Inflationary Flows: Calibrated Bayesian Inference with Diffusion-Based Models

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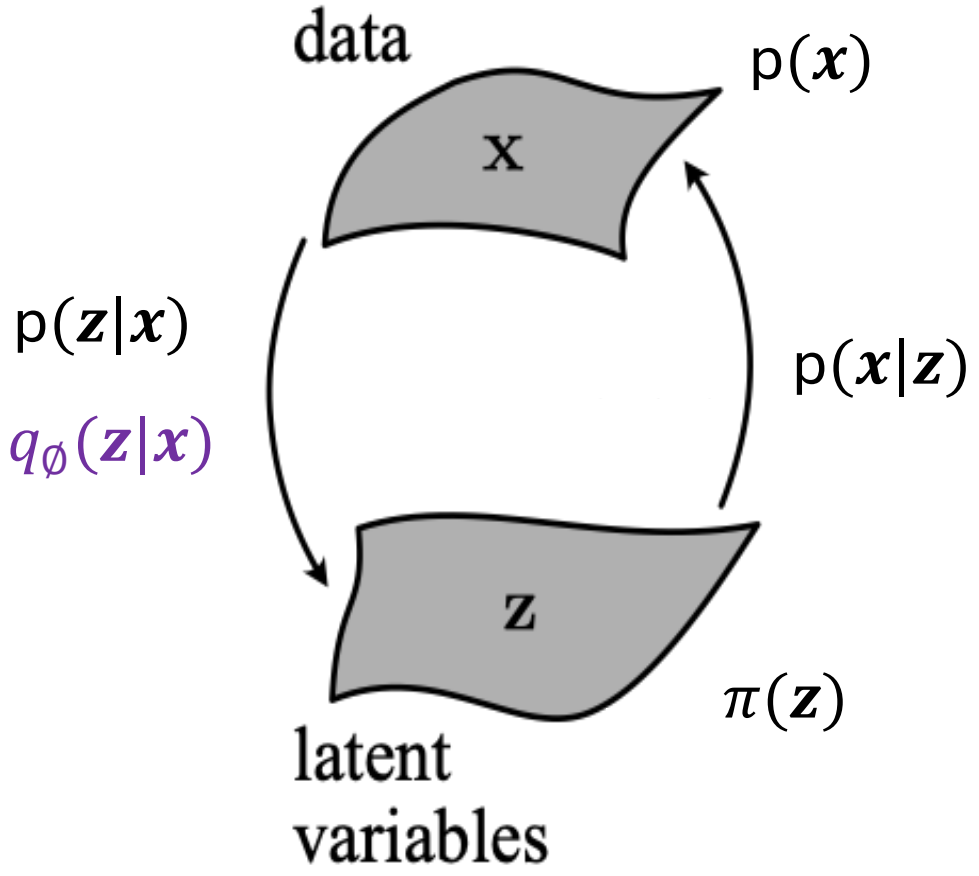
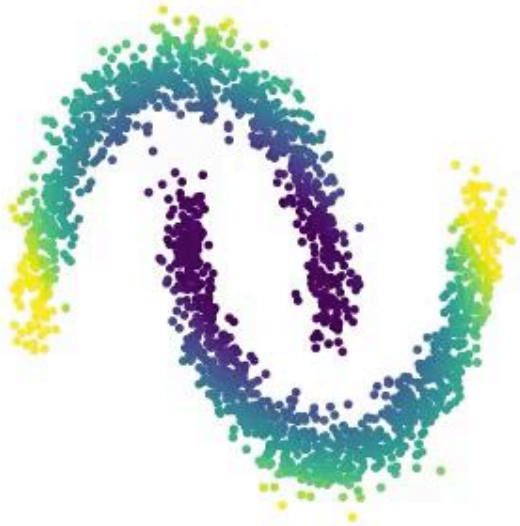
Bayesian Inference with Deep Generative Models: What's Wrong?

