Normalizing Flows for data with (and without) Translational and Rotational Symmetry

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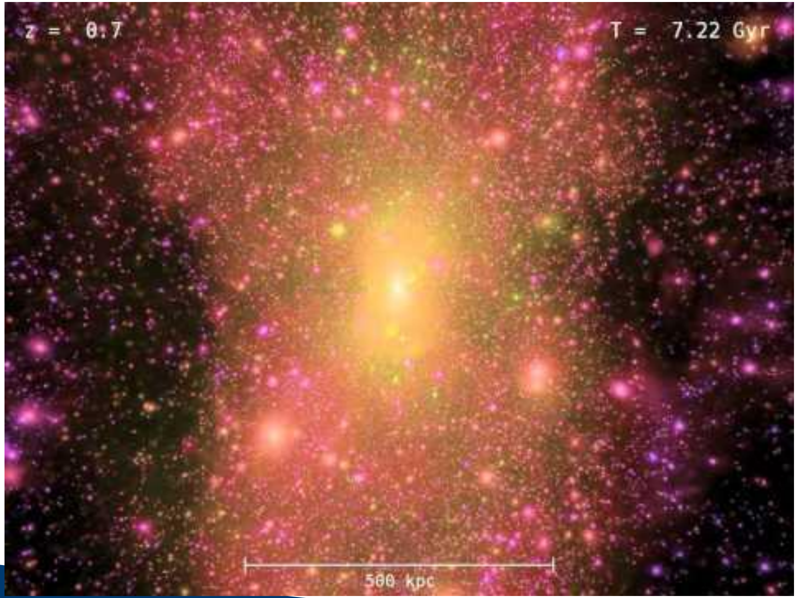
Background

- Numerical simulations are crucial for accurately predicting cosmological observations and understanding the systematic effects in the current and future sky surveys, but they are computationally expensive.

http://www.sdss3.org/press/dr9.php



https://www.youtube.com/watch?v=xfgDoExbu_Q

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Motivations

- Deep generative models have been used in modeling structure formation
  - Predict tSZ signal, HI, dark matter annihilation feedback, super resolution, etc.

- Why not GANs?
  - Pro: Realistic looking samples
  - Con: Mode collapse. Low-dimensional manifold assumption leads to information loss. Potentially introduce systematics in data analysis.

Full dimensional models like **NF**s

- Physical constraints: translational and rotational symmetry
  - What people do now: let the model learn the symmetry by augmenting the training data. Performance not guaranteed. Increase the training work.

Enforce the symmetry in the generative model

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Normalizing Flows

- Bijective mapping f between data x and latent variable z ($z = f(x)$, $z \sim \pi(z)$)
  - Sample: $x = f^{-1}(z)$ ($z \sim \pi(z)$)
  - Evaluate density: $p(x) = \pi(f(x))\, |\det(df/dx)|$
  - $f = f_1 \circ f_2 \circ \ldots \circ f_n$ usually parametrizes with NNs. f should be easy to invert, Jacobian determinant $|\det(df/dx)|$ should be easy to evaluate.
  - Training objective: $\langle \log p(x) \rangle$

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NFs with translational and rotational symmetry

1D function. Model with **cubic splines**

- Convolutional neural networks in Fourier space:
  - Convolution: $\int T(\mathbf{r}-\mathbf{r}')x(\mathbf{r}')d\mathbf{r}' \xrightarrow{\text{FT}} T(\mathbf{k})x(\mathbf{k}) \xrightarrow{\text{rotational symmetry}} T(k)x(\mathbf{k})$
  - Nonlinearity: any monotonic, differentiable functions Ψ

1D function. Model with **rational quadratic splines**, which is continuously differentiable and analytically invertible (Gregory & Delbourgo, 1986)

