



High-dimensional maximum-entropy phase space tomography

Austin Hoover

North American Particle Accelerator Conference

Sacramento, CA, USA

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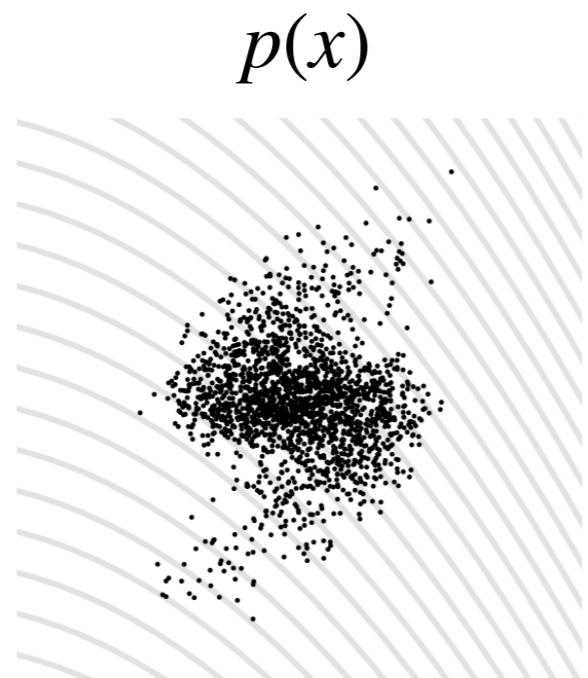
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Outline

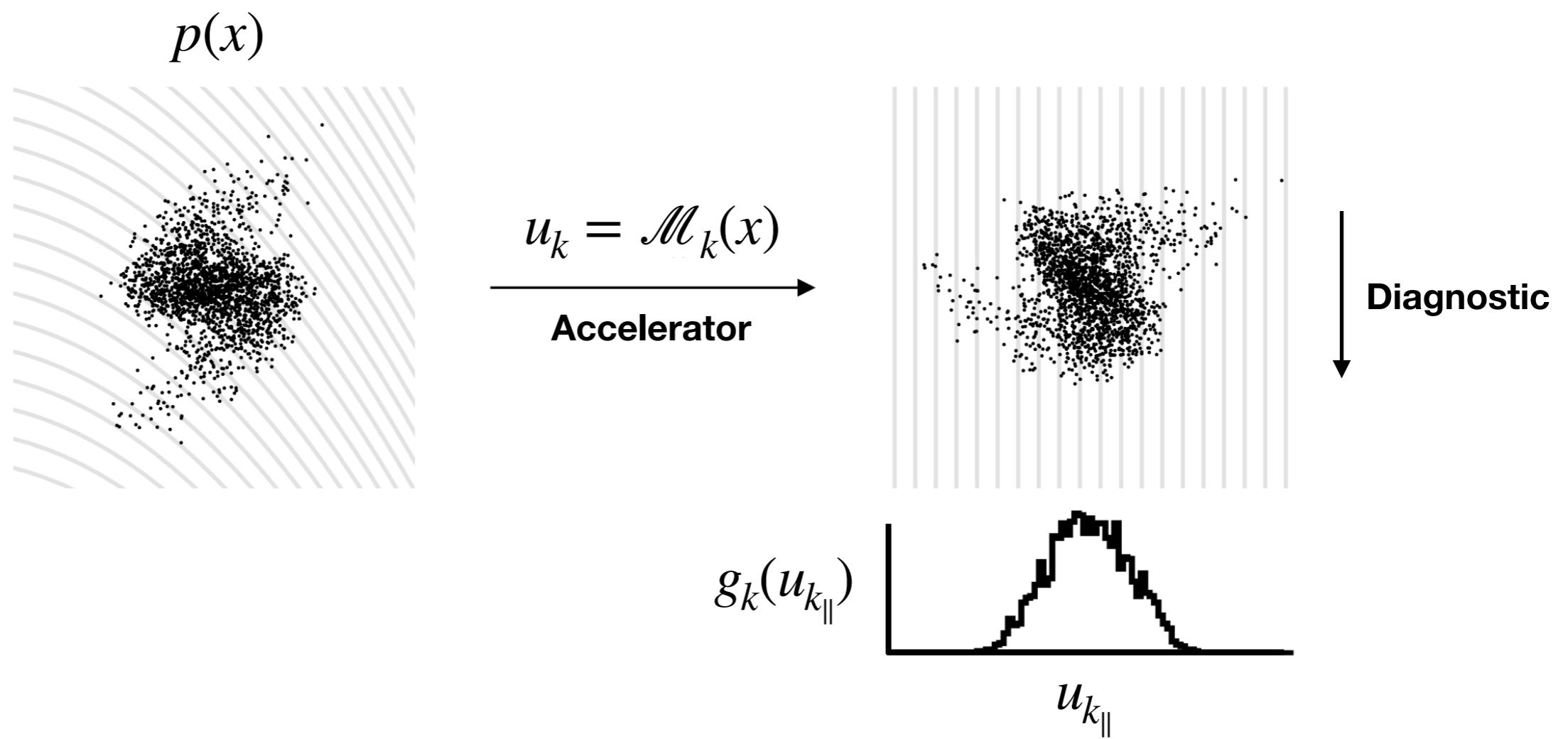
- Phase space tomography and maximum-entropy inference
- Two algorithms:
 - GPSR: generative modeling approach
 - MENT: classical approach
- Conclusion

Background

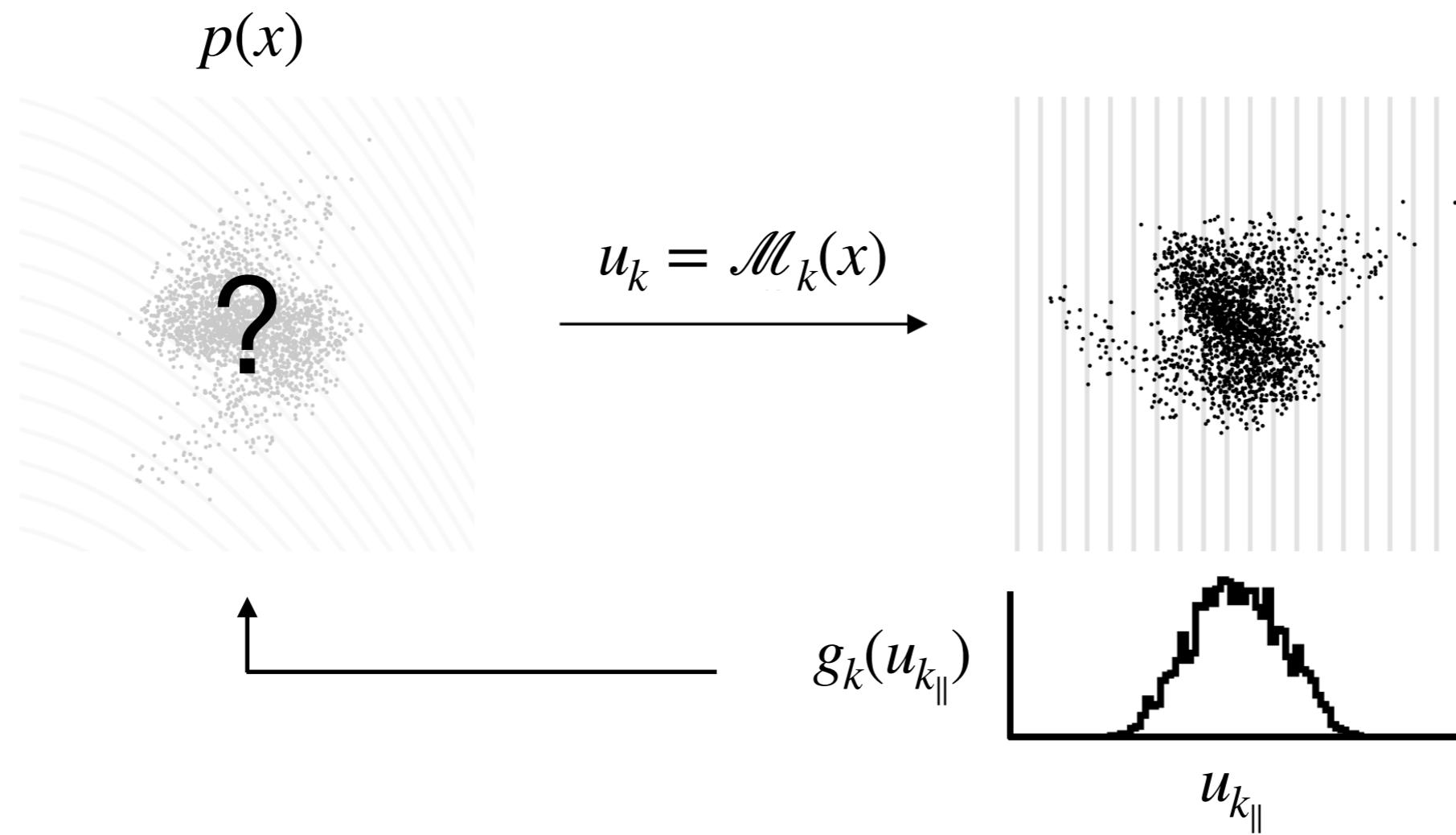
Goal: infer phase space density from measured projections



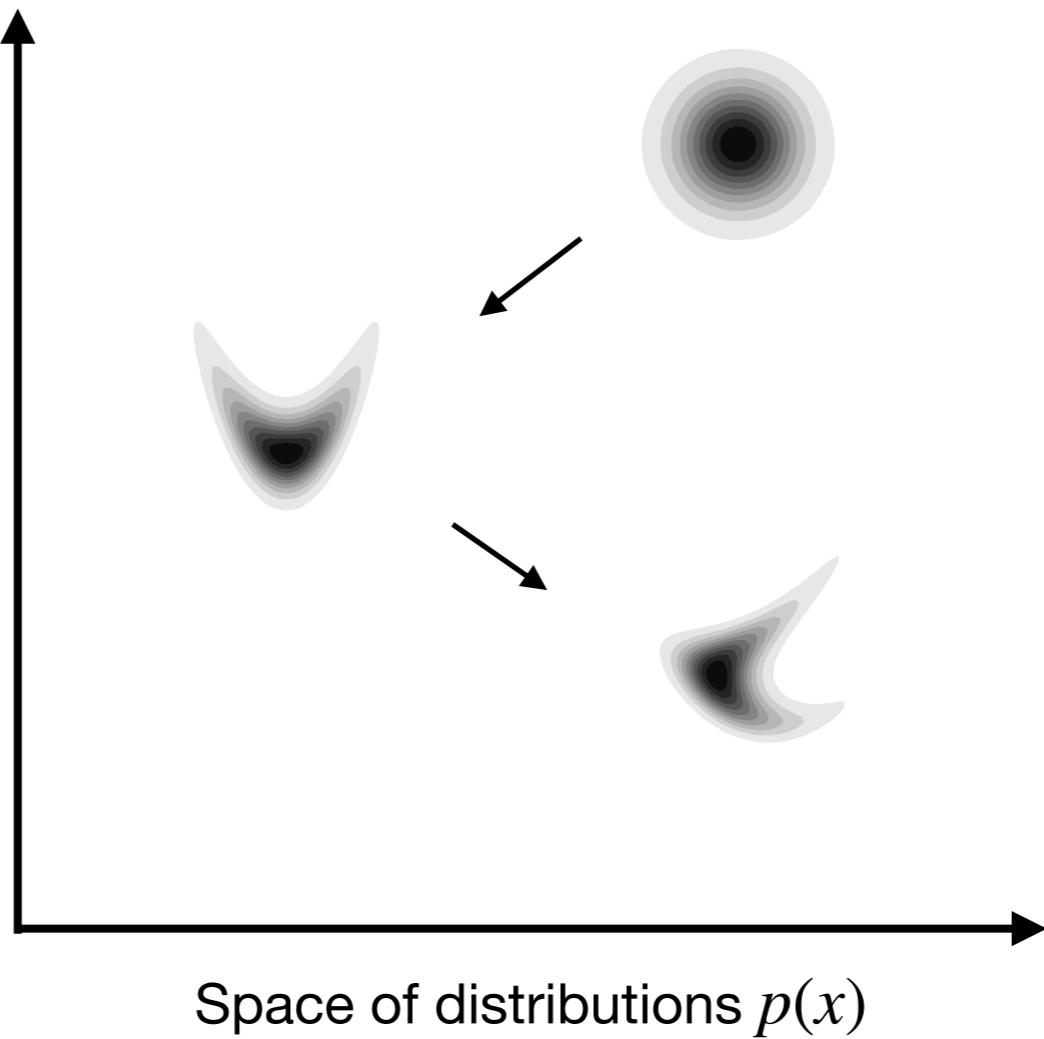
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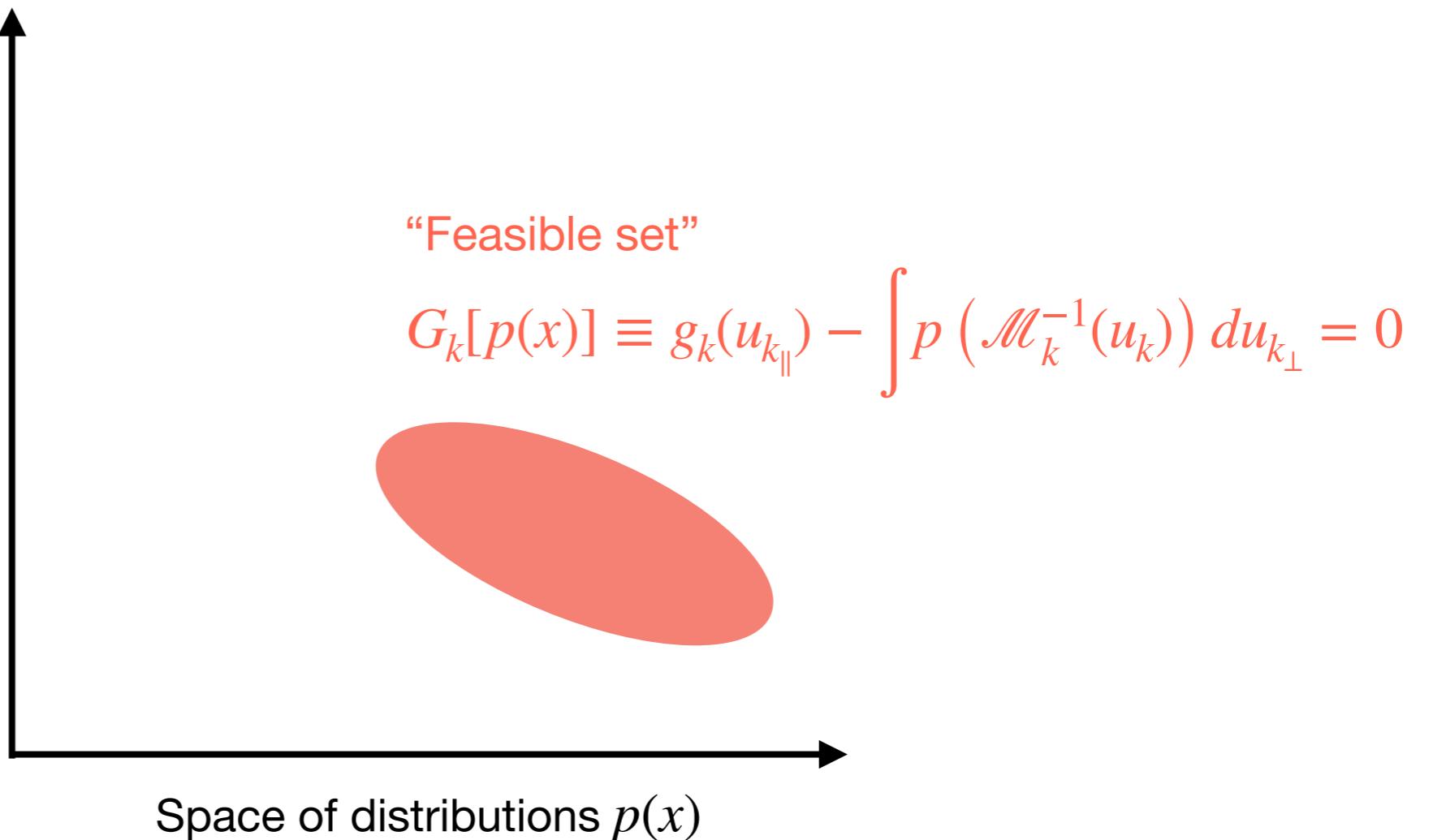
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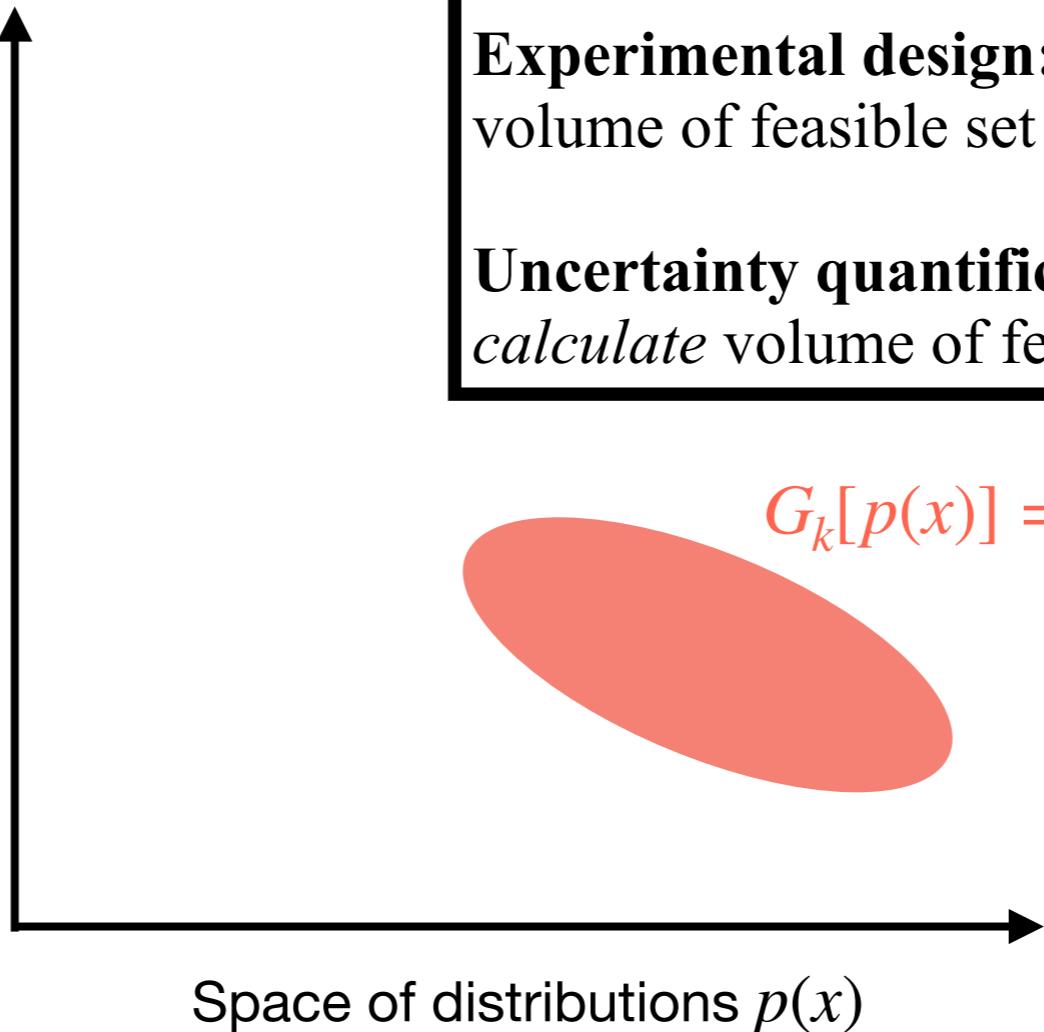
Challenge A: searching the space of distributions



