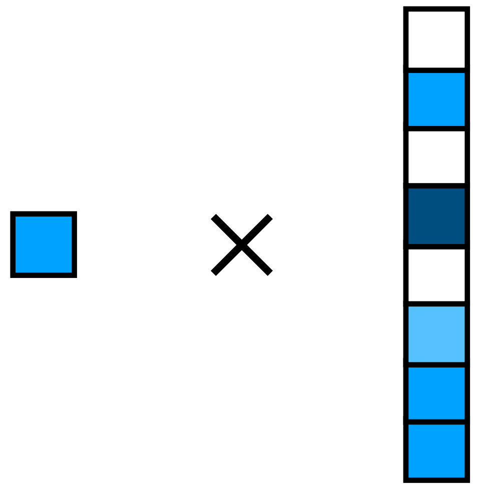

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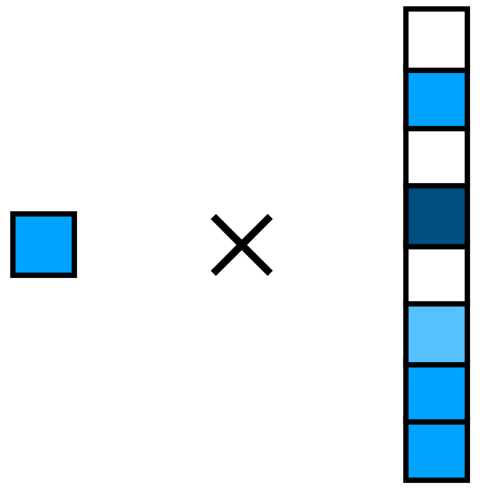

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Gradient Estimation with Discrete Stein Operators

How to choose $\tilde{h}$:

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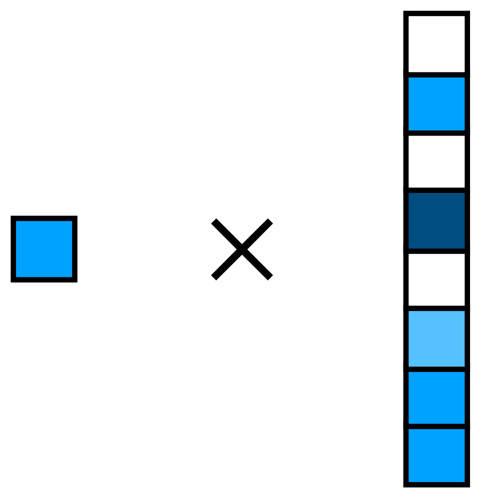

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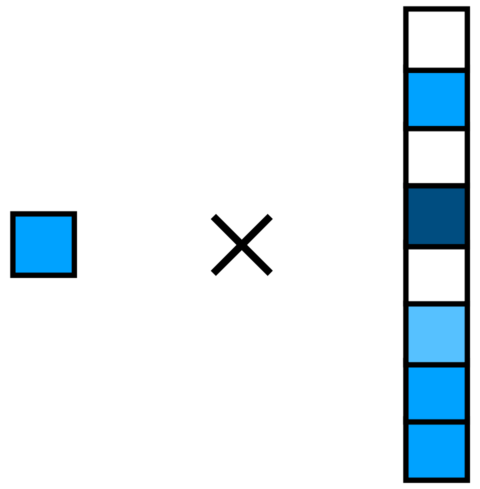

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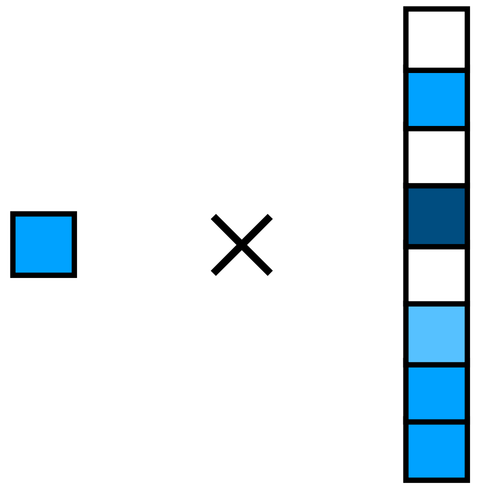

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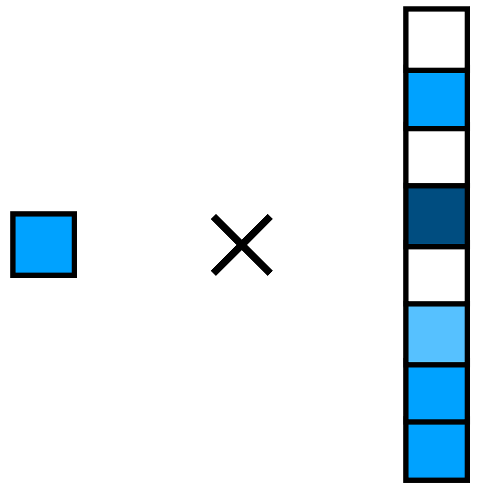

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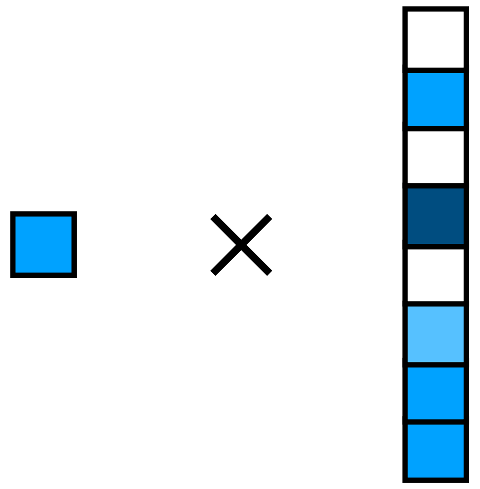

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Theorem When $h = f$, estimators with this $\tilde{h}$ reduce to **Rao-Blackwellization** $K(f\nabla_\eta \log q_\eta)$ which guarantees variance reduction

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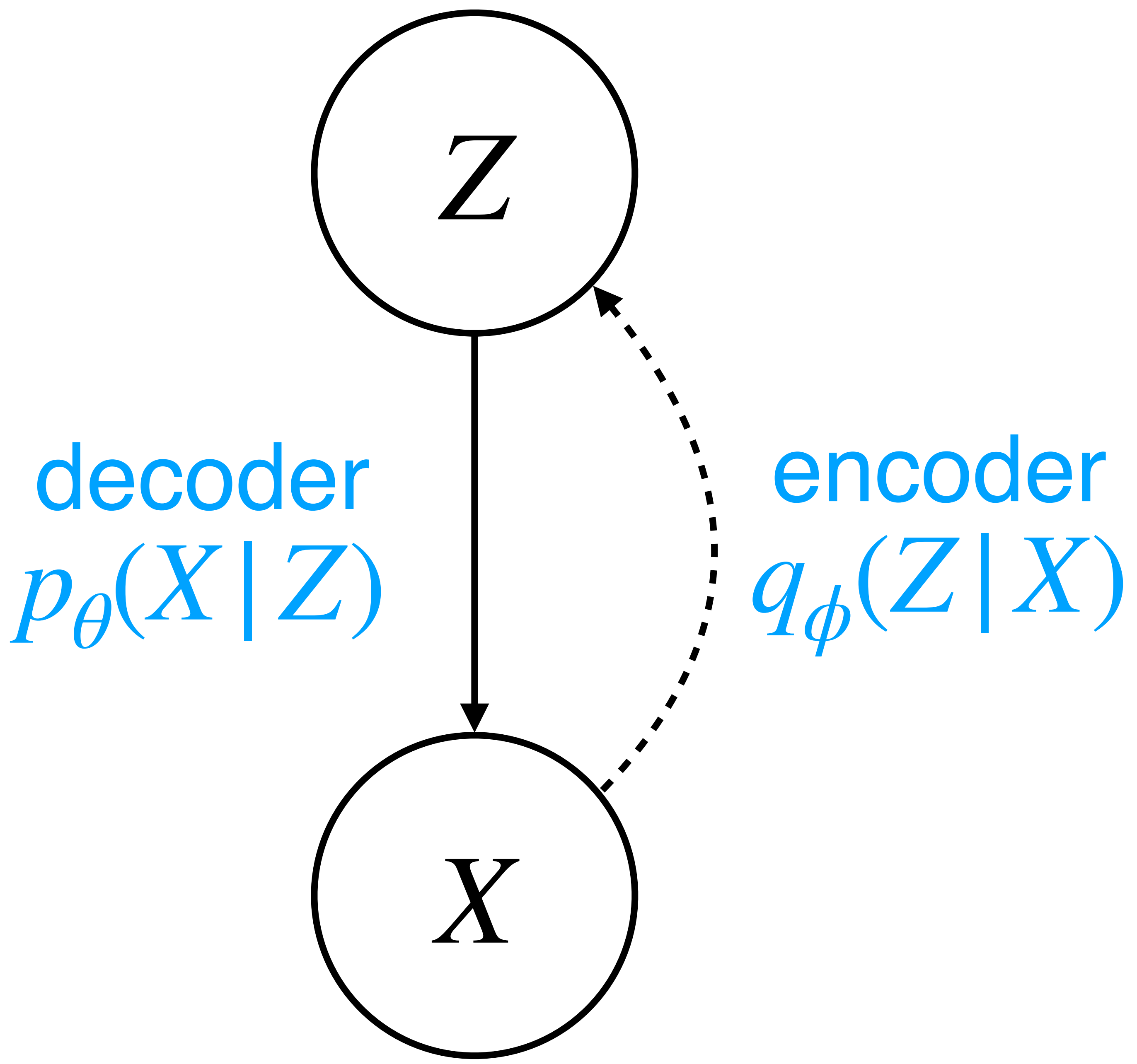
- Replace both "local" and "global" control variates of double CV using discrete Stein operators.

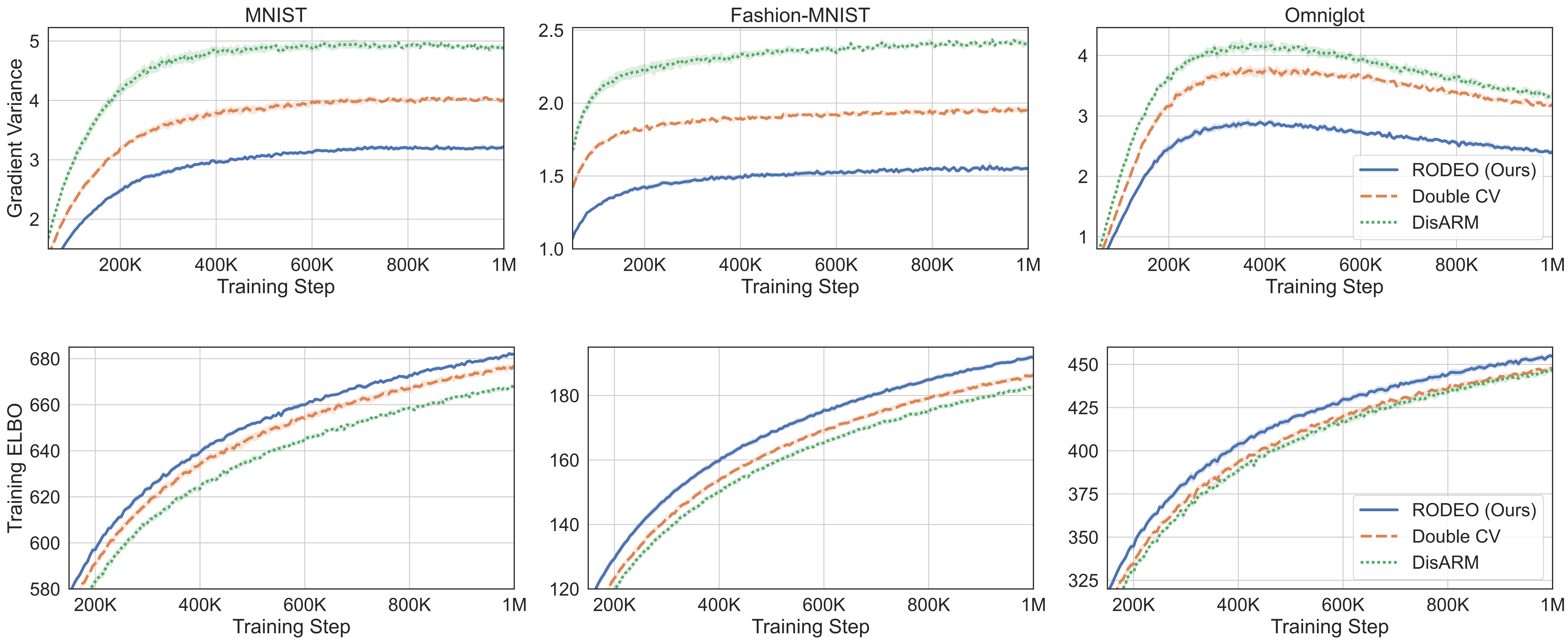
Benchmark: Training Binary Latent VAEs

- Latent-variable model: $p_\theta(X, Z) = p_\theta(X \mid Z)p(Z)$
- Maximizing a lower bound of the log marginal likelihood:

$$\log p_\theta(x) = \log \mathbb{E}_{q_\phi(z|x)}\left[\frac{p_\theta(x, z)}{q_\phi(z \mid x)}\right] \geq \mathbb{E}_{q_\phi(z|x)}\left[\log \frac{p_\theta(x \mid z)p(z)}{q_\phi(z \mid x)}\right]$$