- Want to estimate uncertainty in deep generative model posterior inference.
- Existing methods either produce inaccurate posteriors (e.g., VAEs) or don't allow for dimensionality reduction without substantial added complexity (e.g., injective flows).
- Here, our goal is to combine the flexibility of deep generative models with principled inference.



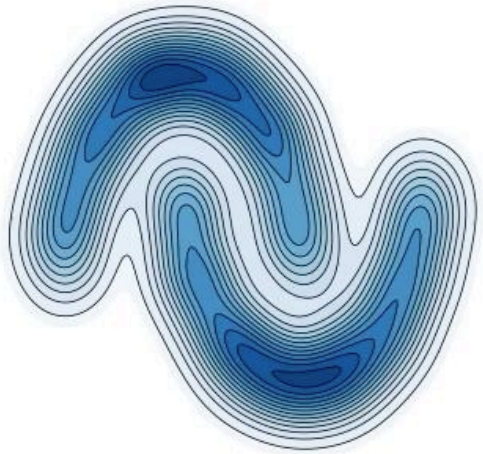
Three Views of Diffusion-Based Models

Diffusion (SDE)



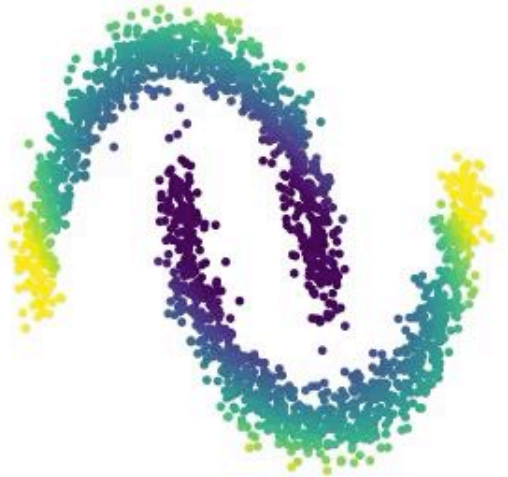
$$d\boldsymbol{x} = \boldsymbol{f}(\boldsymbol{x}, t)dt + \boldsymbol{G}(\boldsymbol{x}, t) \cdot d\boldsymbol{W}$$

Fokker-Planck Equation (FPE)



$$\partial_t\, p = -\nabla \cdot [\boldsymbol{f}p] + \frac{1}{2}\,\partial_i \partial_j \left[\left(\boldsymbol{G}\boldsymbol{G}^{\boldsymbol{T}}\right)_{\boldsymbol{ij}} p\right]$$

Probability Flow ODE (pfODE)



$$d\boldsymbol{x} = \left\{\boldsymbol{f} - \frac{1}{2}\nabla \cdot [\boldsymbol{G}\boldsymbol{G}^{\boldsymbol{T}}] - \frac{1}{2}\boldsymbol{G}\boldsymbol{G}^{\boldsymbol{T}}\nabla \log p_t(\boldsymbol{x})\right\} dt$$

Inflationary Probability Flow ODE

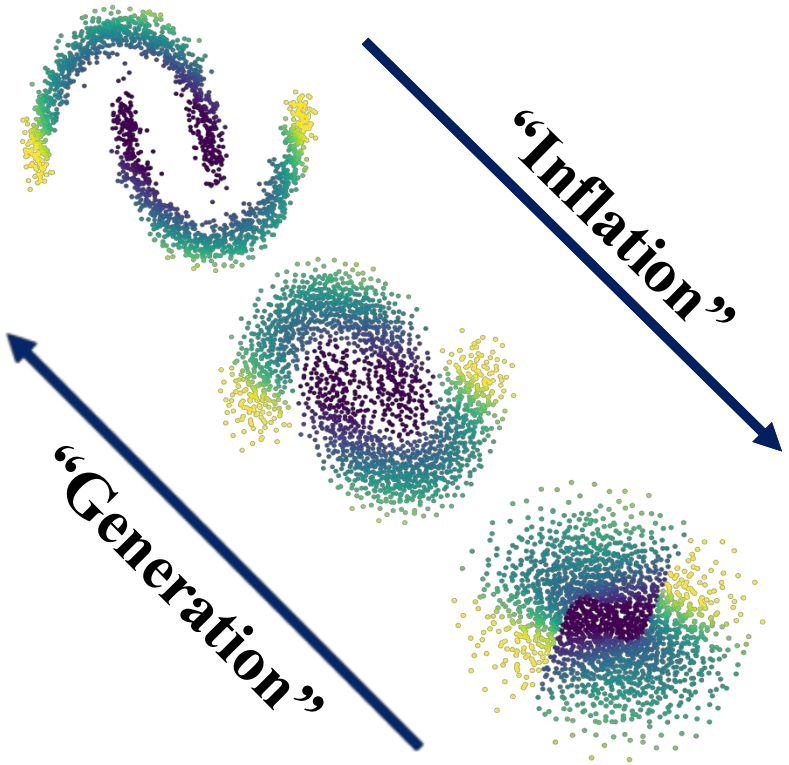
•Convolve data points with Gaussian kernels ($\boldsymbol{C}(t)$) that grow over time → "inflation".