Challenge B: solution is not unique



Challenge B: solution is not unique

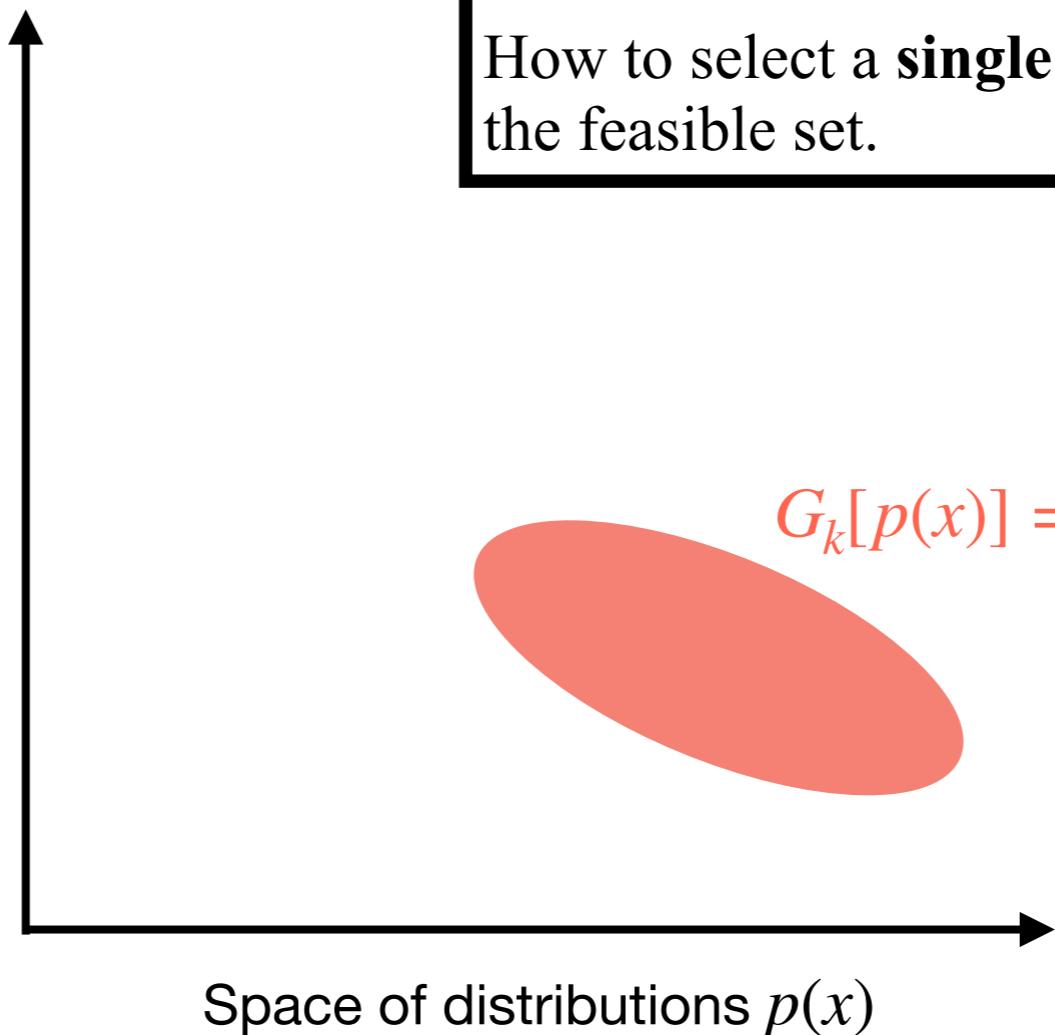


Things I *will not* discuss:

Experimental design: how to *shrink* volume of feasible set

Uncertainty quantification: how to *calculate* volume of feasible set

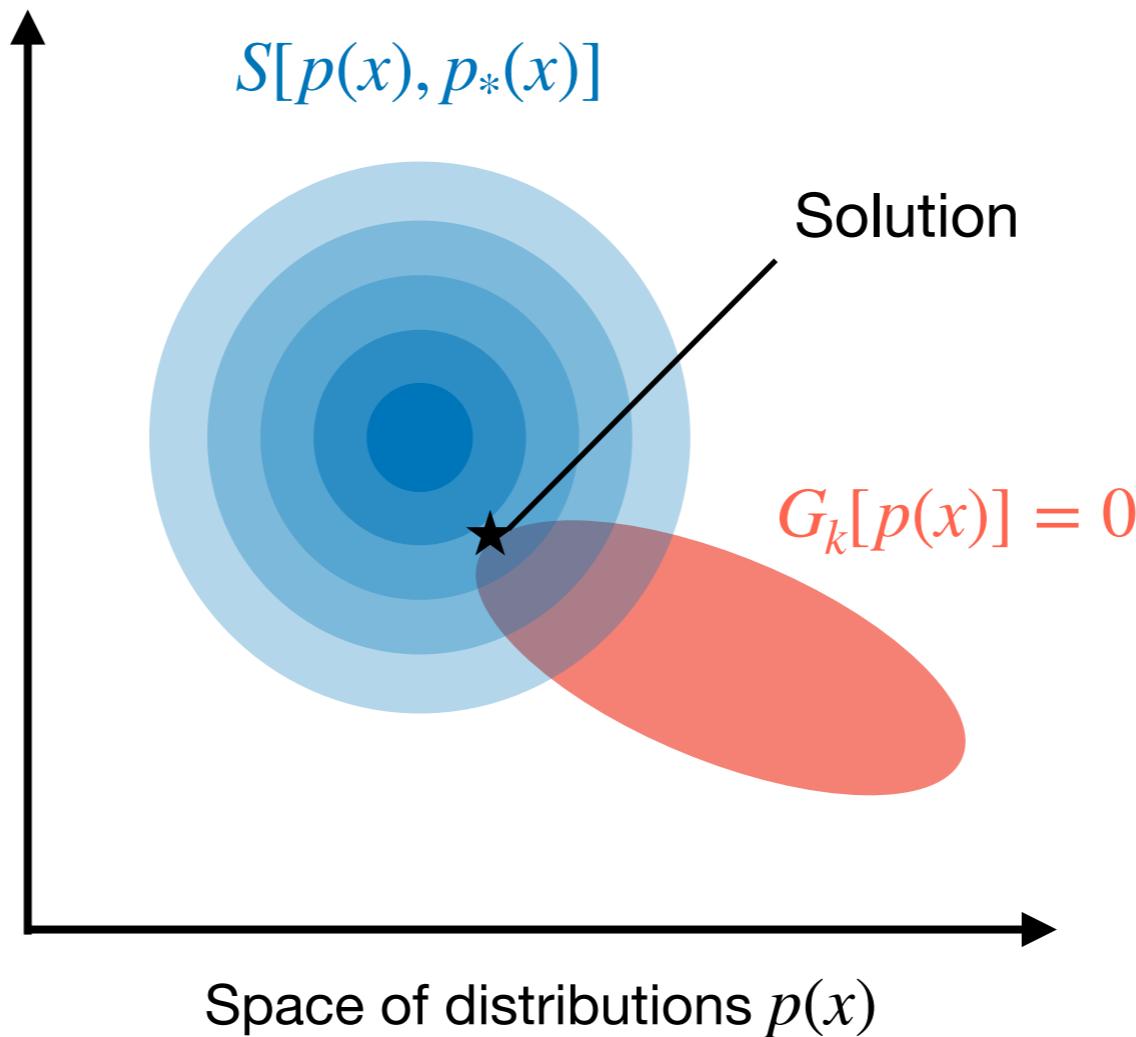
Challenge B: solution is not unique



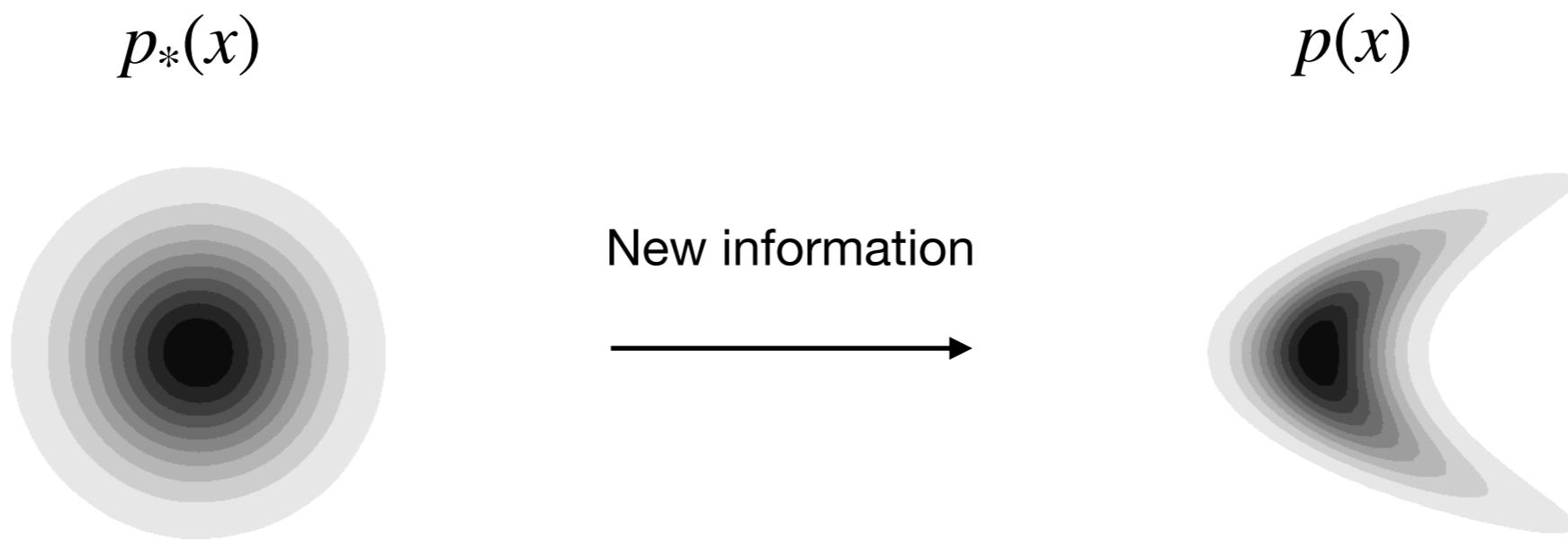
Things I *will* discuss:

How to select a **single distribution** from the feasible set.

MaxEnt: rank solutions by entropy (simplicity) and choose highest ranked solution

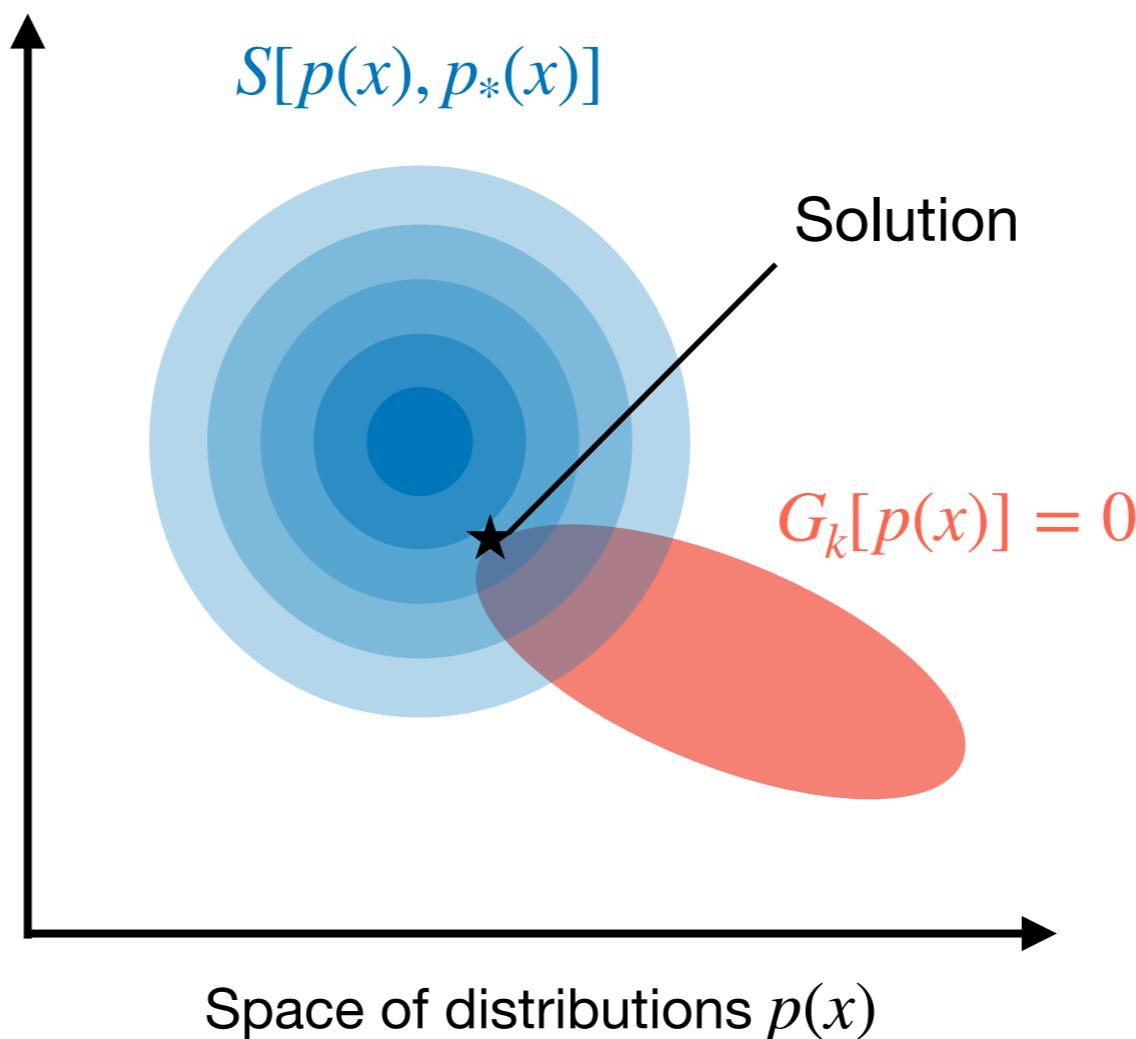


Entropy functional fixed by “Principle of Minimal Updating”



$$S[p(x), p_*(x)] = - \int p(x) \log \left(\frac{p(x)}{p_*(x)} \right) dx$$

MaxEnt solution may be incorrect, but it's the best we can do with the available information



GPSR: generative modeling approach

Generative Phase Space Reconstruction (GPSR)

PHYSICAL REVIEW ACCELERATORS AND BEAMS **27**, 094601 (2024)

Editors' Suggestion

Efficient six-dimensional phase space reconstructions from experimental measurements using generative machine learning

Ryan Roussel¹, Juan Pablo Gonzalez-Aguilera², Eric Wisniewski³, Alexander Ody¹,
Wanming Liu¹, John Power¹, Young-Kee Kim², and Auralee Edelen¹

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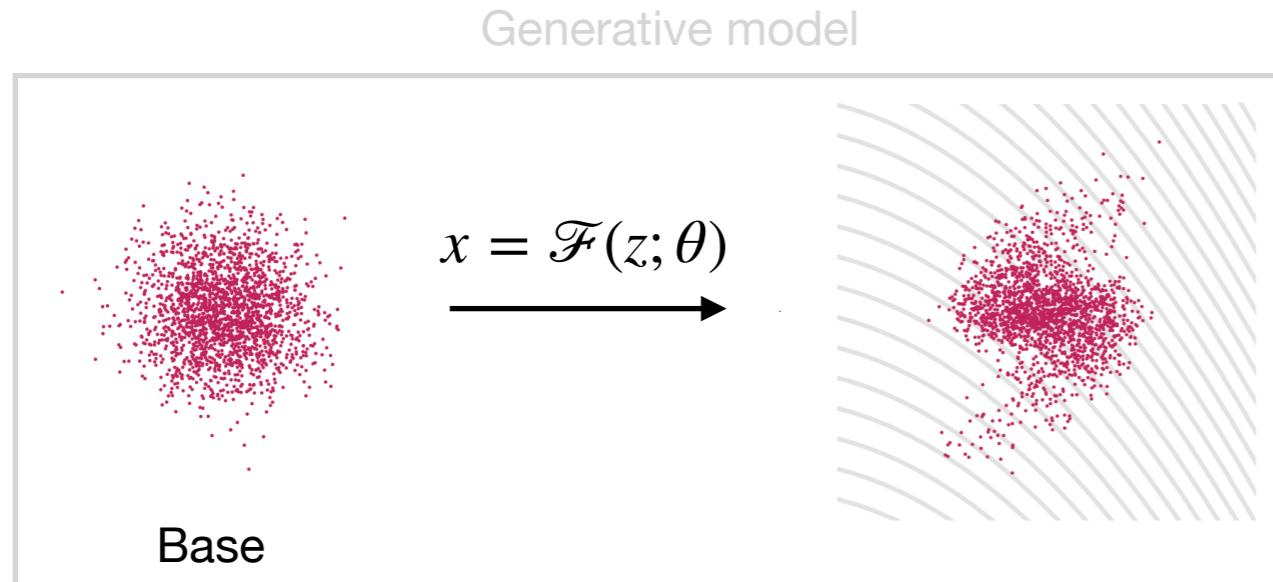
³*Argonne National Laboratory, Lemont, Illinois 60439, USA*



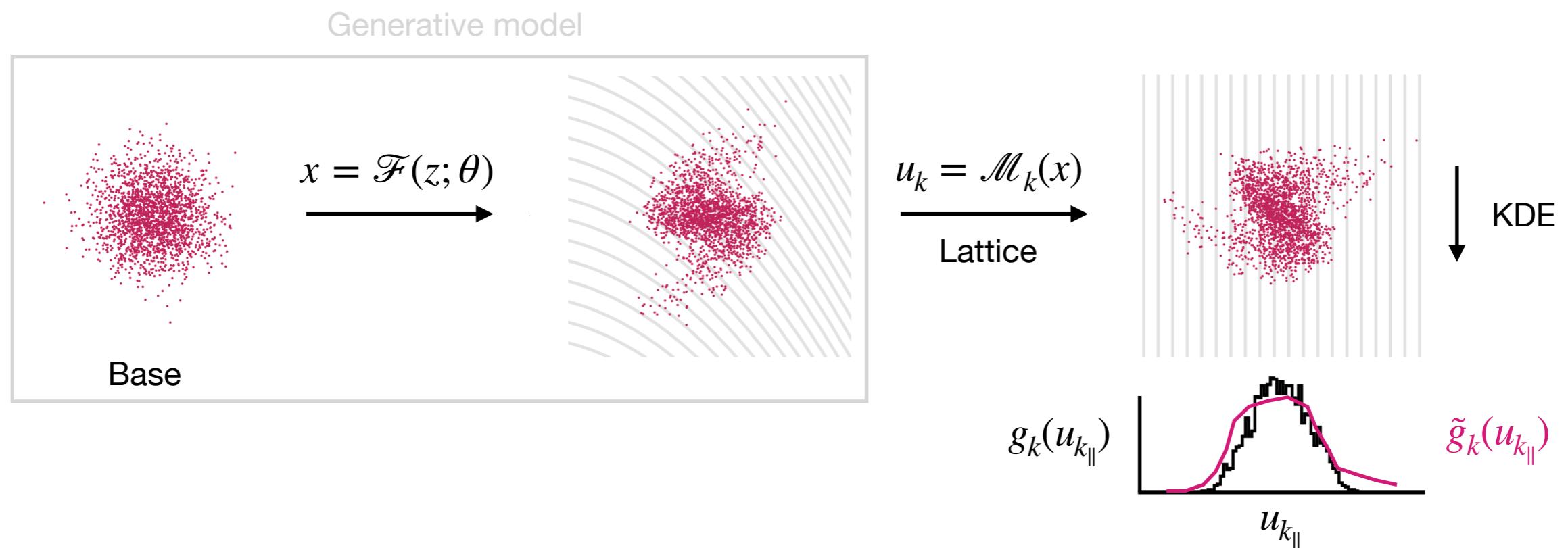
(Received 19 April 2024; accepted 12 August 2024; published 11 September 2024)

- [MOP034] “Efficient 6-dimensional phase space measurements and applications to autonomous monitoring at LCLS-II”
- [MOP029] “Development and Applications of Differentiable Coherent Optical Transition Radiation Simulations”
- [MOP071] “Phase space reconstruction of beams affected by coherent synchrotron radiation”