Benchmark: Training Binary Latent VAEs



$$K = 2, d = 200$$

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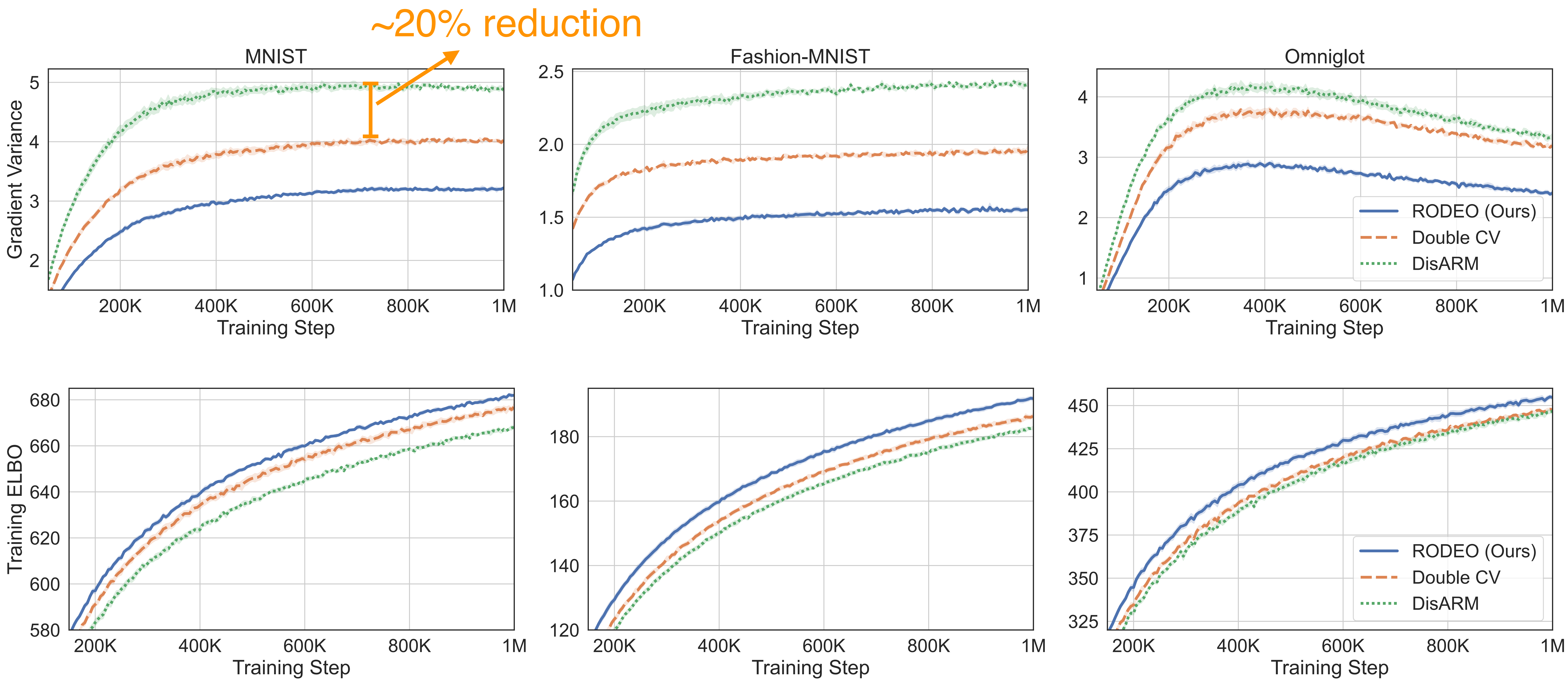

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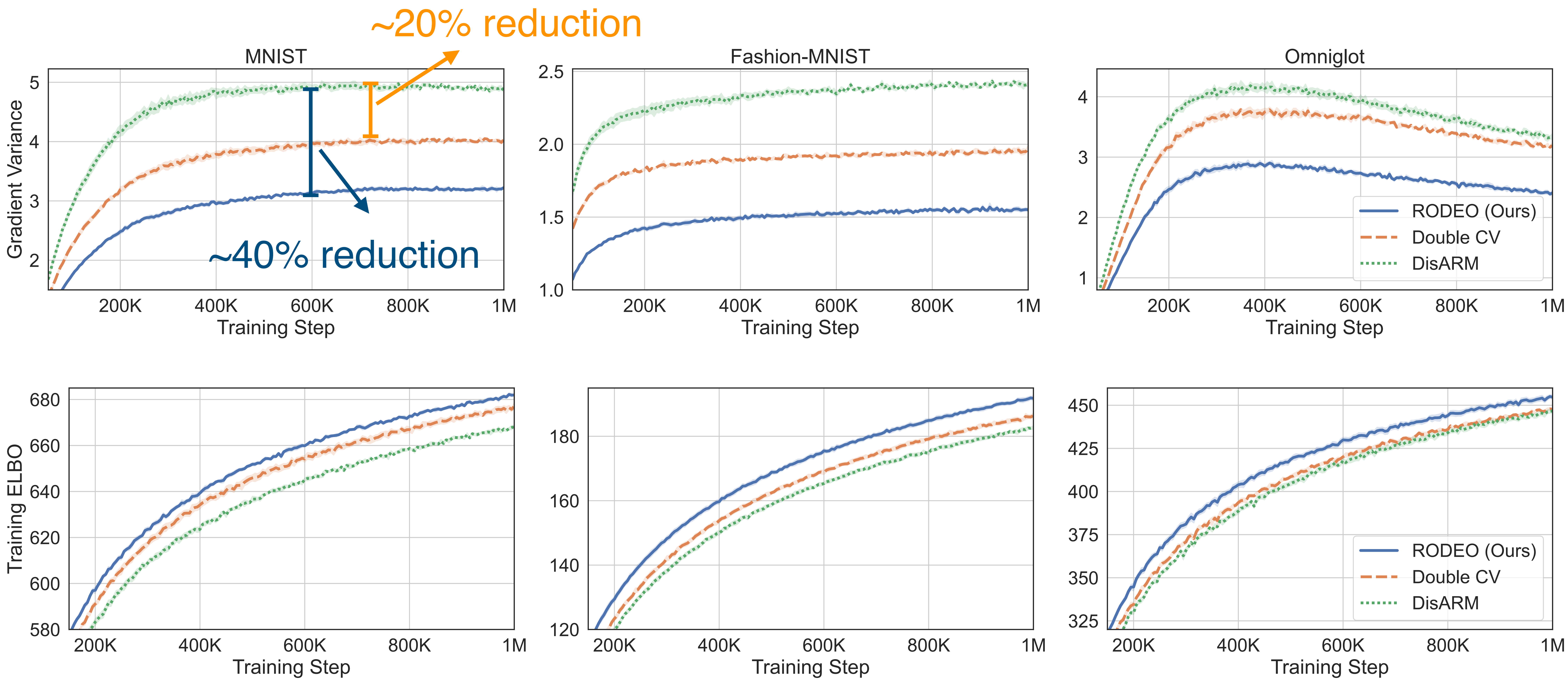

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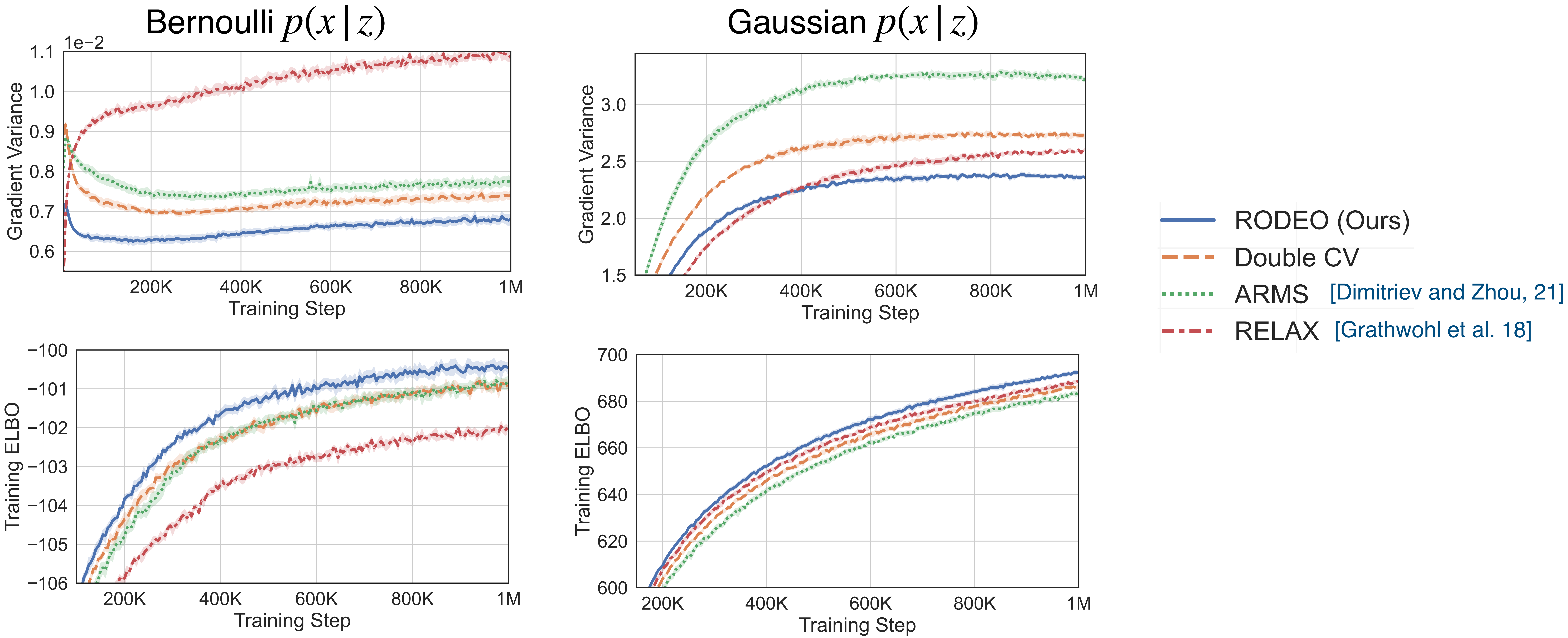

RELAX needs three evaluations of f, $K = 3$ for other estimators

Today's Talk

Gradient estimation for differentiable programming in probabilistic models

- Gradient Estimation for Discrete Expectations
  - Titsias & **Shi**. (AISTATS'22)
  - **Shi**, Zhou, Hwang, Titsias & Mackey. (In Submission)
- Gradient Estimation for Intractable Densities
  - **Shi**, Sun & Zhu. (ICML'18)
  - Zhou, **Shi** & Zhu. (ICML'20)

Motivation

A difficult example in representation learning

representation — data

$Y \longleftarrow \boxed{\text{Encoder NN}_{\phi}} \longleftarrow X \sim P_X$

[Hjelm et al., 19; Tschannen et al., 19]

Motivation

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$$Y \longleftarrow \boxed{\text{Encoder NN}_{\phi}} \longleftarrow X \sim P_X$$

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- learn by maximizing mutual information:

Motivation

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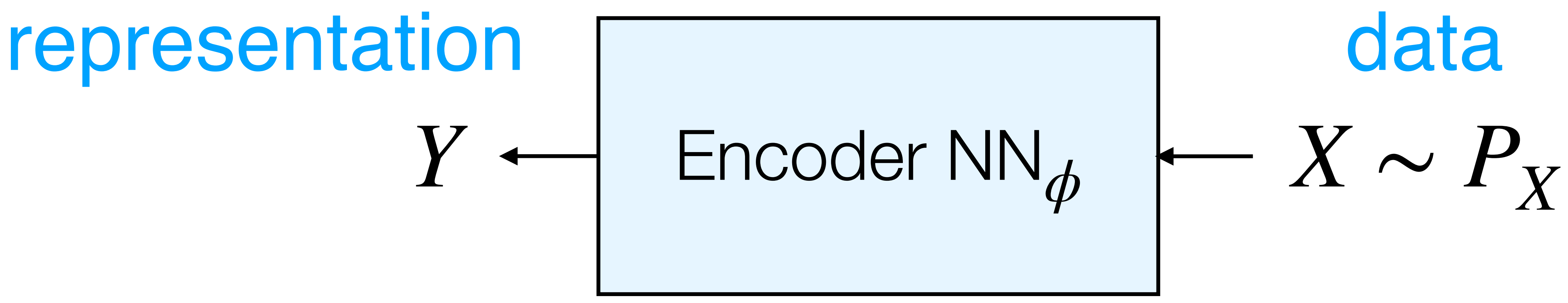

[Hjelm et al., 19; Tschannen et al., 19]

- learn by maximizing mutual information:

$$\max_{\phi} I(X, Y) := \mathrm{KL}(P_{X,Y} \| P_X \otimes P_Y)$$

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Motivation

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Motivation

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representation | | data

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- Often no explicit p_X, and $p_Y, p_{X,Y}$ are intractable
- Prior estimators assume L is computable in $\nabla_{\phi}\mathbb{E}[L(f(X))]$

Motivation

Gradient estimation for KL-divergence

Motivation

Gradient estimation for KL-divergence

$$\nabla_\phi \mathrm{KL}(q_\phi \| p)$$

Motivation

Gradient estimation for KL-divergence

- $q_\phi(\mathbf{x}), p(\mathbf{x})$ are intractable
- easy access to the sample of q_ϕ through $\epsilon \sim \nu$, $\mathbf{x} = g_\phi(\epsilon)$

$$\nabla_\phi \mathrm{KL}(q_\phi \| p)$$

Motivation

Gradient estimation for KL-divergence

- $q_\phi(\mathbf{x}), p(\mathbf{x})$ are intractable
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$$\nabla_\phi \mathrm{KL}(q_\phi \| p) = \mathbb{E}_{\epsilon\sim\nu}[\nabla \log q(\mathbf{x}) \nabla_\phi g_\phi(\epsilon)] - \mathbb{E}_{\epsilon\sim\nu}[\nabla \log p(\mathbf{x}) \nabla_\phi g_\phi(\epsilon)]$$