- Each layer: $\mathbf{f_i(x) = \Psi_i\,(F^{-1}\,T_i(k)\,F\,x)}$
  - Translational and rotational invariant
  - Inverse transform: $f^{-1}_i(x) = F^{-1}\,T_i^{-1}(k)\,F\,\Psi_i^{-1}(x)$
  - Jacobian determinant: $\det(df_i/dx) = d\Psi_i/dx\,\mathbf{\Pi}_k T_i(k)$
- Deep model: $f = f_1 \circ f_2 \circ \ldots \circ f_n$

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NFs with translational and rotational symmetry

- Enforcing translational and rotational symmetry
  - No data augmentation.
  - Fewer parameters: $N_{layer}*(3*N_{\Psi\_knot}+2*N_{T\_knot}) \sim$ O(1000) for d ~ 10^4
  - Faster training.
  - Less overfitting. Better generalization.

- Normalizing Flow structure:
  - Efficient sampling and density estimation.
  - logp training. Better coverage of the data.

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Conditional NFs

- Build generative models conditional on physical parameters y (cosmological parameters, baryon physics parameters, redshift, noise, calibration parameters, etc.)
    - $f(x) = f_y(x)$: $T(x) = T_y(x)$, $\boldsymbol{\Psi}(x) = \boldsymbol{\Psi}_y(x)$
    - Model the conditional dependence: $y \xrightarrow{\text{NN}}$ the knots of T_y and $\boldsymbol{\Psi}_y$
    - Training objective: log-likelihood log p(x|y) $\longrightarrow$ **posterior distribution!**

with non-gaussian information

- $$X \xrightarrow[T_1,\ \boldsymbol{\Psi}_1]{\Psi_1 (F^{-1} T_1(k) F X)} X_1 \xrightarrow[T_2,\ \boldsymbol{\Psi}_2]{\Psi_2 (F^{-1} T_2(k) F X_1)} X_2 \xrightarrow[T_3,\ \boldsymbol{\Psi}_3]{\Psi_3 (F^{-1} T_3(k) F X_2)} \ldots\ldots \xrightarrow[T_N,\ \boldsymbol{\Psi}_N]{\Psi_N (F^{-1} T_N(k) F X_{N-1})} Z$$

$$y \xrightarrow{\text{NN}} T_1, \boldsymbol{\Psi}_1 \qquad y \xrightarrow{\text{NN}} T_2, \boldsymbol{\Psi}_2 \qquad y \xrightarrow{\text{NN}} T_3, \boldsymbol{\Psi}_3 \qquad y \xrightarrow{\text{NN}} T_N, \boldsymbol{\Psi}_N$$

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Experiments

- Data: 2D dark matter overdensity field at redshift 0
  - 512 h^{-1}Mpc Box, 128 h^{-1}Mpc slice, 128 x 128 mesh.
  - Vary cosmology parameters $\Omega_m \in [0.2, 0.5]$ and $\sigma_8 \in [0.5, 1.1]$ (conditional variable y).
  - Generated by N-body solver FastPM.

- Model: convolutional rotation/translation invariant normalizing flow
  - $N_{layer} = 5$, $N_{\Psi\_knot} = 8$, $N_{T\_knot} = 128$
  - Conditional NN: MLP with 2 hidden layers of $N_{neuron} = 512$

