Bayesian Computation with Generative Diffusion Models via Multilevel Monte Carlo

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Outline

Motivation: The Promise of Diffusion Models

- **Diffusion Models:** Class of stochastic samplers that rely on neural networks to generate samples from a posterior distribution.
- **High-quality sampling**: DMs provide state-of-the-art sample quality for complex distributions.
- **Flexible conditioning**: Handle diverse inverse problems (denoising, inpainting, super-resolution) through unified framework.
- Well-defined **probability model** enables proper UQ.

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The Computational Challenge

- **Large-scale UQ**: Reliable uncertainty estimates may require 10^4-10^6 samples, especially when variability is significant.
- **Slow sampling**: Typical DM requires 10^2-10^3 neural function evaluations (NFEs) per sample.
- **Prohibitive cost**: Full UQ analysis can require 10^7-10^9 NFEs.

Motivation: Why Diffusion Models for UQ?

The need for speed

- **Practical deployment** in time-sensitive applications (medical imaging, real-time systems).
- **Large-scale uncertainty studies** (global sensitivity analysis, robust optimization).
- **Hyperparameter tuning** (prior selection, likelihood calibration).

Solutions:

- Reduce cost per NFE (pruning, quantization).
- Reduce number of NFE's per sample (distillation).
- Reduce number of NFE's per statistic computation.

Bayesian framework

- Aim of a Machine Learning algorithm: Estimate $x \in \mathbb{R}^n$, $n \gg 1$, give observed data y.

- Bayesian framework: $Y \sim \mathcal{P}(\mathcal{A}(x))$, conditional on $X = x$.

- Sampling from the conditional density of X, $p(\cdot|y) \propto \mathcal{L}(y|\cdot)\pi(\cdot)$, for likelihood $\mathcal{L}$ and prior π.

- Our goal is to quantify the uncertainty that such a probability distribution entails.

Denoising Diffusion Probabilistic Models

- **Finite sequence of noising kernels**, or a continuous-time SDE.
- Build sequence of states $\{X_i\}_{i=0}^{T}$ with $X_0 = X$.
- Sample from the joint density of $(X_0, \ldots X_T)$ given $Y = y$; joint density admits the desired conditional density as marginal.
- Write

$$p_{0:T}(x_0, \ldots, x_T|y) = \left(\prod_{t=1}^{T} \widehat{\reflectbox{λ}}_{t-1}(x_{t-1}|x_t, y) \right) p_T(x_T|y),$$

  for **reverse transition kernels**, $(\widehat{\reflectbox{$\lambda$}}_t)_{t=0}^{T-1}$, and a *pre-determined* posterior density $p_T(\cdot|y)$ of the final state X_T.
- For example, $p_T(\cdot \mid y) \in \{\phi_n(\cdot),\ \delta_y(\cdot),\ \phi_n(\cdot; (\mathbb{I}_n - \mathbb{M})y, \mathbb{M})\}$.

DDPMs: Forward transition kernels, K

Gaussian, Markovian forward process:

$$K_t(x|x_{t-1}) = \phi_n\left(x; \sqrt{\frac{\gamma_t}{\gamma_{t-1}}}x_{t-1}, \left(1 - \frac{\gamma_t}{\gamma_{t-1}}\right)\mathbb{I}_n\right),$$

for $x \in \mathbb{R}^n$ and where $1 = \gamma_0 > \gamma_1 > \ldots > \gamma_T > 0$.
Hence

$$K_{t;0}(x|x_0) = \phi_n(x; \sqrt{\gamma_t}x_0, (1-\gamma_t)\mathbb{I}_n), \quad 1 \le t \le T,$$

and we define the score function, for any $x \in \mathbb{R}^n$,

$$\nabla \log K_{t;0}(x_t|x_0) = (\sqrt{\gamma_t}x_0 - x_t)/(1-\gamma_t),$$

and we solve for x_0

$$x_0(x_t; y, t) = \frac{1}{\sqrt{\gamma_t}}(x_t + (1-\gamma_t)\nabla \log K_{t;0}(x_t|x_0))$$

DDPMs: Reverse Kernel, ⅄

By conditioning on the initial state and assuming intermediate states are independent of the observation Y,

$$\widehat{\lambda}_{t-1}(x|x_t, y) = \int_{\mathbb{R}^n} \lambda_{t-1;0,t}(x|x_0, x_t)\widehat{\lambda}_{0;t}(x_0|x_t, y)dx_0.$$

We use

$$\widehat{\lambda}_{0;t}(\cdot|x_t, y) = \delta_{\hat{x}_0}(\cdot)$$

where

$$\widehat{x}_0(x_t; y, t \quad) = \frac{1}{\sqrt{\gamma_t}}(x_t + (1-\gamma_t)\nabla \log K_{t;0}(x_t|x_0))$$

Finally,

$$\lambda_{t-1;0,t}(x|x_0, x_t) = \phi_n(\cdot, \mu_{t-1;0,t}, \sigma^2_{t-1;0,t}\mathbb{I}_n)$$

for some known mean and variance.