Motivation

Gradient estimation for KL-divergence

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Score function

Motivation

Gradient estimation for KL-divergence

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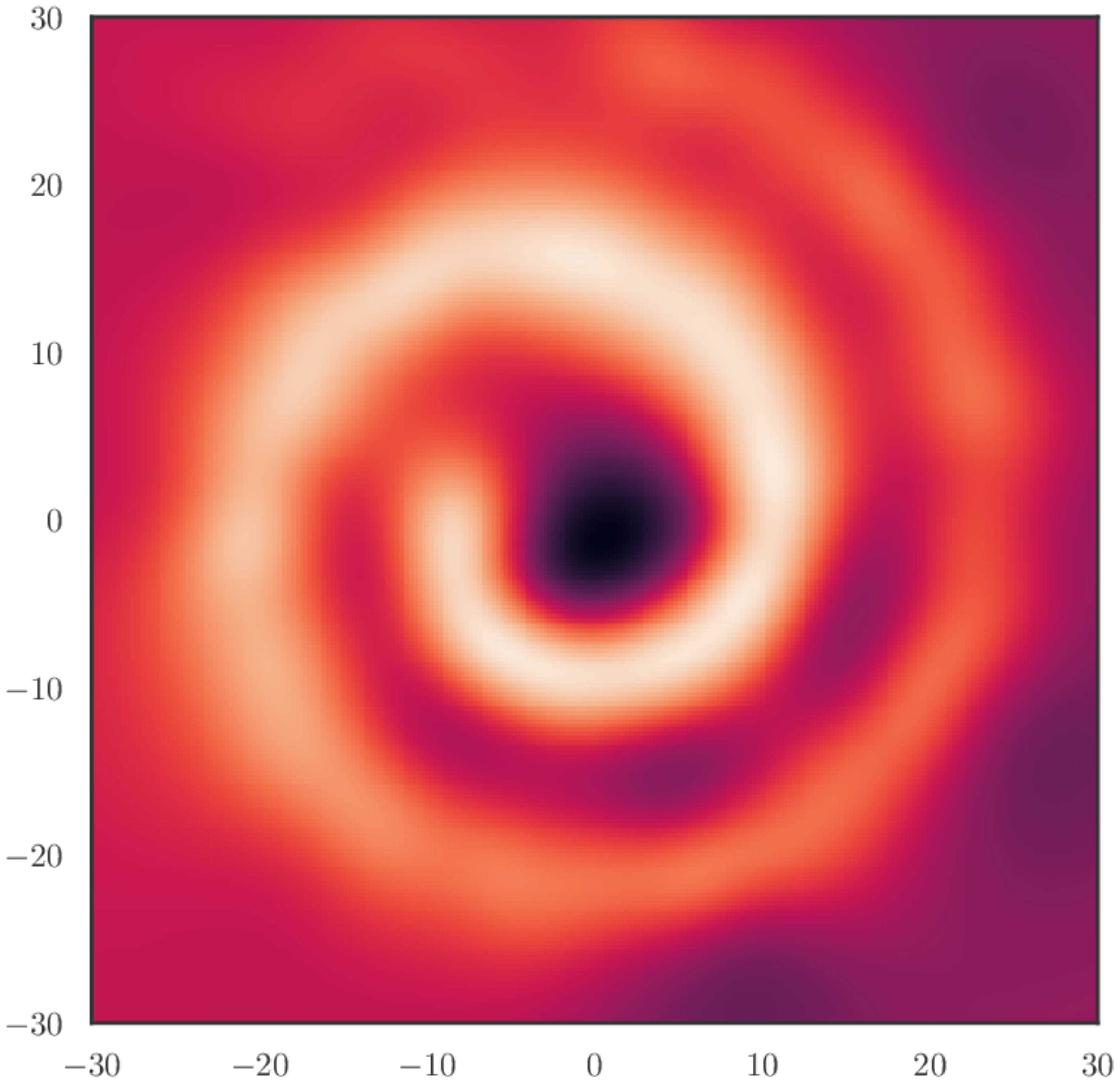
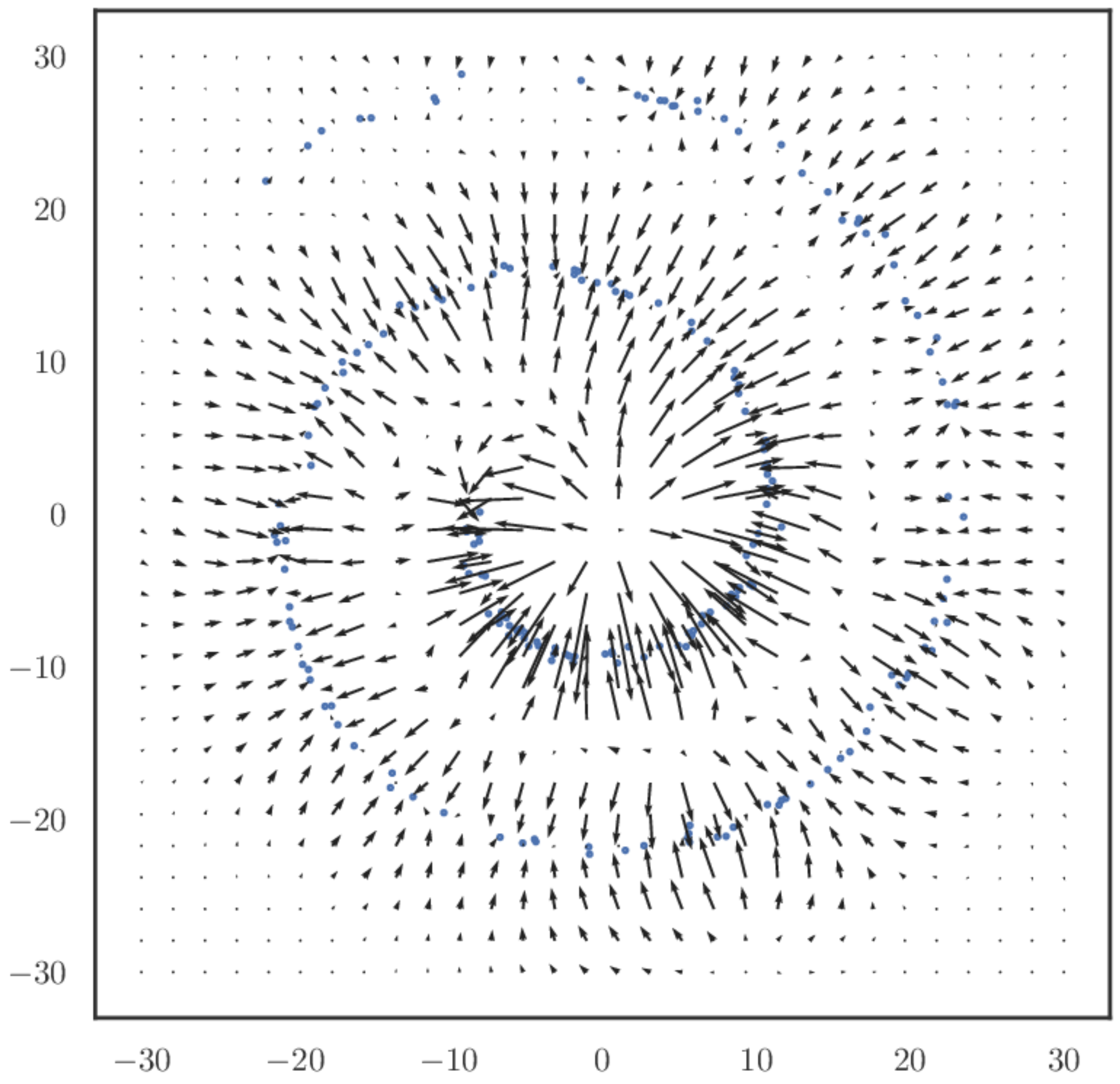
Score function

$$\{\mathbf{x}^j\}_{j=1}^M \overset{\text{i.i.d.}}{\sim} q \longrightarrow \nabla \log q(\mathbf{x})$$

Score Estimation



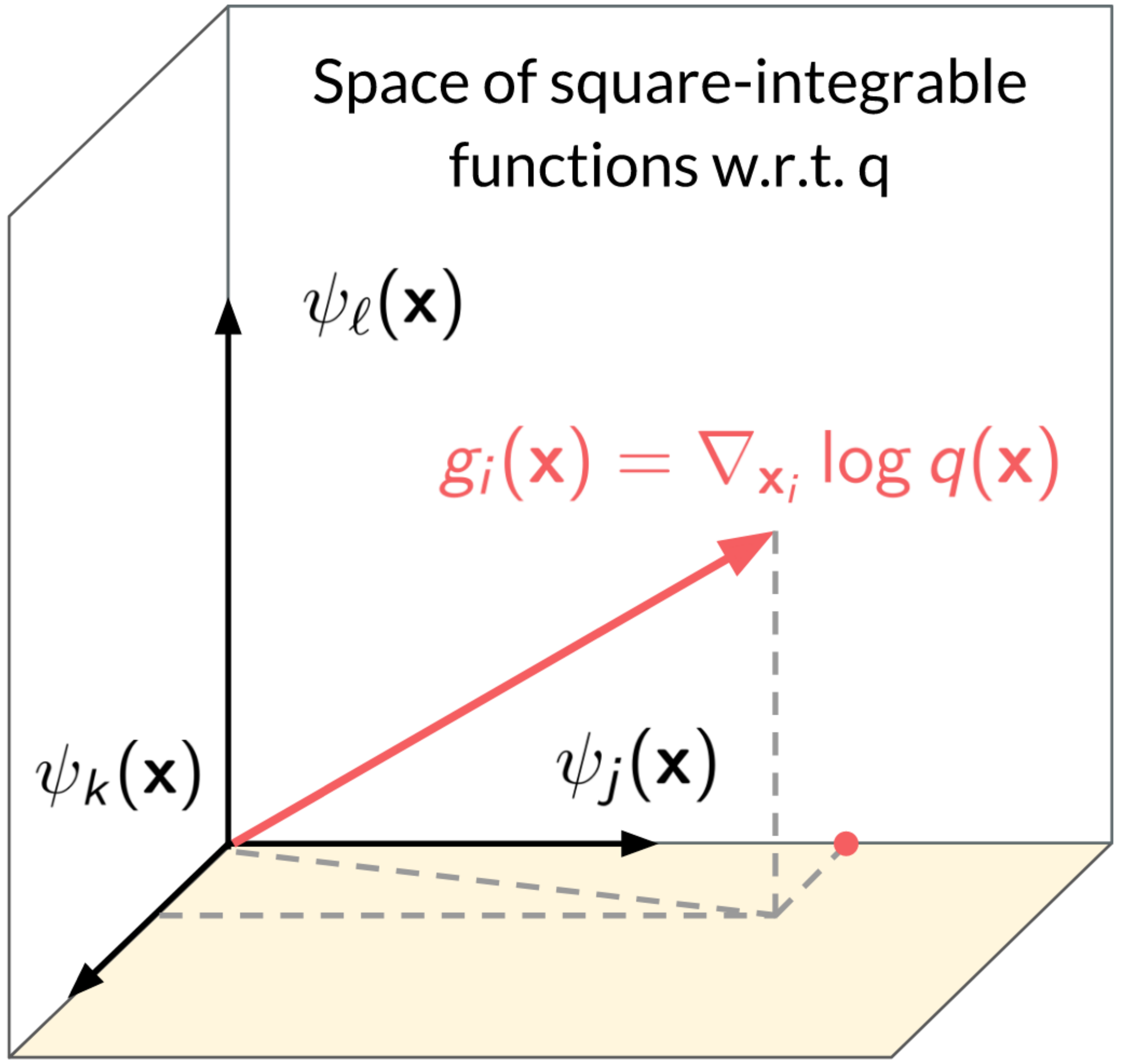
$q(\mathbf{x})$



$\nabla \log q(\mathbf{x})$

A Spectral Estimator

Main result



$$\mathbb{E}_{\mathbf{x}' \sim q}[k(\mathbf{x}, \mathbf{x}')\psi_j(\mathbf{x}')] = \lambda_j \psi_j(\mathbf{x})$$

- Under mild conditions

$$\nabla_{x_i} \log q(\mathbf{x}) = -\sum_{j \geq 1} \mathbb{E}_q \left[\nabla_{x_i} \psi_j(\mathbf{x}) \right] \psi_j(\mathbf{x})$$

- Nyström methods for estimating ψ_j and its derivatives
- Truncating the series at small eigenvalues

Shi et al. A spectral approach to gradient estimation for implicit distributions. ICML 2018

A Spectral Estimator

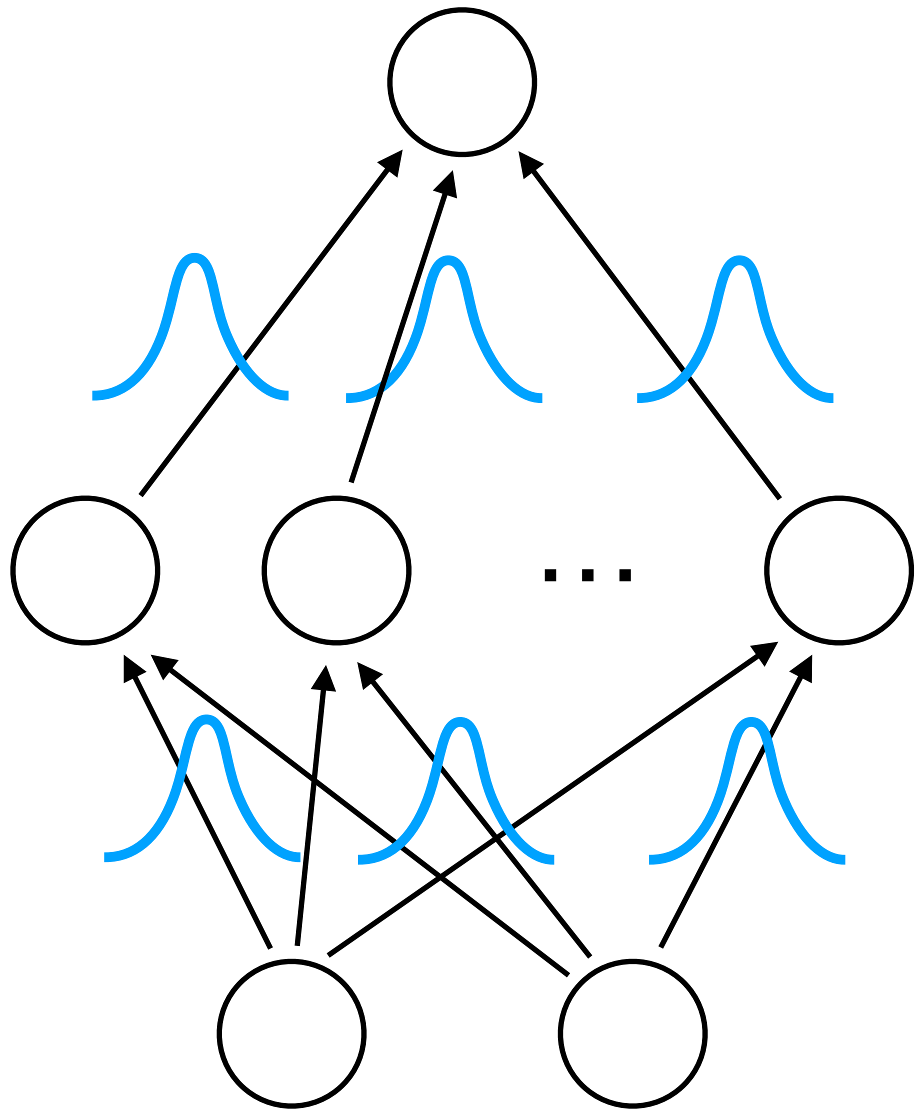
Properties

	Alain & Bengio, 14	Sriperumbudur et al., 13	Li & Turner, 17	This work
Closed-form	**N**	**Y**	**Y**	**Y**
Complexity scales linearly w/ d	**Y**	**N**	**Y**	**Y**
Principled out-of-sample prediction	**Y**	**Y**	**N**	**Y**
Convergence rates	-	[1/4, 1/3]	-	[1/4, 1/2)
	need training	cubic scaling	only in-sample prediction	