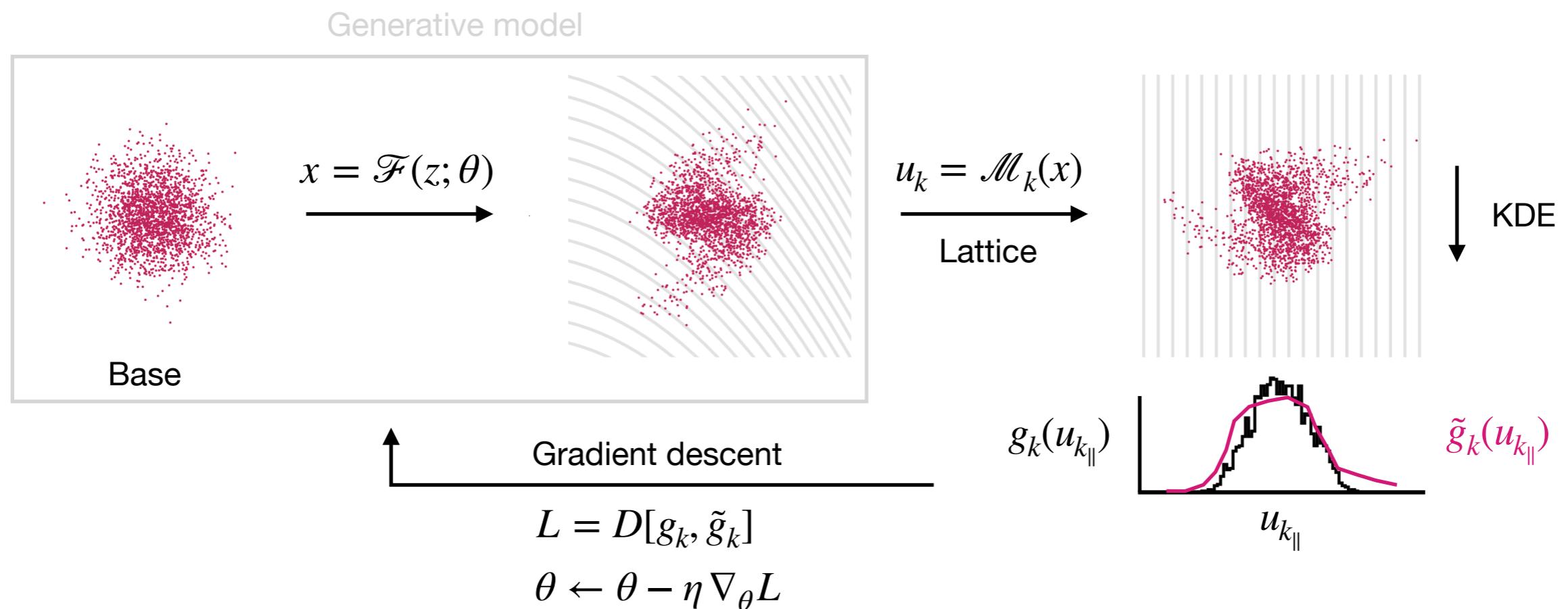
Generative Phase Space Reconstruction (GPSR)



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Generative Phase Space Reconstruction (GPSR)

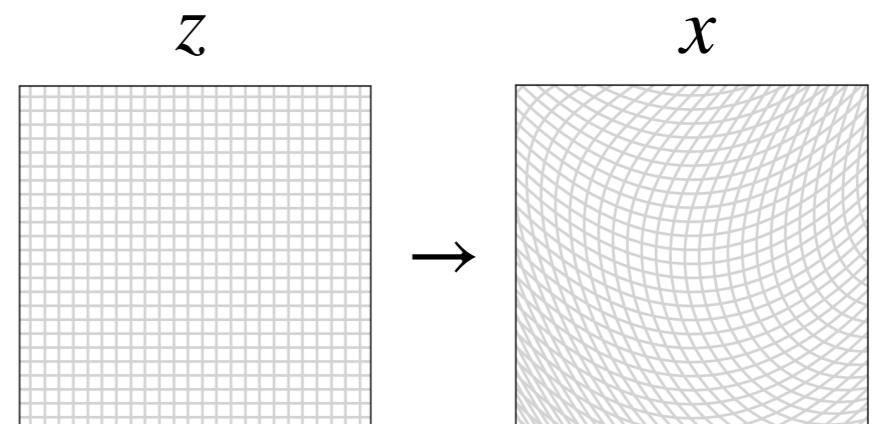


Normalizing flows enable simultaneous sampling and density evaluation

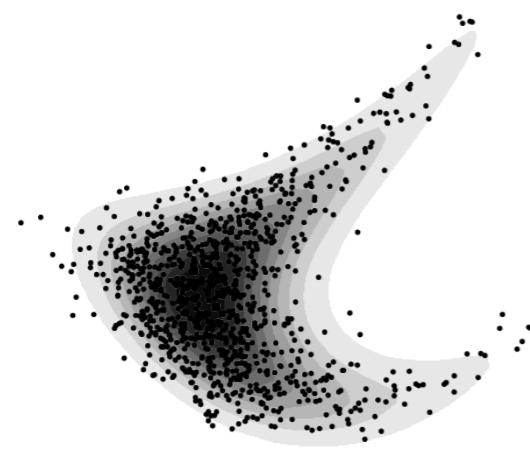
$\mathcal{F} : \mathbb{R}^N \rightarrow \mathbb{R}^N$ is differentiable, invertible map from z to x .

$$\log p(x) = \log p(z) - \log |J_{\mathcal{F}}(z)|$$

$$J_{\mathcal{F}} = \frac{dx}{dz} = \begin{bmatrix} \frac{\partial x_1}{\partial z_1} & \cdots & \frac{\partial x_1}{\partial z_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial x_N}{\partial z_1} & \cdots & \frac{\partial x_N}{\partial z_N} \end{bmatrix}$$



Normalizing flows can estimate entropy



$$\{x^{(i)}\} \sim p(x)$$

$$\begin{aligned} S[p(x), p_*(x)] &= - \int p(x) \log(p(x)/p_*(x)) dx \\ &= - \mathbb{E}_{p(x)} [\log(p(x)/p_*(x))] \\ &\approx - \frac{1}{N} \sum_{i=1}^N \log(p(x^{(i)})/p_*(x^{(i)})) \end{aligned}$$

Normalizing flows can estimate entropy

Published as a conference paper at ICLR 2017

MAXIMUM ENTROPY FLOW NETWORKS

Gabriel Loaiza-Ganem*, Yuanjun Gao* & John P. Cunningham

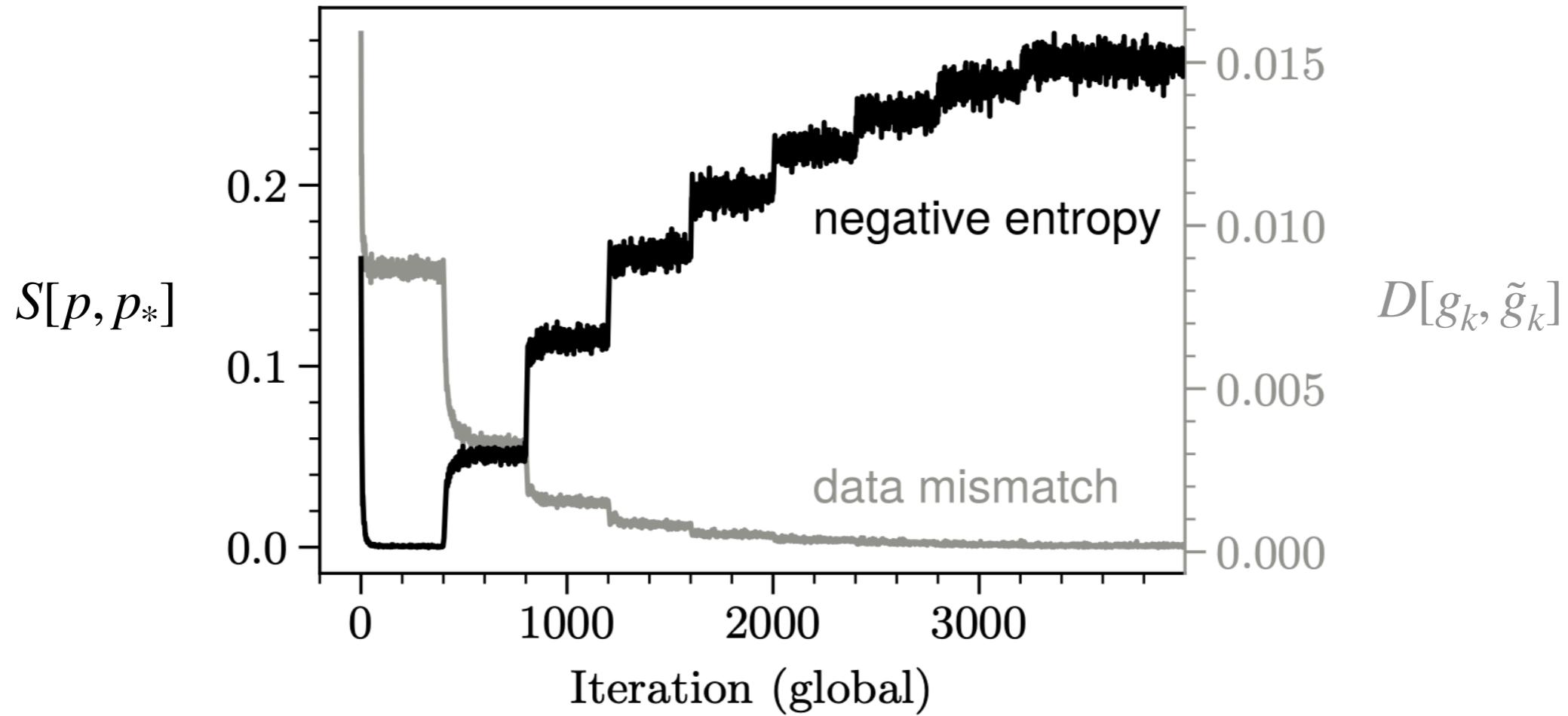
Department of Statistics
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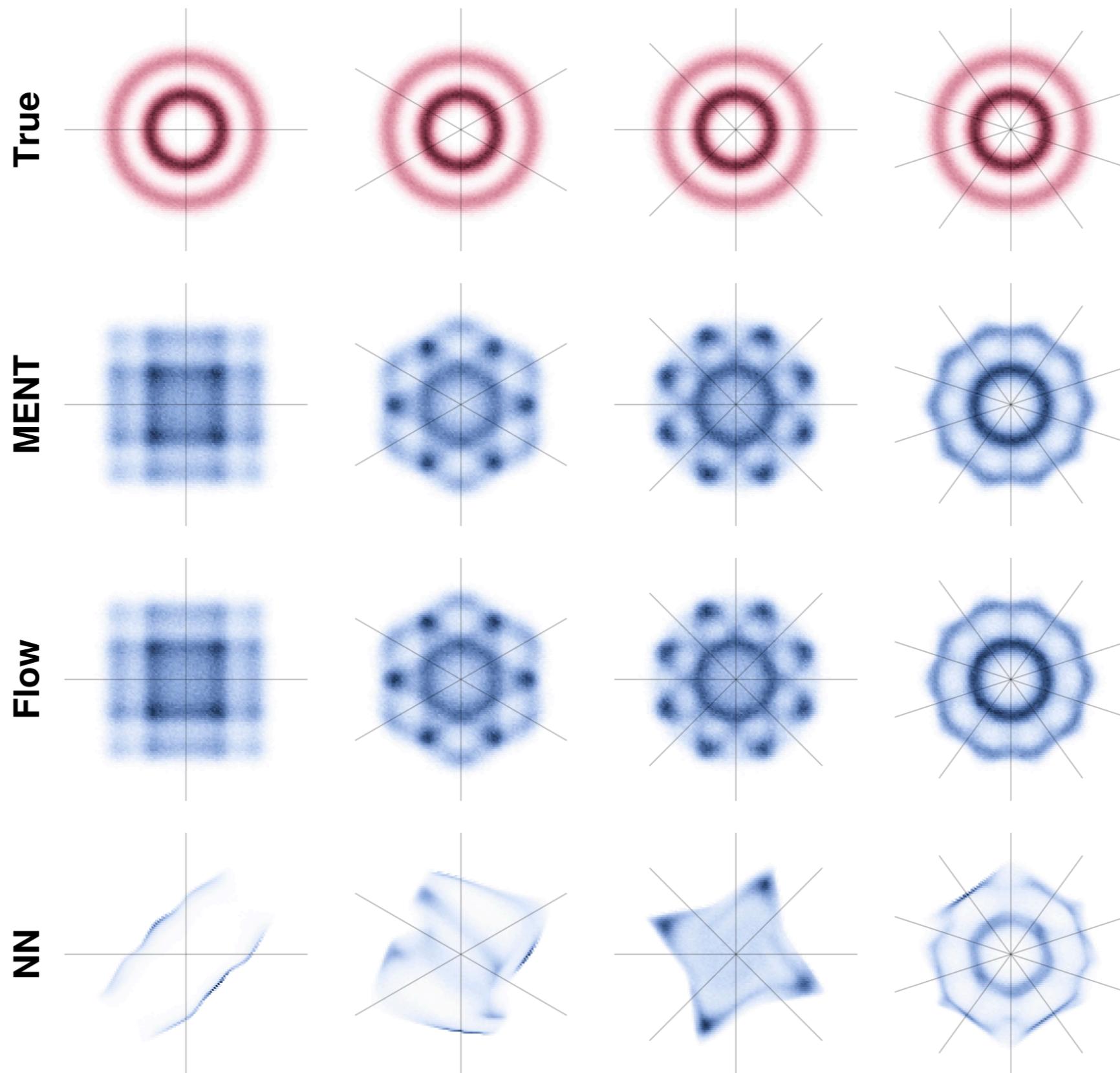
ABSTRACT

Maximum entropy modeling is a flexible and popular framework for formulating statistical models given partial knowledge. In this paper, rather than the traditional method of optimizing over the continuous density directly, we learn a smooth and invertible transformation that maps a simple distribution to the desired maximum entropy distribution. Doing so is nontrivial in that the objective being maximized (entropy) is a function of the density itself. By exploiting recent developments in normalizing flow networks, we cast the maximum entropy problem into a finite-dimensional constrained optimization, and solve the problem by combining stochastic optimization with the augmented Lagrangian method. Simulation results demonstrate the effectiveness of our method, and applications to finance and computer vision show the flexibility and accuracy of using maximum entropy flow networks.

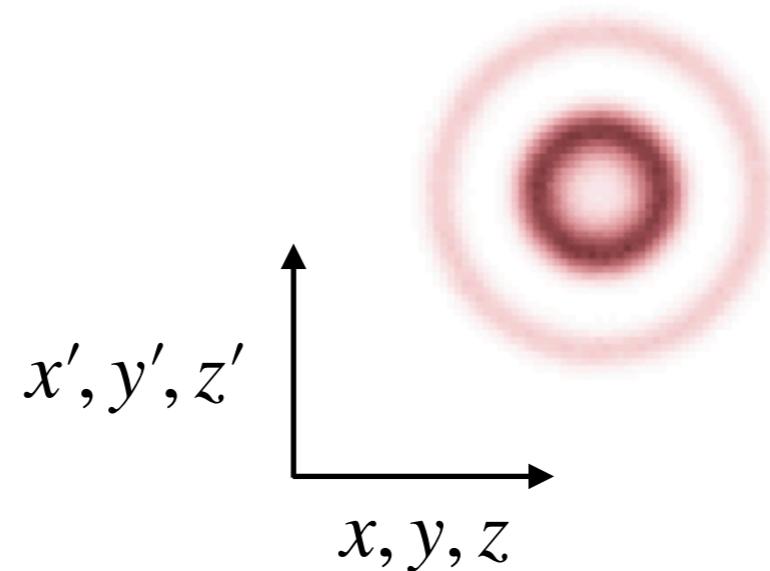
Penalty method not ideal but (in my experience) can generate pretty good solutions

$$L = -S[p, p_*] + \mu D[g_k, \tilde{g}_k]$$

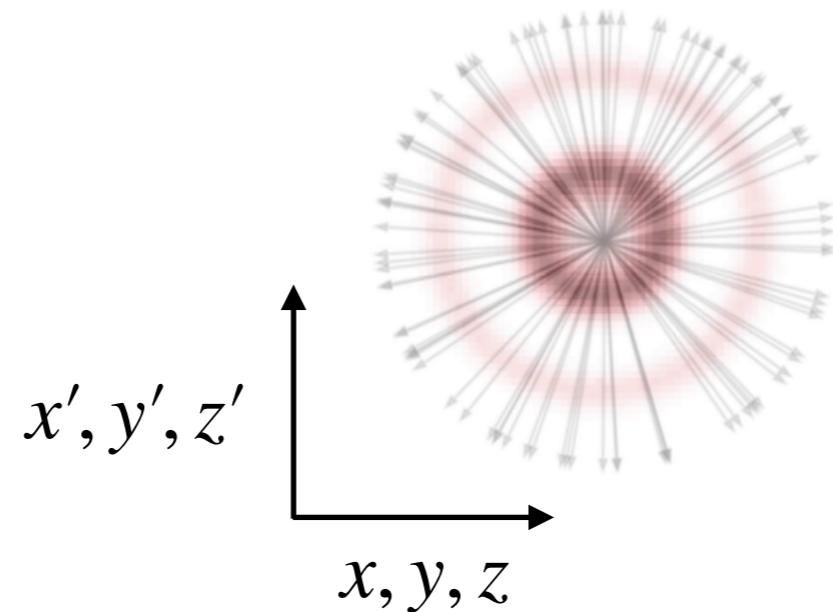




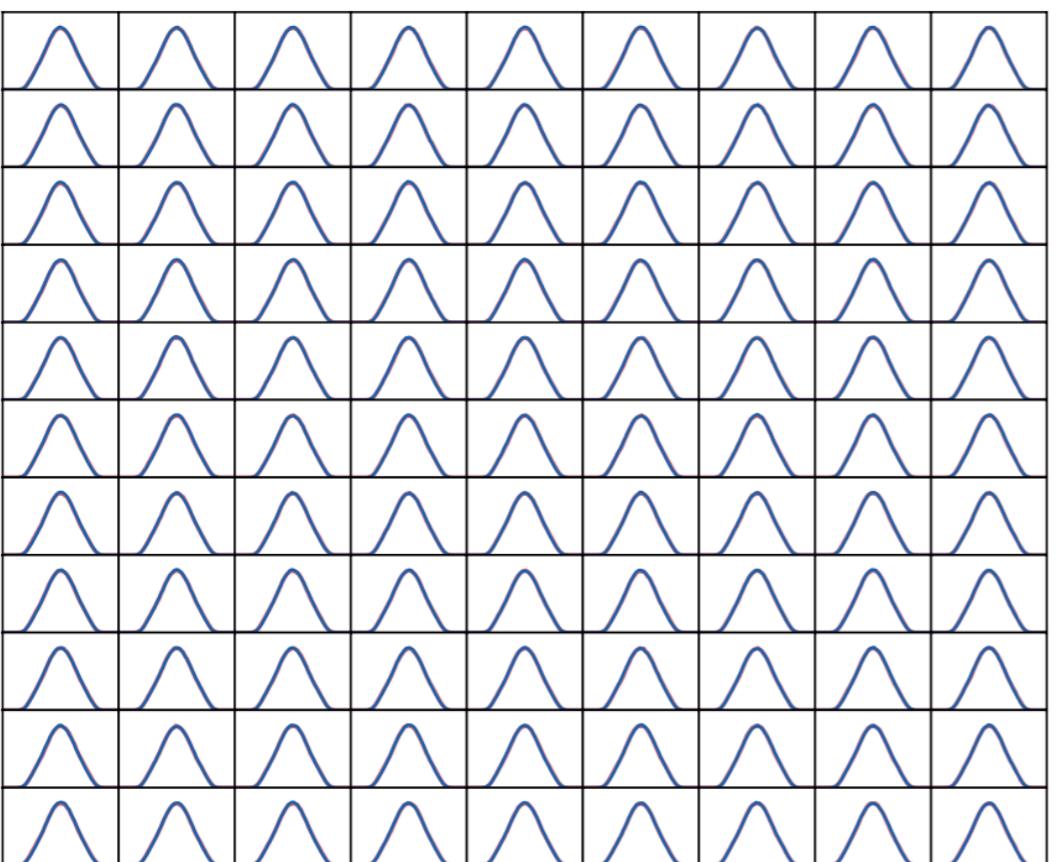
Toy problem: 6D “rings” distribution projected along random 1D directions