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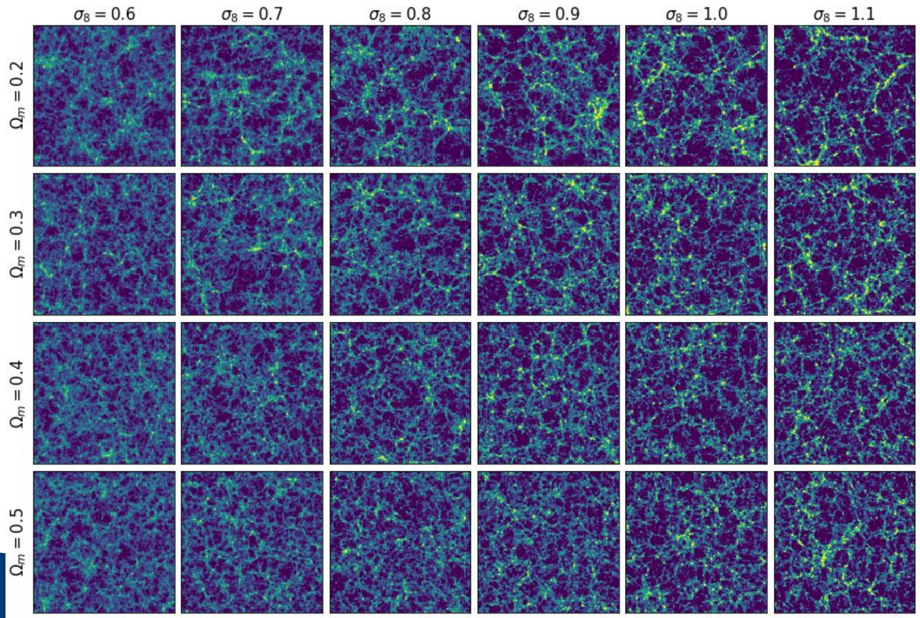
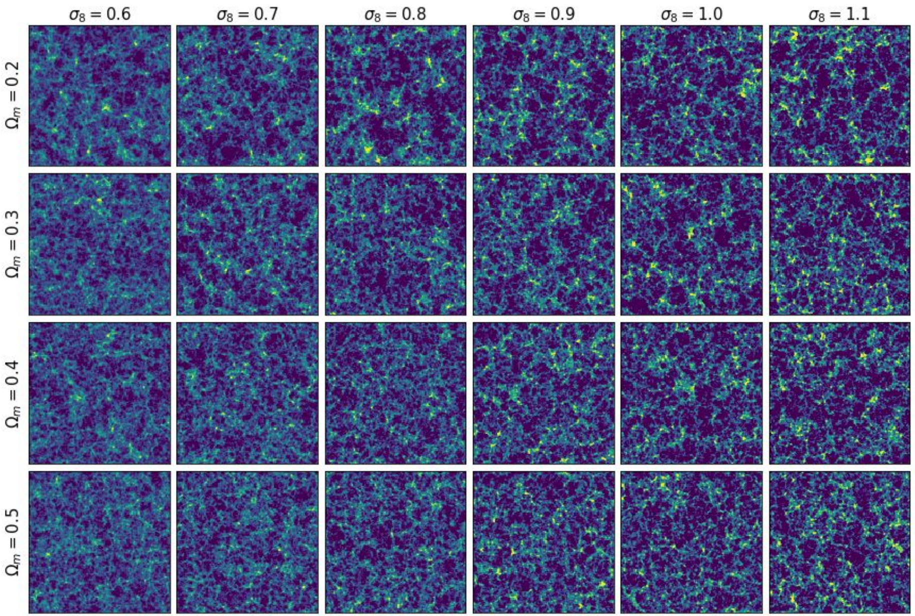
Preliminary Results -- Samples

- data:



- sample:



more clustering

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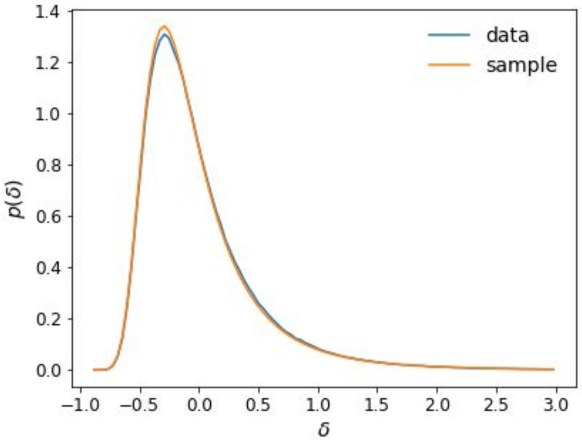
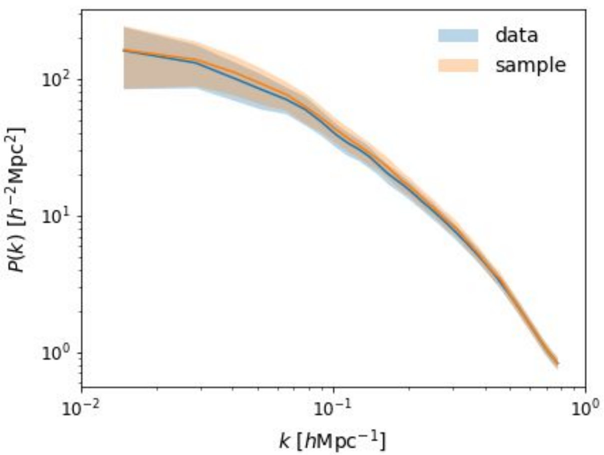
Preliminary Results -- Samples

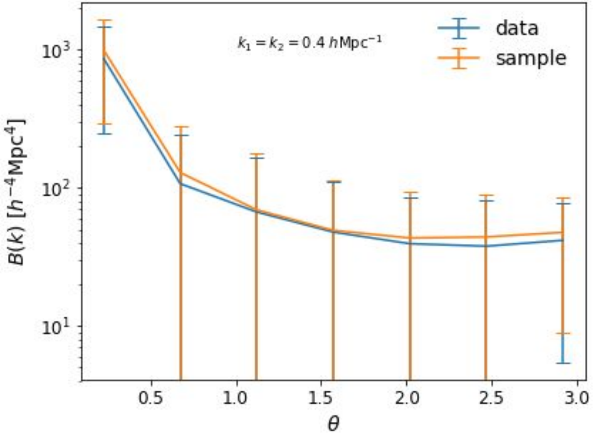
- 1-D probability distribution function



- power spectrum:



- bispectrum:



Measured over 10000 samples

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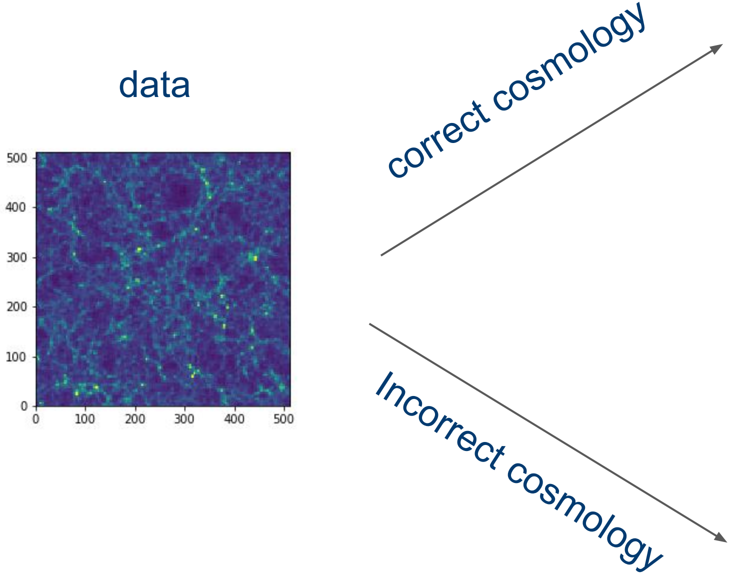
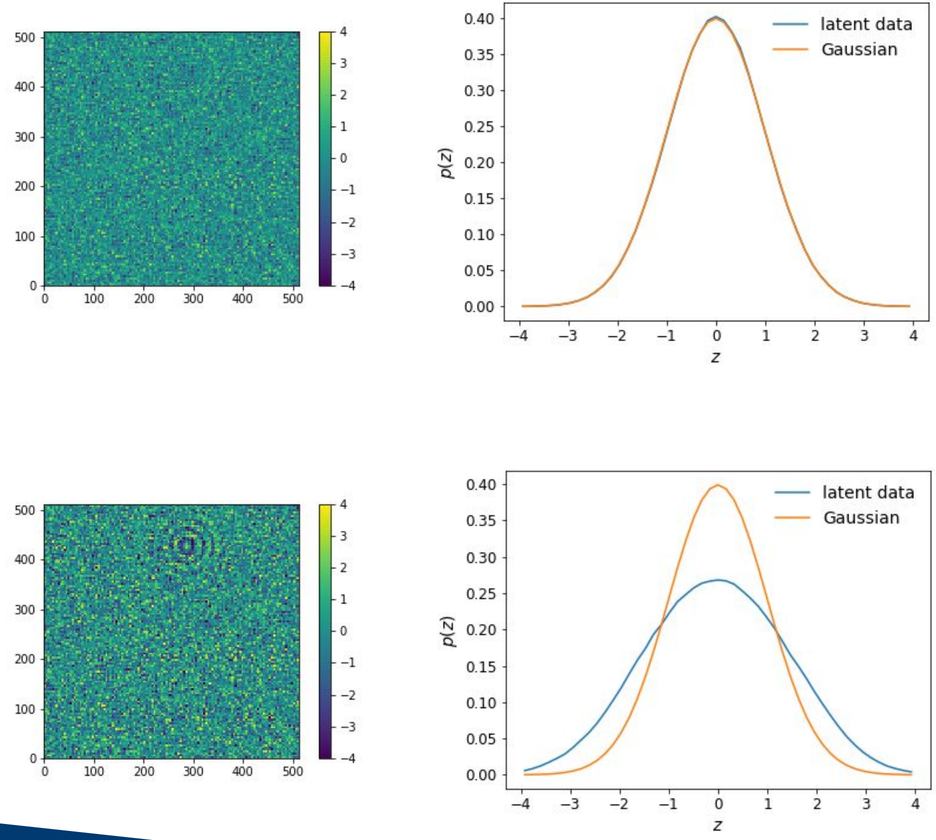
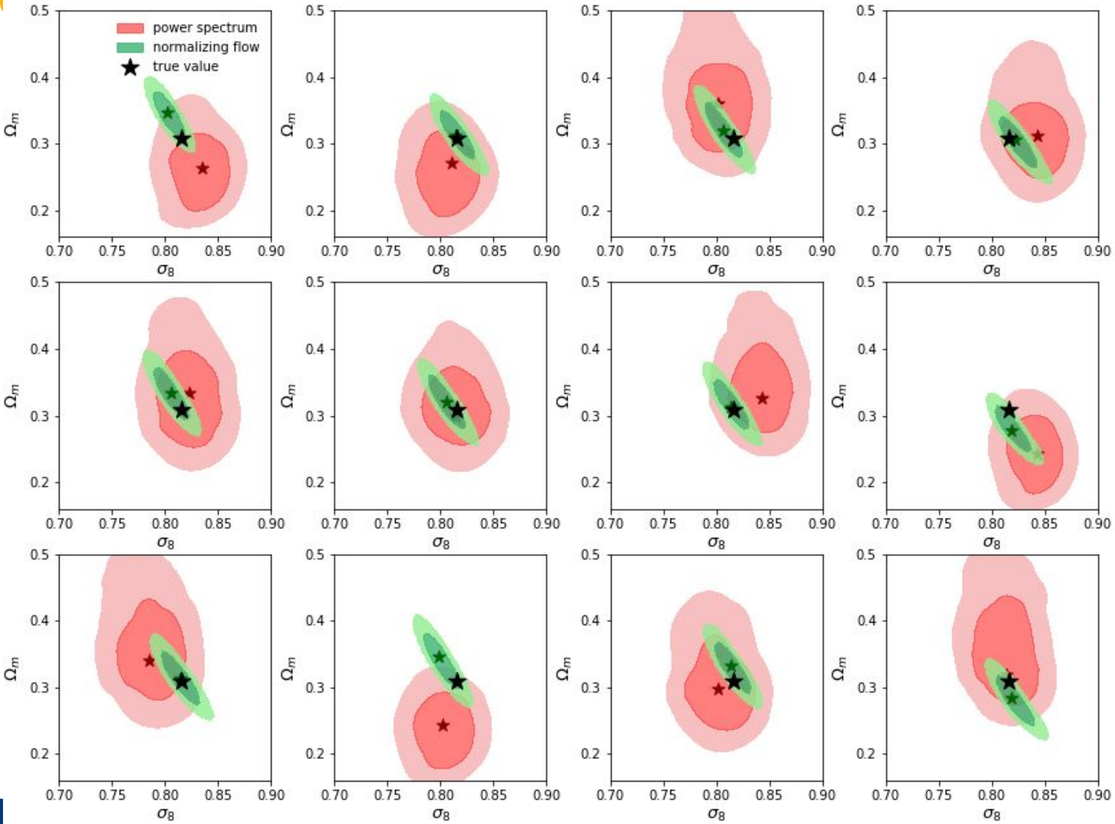
Preliminary Results -- Latent variables





