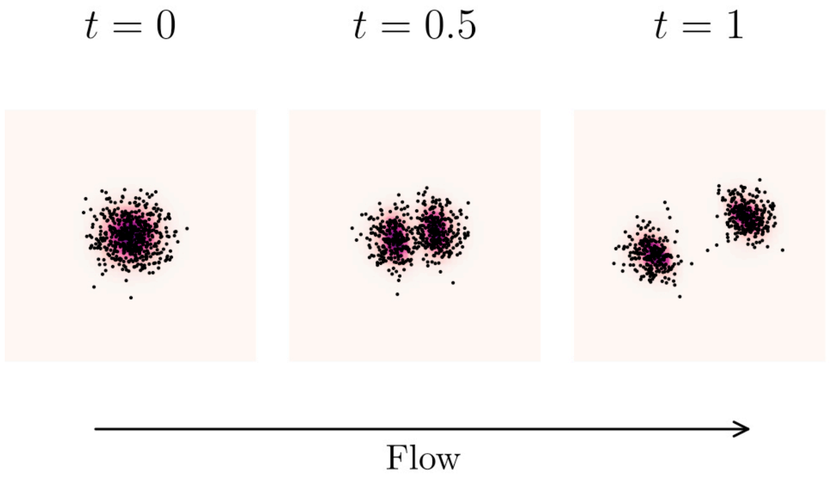
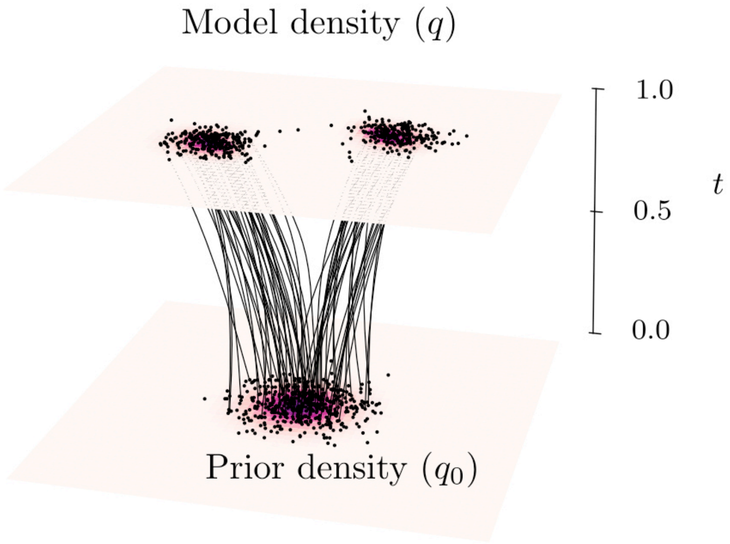
Normalizing flows for Lattice gauge theory





Gurtej Kanwar
Chancellor's Fellow in AI & Datascience
University of Edinburgh

Jul 28 - Aug 1, 2025
MITP Summer School

Lecture 1

Markov chains

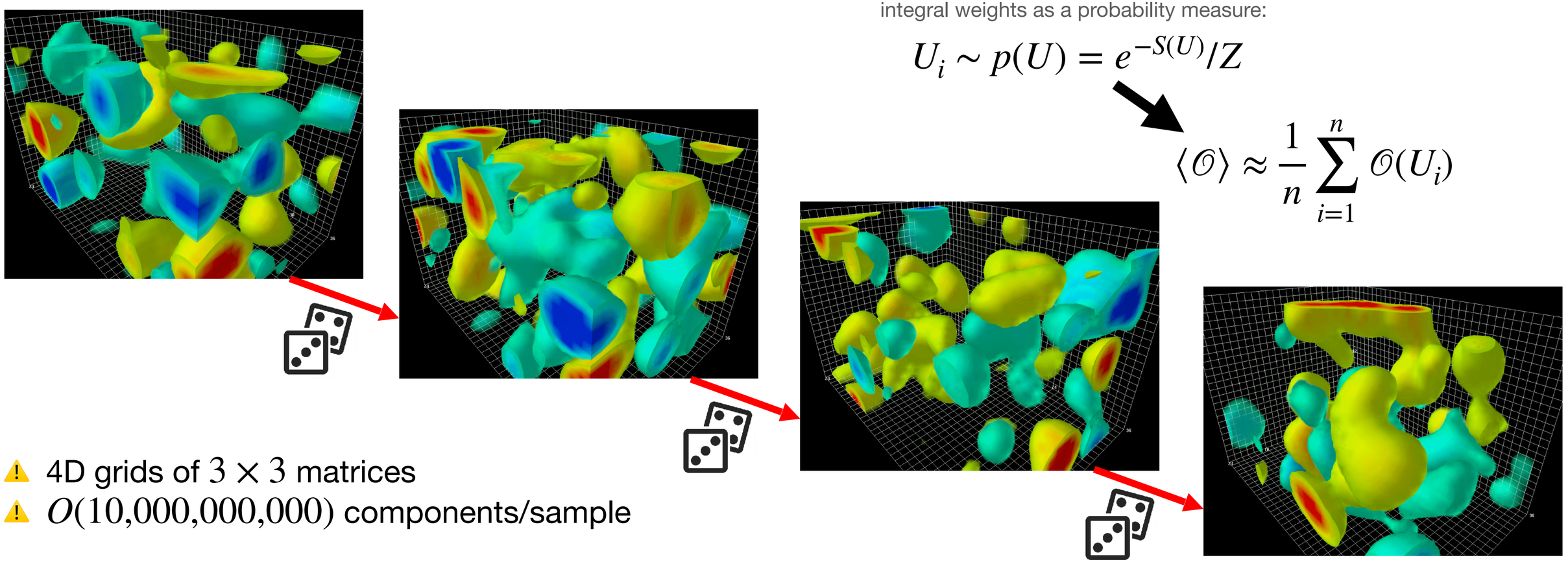
$$\langle \mathcal{O} \rangle = \left[\prod_{x,\mu} \int dU_\mu(x) \right] \mathcal{O}(U)\, e^{-S(U)}/Z$$

Estimate observables by averaging over Markov chain Monte Carlo samples.

Positive integrand allows interpreting path integral weights as a probability measure:

$$U_i \sim p(U) = e^{-S(U)}/Z$$

$$\langle \mathcal{O} \rangle \approx \frac{1}{n} \sum_{i=1}^{n} \mathcal{O}(U_i)$$



- ⚠ 4D grids of 3×3 matrices
- ⚠ $O(10{,}000{,}000{,}000)$ components/sample

Image credit: Leinweber, et al.

Critical slowing down (CSD)

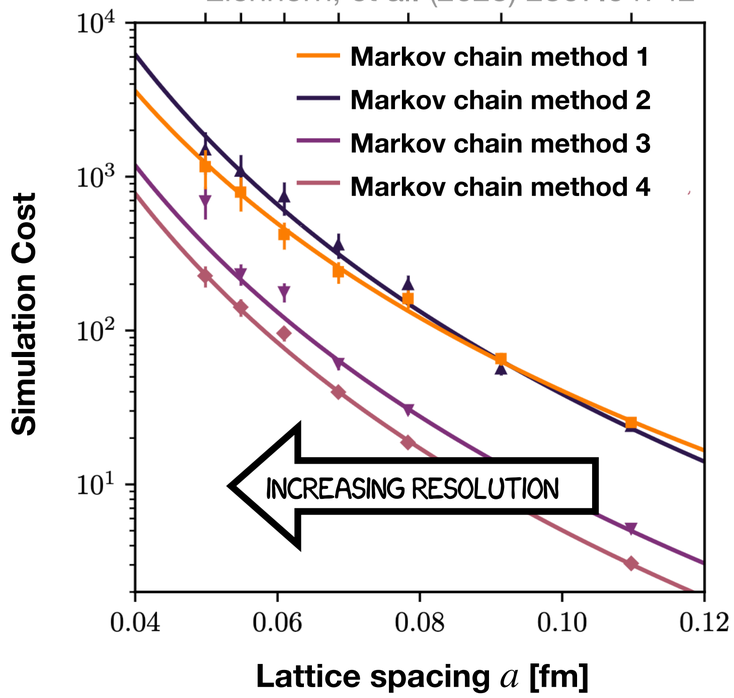
Markov chains are typically **inefficient** as $a \to 0$