Toy problem: 6D “rings” distribution projected along random 1D directions

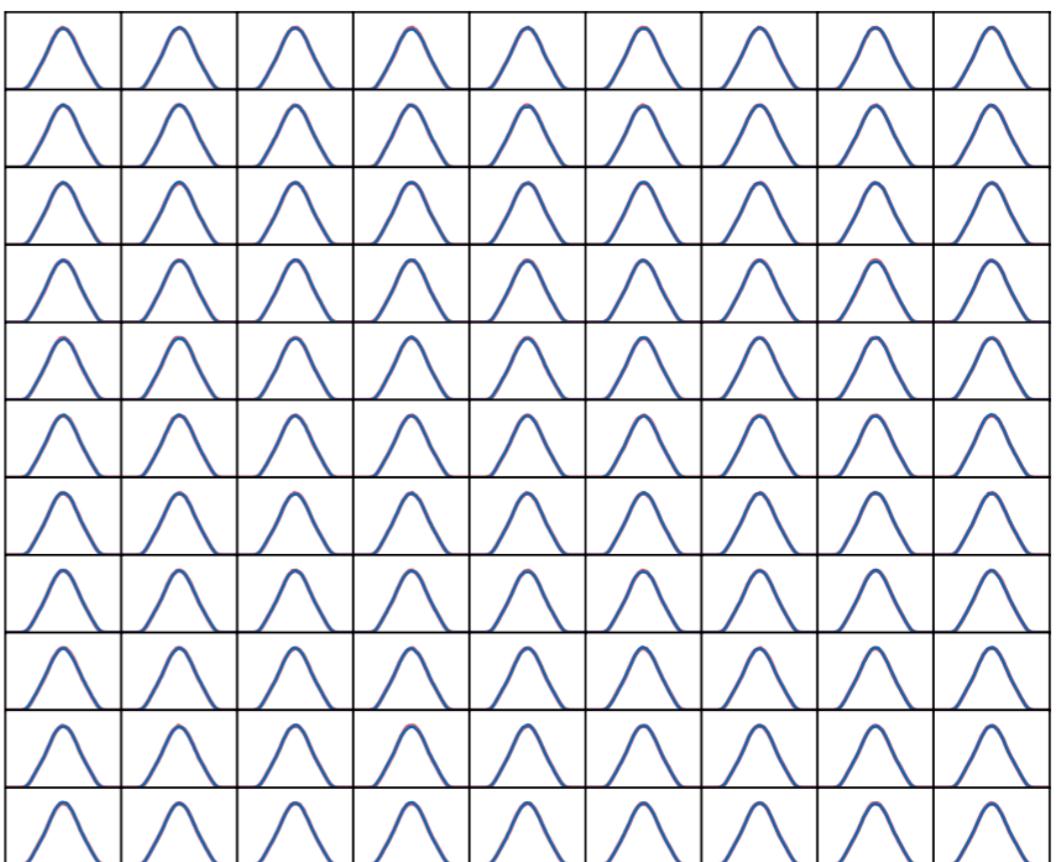


FLOW

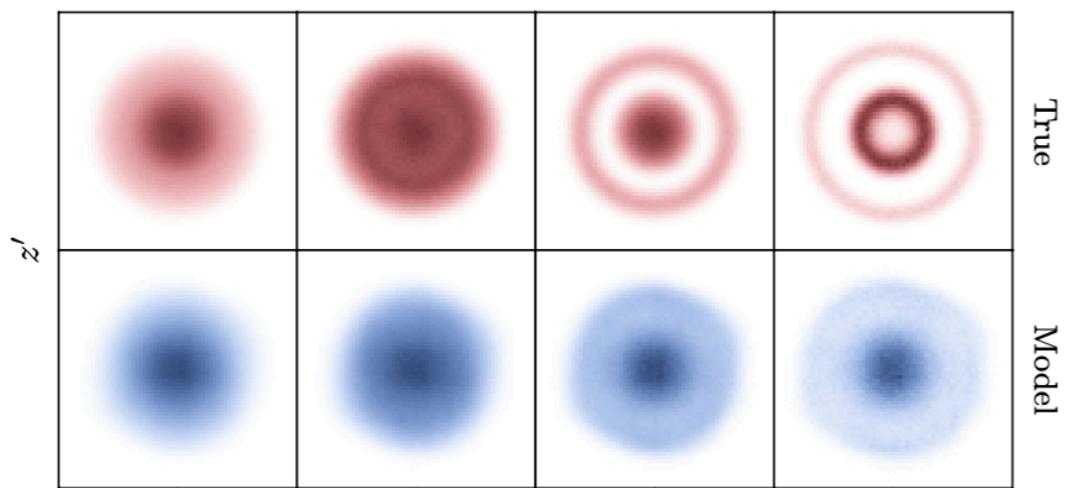
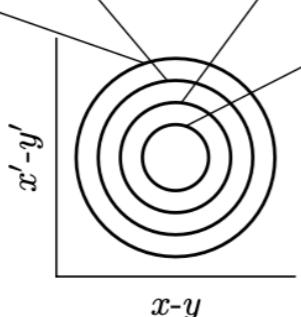


(a)

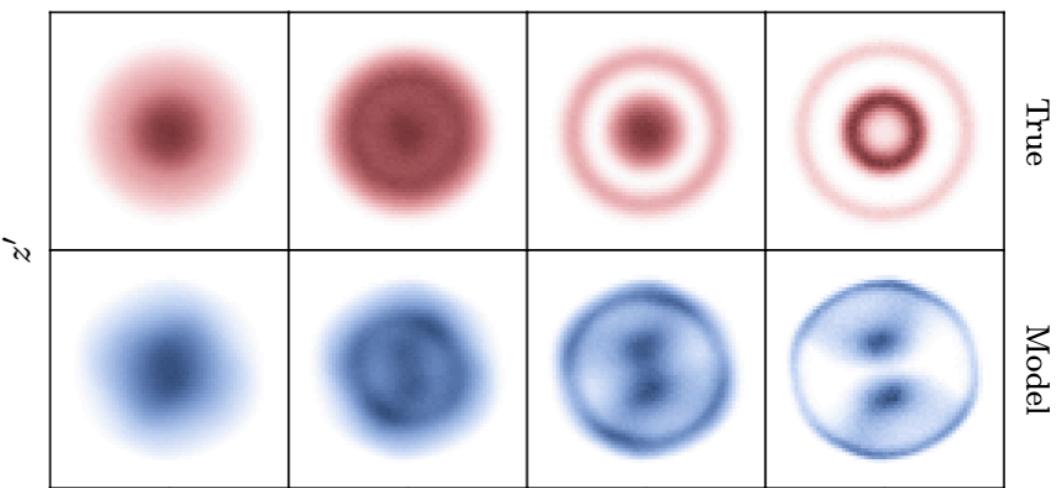
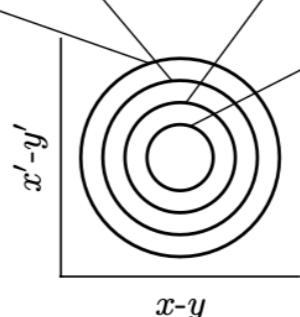
NN



(b)

 $\rho(z, z' | r_\perp < \tilde{r}_\perp)$ True
Model

(c)

 $\rho(z, z' | r_\perp < \tilde{r}_\perp)$ True
Model

(d)

High-dimensional maximum-entropy phase space tomography using normalizing flows

Austin Hoover^{id*}

Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, USA

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Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China



(Received 31 May 2024; accepted 27 July 2024; published 12 August 2024)

Particle accelerators generate charged-particle beams with tailored distributions in six-dimensional position-momentum space (phase space). Knowledge of the phase space distribution enables model-based beam optimization and control. In the absence of direct measurements, the distribution must be tomographically reconstructed from its projections. In this paper, we highlight that such problems can be severely underdetermined and that entropy maximization is the most conservative solution strategy. We leverage *normalizing flows*—invertible generative models—to extend maximum-entropy tomography to six-dimensional phase space and perform numerical experiments to validate the model’s performance. Our numerical experiments demonstrate consistency with exact two-dimensional maximum-entropy solutions and the ability to fit complicated six-dimensional distributions to large measurement sets in reasonable time.

DOI: [10.1103/PhysRevResearch.6.033163](https://doi.org/10.1103/PhysRevResearch.6.033163)

Summary of GPSR

- Efficient method to optimize high-dimensional distributions when differentiable simulations are available.
- Flexible – different kinds of data.
- Future: more sophisticated constrained optimization
- Future: better/non-invertible flows

MENT: classical approach

Maximum-entropy PDF is exponential of product of Lagrange Multipliers

Lagrangian:

$$\Psi = S[p(x), p_*(x)] + \sum_k \int G_k[p(x)] \lambda_k(u_{k\parallel}) du_{k\parallel}$$

Enforce $\delta\Psi = 0$ with respect to p and λ_k :

$$p(x) = p_*(x) \prod_k \exp \left[\lambda_k(u_{k\parallel}(x)) \right]$$

$$p(x) = p_*(x) \prod_k h_k(u_{k\parallel}(x))$$

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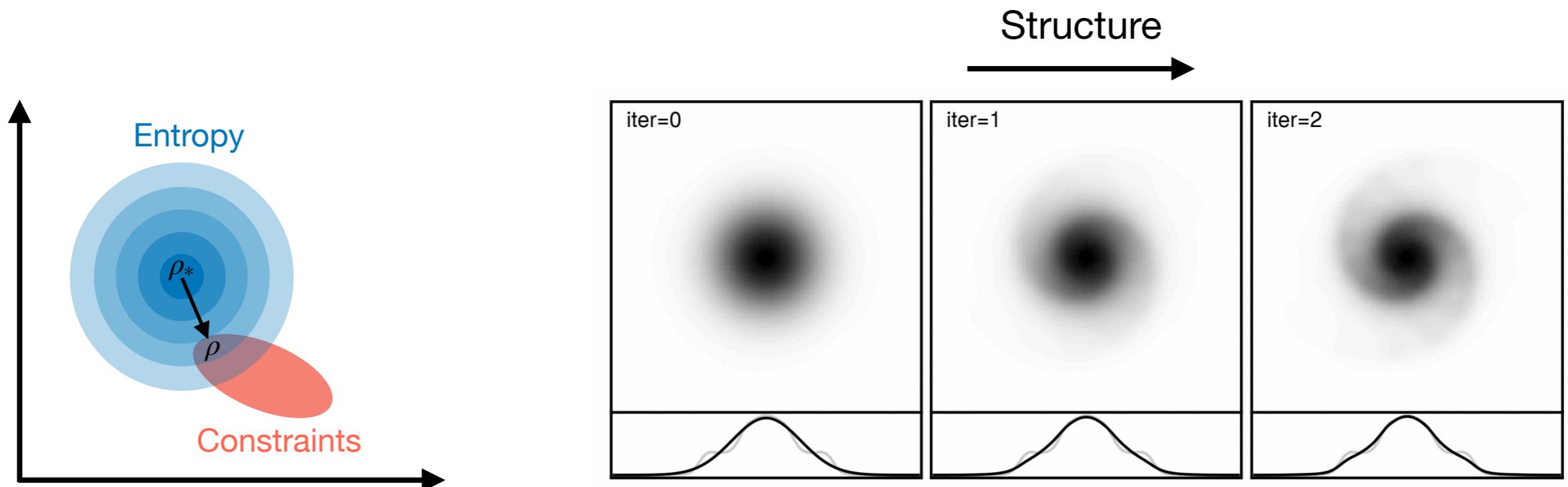
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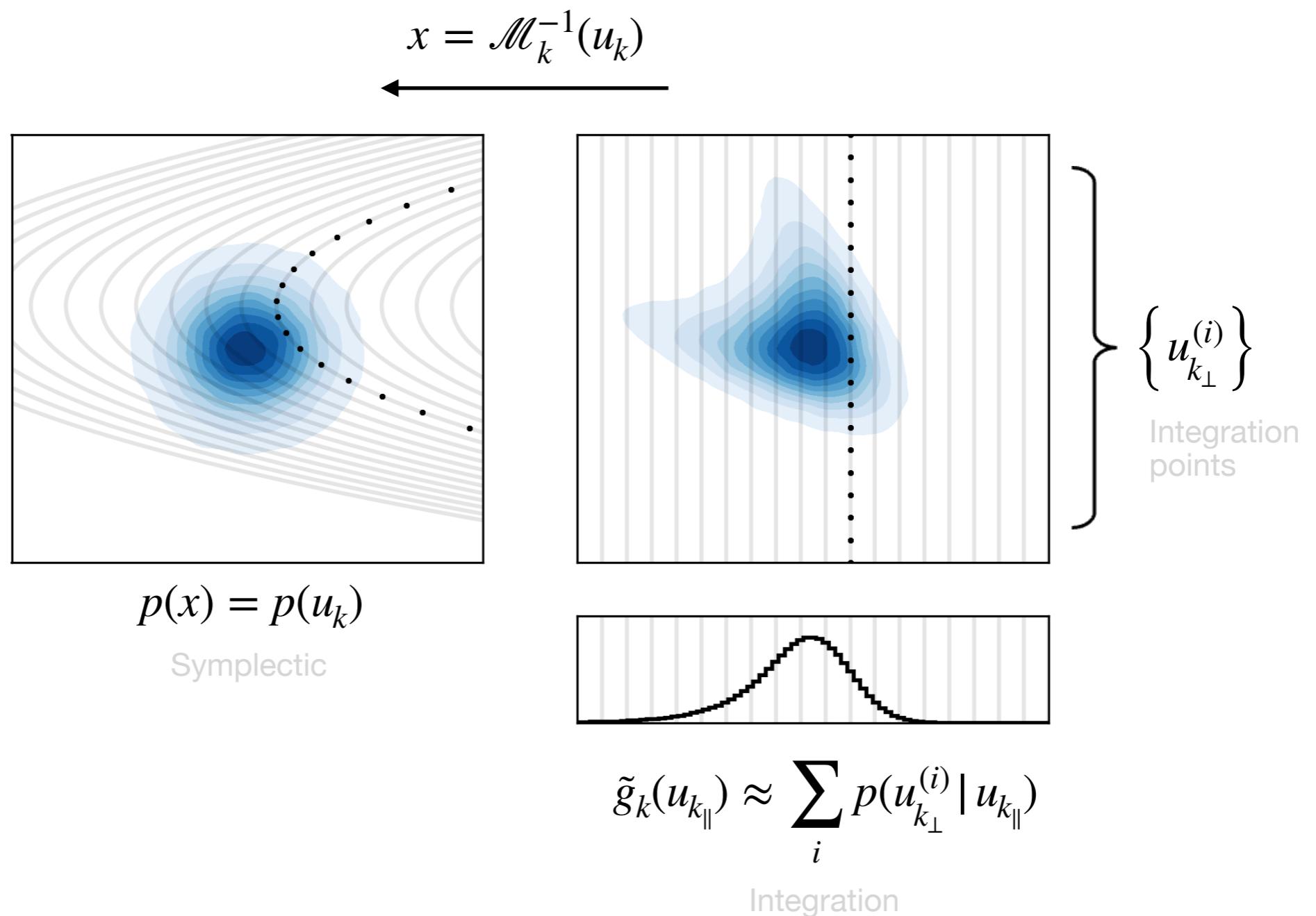
Prior Positive functions defined on measurement axes

Nonlinear Gauss-Seidel iterations used to solve for unknown functions: simple algorithm!

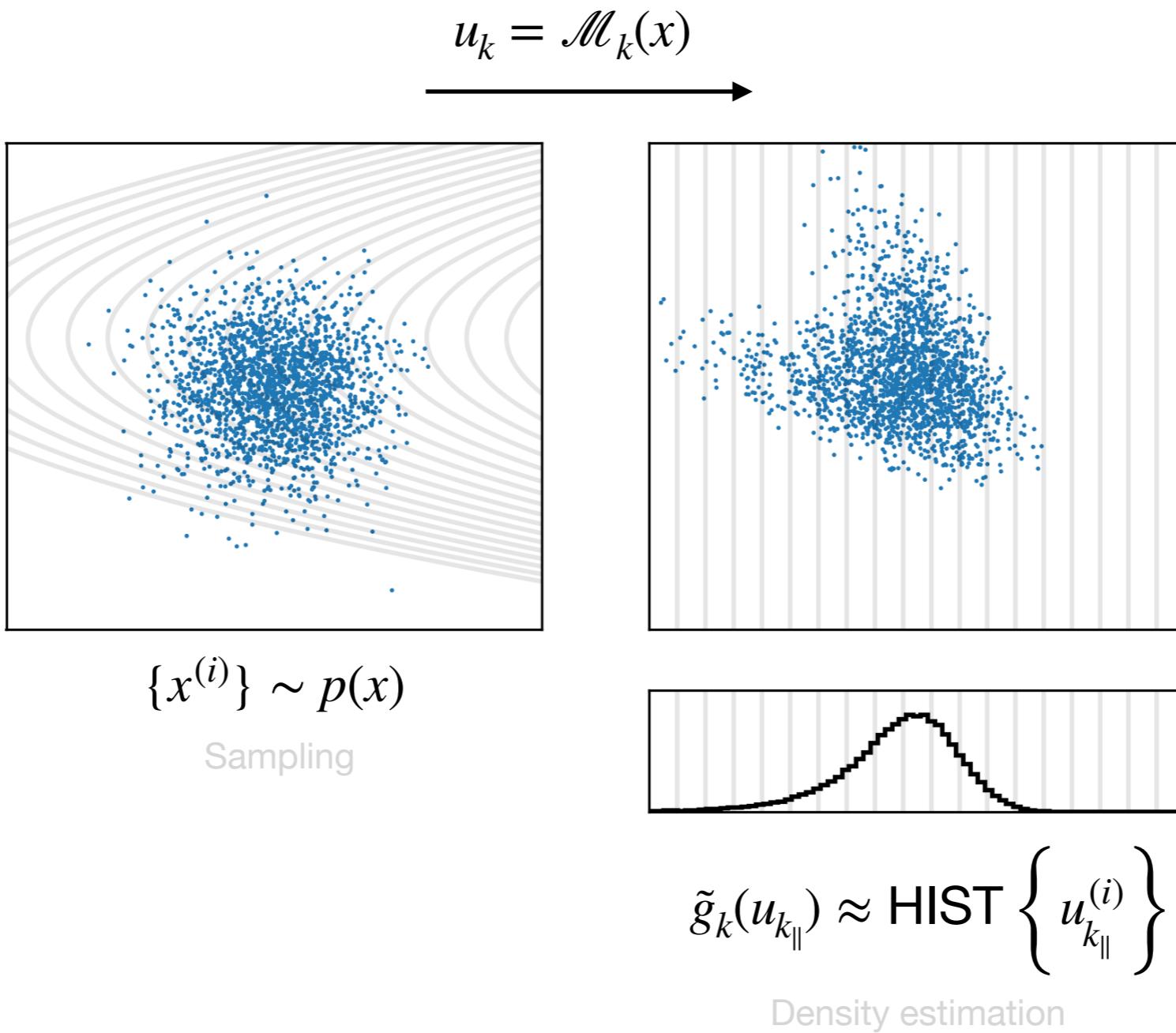
$$h_k^{(i+1)} = h_k^{(i)} \left[(1 - \omega) + \omega \left(g_k / \tilde{g}_k \right) \right]$$



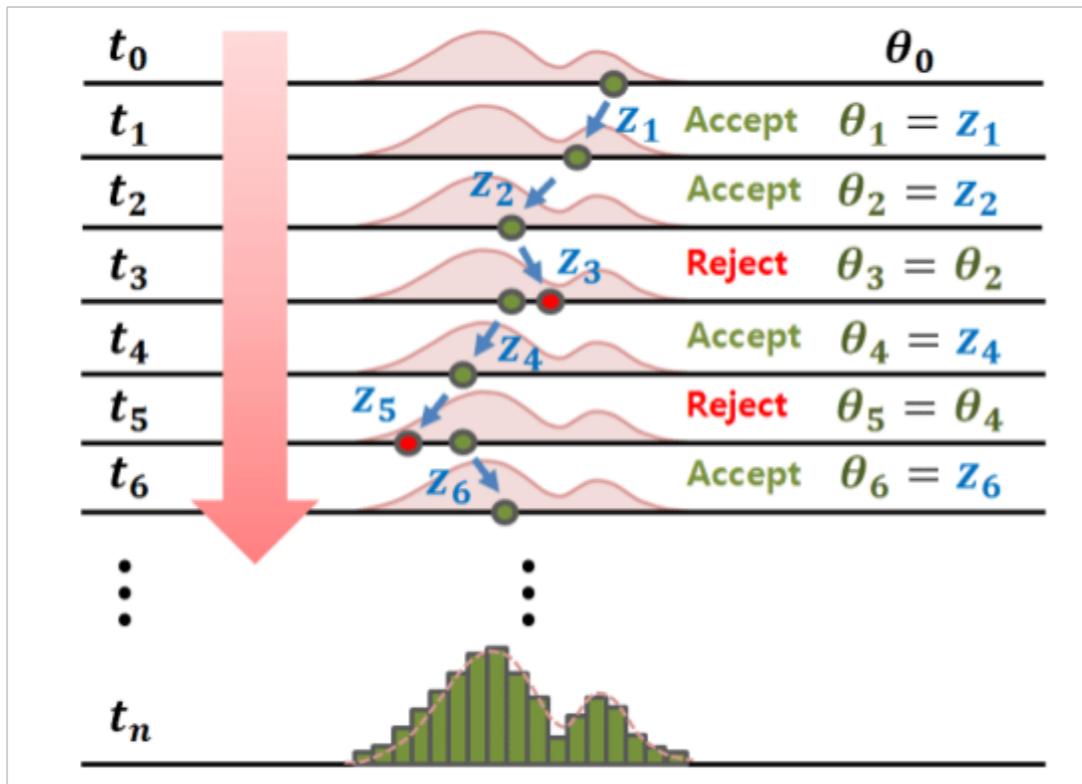
Standard implementation uses numerical integration (**reverse mode**) to compute projections



I propose particle sampling (**forward mode**) for high-dimensional problems



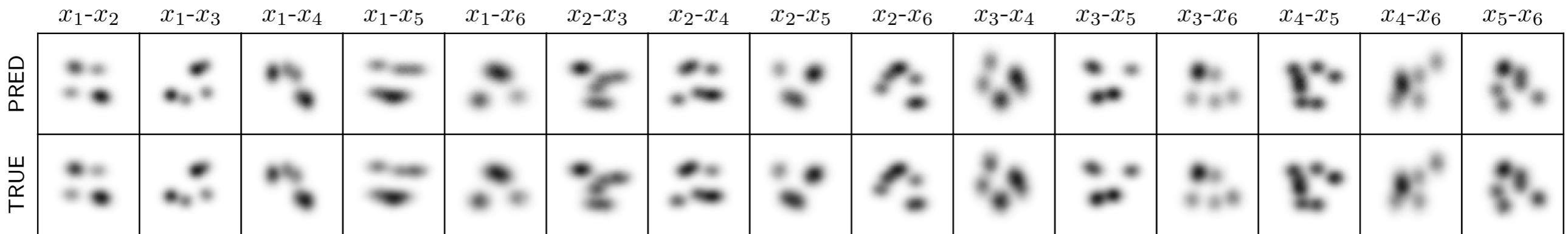
Metropolis-Hastings is gridless sampling algorithm with long-run guarantees



Requires hand-tuning of jumping distribution, and it's not always clear when it converges...