Applications

Functional Bayesian Neural Networks

Bayesian Neural Networks



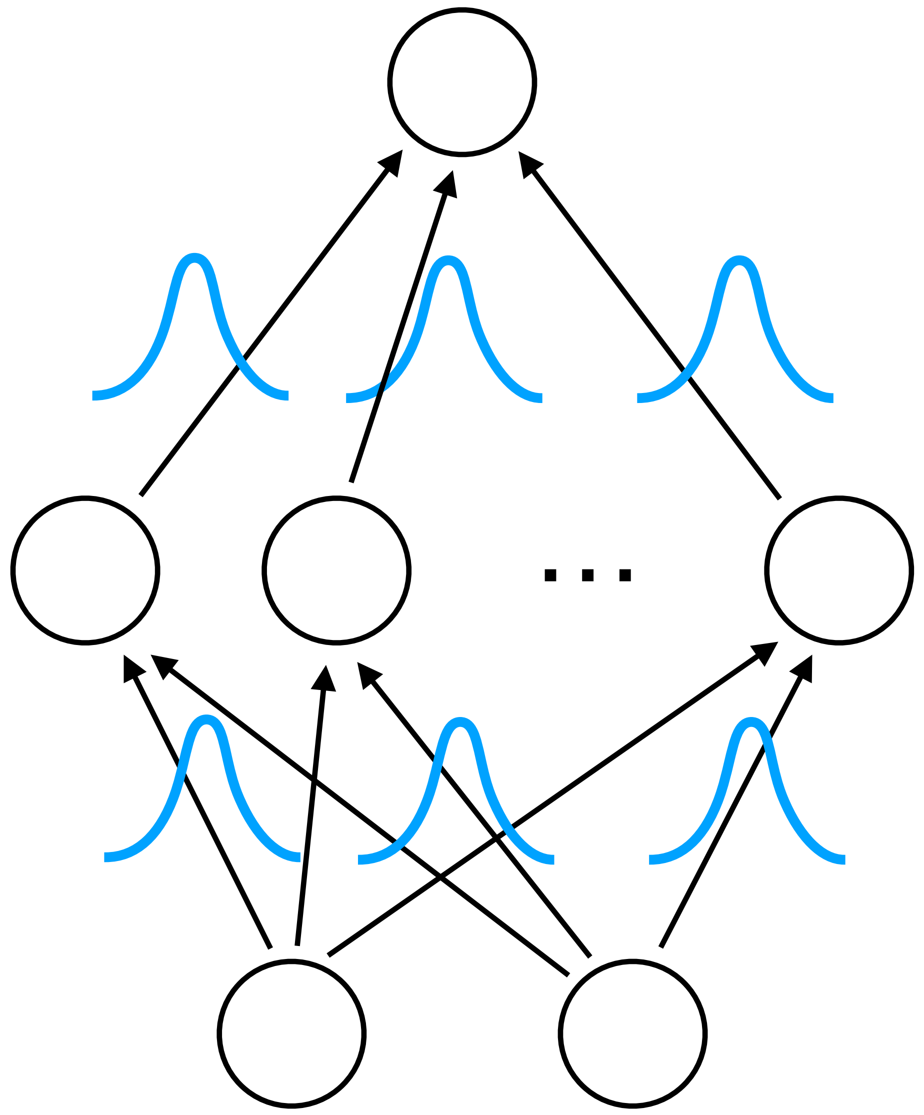
$$p(w \mid \mathbf{X}, \mathbf{y}) \propto \prod_{i=1}^{n} p(y_i \mid f(\mathbf{x}_i; \mathbf{w}))p(\mathbf{w})$$

Sun*, Zhang*, **Shi***, Grosse. Functional variational Bayesian neural networks. ICLR 2019

Applications

Functional Bayesian Neural Networks

Bayesian Neural Networks



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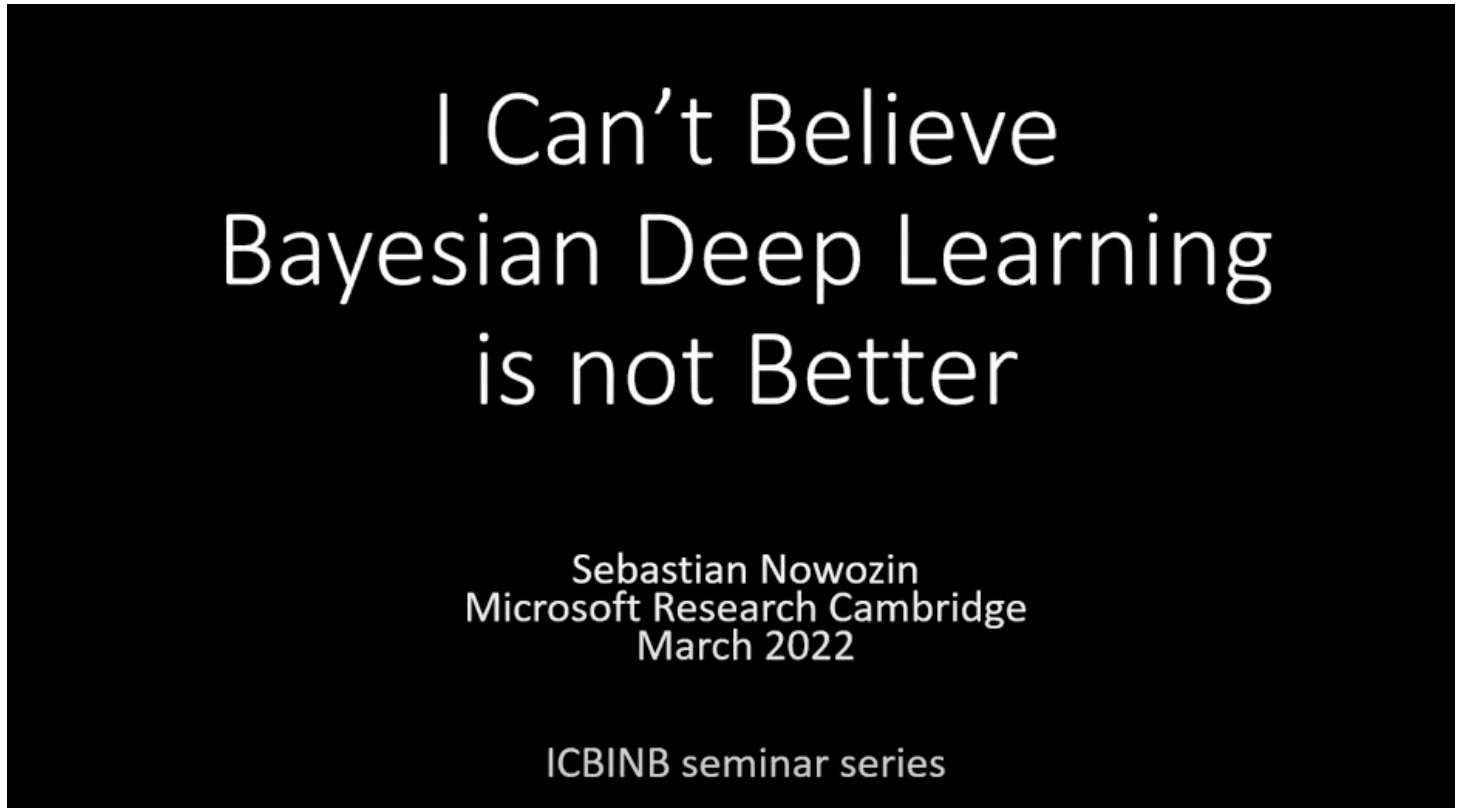

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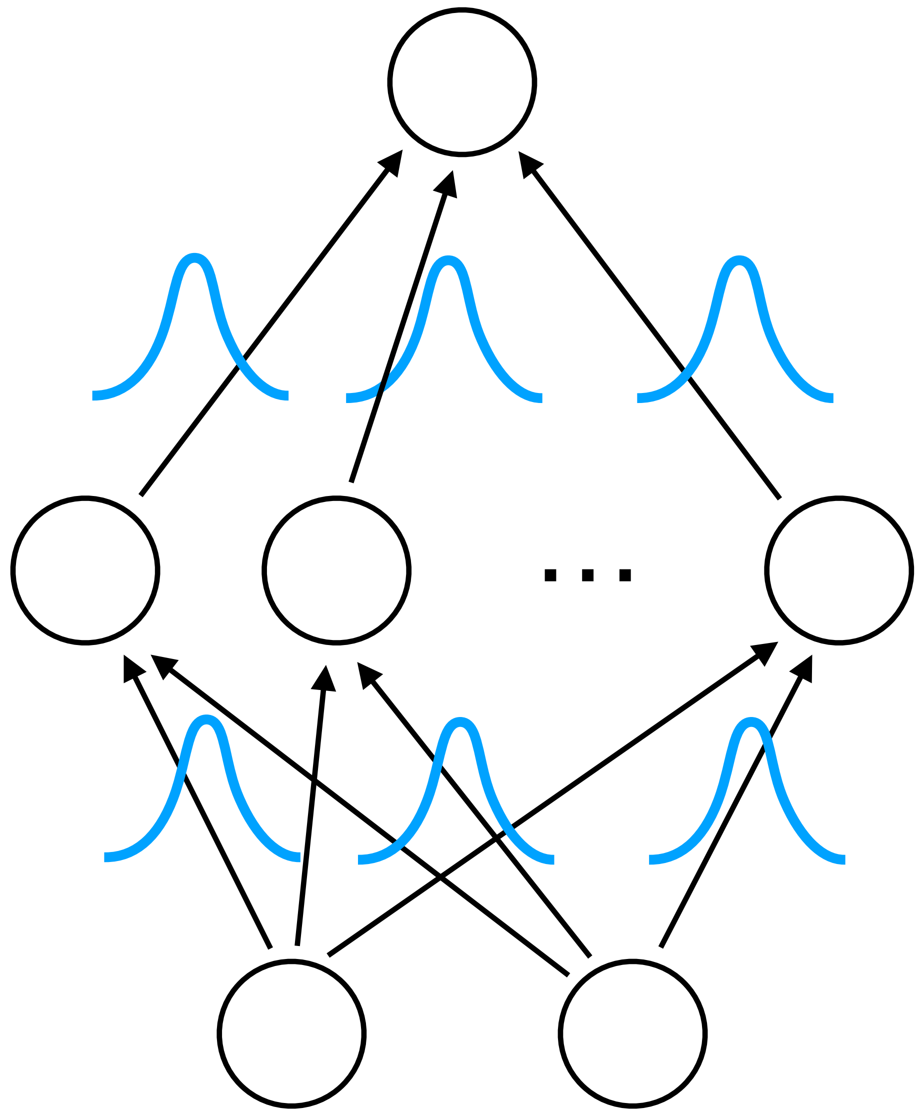