- Information transfer is local while correlations grow
- **CSD:** diverging autocorrelation time
- **Topological freezing:** Markov chain gets “stuck”

This **limits the physics results:**

- Heavy quarks (short-range interactions)
- Systematic uncertainties

Eichhorn, et al. (2023) 2307.04742

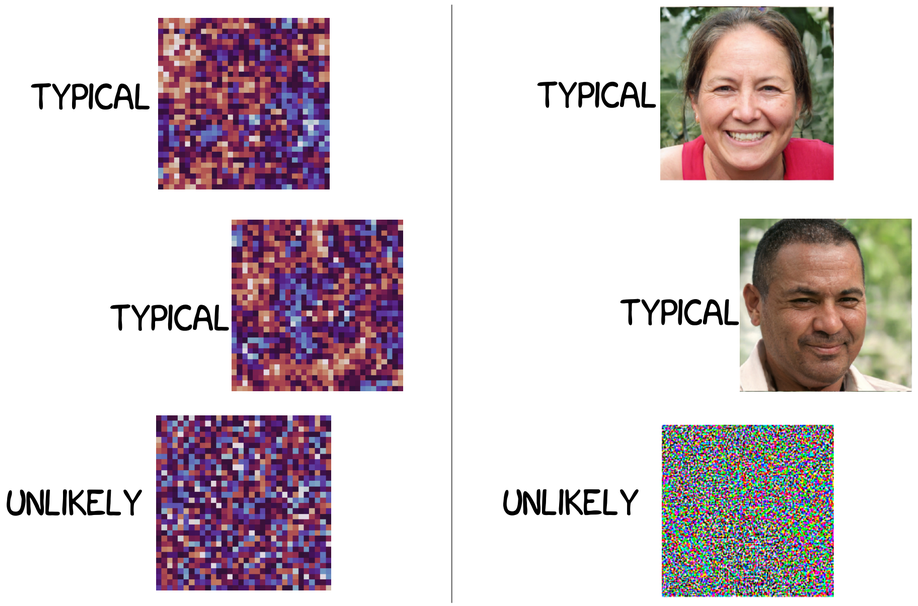


Lattice Monte Carlo ~ Image generation

Generative models can directly produce "typical" samples

Lattice sampling vs. Generative AI

Karras, Lane, Aila (NVIDIA) 1812.04948

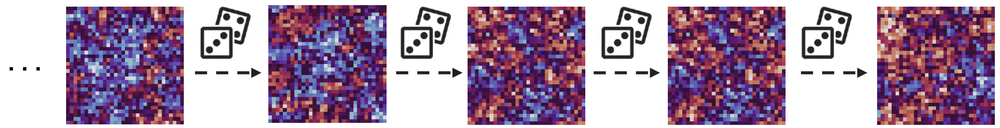


Unique features:

- ⚠ Demand **unbiased results**
- ⚠ Not much **existing training data**
  … $O(1000)$ samples at finest resolutions
  … $O(10{,}000{,}000{,}000)$ components/sample
- ✓ Know **target probability density**
- ✓ Know **physical symmetries**

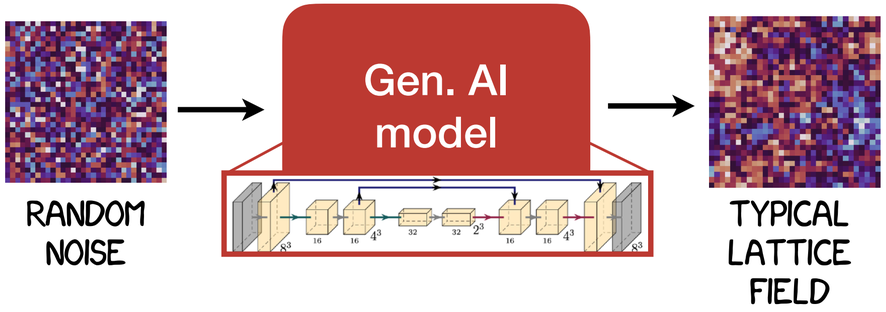
Can we use **Generative AI** to solve critical slowing down?

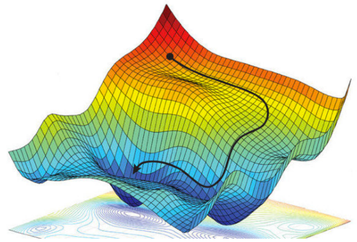
Replace or augment **Markov Chain Monte Carlo**…

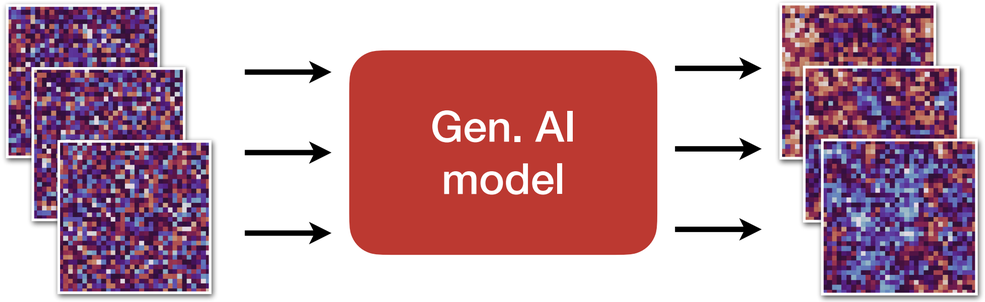


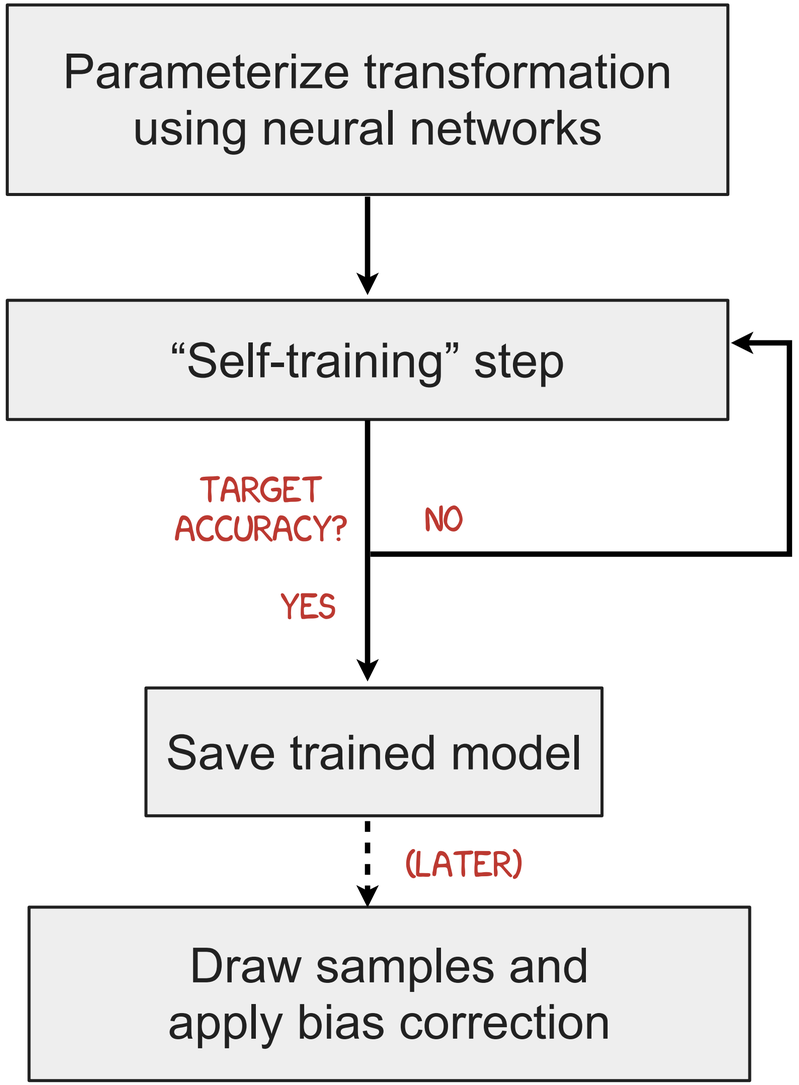
… with generated samples?