But let's try it.

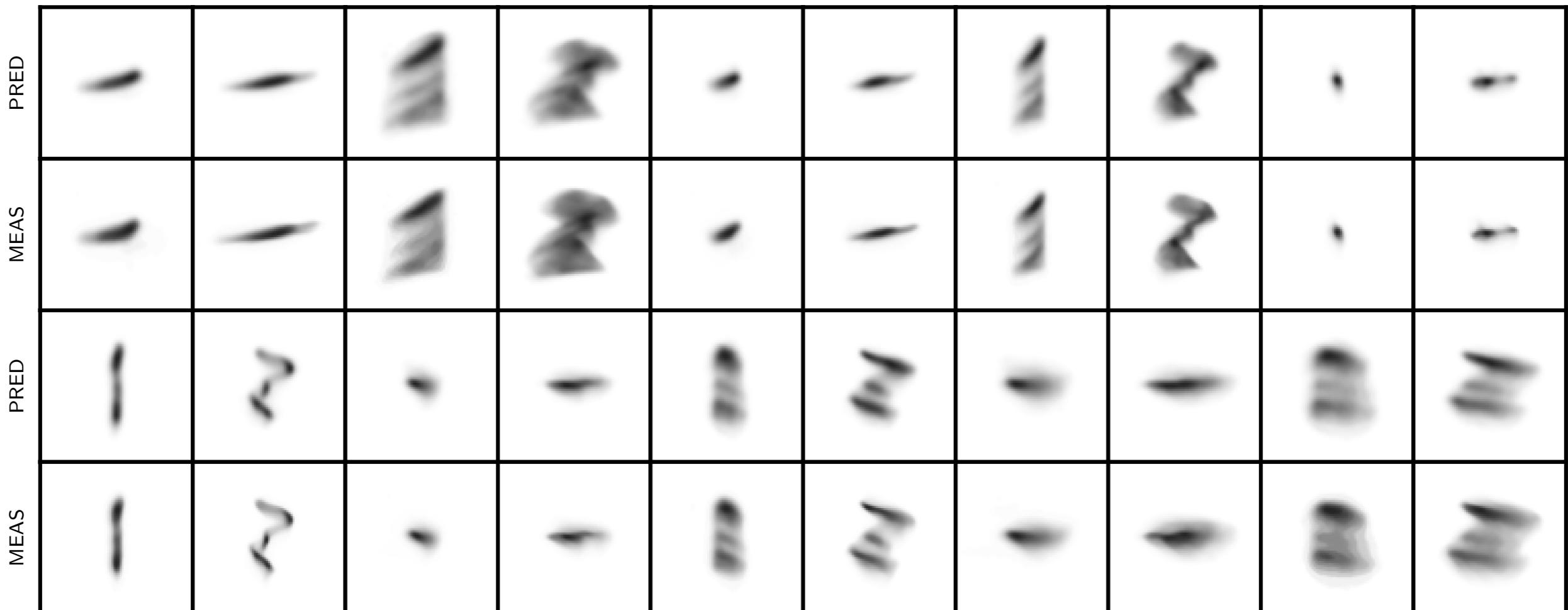
Test: 6D Gaussian mixture distribution



Reverse (50^4 integration, 50^2 measurement grid): **24 hour** / iteration

Forward (500,000 samples, 1000 chains) : **30 sec** / iteration

Test: 6D Argonne Wakefield Accelerator dataset



N-dimensional maximum-entropy tomography via particle sampling

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(Received 4 October 2024; accepted 14 May 2025; published 7 August 2025)

We propose a modified maximum-entropy (MENT) algorithm for six-dimensional phase space tomography. The algorithm uses particle sampling and low-dimensional density estimation to approximate large sets of high-dimensional integrals in the original MENT formulation. We implement this approach using Markov Chain Monte Carlo (MCMC) sampling techniques and demonstrate convergence of six-dimensional MENT on both synthetic and measured data.

DOI: [10.1103/2h-3v32](https://doi.org/10.1103/2h-3v32)

Summary of MENT

- Elegant – minimal storage, simple algorithm.
- Flexible – no restrictions on distribution or transformations.
- Future: new sampling algorithm / tuning
- Future: GPU + parallel

Conclusion

Conclusion

- Several MaxEnt algorithms running in 2D/4D/6D.
- Algorithm improvements possible
- Currently working on uncertainty quantification (UQ), improved dynamic range (DR), self-fields

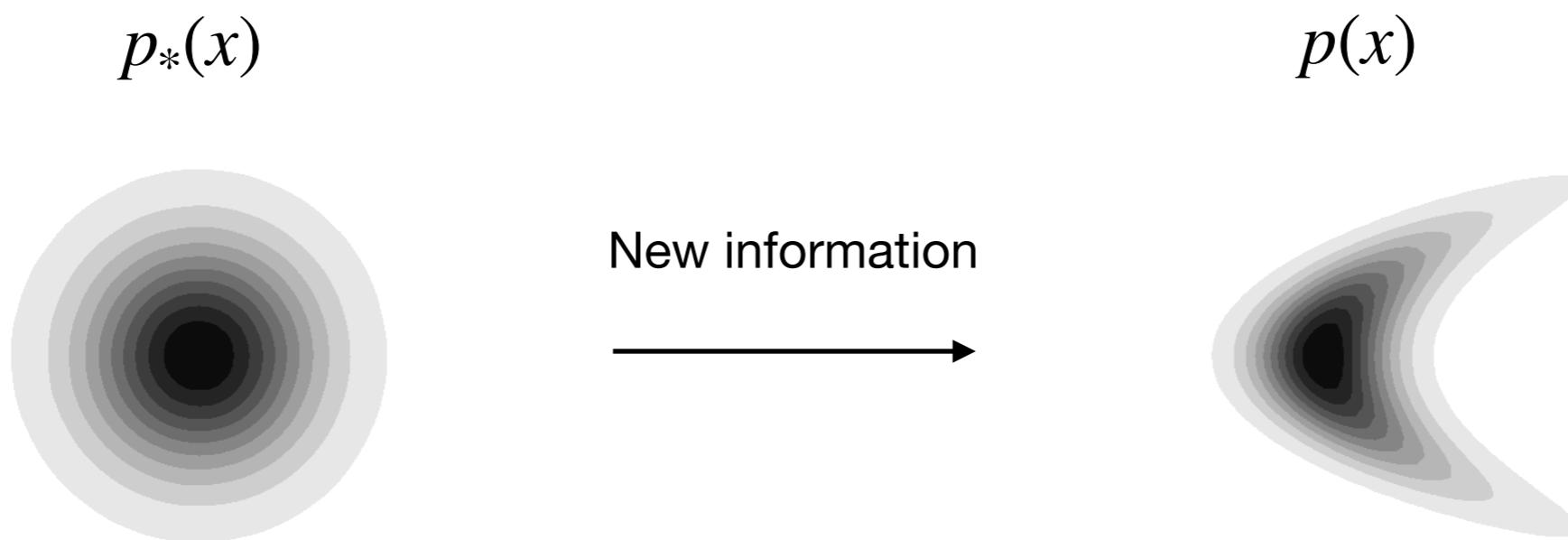
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- <https://github.com/austin-hoover/ment>
- <https://github.com/roussel-ryan/gpsr>
- Zenodo repositories linked in papers

Conclusion

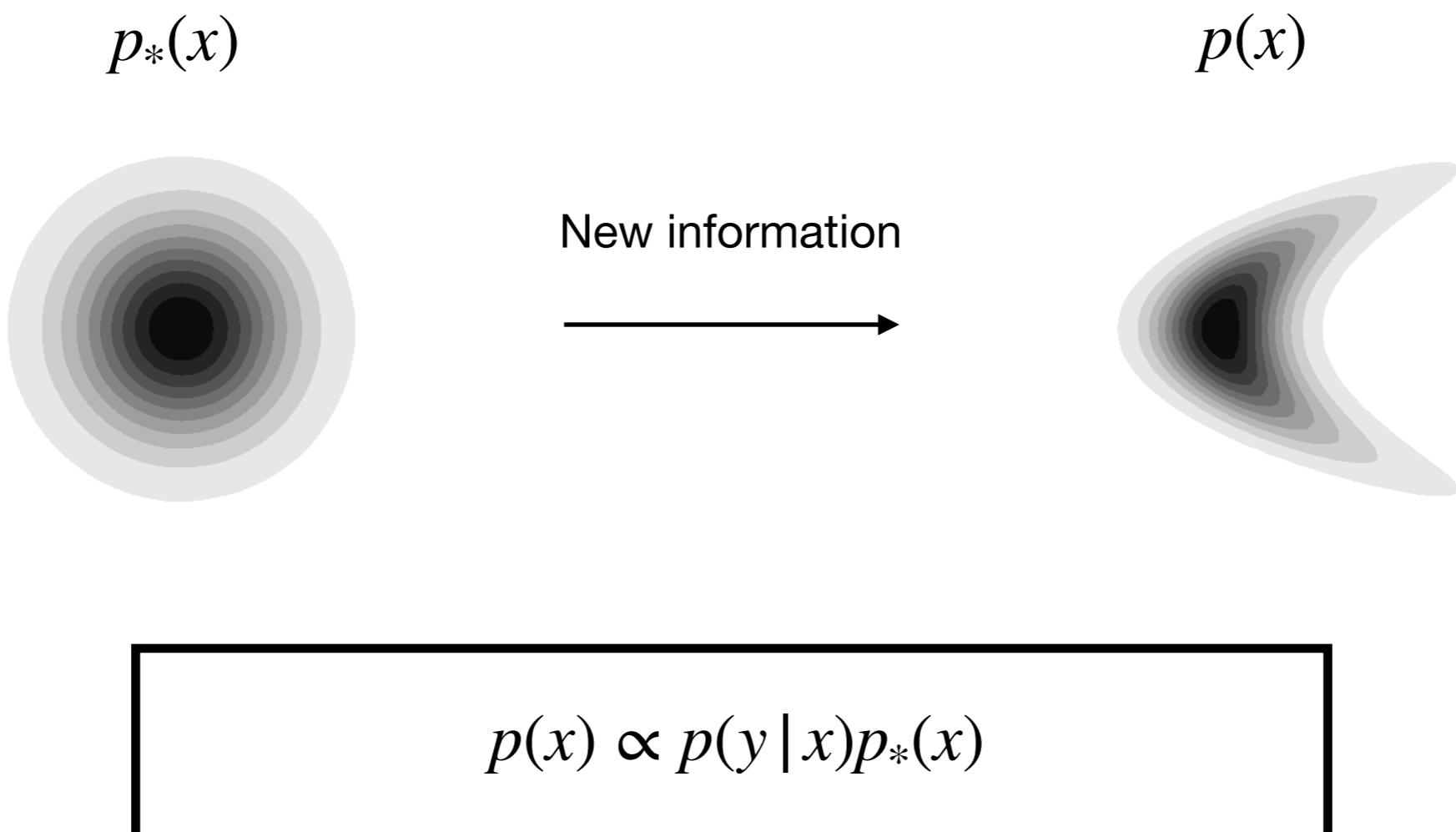
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- Zenodo repositories linked in papers
- Thanks for listening!
- **hooveram@ornl.gov**

MaxEnt updates prior to posterior given constraints on posterior



$$\max_{p(x)} S[p(x), p_*(x)] \quad \text{s.t.} \quad \{G_k[p(x)] = 0\}$$

Given a likelihood function, MaxEnt becomes Bayesian inference



Kangaroos



Kangaroos

Table 1: Results for currently advertised functionals

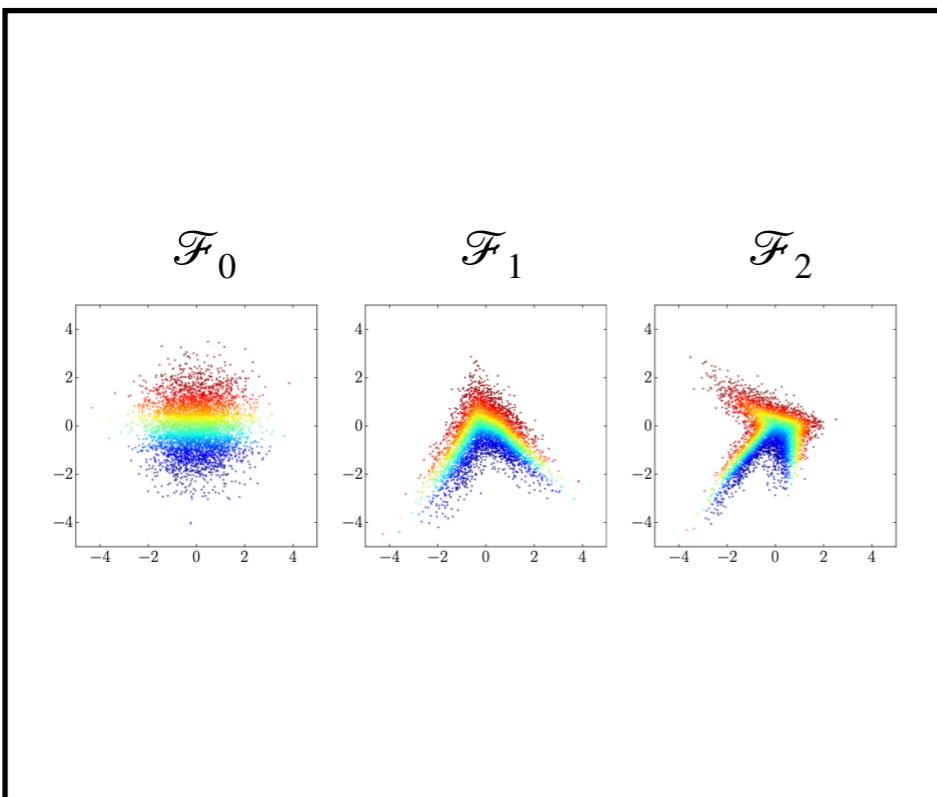
Function	p (blue-eyes and left-handed)	Correlation
$-\sum p \log p$	$1/9 = 0.11111$	uncorrelated
$-\sum p^2$	$1/12 = 0.08333$	negative
$\sum \log p$	0.13013	positive
$\sum p^{1/2}$	0.12176	positive

Two ways to build flows: discrete vs. continuous

Discrete

$$x = \mathcal{F}(z; \theta)$$

$$\mathcal{F} = \mathcal{F}_T \circ \mathcal{F}_{T-1} \circ \dots \circ \mathcal{F}_2 \circ \mathcal{F}_1$$