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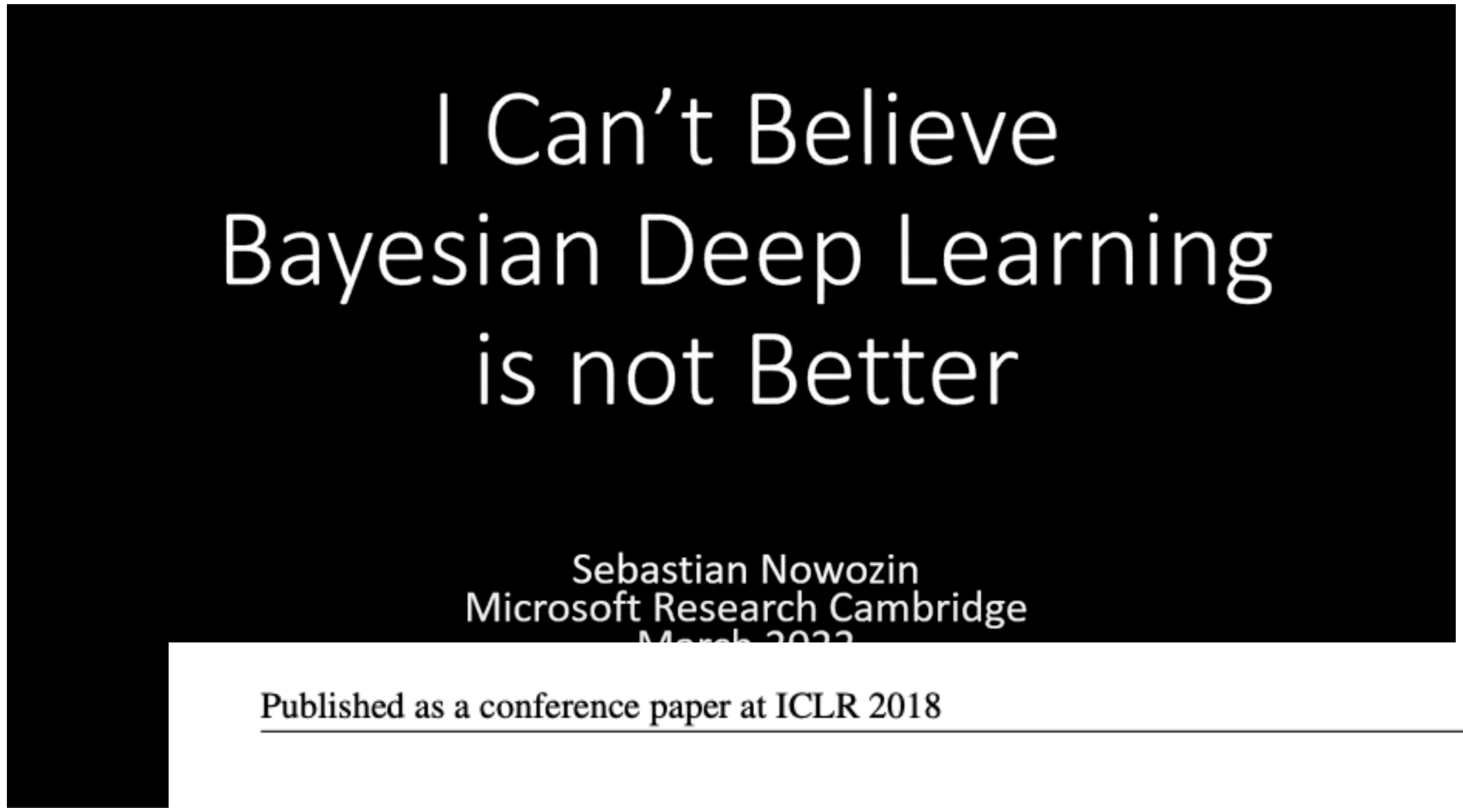
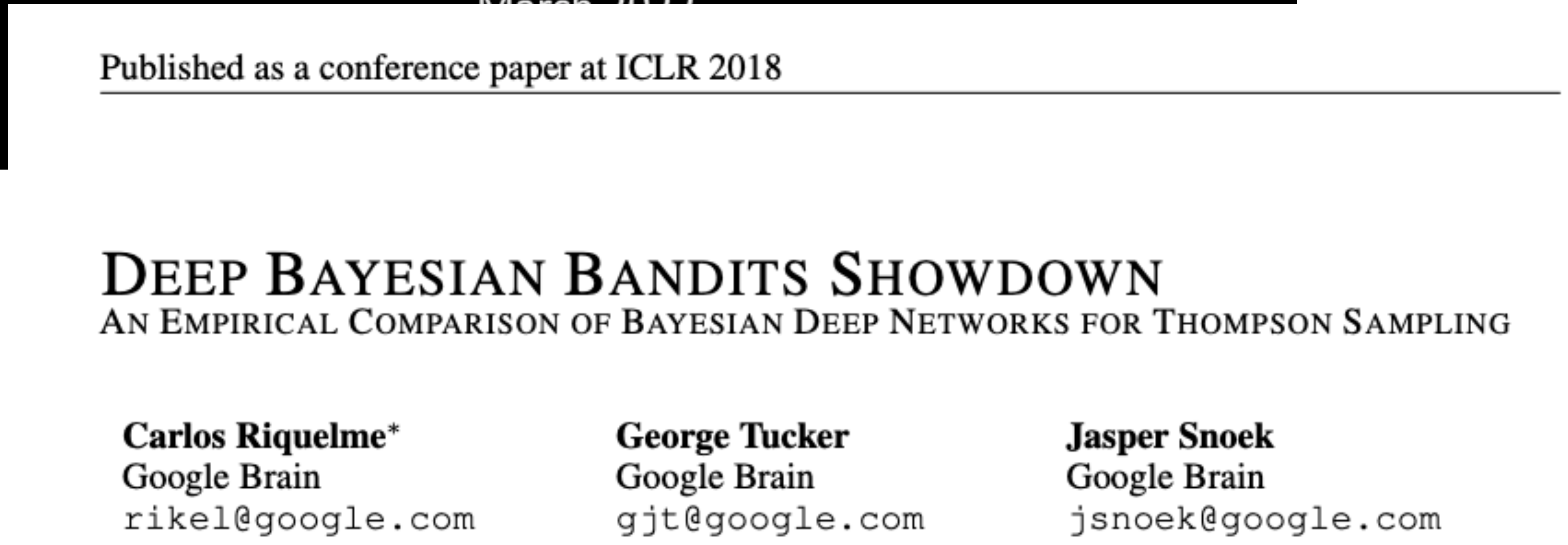


I Can't Believe
Bayesian Deep Learning
is not Better

Sebastian Nowozin
Microsoft Research Cambridge



Published as a conference paper at ICLR 2018

DEEP BAYESIAN BANDITS SHOWDOWN

AN EMPIRICAL COMPARISON OF BAYESIAN DEEP NETWORKS FOR THOMPSON SAMPLING

Carlos Riquelme* Google Brain rikel@google.com

George Tucker Google Brain gjt@google.com

Jasper Snoek Google Brain jsnoek@google.com

Sun*, Zhang*, **Shi***, Grosse. Functional variational Bayesian neural networks. ICLR 2019

Applications

Functional Bayesian Neural Networks

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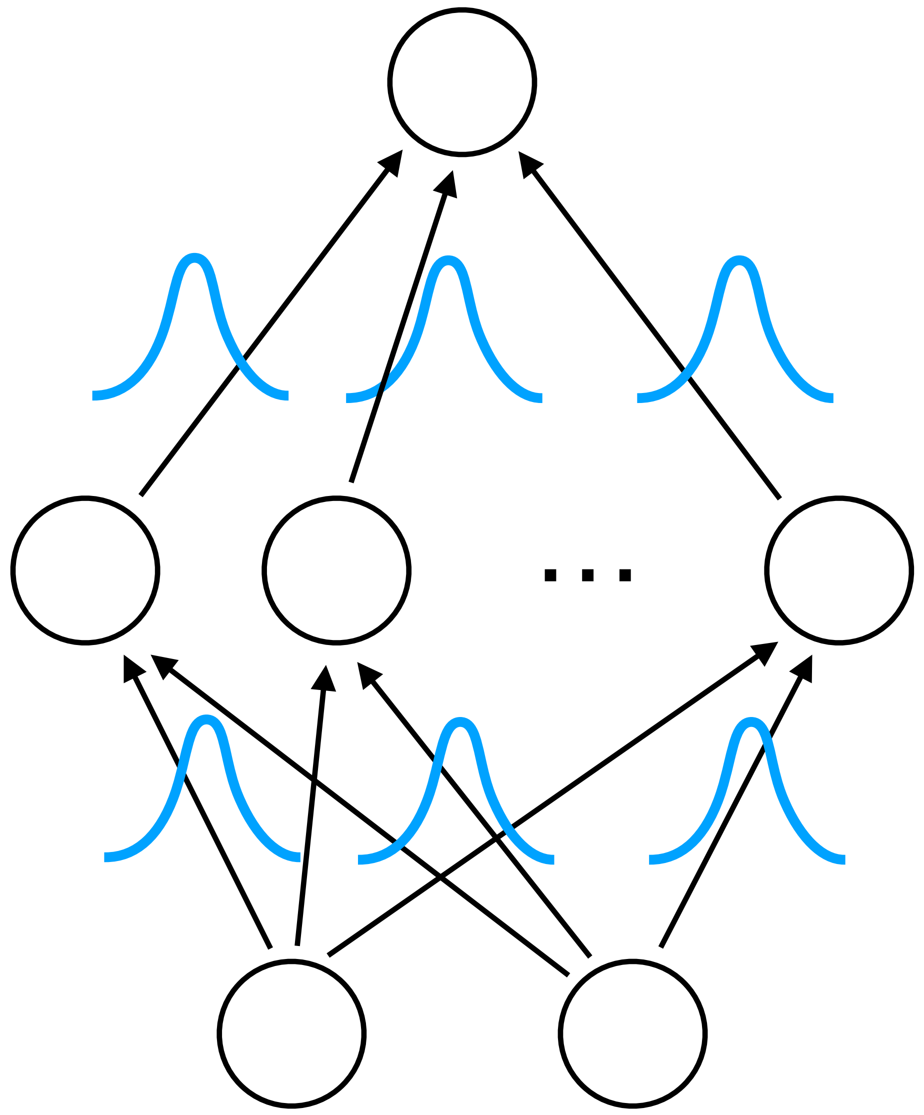

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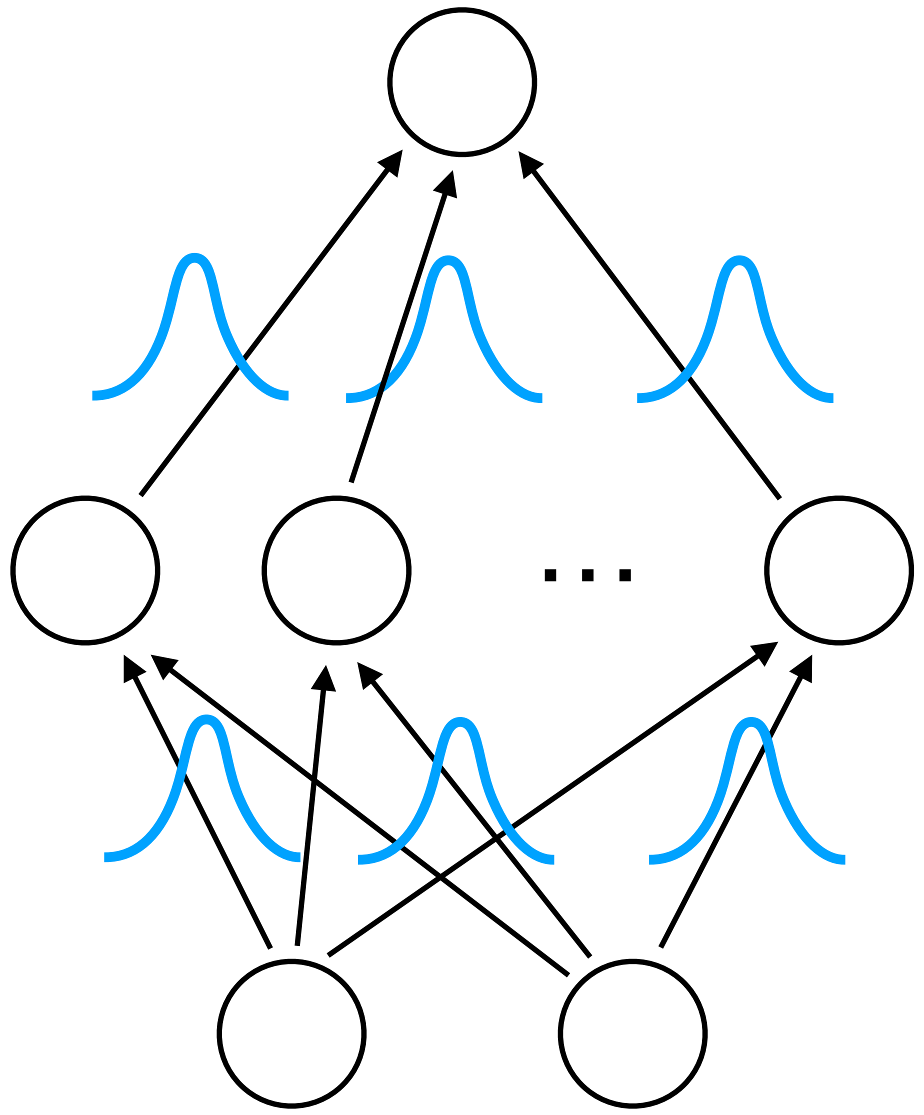
Sun*, Zhang*, **Shi***, Grosse. Functional variational Bayesian neural networks. ICLR 2019

Applications

Functional Bayesian Neural Networks

Bayesian Neural Networks



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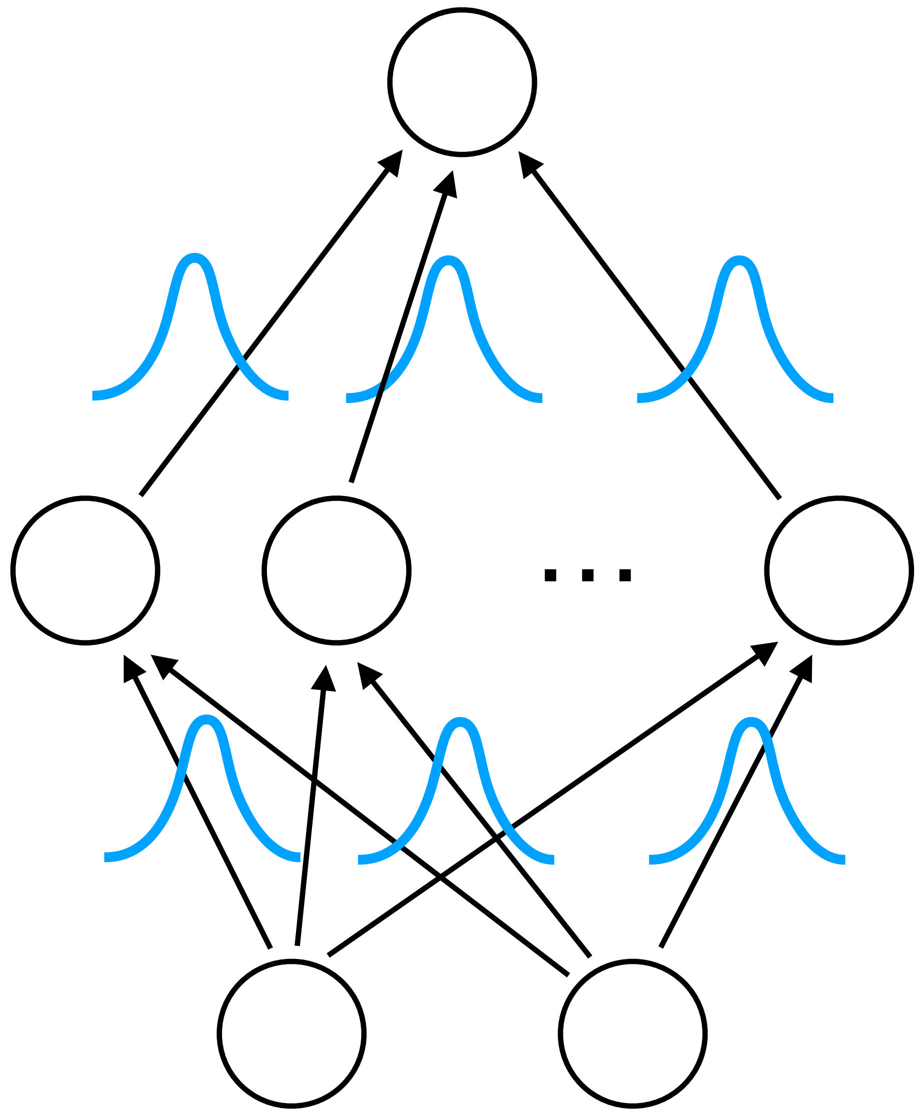
Applications