Generative AI models for Lattice QCD









Survey of image models

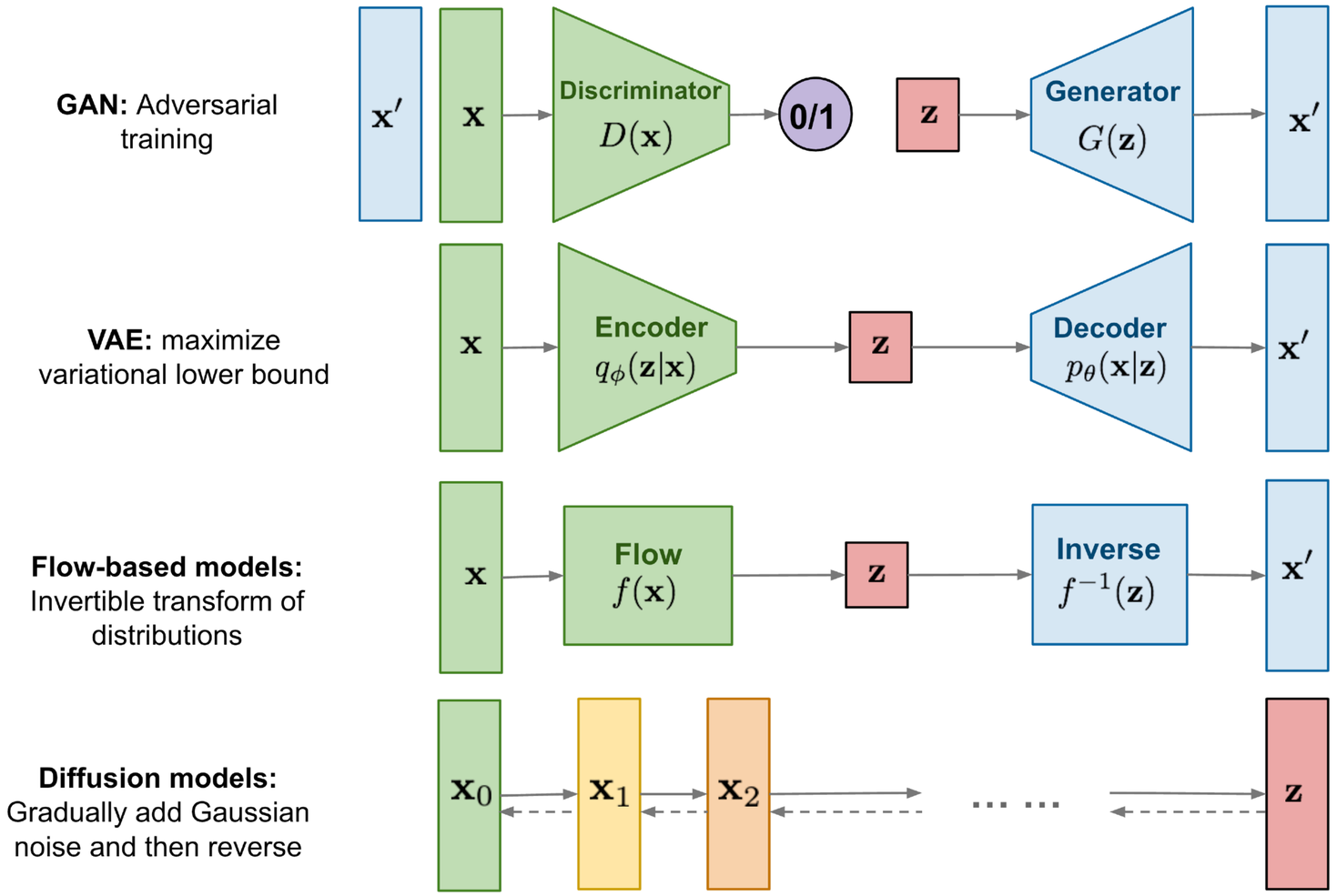
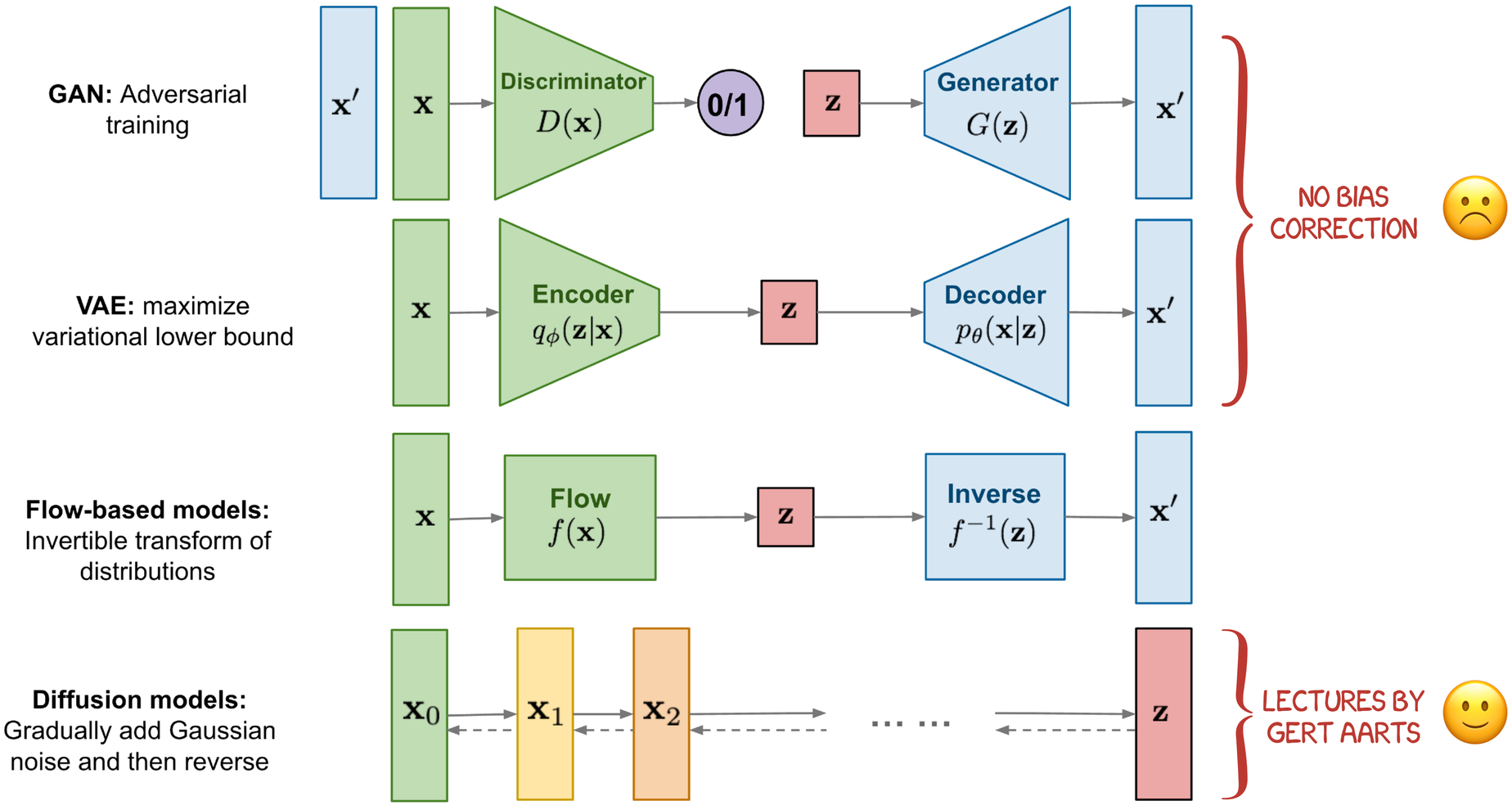