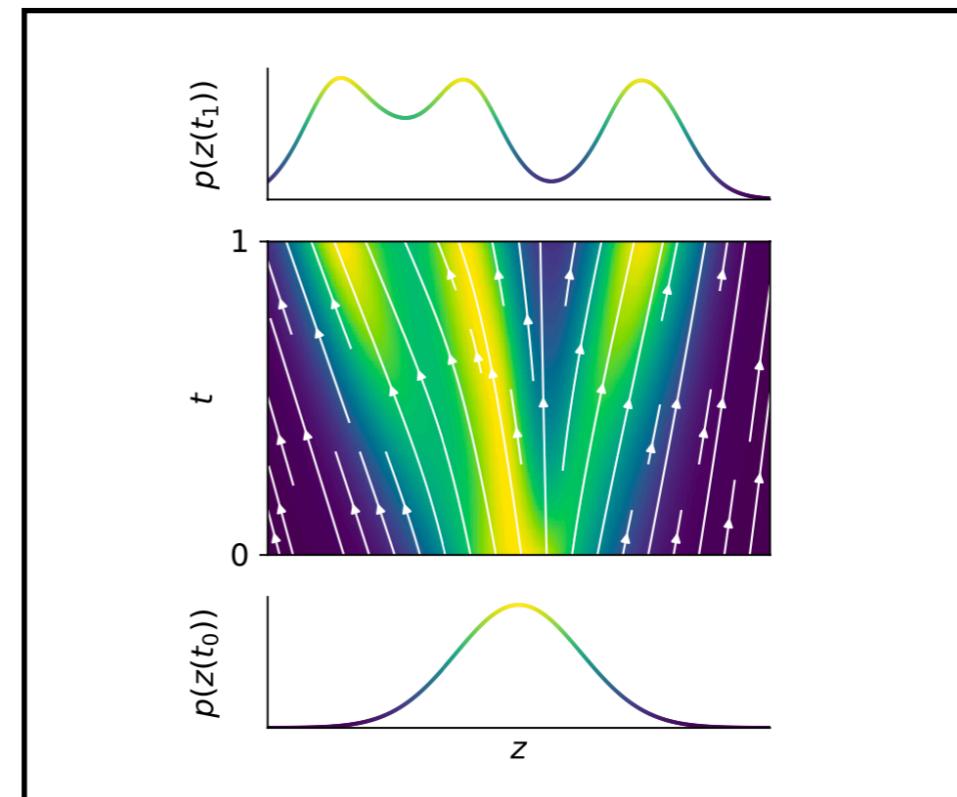


<https://arxiv.org/abs/1912.02762>

Continuous

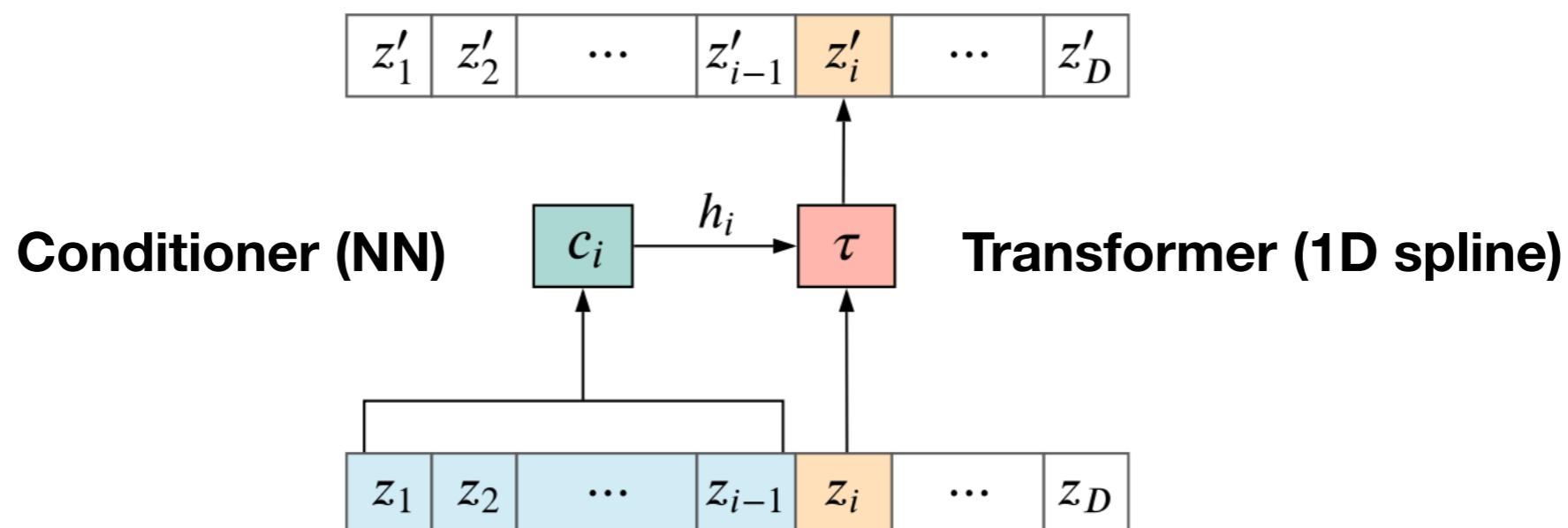
$$\partial_t z = v(z, t; \theta)$$

$$x \equiv z(t = T)$$



<https://arxiv.org/abs/1810.01367>

Autoregressive flow architecture



Rational-quadratic spline transformer

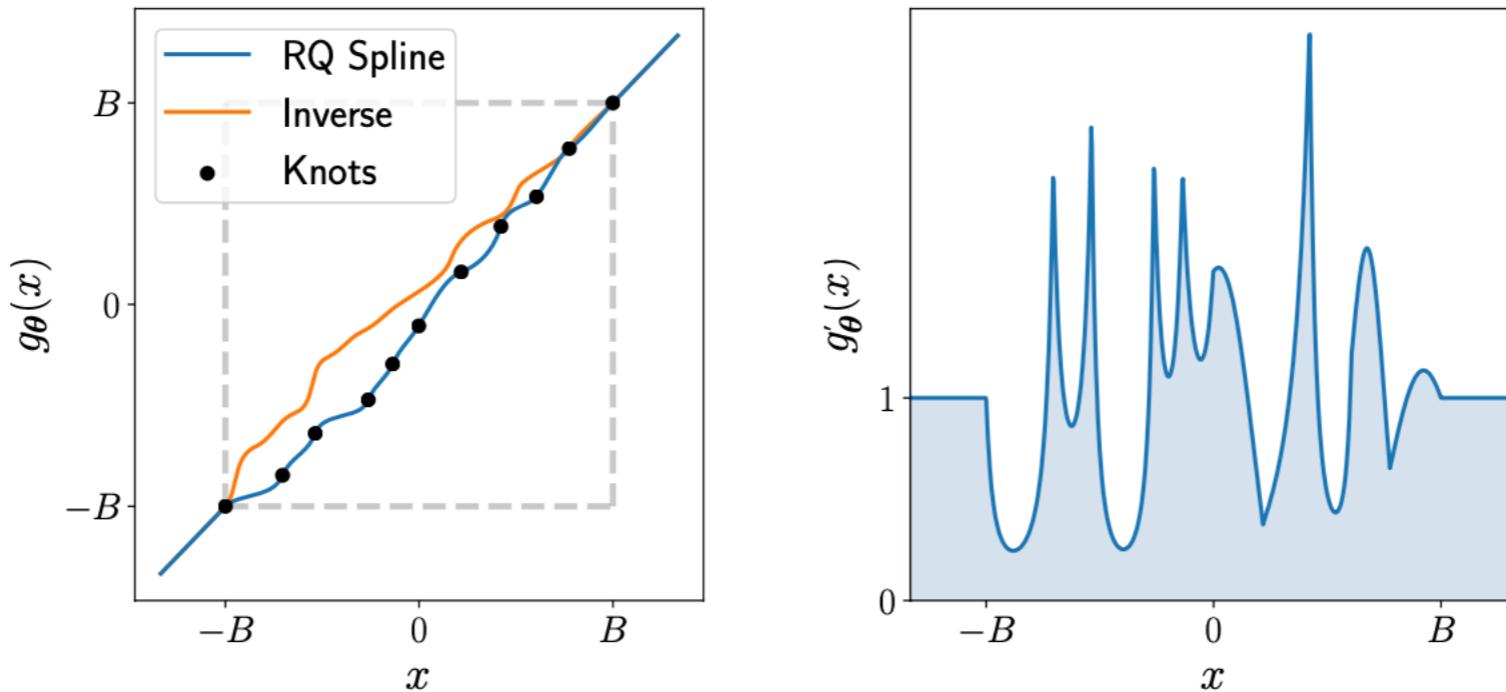
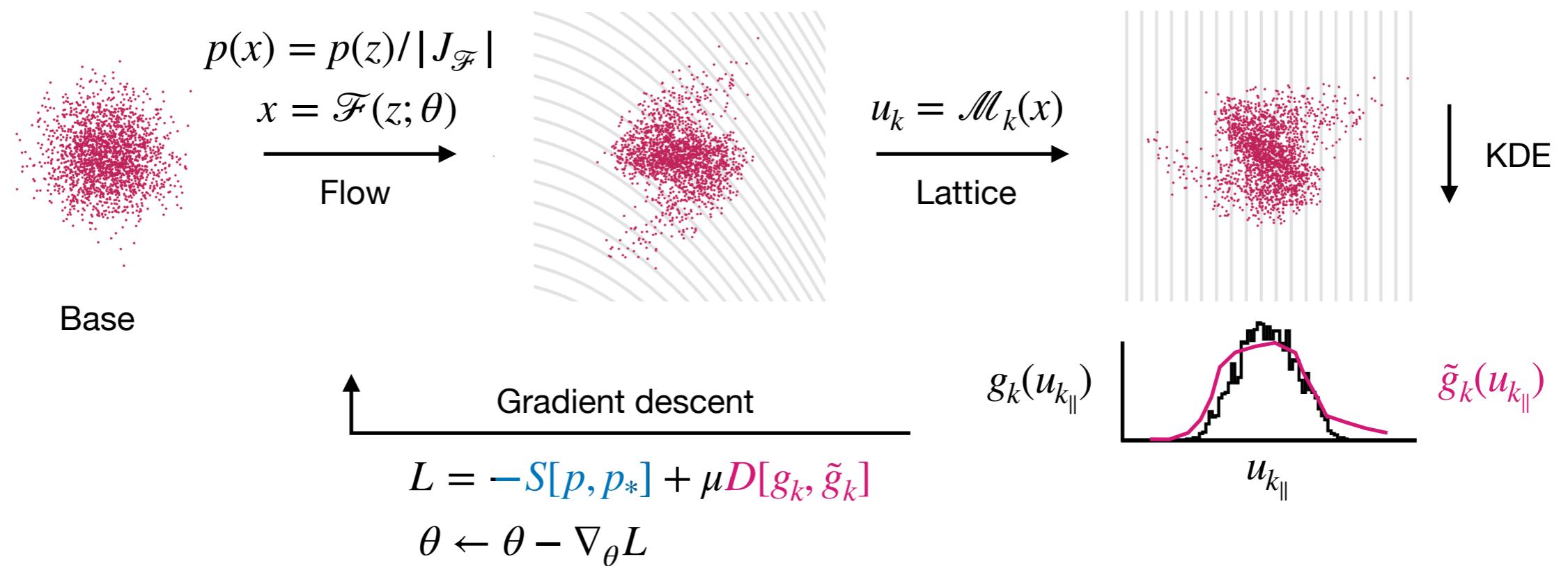
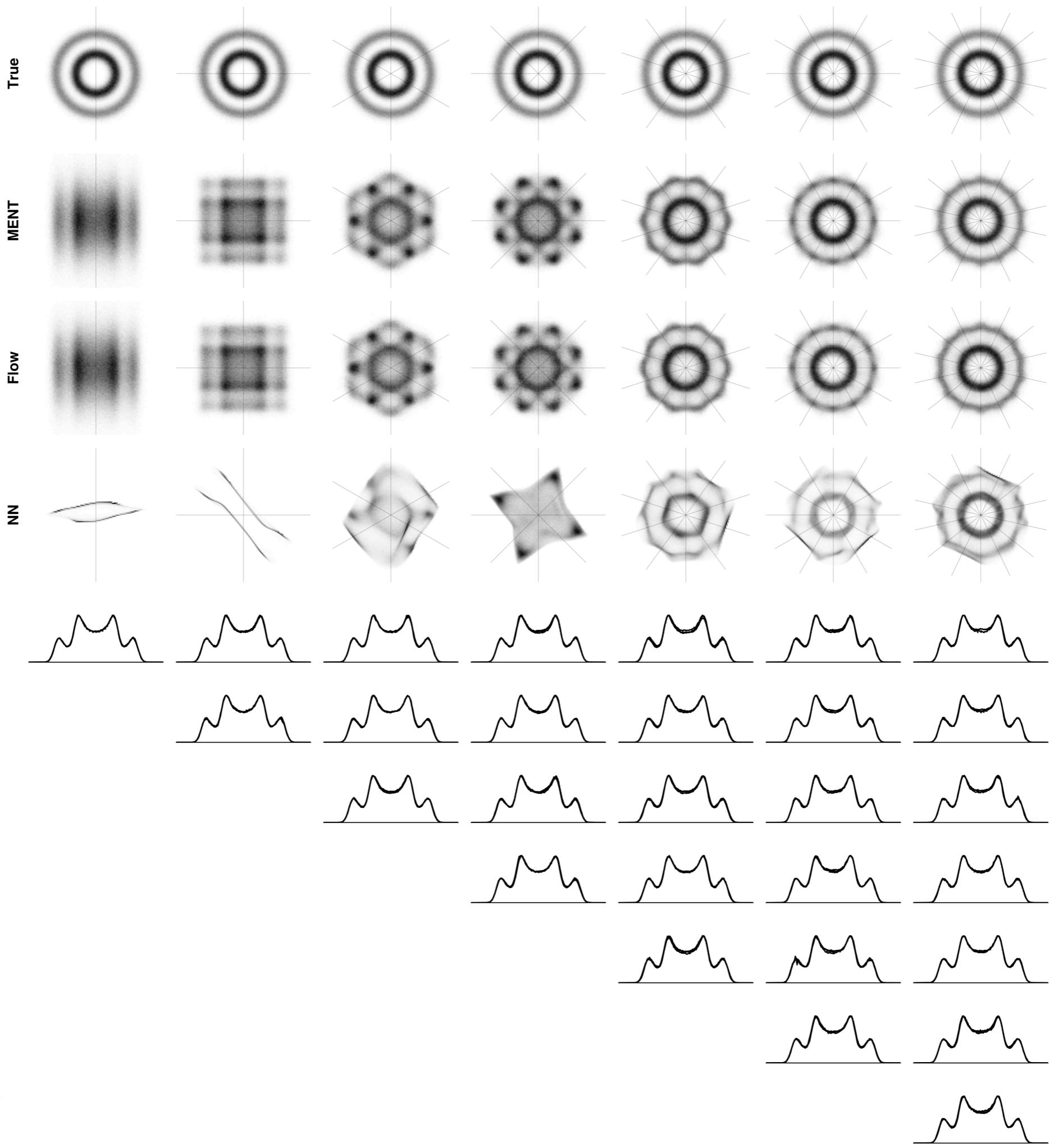
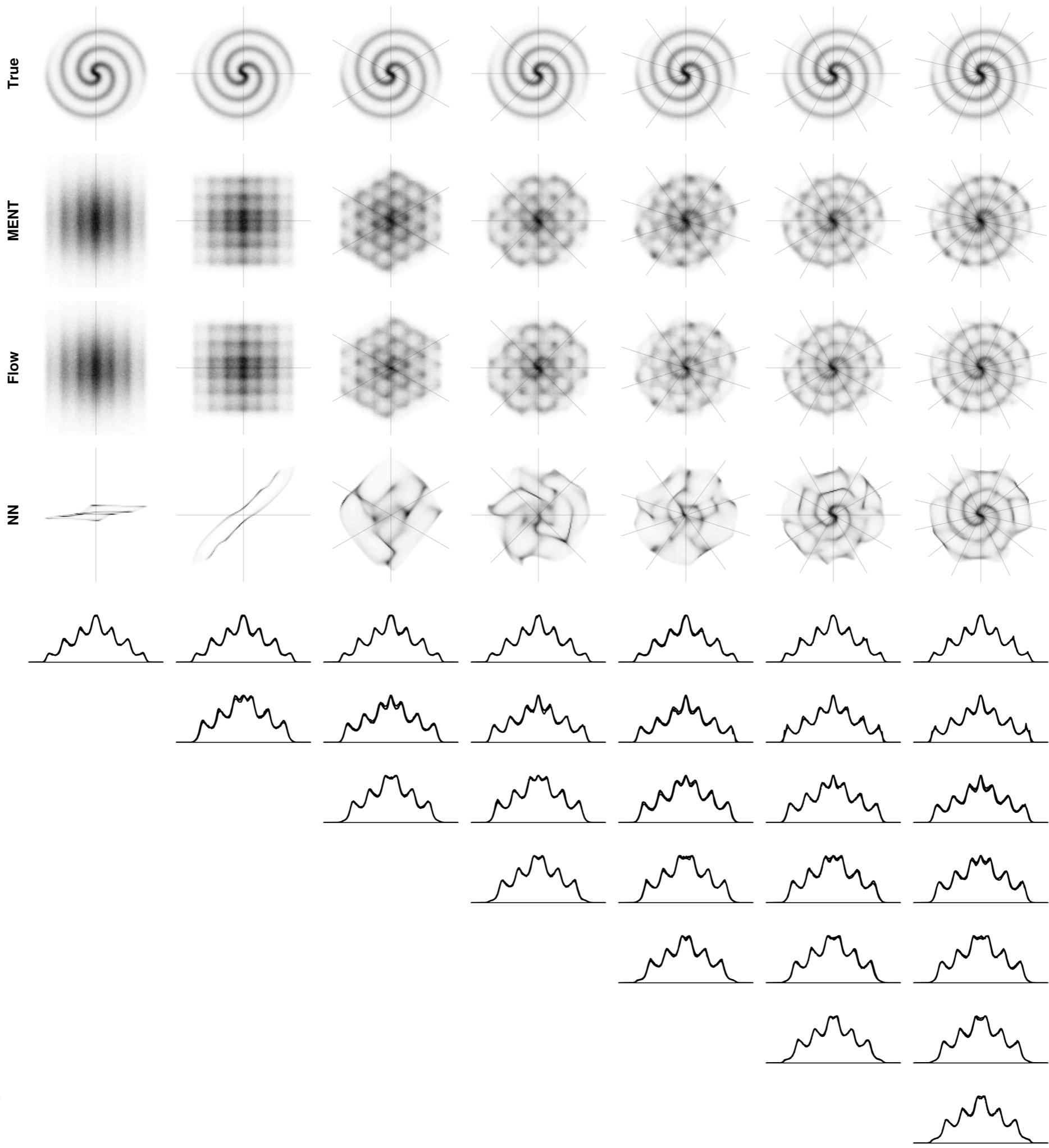


Figure 1: Monotonic rational-quadratic transforms are drop-in replacements for additive or affine transformations in coupling or autoregressive layers, greatly enhancing their flexibility while retaining exact invertibility. **Left:** A random monotonic rational-quadratic transform with $K = 10$ bins and linear tails is parameterized by a series of $K + 1$ ‘knot’ points in the plane, and the $K - 1$ derivatives at the internal knots. **Right:** Derivative of the transform on the left with respect to x . Monotonic rational-quadratic splines naturally induce multi-modality when used to transform random variables.

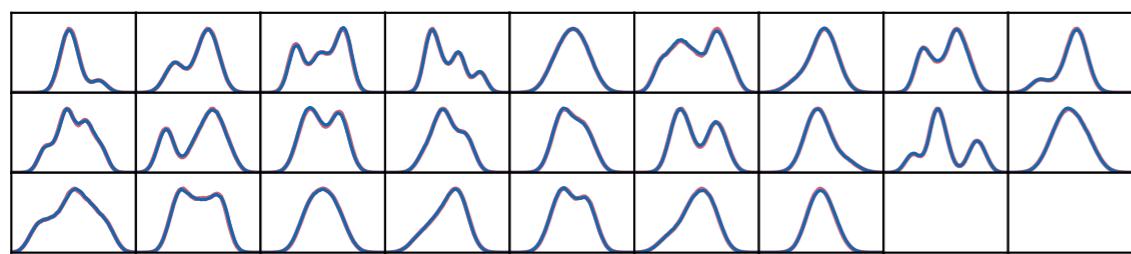
Find approximate constrained maximum using Penalty Method (PM) in outer loop



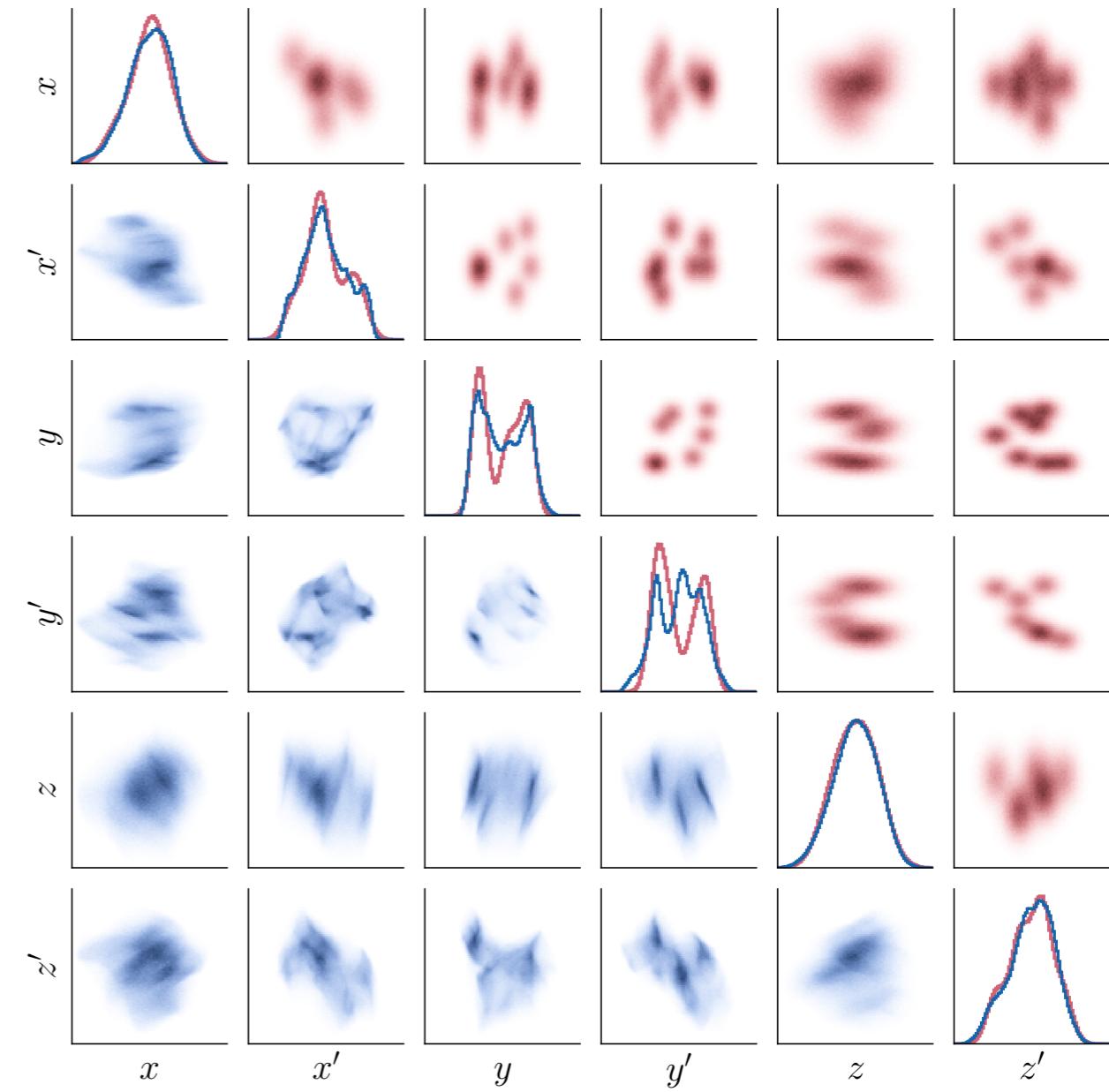
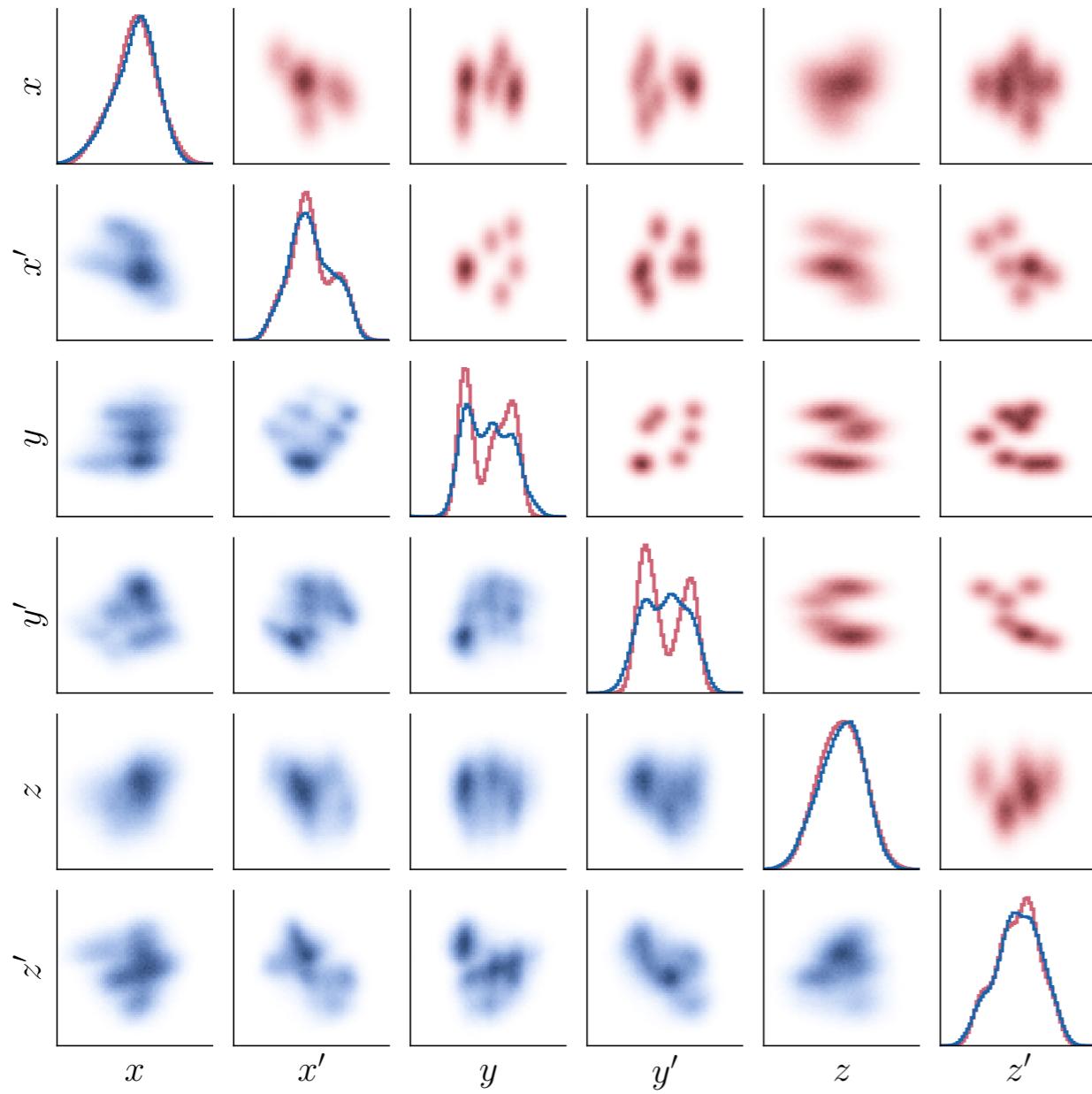
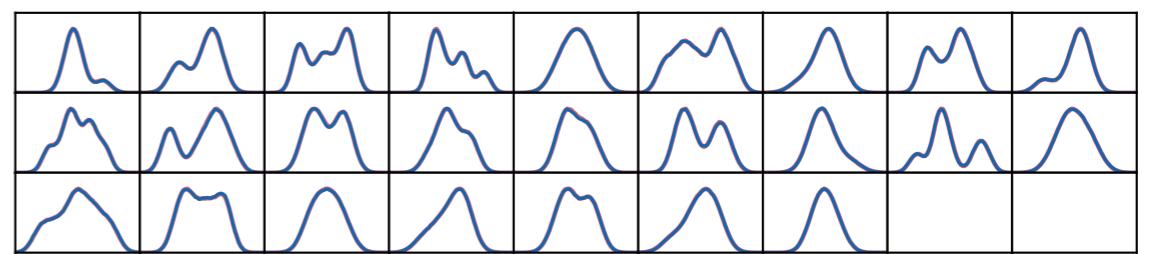