Preliminary Results – Posterior analysis

- This approach learns likelihood p(x|y) directly: full posterior distribution via p(y|x)=p(x|y)p(y)/p(x)
- Aims to capture all the information of the data ⟶ **optimal posterior analysis**
- This is very different from Likelihood Free Inference or ABC, which use suboptimal summary statistics S and build their p(y|S) or p(S|y)
- Figure of merit (inverse of the area of the 68% confidence region):
  - power spectrum: ~ 176
  - normalizing flow: ~ 1065



Discussion

- Current and future works:
  - Apply the model to other (noisy) observables (weak lensing, galaxies, tSZ, etc.). Adding translational / rotational invariant noise is easy (train with noise).
  - Use this model to learn the relation / mapping between baryon and DM.
  - Explore training with $p(y|x)$.

- Challenges: the translational and rotational symmetry is broken
  - Redshift space distortion: $T(k) \longrightarrow T(k_r, k_z)$
  - Survey window function: adding non convolutional layers (e.g. add SINF)

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Conclusions

- We introduce a NF model that explicitly satisfies the **translational and rotational symmetry**. These symmetries reduce the degrees of freedom and enable the model to scale well to high dimensions.

- Compared to other generative models like GANs, this model is **bijective (no information loss), is easier and faster to train, has better coverage of the data, and allows exact density (likelihood) evaluation p(x|y)**.

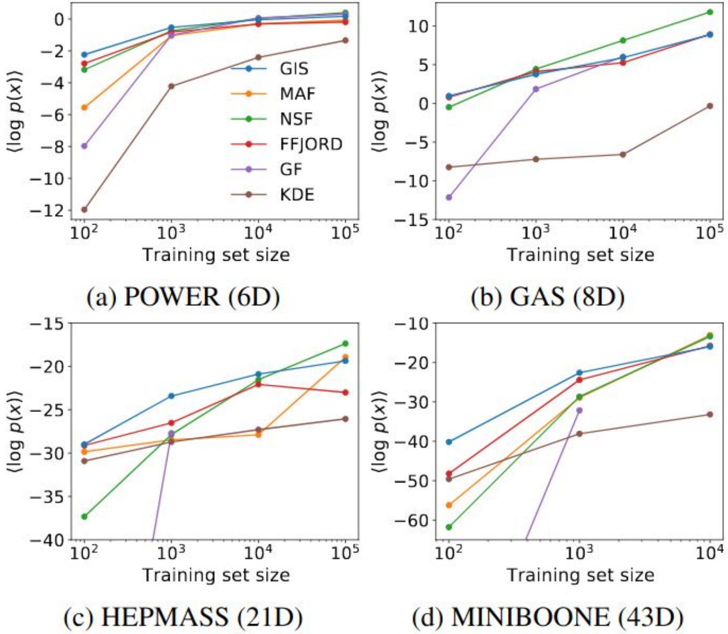
- We apply the model for generating DM density field conditional on Ω_m and σ_8. We show it is able to generate **realistic samples** that agree well with the data on various summary statistics, and the data is visually mapped to a Gaussian. We show that its likelihood gives **much tighter constraints on cosmological parameters** than standard power spectrum analysis. If NF maps to a perfect Gaussian then p(x|y) enables **optimal posterior analysis** of cosmological data.