Image credit: Lilian Weng

Survey of image models



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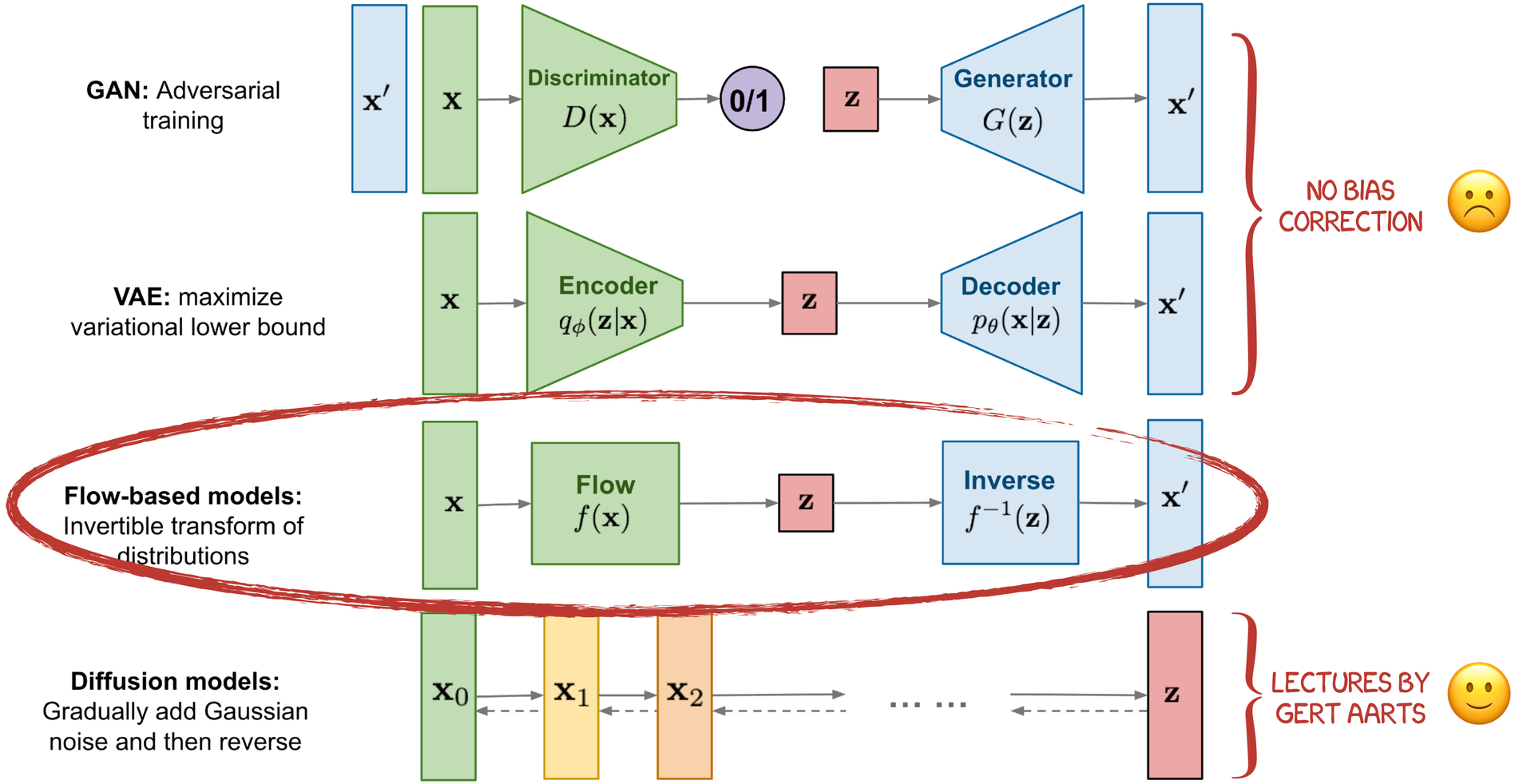
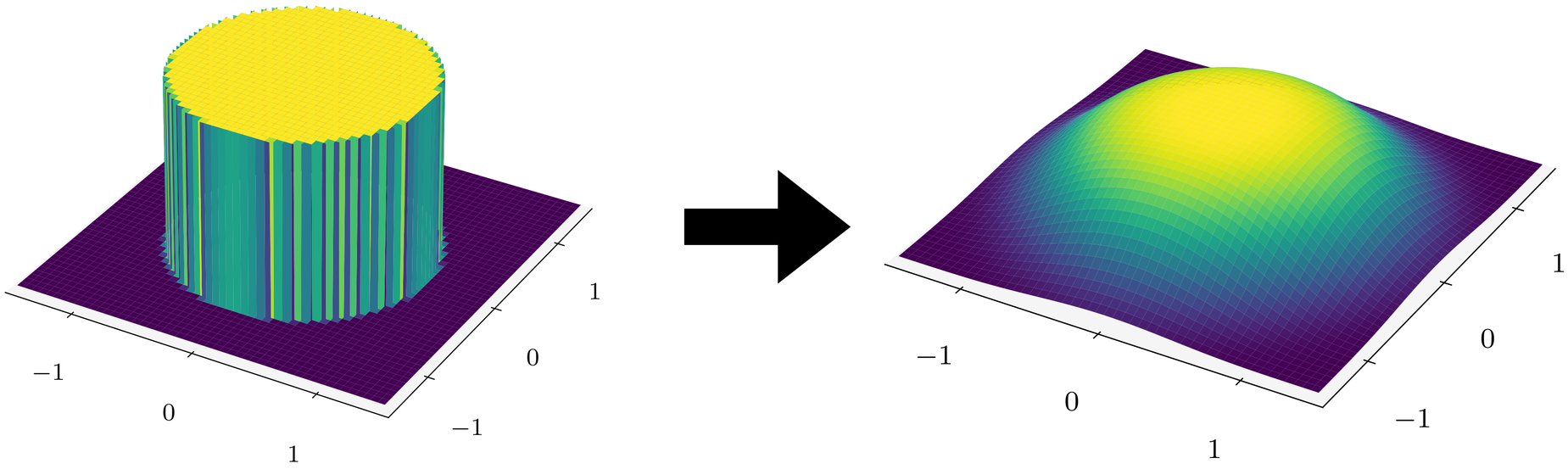