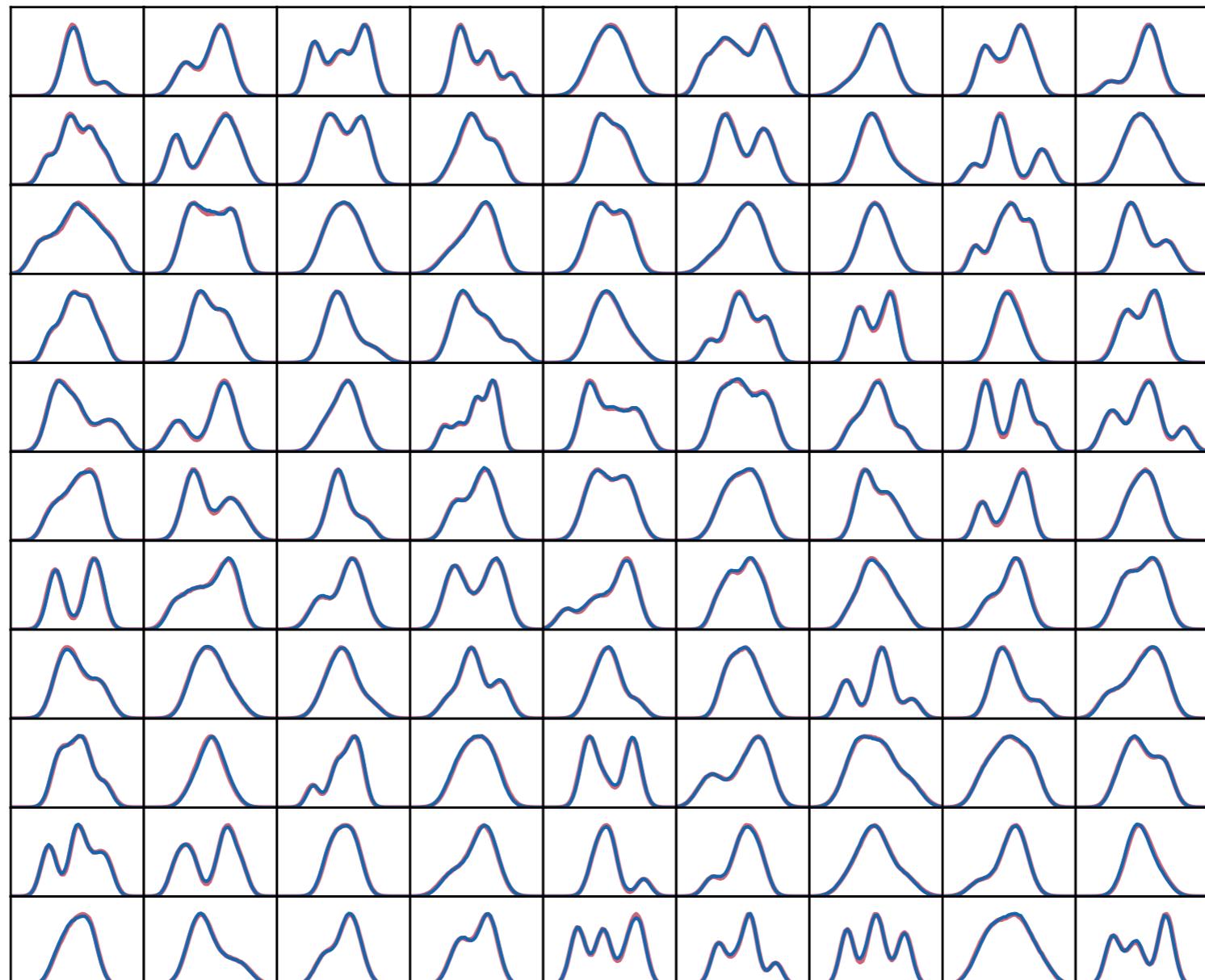
FLOW



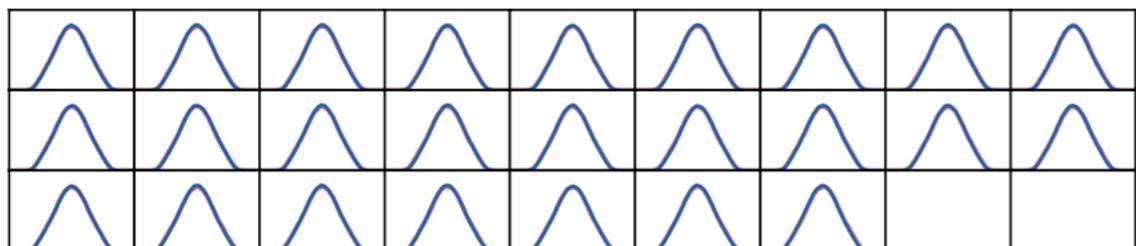
NN



FLOW

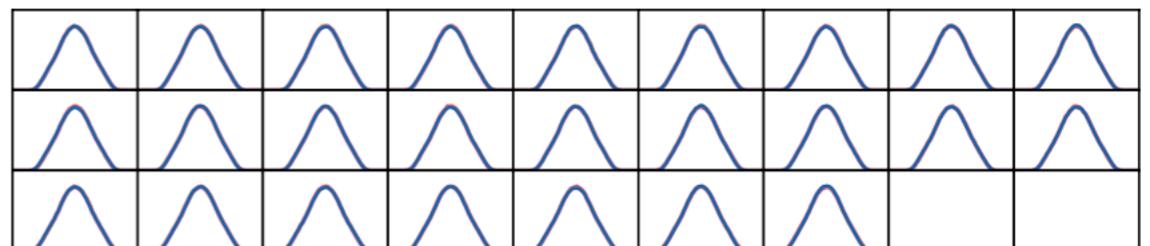


FLOW



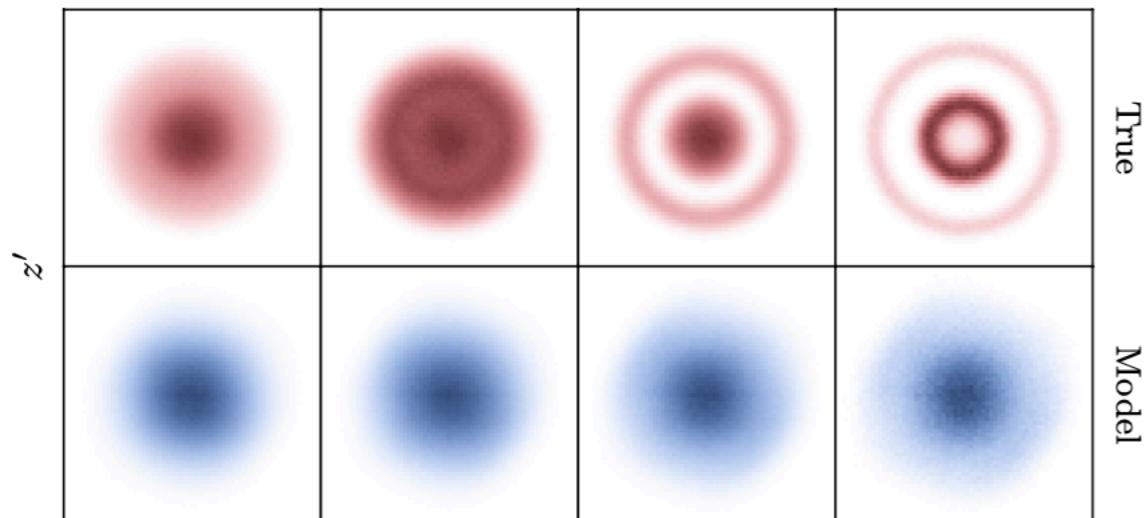
(a)

NN

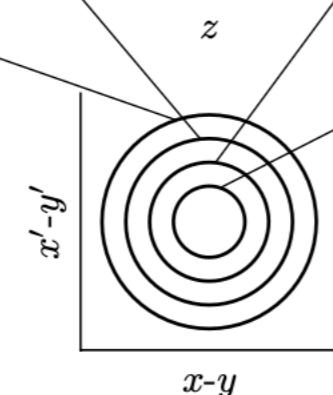


(b)

$$\rho(z, z' | r_{\perp} < \tilde{r}_{\perp})$$

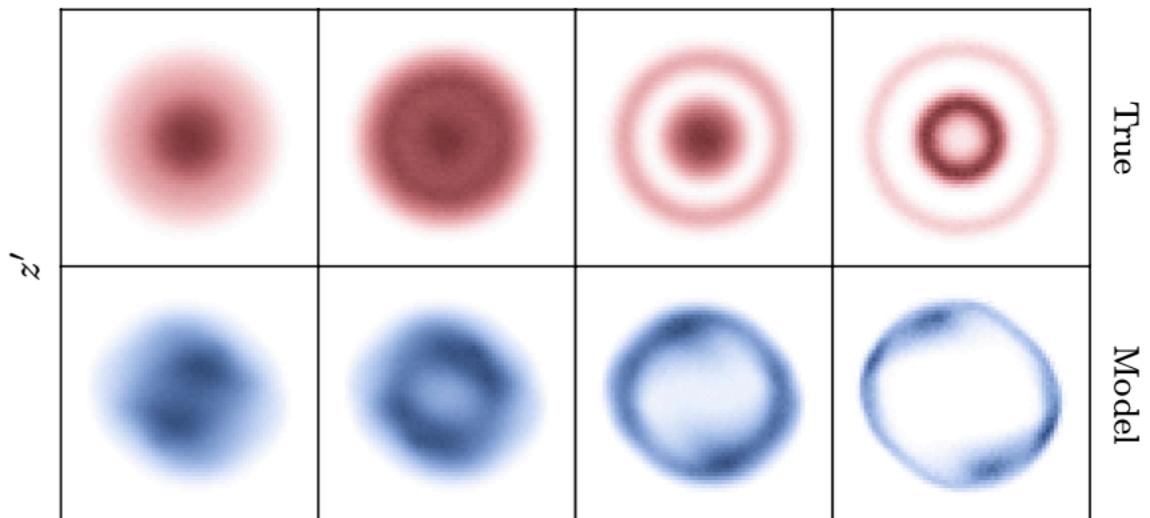


True
Model

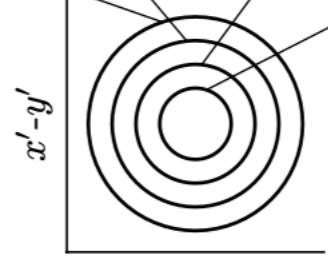


(c)

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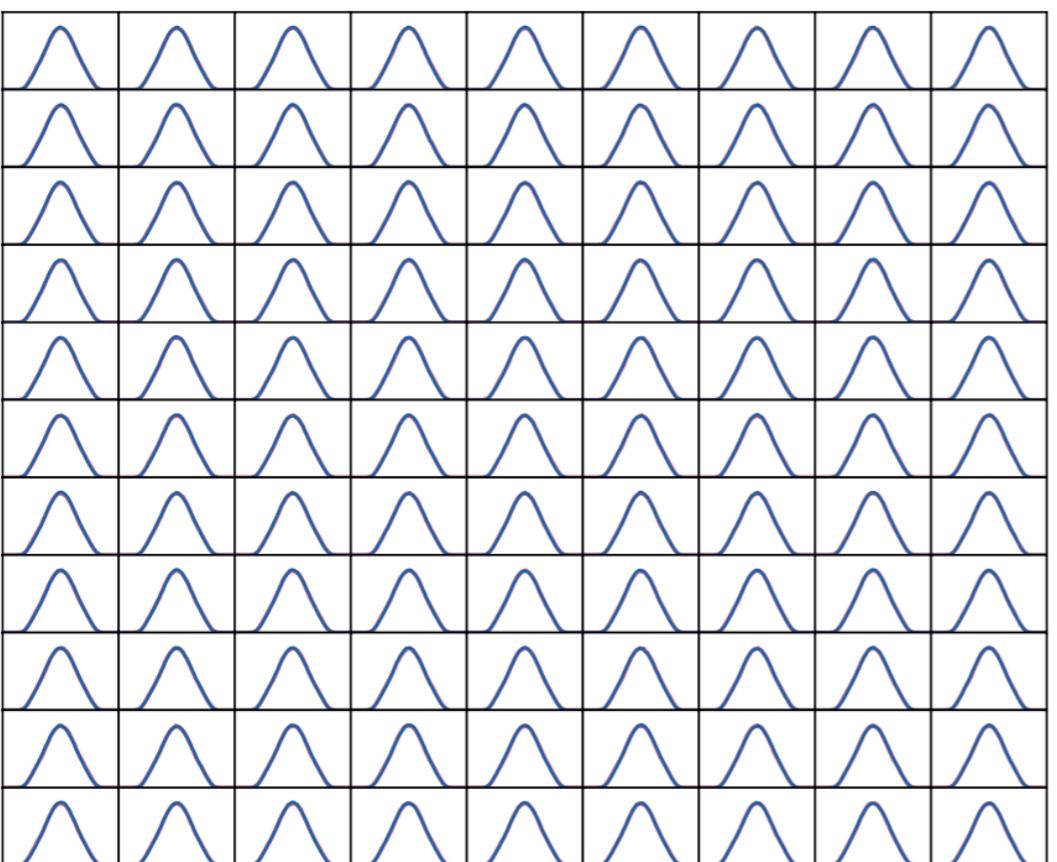


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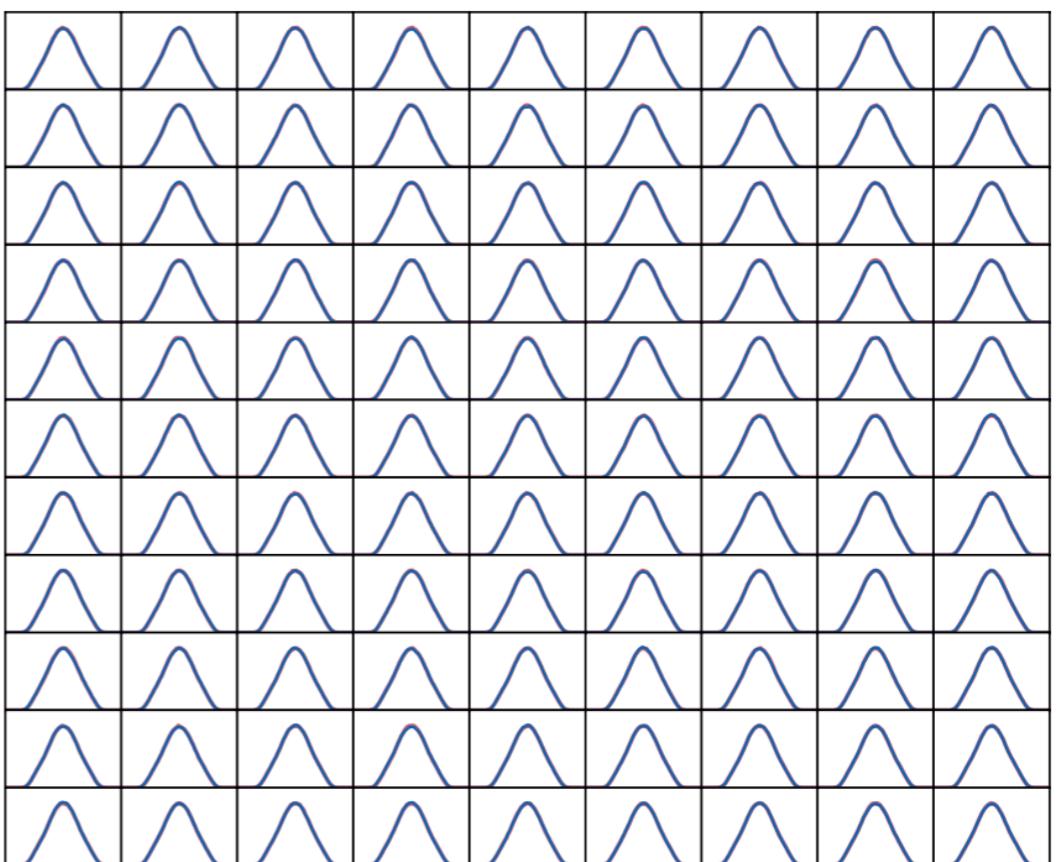
(d)