Functional Bayesian Neural Networks

Bayesian Neural Networks



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Applications

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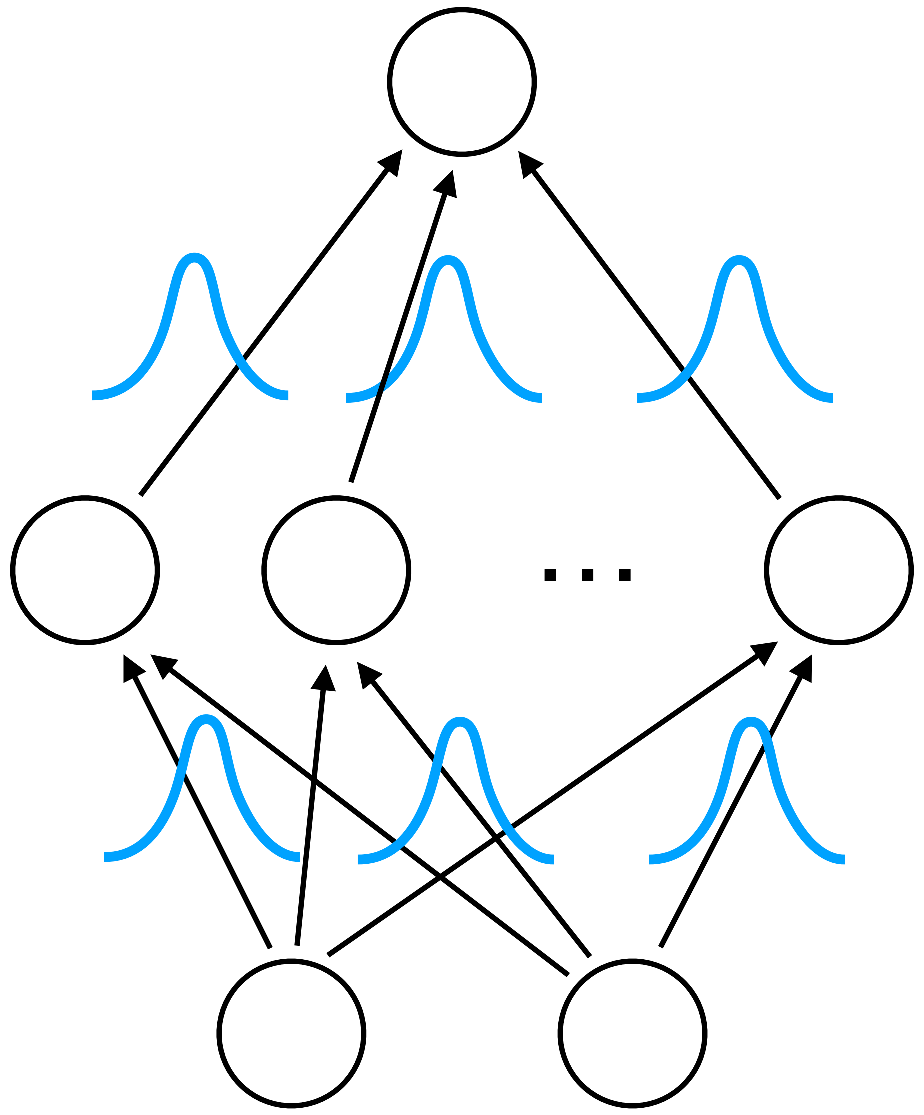

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Applications

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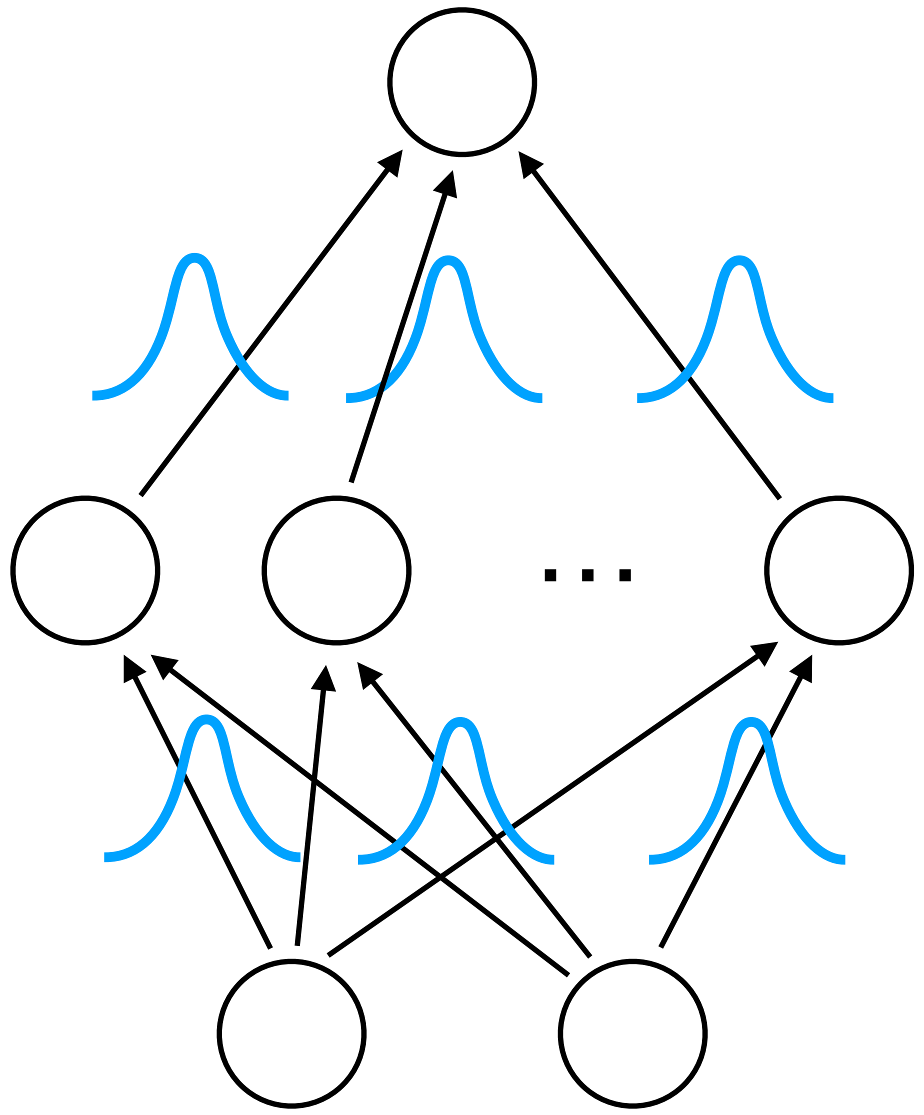

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Applications

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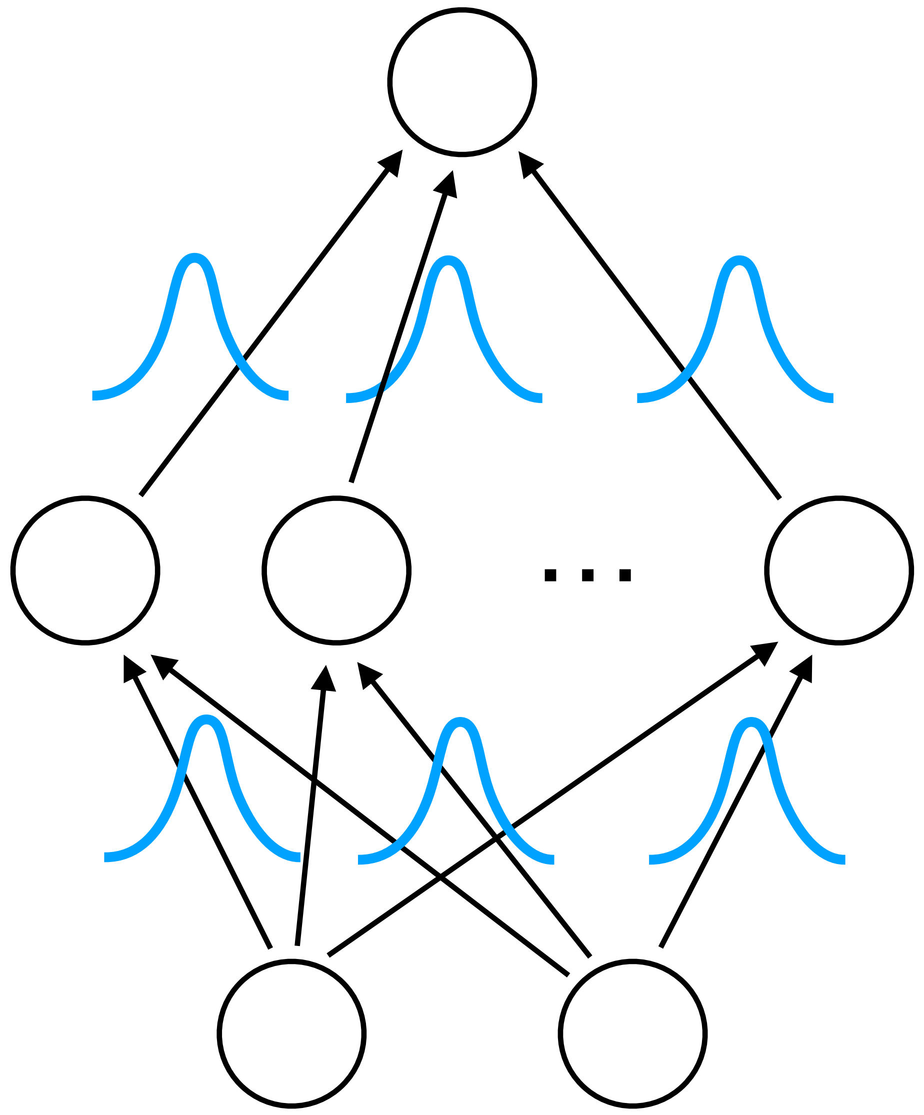

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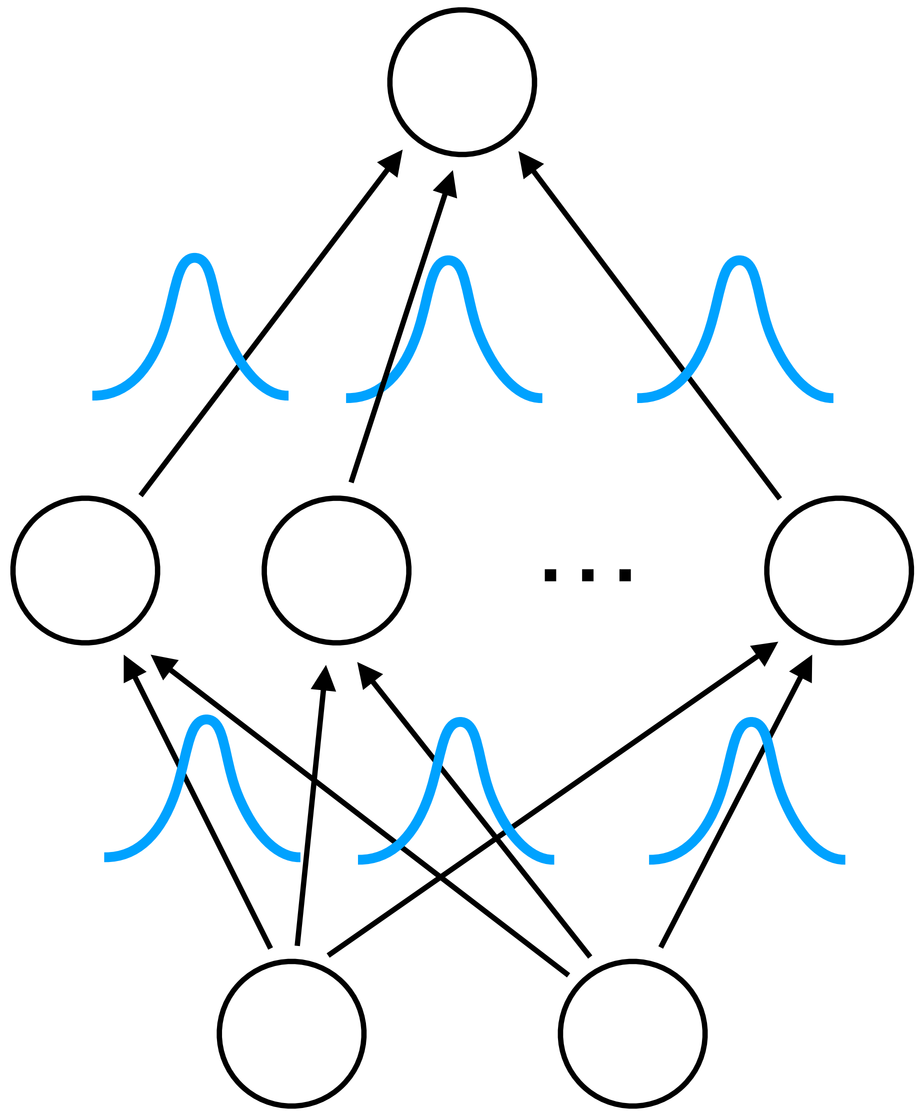