Image credit: Lilian Weng

Sampling using flows

Box-Muller transform to map $\mathrm{Unif}[\mathrm{circle}] \to \mathcal{N}(0,1)^2$

$$x' = \frac{x}{r}\sqrt{-2\ln r^2} \qquad y' = \frac{y}{r}\sqrt{-2\ln r^2}$$



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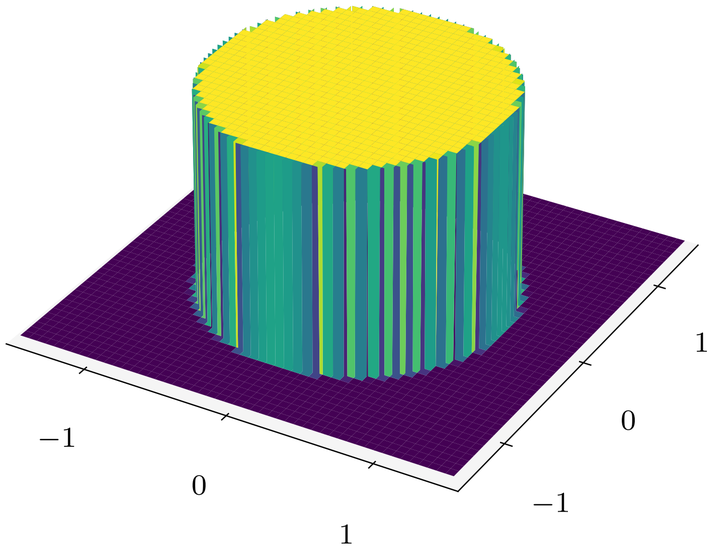
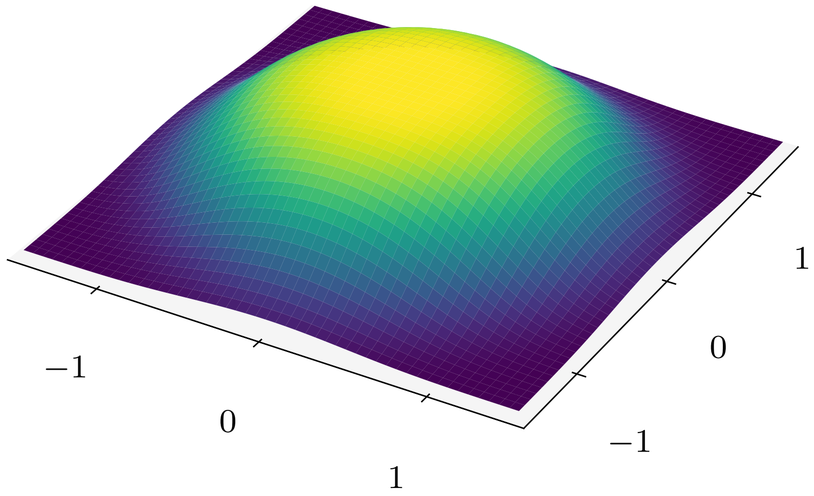


(Simple) Prior density:
$r(x, y)$

Flow f



(More complex) Output density:
$q(x', y') = r(x, y)\,|\det J|^{-1}$

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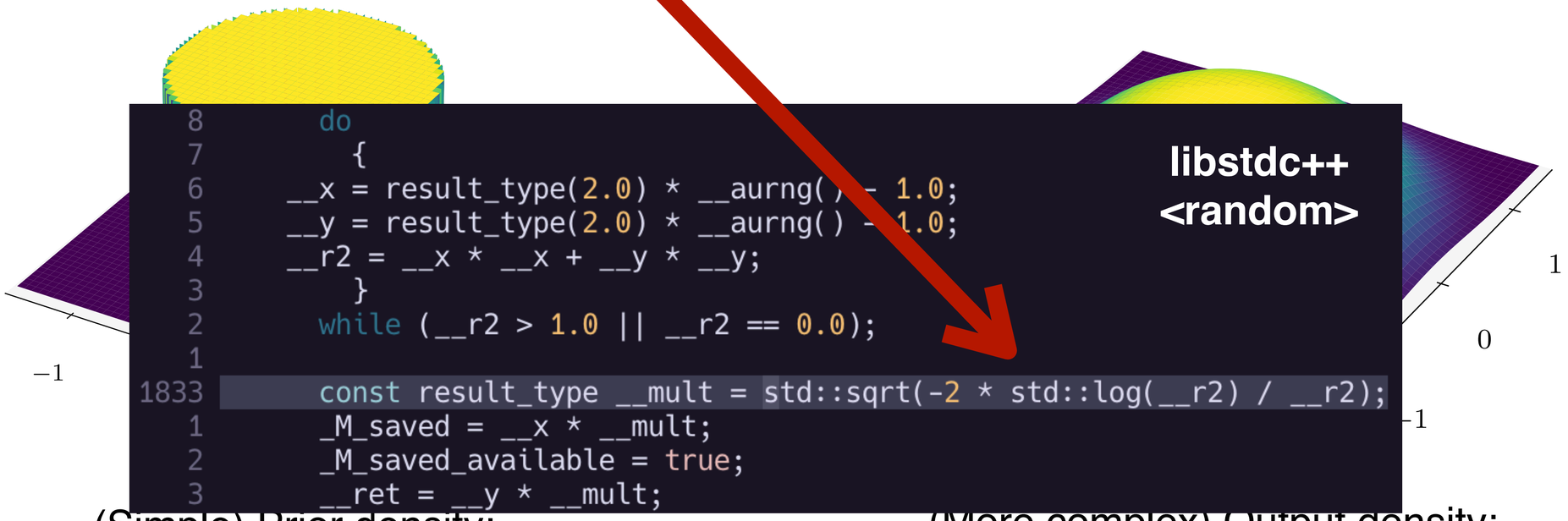


```
      do
        {
      __x = result_type(2.0) * __aurng() - 1.0;
      __y = result_type(2.0) * __aurng() - 1.0;
      __r2 = __x * __x + __y * __y;
        }
      while (__r2 > 1.0 || __r2 == 0.0);

      const result_type __mult = std::sqrt(-2 * std::log(__r2) / __r2);
      _M_saved = __x * __mult;
      _M_saved_available = true;
      __ret = __y * __mult;
```

libstdc++ <random>

(Simple) Prior density:

$r(x, y)$

(More complex) Output density:

$q(x', y') = r(x, y)\,|\det J|^{-1}$

Flow-based generative models

Tabak & Vanden-Eijnden CMS8 (2010) 217
Tabak & Turner CPA66 (2013) 145
Rezende & Mohamed (2015) PMLR 37, 1530