Sliced Iterative Normalizing Flows (SINF)

- This is for data without translational/rotational invariance
- Iteratively building the NF based on optimal transport on 1D slices
- GIS trains in Gaussian space: achieves **the best density estimation results on small training sets**.
- One line code:

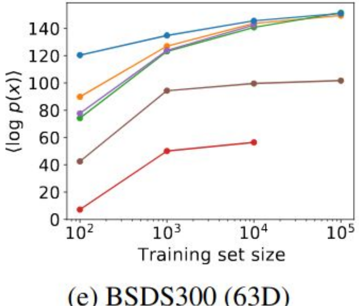
```
model = GIS(data_train, data_validate)

logp_test = model.evaluate_density(data_test)
sample, logp_sample = model.sample(nsample=100)
```



(a) POWER (6D) (b) GAS (8D)
(c) HEPMASS (21D) (d) MINIBOONE (43D)

2007.00674
https://github.com/biweidai/SIG_GIS



(e) BSDS300 (63D)

Sliced Iterative Normalizing Flows (SINF)

- (SIG) trains in data space: allows directly optimizing the distribution of samples

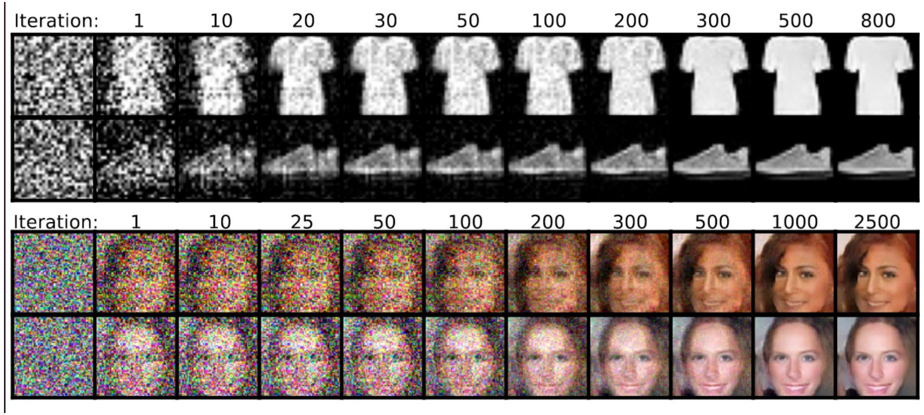


Table 2. FID scores on different datasets (lower is better). The errors are generally smaller than the differences.

	Method	MNIST	Fashion	CIFAR-10	CelebA
iterative	SWF	225.1	207.6	-	-
	SIG ($T = 1$) (this work)	**4.5**	**13.7**	66.5	37.3
adversarial training	Flow-GAN (ADV)	155.6	216.9	71.1	-
	WGAN	6.7	21.5	**55.2**	41.3
	WGAN GP	20.3	24.5	55.8	**30.0**
	Best default GAN	~ 10	~ 32	~ 70	~ 48
AE based	SWAE	29.8	74.3	141.9	53.9
	CWAE	23.6	57.1	120.0	49.7
	PAE	-	28.0	-	49.2
	two-stage VAE	12.6	29.3	96.1	44.4
	Best default VAE	16.6	43.6	-	53.3

2007.00674
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