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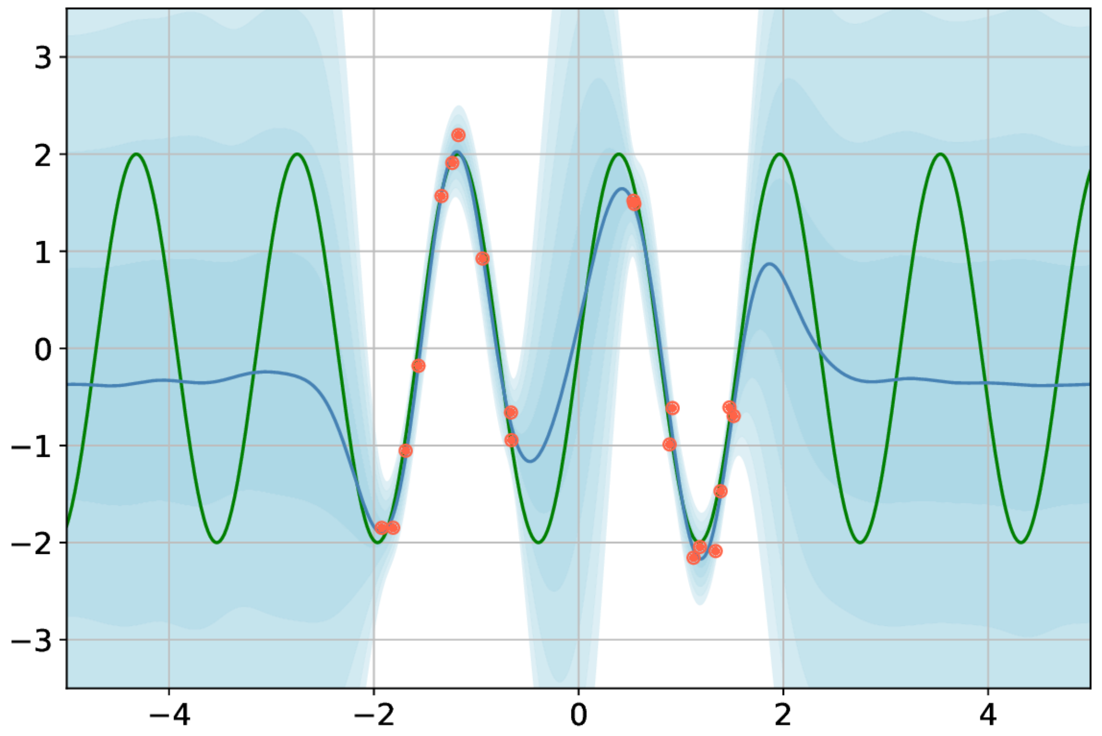
intractable

Sun*, Zhang*, **Shi***, Grosse. Functional variational Bayesian neural networks. ICLR 2019

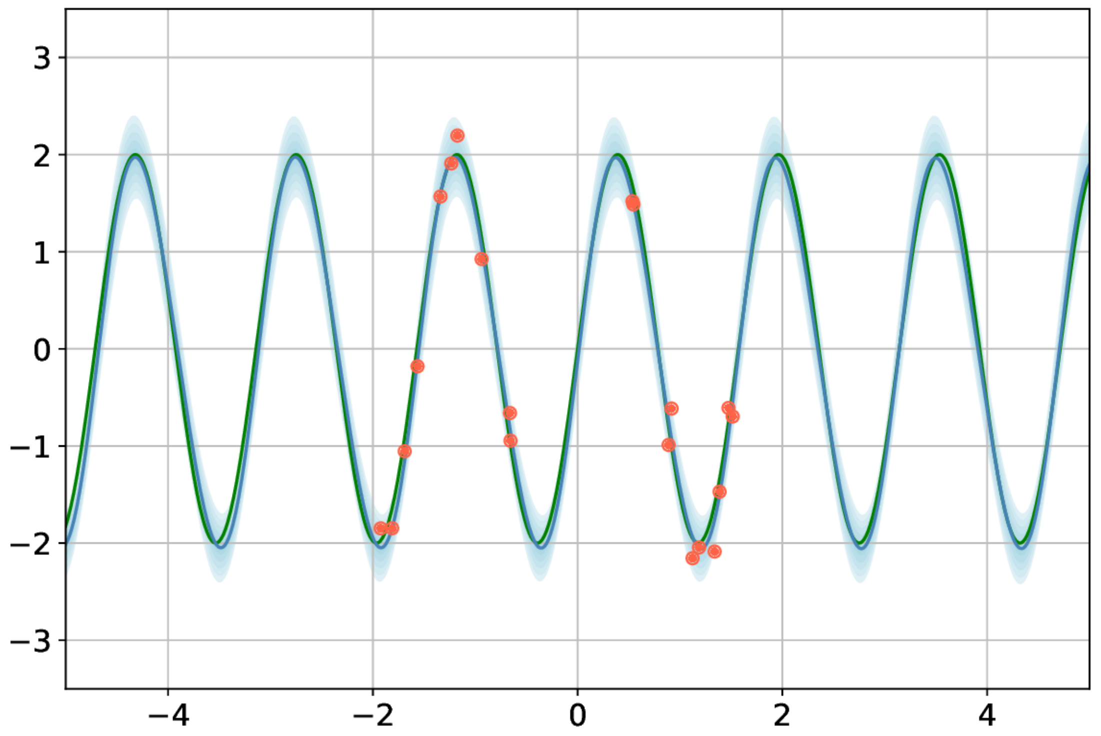
Applications

Functional Bayesian Neural Networks

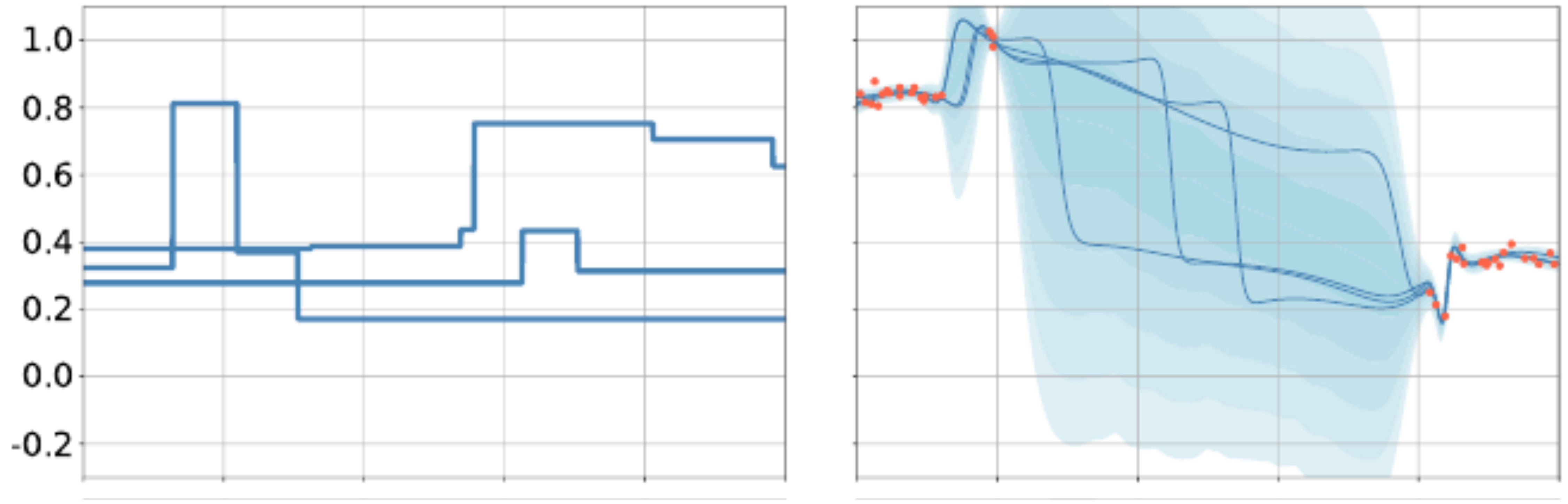
Locally smooth



Periodic



Piecewise constant



	M. Rank	M. Value	MushRoom	Statlog	Covertype	Financial	Jester	Adult
FBNN 1×50	4.7	41.9	21.38 ± 7.00	8.85 ± 4.55	47.16 ± 2.39	9.90 ± 2.40	75.55 ± 5.51	$\mathbf{88.43 \pm 1.95}$
FBNN 2×50	6.5	43.0	24.57 ± 10.81	10.08 ± 5.66	49.04 ± 3.75	11.83 ± 2.95	73.85 ± 6.82	88.81 ± 3.29
FBNN 3×50	7	45.0	34.03 ± 13.95	7.73 ± 4.37	50.14 ± 3.13	14.14 ± 1.99	74.27 ± 6.54	89.68 ± 1.66
FBNN 1×500	**3.8**	41.3	21.90 ± 9.95	6.50 ± 2.97	47.45 ± 1.86	$\mathbf{7.83 \pm 0.77}$	74.81 ± 5.57	89.03 ± 1.78
FBNN 2×500	4.2	41.2	23.93 ± 11.59	7.98 ± 3.08	46.00 ± 2.01	10.67 ± 3.52	$\mathbf{68.88 \pm 7.09}$	89.70 ± 2.01
FBNN 3×500	4.2	**40.9**	19.07 ± 4.97	10.04 ± 5.09	$\mathbf{45.24 \pm 2.11}$	11.48 ± 2.20	69.42 ± 7.56	90.01 ± 1.70
MultitaskGP	4.3	41.7	20.75 ± 2.08	7.25 ± 1.80	48.37 ± 3.50	8.07 ± 1.13	76.99 ± 6.01	88.64 ± 3.20
BBB 1×50	10.8	52.7	24.41 ± 6.70	25.67 ± 3.46	58.25 ± 5.00	37.69 ± 15.34	75.39 ± 6.32	95.07 ± 1.57
BBB 1×500	13.7	66.2	26.41 ± 8.71	51.29 ± 11.27	83.91 ± 4.62	57.20 ± 7.19	78.94 ± 4.98	99.21 ± 0.79
BBAlphaDiv	15	83.8	61.00 ± 6.47	70.91 ± 10.22	97.63 ± 3.21	85.94 ± 4.88	87.80 ± 5.08	99.60 ± 1.06
ParamNoise	10	47.9	20.33 ± 13.12	13.27 ± 2.85	65.07 ± 3.47	17.63 ± 4.27	74.94 ± 7.24	95.90 ± 2.20
NeuralLinear	10.8	48.8	16.56 ± 11.60	13.96 ± 1.51	64.96 ± 2.54	18.57 ± 2.02	82.14 ± 3.64	96.87 ± 0.92
LinFullPost	8.3	46.0	14.71 ± 0.67	19.24 ± 0.77	58.69 ± 1.17	10.69 ± 0.92	77.76 ± 5.67	95.00 ± 1.26
Dropout	5.5	41.7	$\mathbf{12.53 \pm 1.82}$	12.01 ± 6.11	48.95 ± 2.19	14.64 ± 3.95	71.38 ± 7.11	90.62 ± 2.21
RMS	6.5	43.9	15.29 ± 3.06	11.38 ± 5.63	58.96 ± 4.97	10.46 ± 1.61	72.09 ± 6.98	95.29 ± 1.50
BootRMS	4.7	42.6	18.05 ± 11.20	$\mathbf{6.13 \pm 1.03}$	53.63 ± 2.15	8.69 ± 1.30	74.71 ± 6.00	94.18 ± 1.94
Uniform	16	100	100.0 ± 0.0	100.0 ± 0.0	100.0 ± 0.0	100.0 ± 0.0	100.0 ± 0.0	100.0 ± 0.0

Exploration using posterior uncertainty in contextual bandits

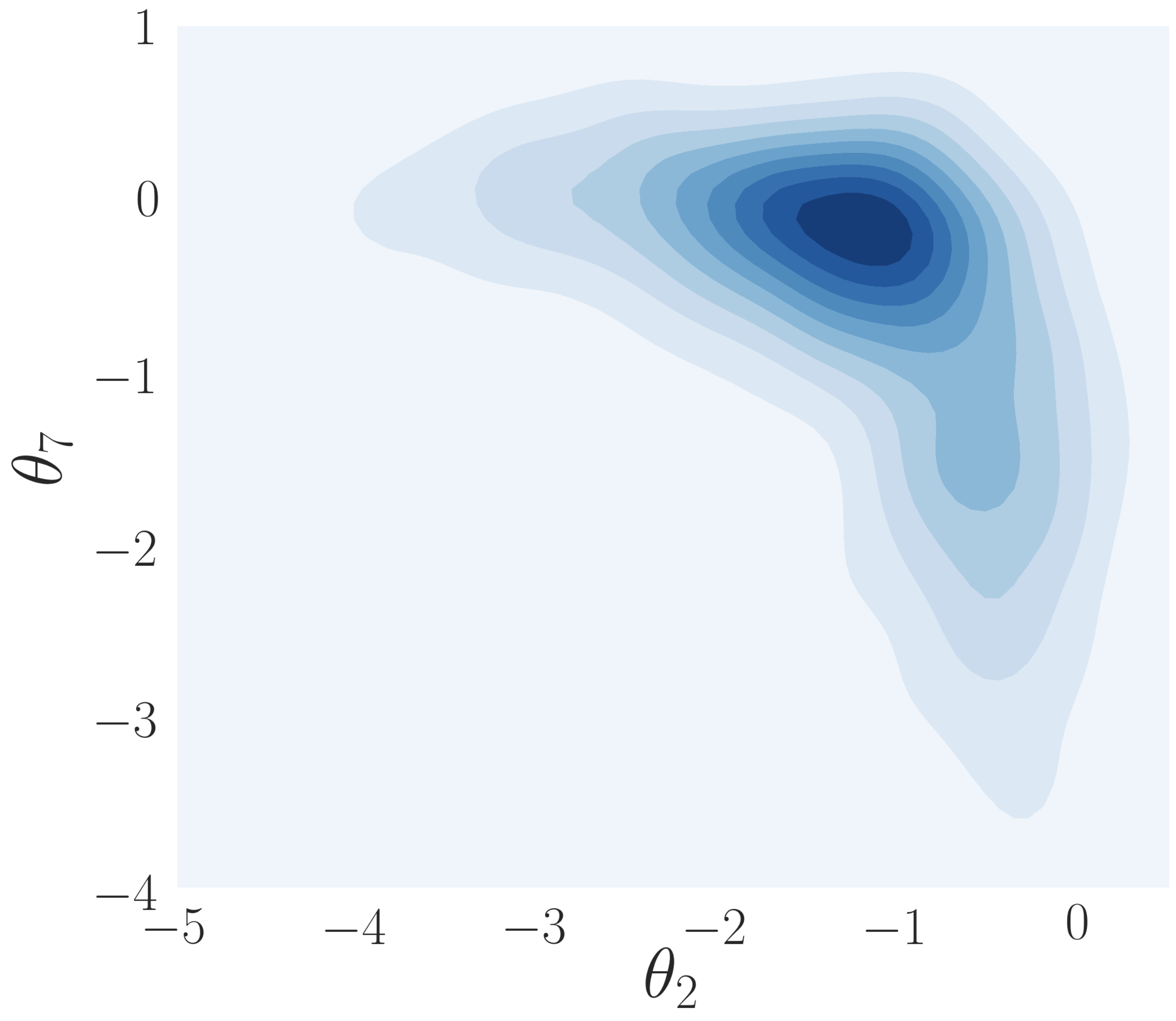
[Sun*, Zhang*, **Shi*** & Grosse, ICLR'19]