•To keep bounds finite, adopt a coordinate rescaling $\tilde{\boldsymbol{x}} = \boldsymbol{A}(t) \cdot \boldsymbol{x}(t)$.

•This is equivalent to the original pfODE formulation (Song et al., 2021) for some specific choices of $\boldsymbol{f}$ and $\boldsymbol{G}$.

•Need only to construct $\boldsymbol{C}(t)$ and $\boldsymbol{A}(t)$ to preserve (or reduce) "intrinsic dimensionality".

Inflationary pfODE



A Measure of Intrinsic Dimensionality: Participation Ratio

•Gao et al., 2017 define the *participation ratio* (PR), in terms of the data covariance $\boldsymbol{\Sigma}$:

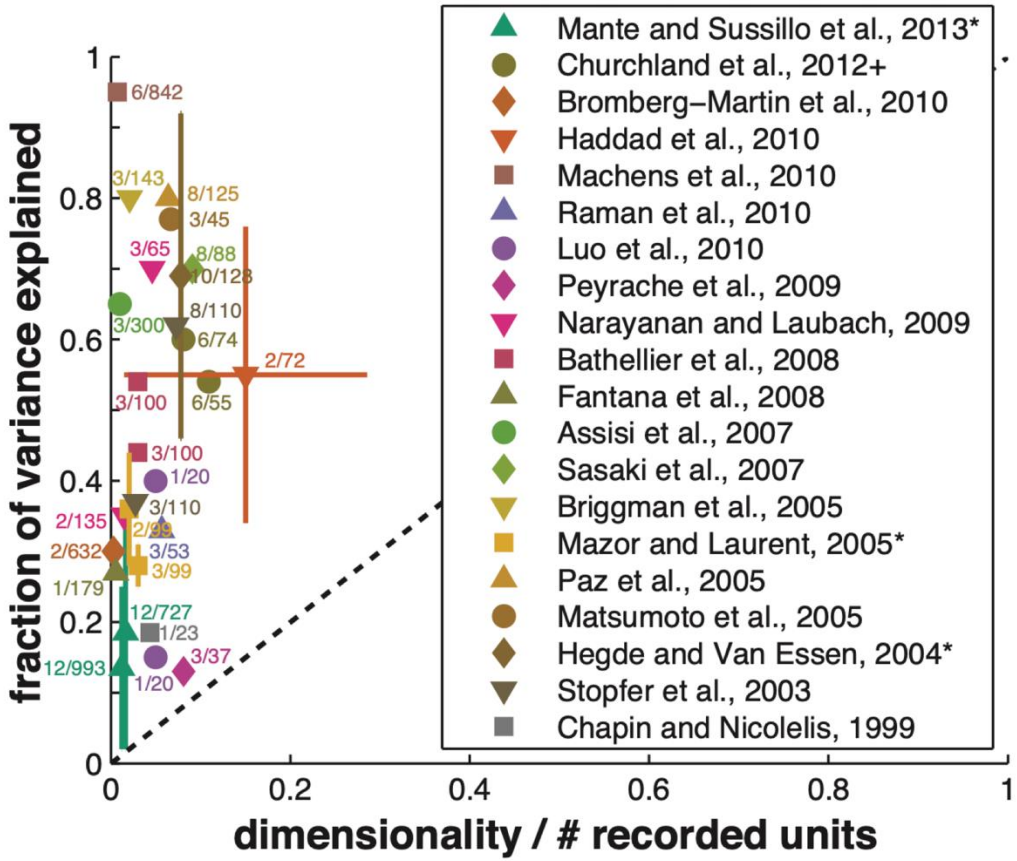
$$R(\boldsymbol{\Sigma}) = \frac{Tr(\boldsymbol{\Sigma})^2}{Tr(\boldsymbol{\Sigma}^2)}$$