1. Sample from “easy” prior density

$$V \sim r(V)$$

2. Apply parametrized diffeomorphism (the “flow”)

$$U = f(V)$$

3. Output samples follow new “model density” thanks to **change of measure** formula

$$q(U) = r(V)\,|\det \partial U/\partial V|^{-1} = r(V)\,J_f(V)^{-1}$$

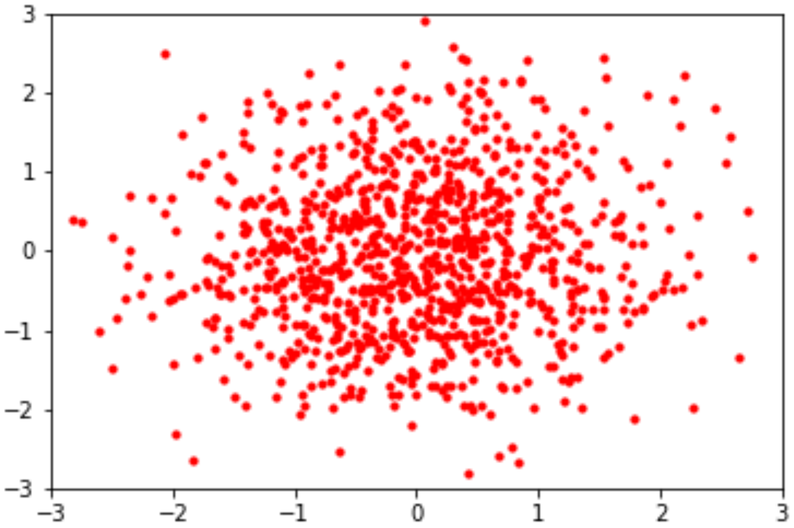

Image credit: blog.evjang.com/2019/07/nf-jax.html

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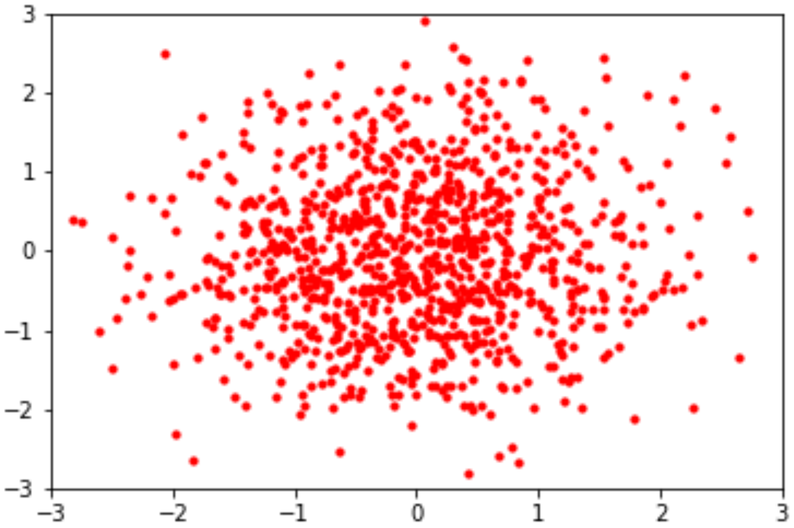

Image credit: blog.evjang.com/2019/07/nf-jax.html

Learned flows

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Approximate more complicated distributions by optimizing flexible ansatz f.

(E.G. USING ML METHODS)

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Approximate more complicated distributions by optimizing flexible ansatz f.

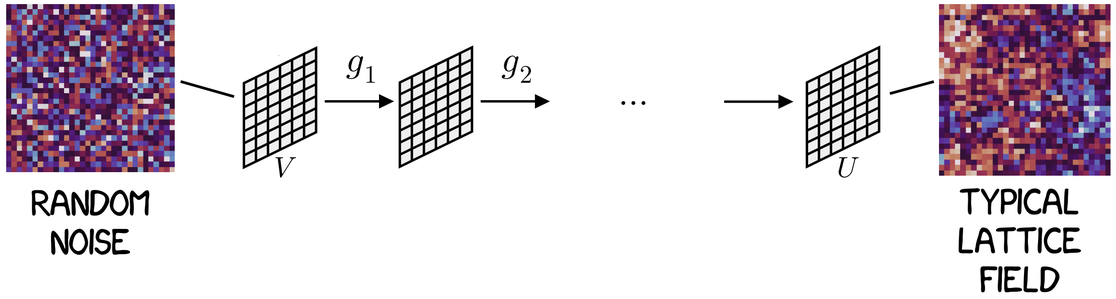
(E.G. USING ML METHODS)

- Discrete coupling layers:

  Dinh, et al (2014) 1410.8516; Dinh, et al (2016) 1605.08803

FLOW $f = g_1 \circ \ldots \circ g_n$

JAC. $\det J = \det J_1 \cdot \ldots \cdot \det J_n$



Learned flows

Approximate more complicated distributions by optimizing flexible ansatz f.

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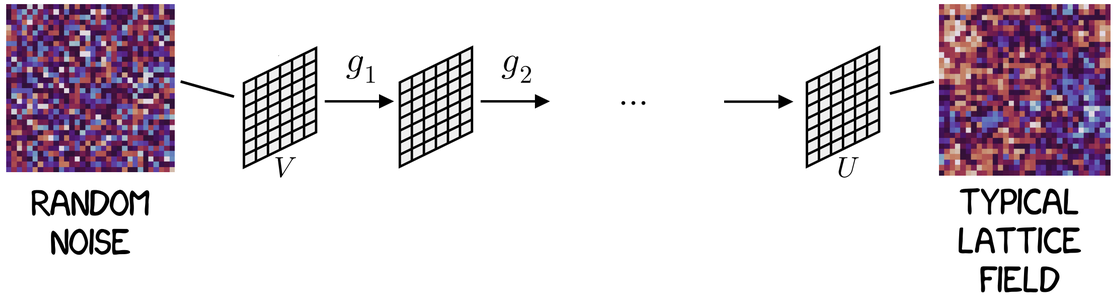


- Continuous flows:

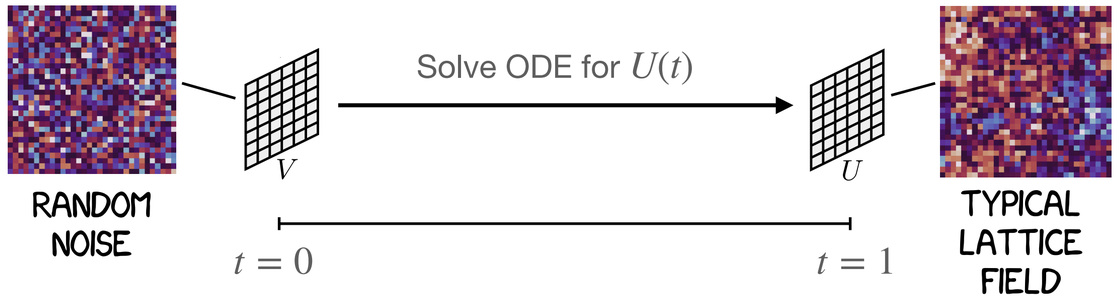
  Chen, et al (2018) 1806.07366; Zhang, et al (2018) 1809.10188

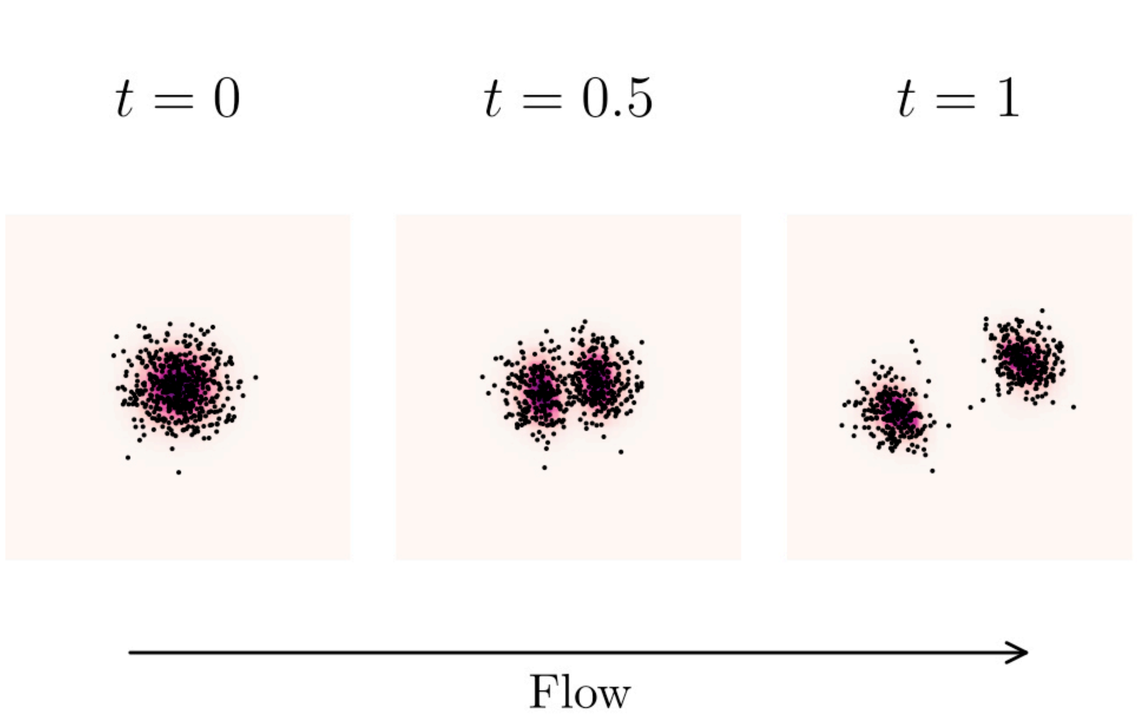
  FLOW $\dot{U}(t) = \nabla\varphi(U(t);t)\,U(t)$