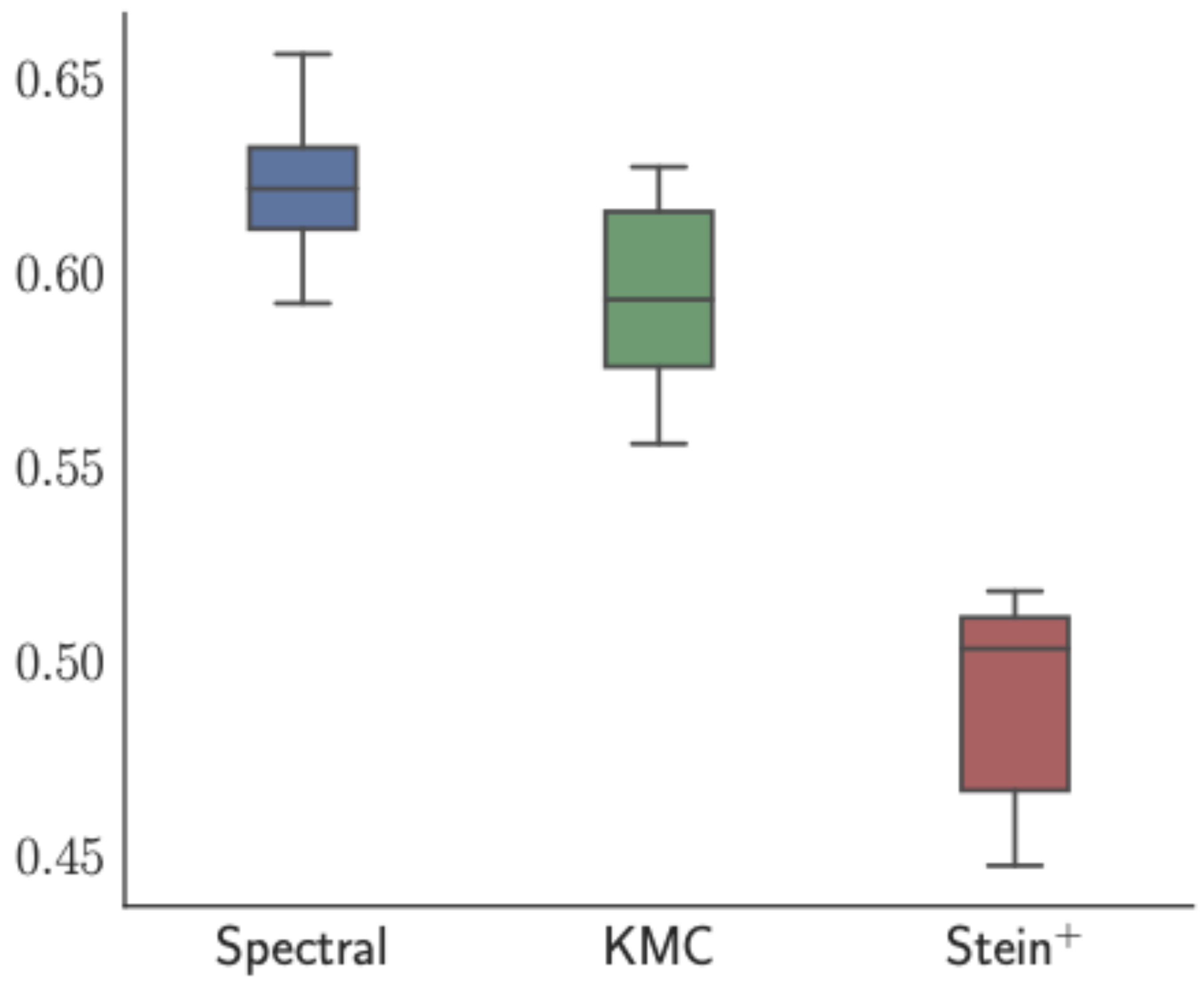
Applications

Learning Wasserstein Autoencoders

[Zhou, **Shi** & Zhu, ICML’20]

Gradient-free Hamiltonian Monte Carlo





[**Shi** et al., ICML’18]

Applications

Mutual Information Gradient Estimation

Performance of Learned Representations

Model	CIFAR-10			CIFAR-100		
	conv	fc(1024)	Y(64)	conv	fc(1024)	Y(64)
DIM (JSD)	55.81%	45.73%	40.67%	28.41%	22.16%	16.50%
DIM (JSD + PM)	52.2%	52.84%	43.17%	24.40%	18.22%	15.22%
DIM (infoNCE)	51.82%	42.81%	37.79%	24.60%	16.54%	12.96%
DIM (infoNCE + PM)	56.77%	49.42%	42.68%	25.51%	20.15%	15.35%
MIGE	**57.95%**	**57.09%**	**53.75%**	**29.86%**	**27.91%**	**25.84%**

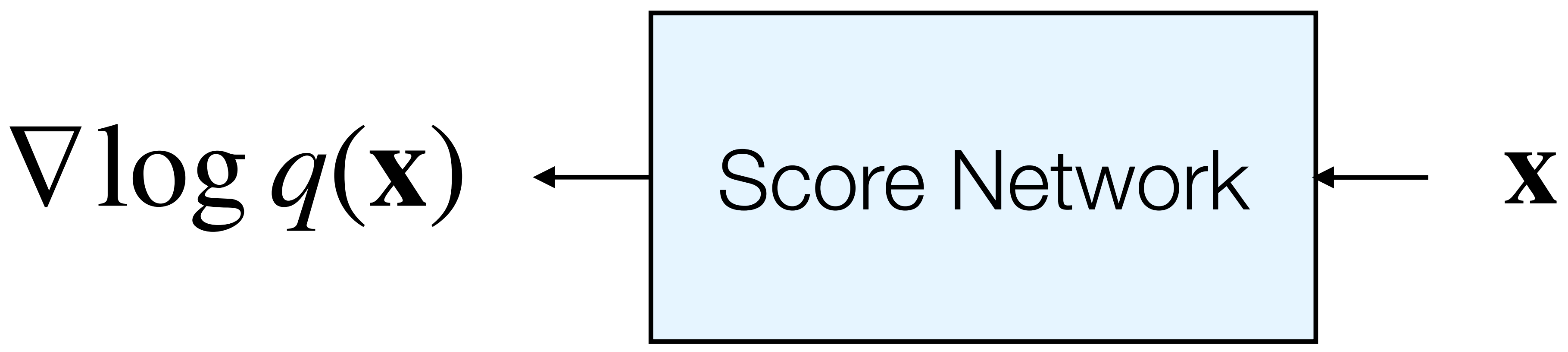
[Wen et al., ICLR’20]

Concluding Remarks

Gradient estimation for differentiable programming in probabilistic models

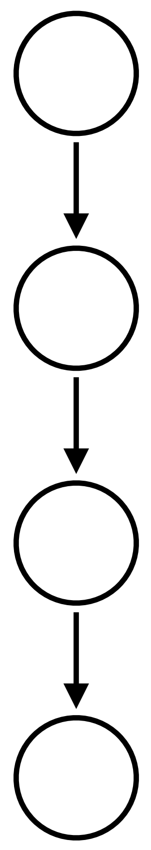
- Gradient Estimation for Discrete Expectations
  - Double control variates—a new framework for variance reduction in REINFORCE-type estimators
  - Discrete Stein operators—a general recipe for constructing flexible control variates for discrete distributions
- Gradient Estimation for Intractable Densities
  - Score estimation—a spectral approach and applications

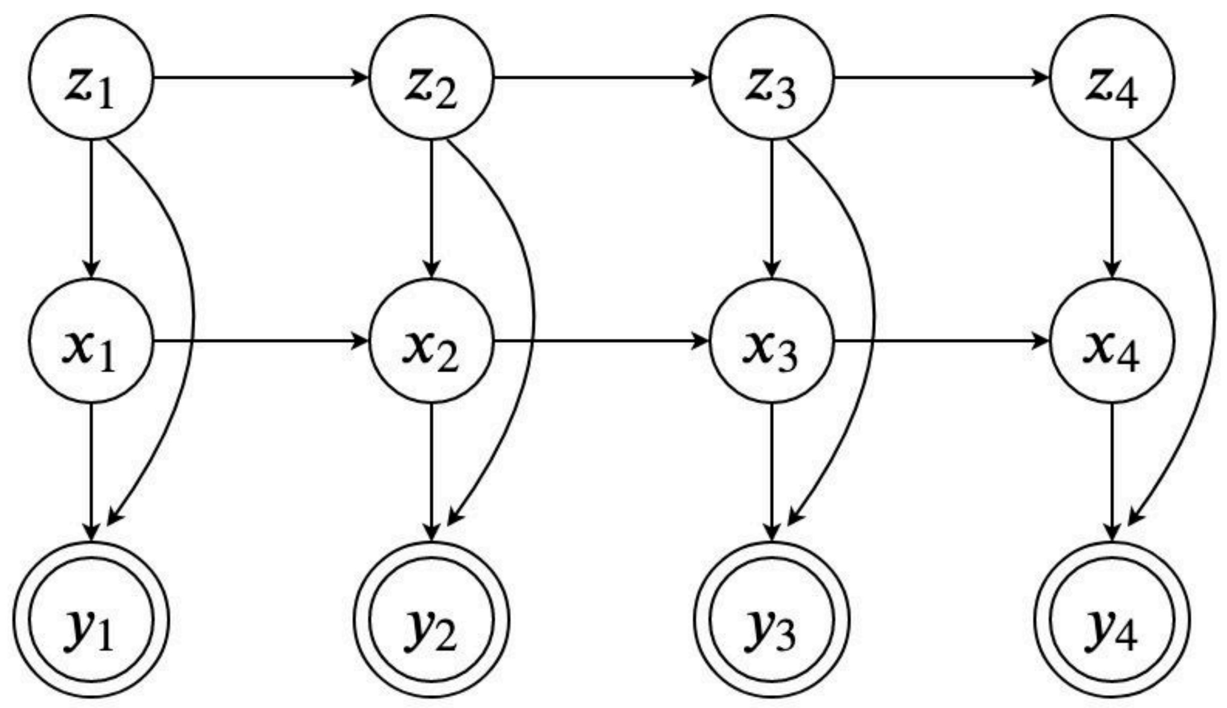
Future Directions



- Score-based probabilistic modeling
  - Parametric score estimators, e.g., sliced score matching [Song, Garg, **Shi**, Ermon, UAI'20]
  - Fit such estimators to data: score-based generative models

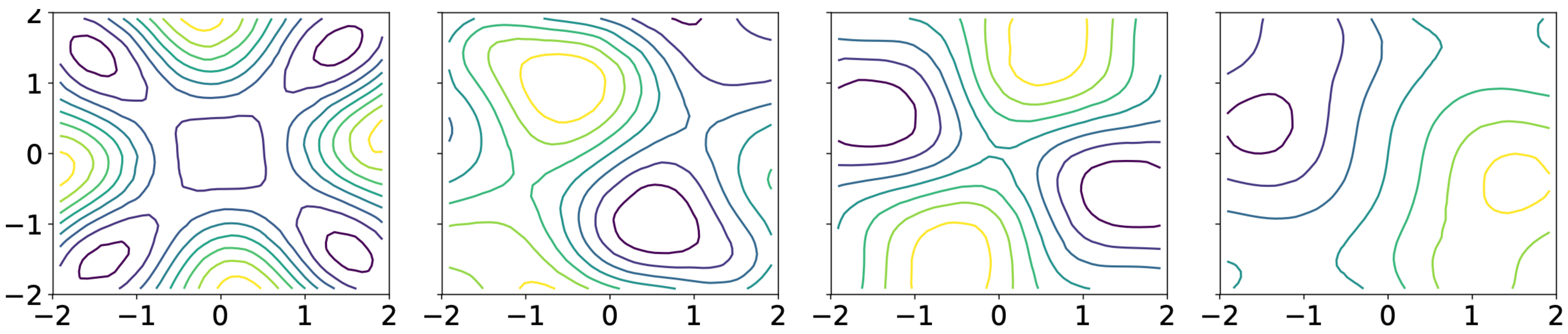
Future Directions





- Gradient estimation for discrete expectations in structured models
    - chains, temporal dependencies, state-space models
    - exploit graphical structure to achieve further variance reduction

Future Directions



[Sun, **Shi,** et al., ICML'21]

- Structured data distribution, symmetry and invariance
  - differentiable programming is good at exploiting invariance/equivariance
  - exploiting such properties in probabilistic inference?

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