•If $\boldsymbol{\Sigma}$ is rank 1, $R = 1$.

•If $\boldsymbol{\Sigma} \propto \mathbb{I}_{dxd}$, $R = d$.

•PR is invariant to linear transforms and only requires knowledge of second order statistics.

•This is the measure of dimensionality we will work with.



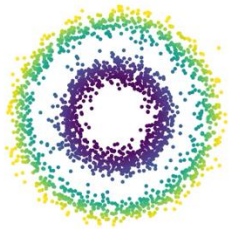
Gao et al., bioRxiv (2017)

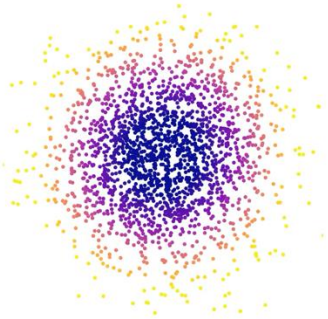
Dimension-Preserving Flows

Inflation

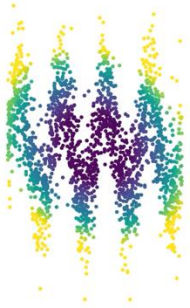
Generation

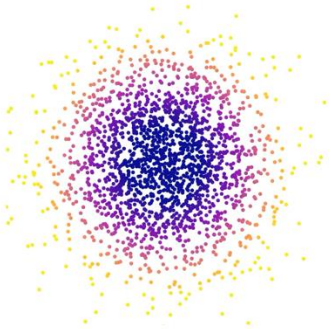
Circles



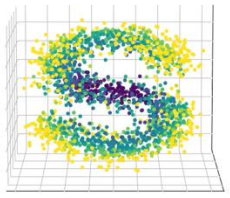


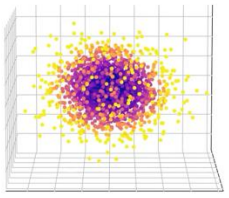
Sine





S-Curve



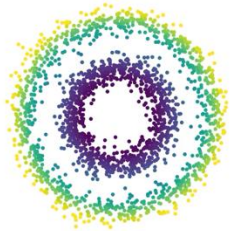


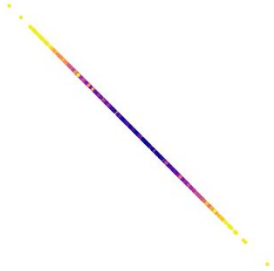
Dimension-Reducing Flows

Inflation

Generation

Circles





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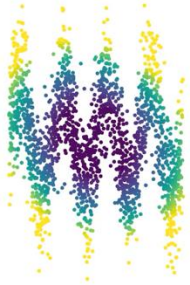
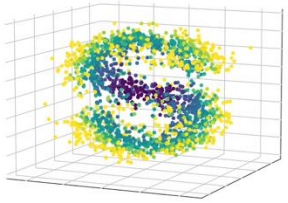
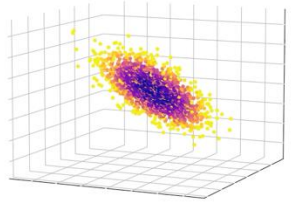


S-Curve





Thank You!

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