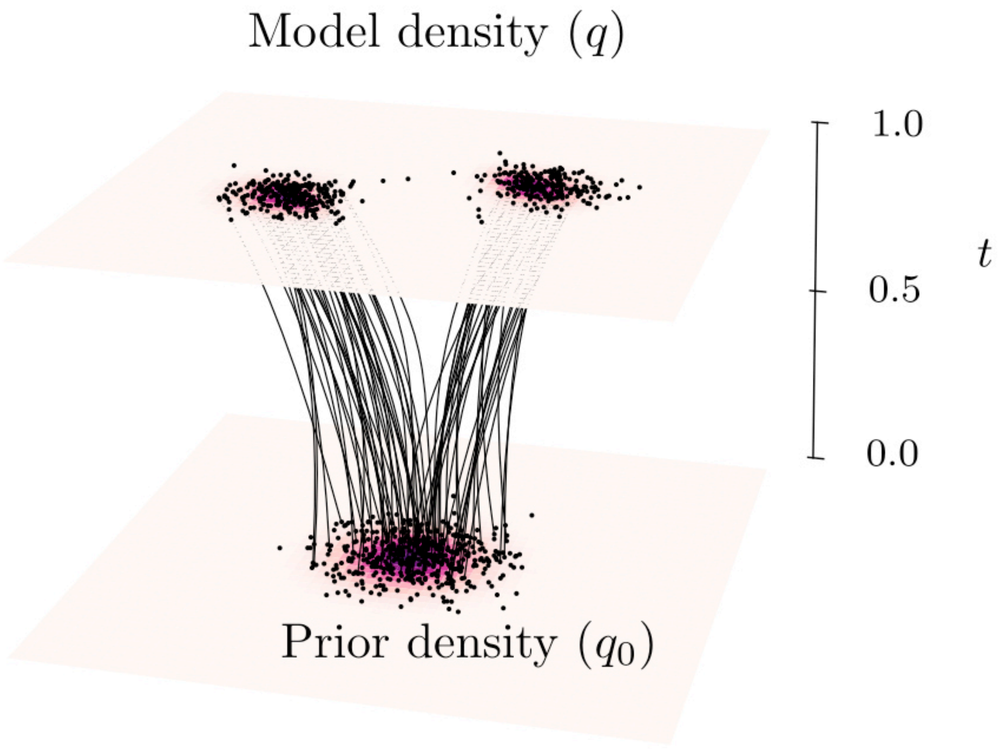
  with $f(V) := U(t=1)$

  JAC. $\ln\det J = -\int_0^1 dt\,\nabla^2\varphi(U(t);t)$

(NOTE: DERIVATIVE ∇ EVALUATED IN LIE ALGEBRA)



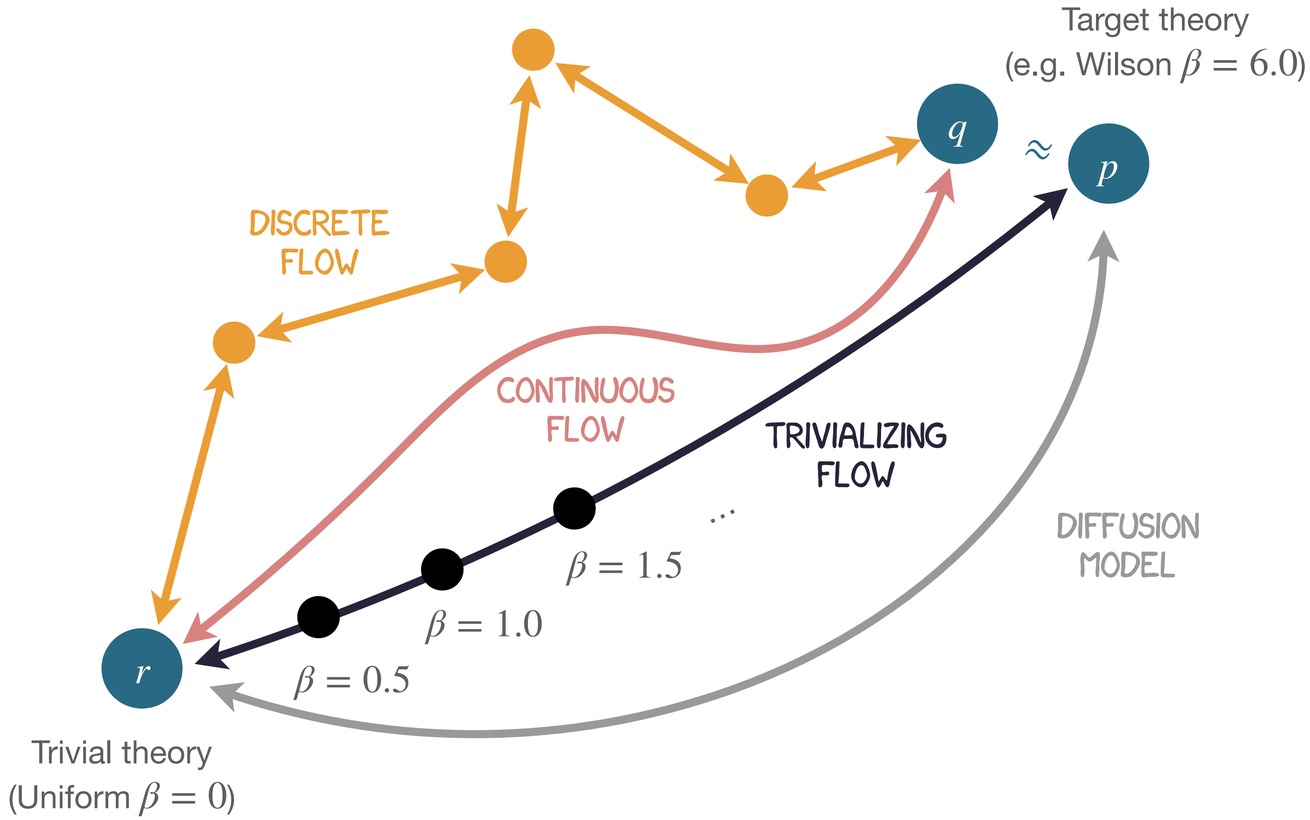

$t = 0$
$t = 0.5$
$t = 1$
Flow


Model density (q)
1.0
0.5
0.0
t
Prior density (q_0)

Flow-based sampling strategies

Various possible paths through space of distributions:

- **Freely learnable**
  - E.g. discrete / continuous flow models
- **Explicit fixed path**
  - Define $S_t(U)$ for $t \in [0,1]$
  - E.g. Lüscher's trivializing flow
- **Implicit fixed path**
  - Interpolation on samples
  - E.g. diffusion models, flow matching



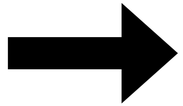
Exactness

Samples from model are from **biased distribution** $q(U) \neq p(U)$, but…

For each U_i drawn from the model, we know $q(U_i)$ and $p(U_i)$

Flow-based models provide this.

Known in terms of the lattice action.