FLOW

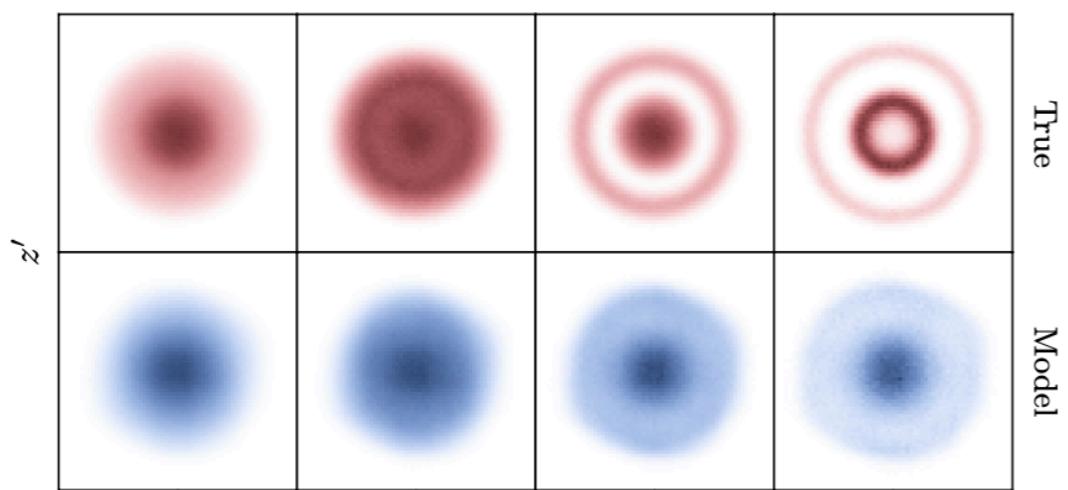
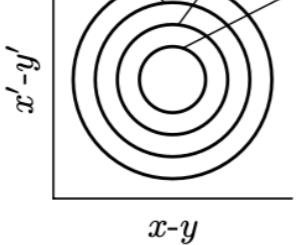


(a)

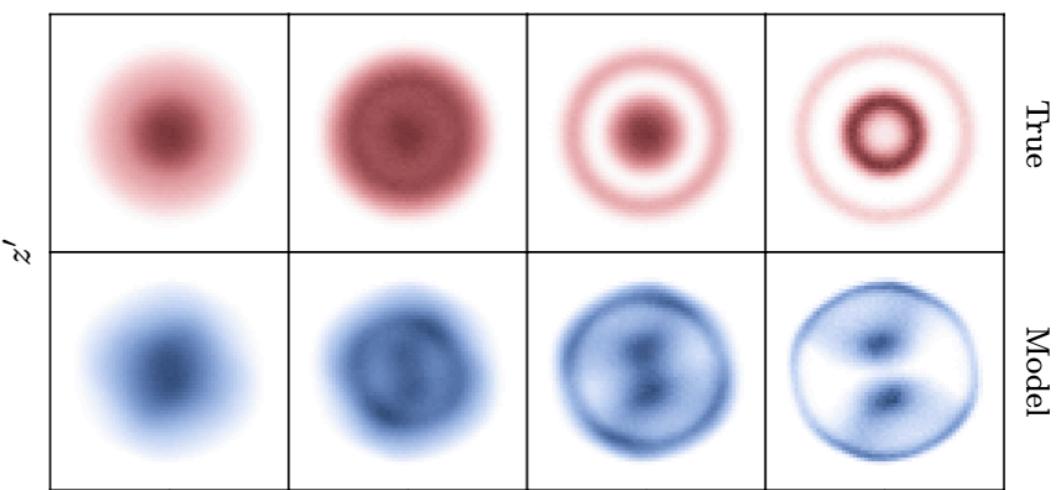
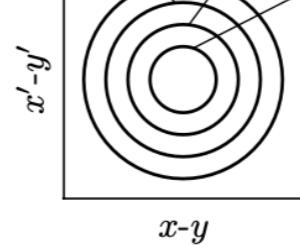
NN



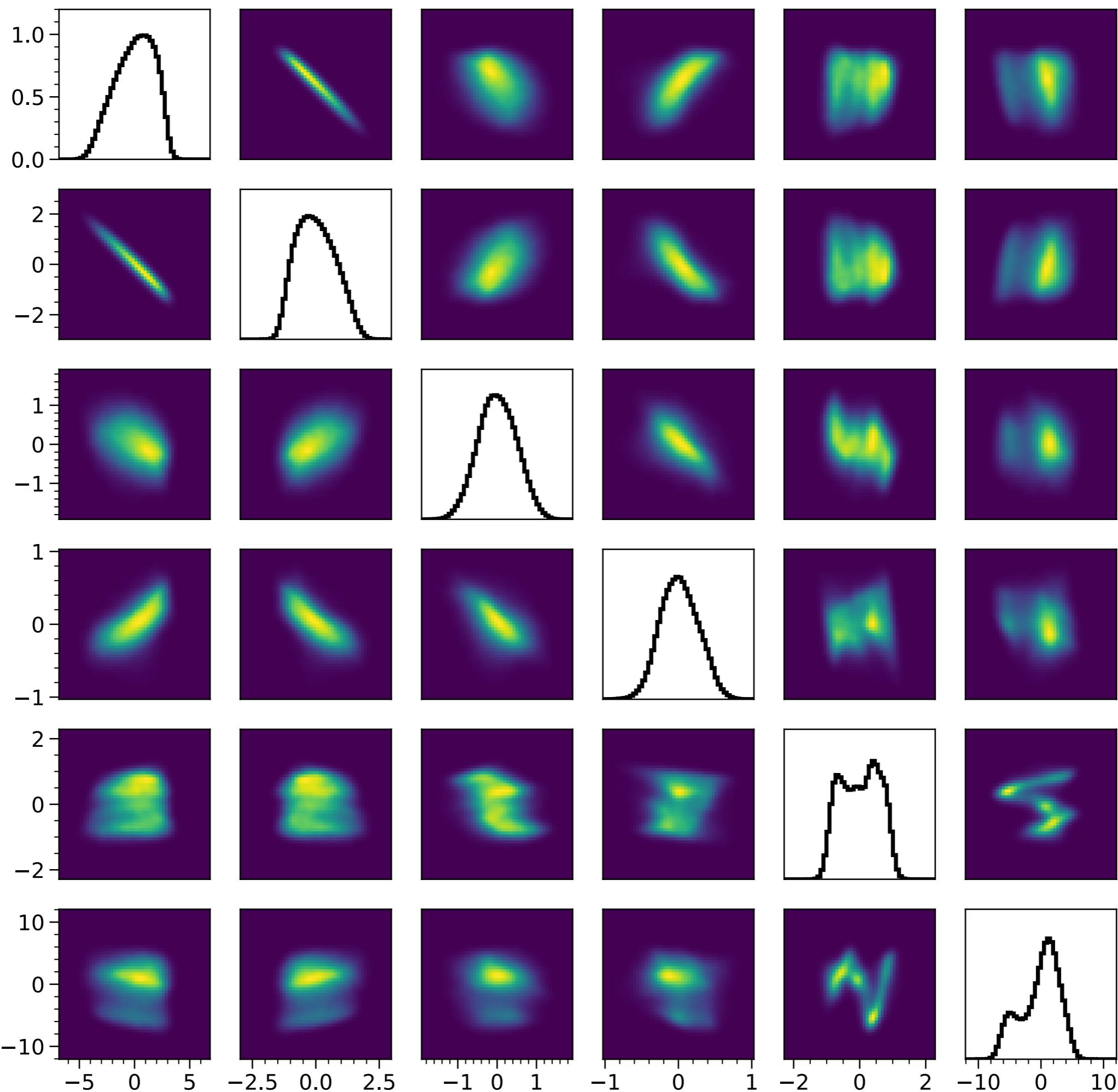
(b)

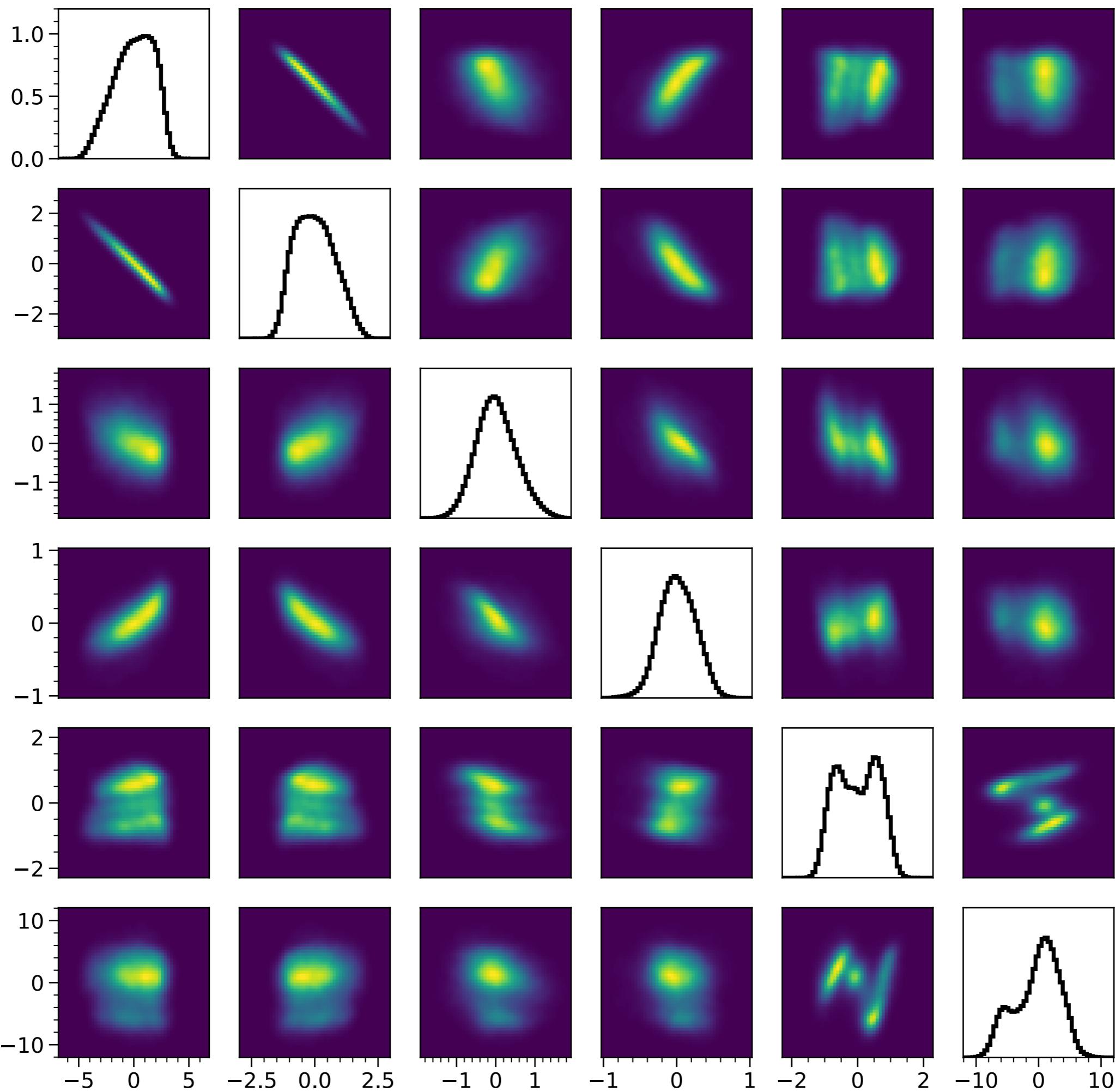
 $\rho(z, z' | r_\perp < \tilde{r}_\perp)$ True
Model

(c)

 $\rho(z, z' | r_\perp < \tilde{r}_\perp)$ True
Model

(d)





First 4D MENT demonstration in 1981!

IEEE Transactions on Nuclear Science, Vol. NS-28, No. 3, June 1981

FOUR-DIMENSIONAL BEAM TOMOGRAPHY*

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Summary

A computer code has been developed to reconstruct the 4-D transverse phase-space distribution of an accelerator beam from a set of linear profiles measured at different angles at three or more stations along the beam line. The code was applied to wire-scan data obtained on the low-intensity H⁻ beam of the LAMPF accelerator. A 4-D reconstruction was obtained from 10 wire-scan profiles; 2-D projections of the reconstruction agree fairly well with slit-and-collector measurements of the horizontal and vertical emittance distributions.

We assume, for simplicity that f has been normalized and centered as follows:

$$\int d^4v f(v) = 1, \int d^4v v_n f(v) = 0, \quad n = 1, \dots, 4.$$

The transfer matrices have $\det T_j = 1$ under very general conditions, hence the g_j will also be normalized and centered. We define b_j , the RMS width of g_j , by

$$b_j^2 = \int du u^2 g_j(u), \quad j = 1, \dots, J. \quad (3)$$

The covariance matrix σ of f is defined as

MENT recently applied to 4D reconstructions in SNS accelerator at ORNL

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4D transverse phase space tomography of an operational hydrogen ion beam via noninvasive 2D measurements using laser wires

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PHYSICAL REVIEW ACCELERATORS AND BEAMS **27**, 122802 (2024)

Four-dimensional phase space tomography from one-dimensional measurements of a hadron beam

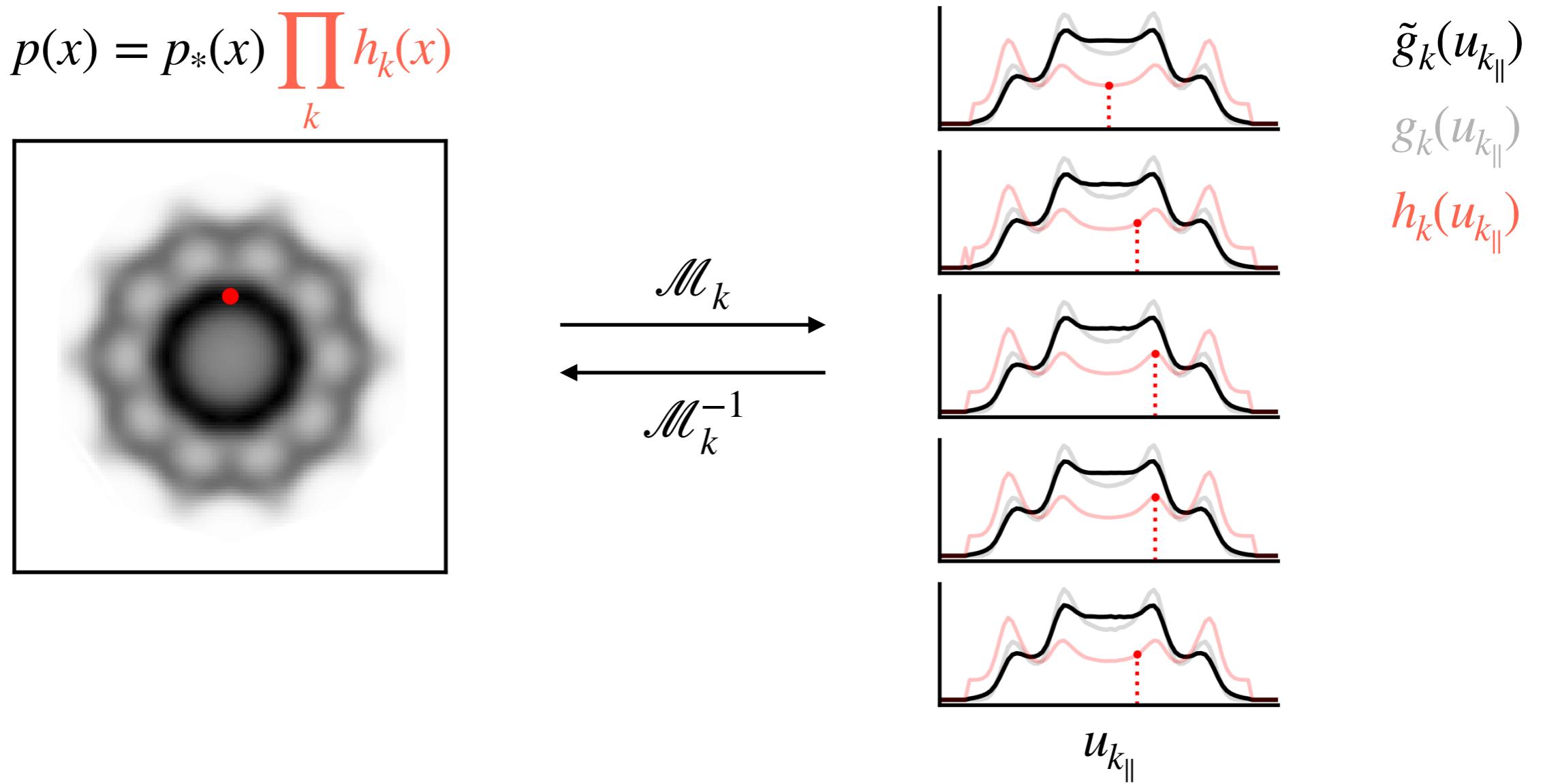
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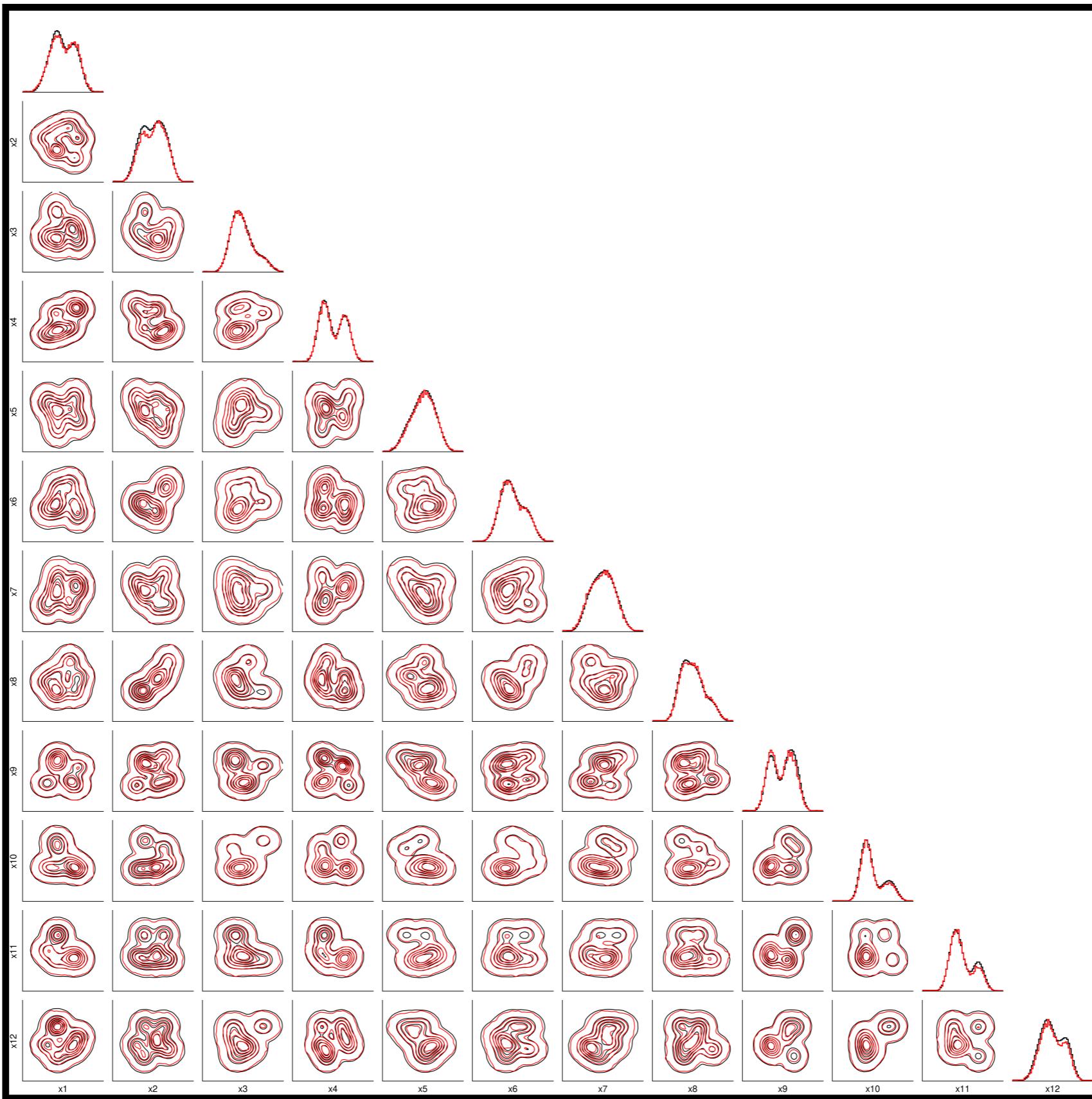


(Received 4 September 2024; accepted 4 December 2024; published 26 December 2024)

MENT requires map between PDF and projections



Test: 12D Gaussian Mixture distribution



6D phase space distribution can strongly influence beam evolution!