Exact bias correction possible
(e.g. “flow-based MCMC” or reweighting)

$$\langle \mathcal{O} \rangle_p = \frac{\langle \mathcal{O}(U)\, p(U)/q(U) \rangle_q}{\langle p(U)/q(U) \rangle_q}$$

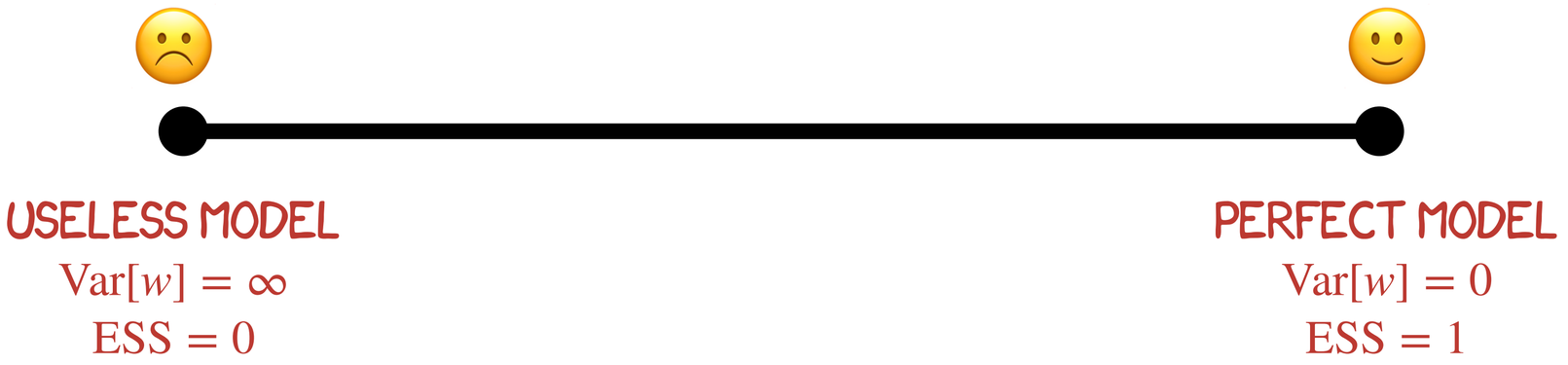
Note: *Efficiency* of bias correction depends on how close q and p are.

Measuring model quality

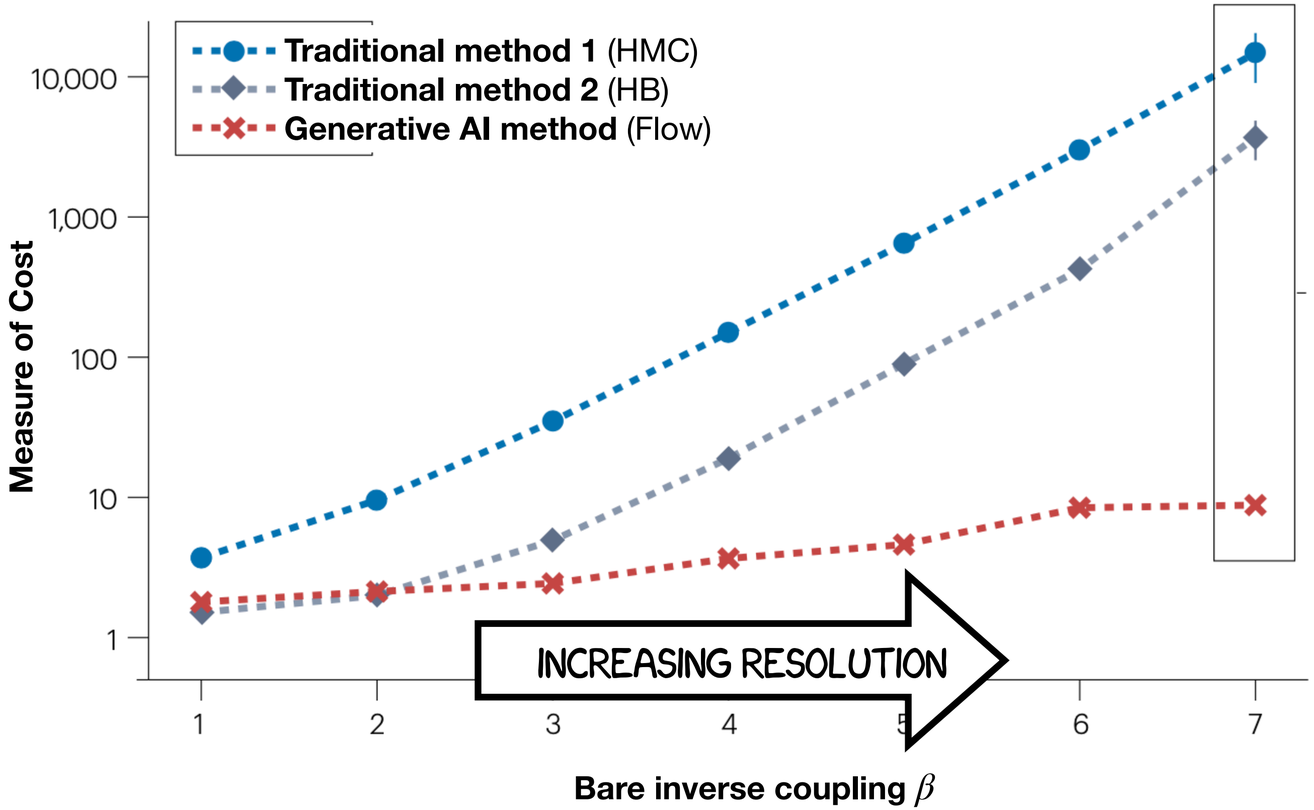
Variance of reweighting factors $\mathrm{Var}[w]$, where $w(U) := p(U)/q(U)$

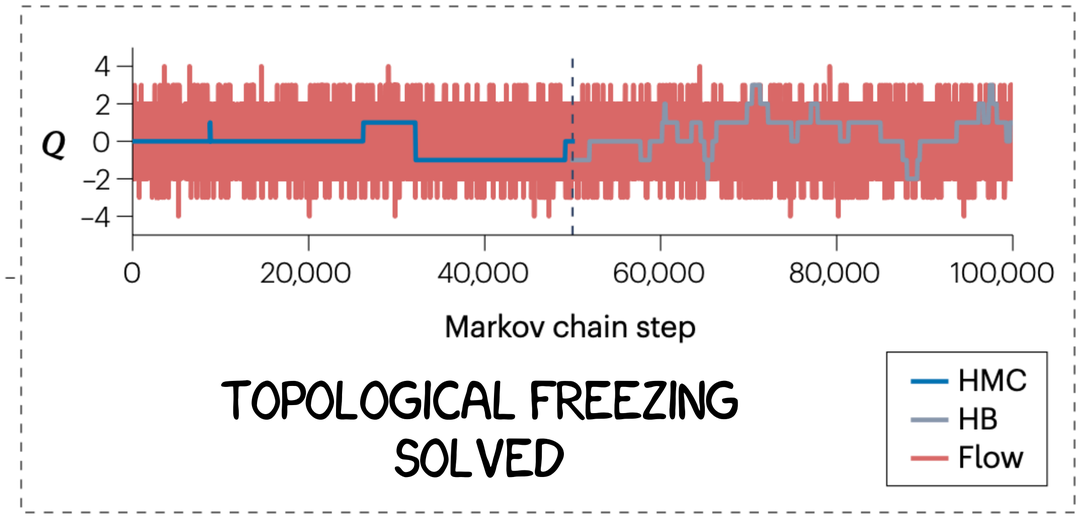
Effective sample size, $\mathrm{ESS} := \langle w \rangle_q^2 / \langle w^2 \rangle_q$

- "Fraction samples from q that are effective samples of p"



Preview: Very effective in some cases!





Cranmer, GK, Racanière, Rezende, Shanahan
Nature Reviews Physics 5 (2023) 526

Hands-on coding

github.com/gkanwar/flow-lectures

- Set up your env and follow along (if you want!)
- Implement HMC for ϕ^4 theory, observe slowing down
- Implement a toy flow-based sampler
- Explore this code further in the exercises