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We use

$$\widehat{\text{ꓘ}}_{0;t}(\cdot|x_t, y) = \delta_{\hat{x}_0}(\cdot)$$

where

$$\widehat{x}_0(x_t; y, t, \theta) = \frac{1}{\sqrt{\gamma_t}}(x_t + (1-\gamma_t) \quad s_\theta(x_t, y, t) \quad)$$

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for some known mean and variance.

DDPMs: Four Sources of Errors

$$
\begin{aligned}
x_{t-1} &= \sqrt{\frac{\gamma_{t-1}}{\gamma_t}}x_t - \sqrt{\frac{\gamma_t}{\gamma_{t-1}}}\left(\Gamma_{t-1} - \frac{\gamma_{t-1}}{\gamma_t}\Gamma_t\right) s_\theta(x_t, y, t) \\
&\quad + \sqrt{\frac{\Gamma_{t-1}}{\Gamma_t}\left(1 - \frac{\gamma_t}{\gamma_{t-1}}\right)}\xi_t, \qquad \text{where } \Gamma_t = 1 - \gamma_t
\end{aligned}
$$

- **Model error**: From imperfect score network training based on a finite training-set.
- **Finite-time error**: We have to choose $\gamma_T > 0$ (to ensure γ_{t-1}/γ_t is small), hence X_T will not be exactly Gaussian (not fully diffused).
- **Truncation error**: The posterior $p(\cdot \mid y)$ has smaller support than $p_t(\cdot \mid y)$, leading to blow up in s_θ as $t \to 0$; need to stop early or have a Gaussian approximation independent of the score.
- **Discretization error** (our focus today): We can skip M steps, sampling directly x_{t-M} given x_t.

DDPMs: Four Sources of Errors

$$x_{t-M} = \sqrt{\frac{\gamma_{t-M}}{\gamma_t}} x_t - \sqrt{\frac{\gamma_t}{\gamma_{t-M}}} \left(\Gamma_{t-M} - \frac{\gamma_{t-M}}{\gamma_t} \Gamma_t \right) s_\theta(x_t, y, t)$$
$$+ \sqrt{\frac{\Gamma_{t-M}}{\Gamma_t} \left(1 - \frac{\gamma_t}{\gamma_{t-M}} \right)} \xi_t, \qquad \text{where } \Gamma_t = 1 - \gamma_t$$

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Monte Carlo Estimation

- Goal: Estimate $\mathrm{E}[\,f(X)\,]$, where $X \sim p(\cdot)$.
- Monte Carlo estimator:

$$\mathrm{E}[\,f(X)\,] \approx \mathrm{E}[\,f(\widehat{X})\,] \approx \frac{1}{N}\sum_{i=1}^{N} \widehat{x}^{(i)},$$

- Variance $\frac{1}{N}\mathrm{Var}[\,f(\widehat{X})\,]$, Bias $|\mathrm{E}[\,f(X)\,] - \mathrm{E}[\,f(\widehat{X})\,]|$.
- For RMSE ε: Number of samples grow as $O(\varepsilon^{-2})$ to reduce variance. Cost per sample grows as ε decreases to decrease bias.

Multilevel Monte Carlo: Basic Identity

- Use a hierarchy of approximations: $\widehat{X}_0, \widehat{X}_1, \ldots, \widehat{X}_L$ with increasing cost and accuracy (each adding M intermediate steps compared to the previous approximation).
- Telescoping sum:

$$\mathrm{E}[\, f(\widehat{X}_L)\,] = \mathrm{E}[\, f(\widehat{X}_0)\,] + \sum_{\ell=1}^{L} \mathrm{E}[\, f(\widehat{X}_\ell) - f(\widehat{X}_{\ell-1})\,]$$

- Define level estimators:

$$Y_\ell = \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} \left(f(\widehat{x}_\ell^{(i)}) - f(\widehat{x}_{\ell-1}^{(i)}) \right) \quad \text{with coupled samples}$$

- Total estimator:

$$Y = \sum_{\ell=0}^{L} Y_\ell \quad \text{with } \; Y_0 = \frac{1}{N_0} \sum_{i=1}^{N_0} f(x_0^{(i)})$$

MLMC Efficiency and Complexity

- $$\begin{aligned} \text{Bias:} \quad & \left|\mathrm{E}[\, f(\widehat{X}_\ell) - f(\widehat{X}_{\ell-1})\,]\right| \sim && M^{-\alpha\ell} \\ \text{Variance:} \quad & \mathrm{Var}[\, f(\widehat{X}_\ell) - f(\widehat{X}_{\ell-1})\,] =: V_\ell \sim && M^{-\beta\ell} \\ \text{Sampling cost:} \quad & C_\ell \sim && M^{\ell} \end{aligned}$$
- Optimal total cost: Choosing N_ℓ to minimize cost, yields

$$\begin{aligned} C_{\mathrm{MLMC}} &\lesssim \quad \varepsilon^{-2} \left(\sum_{\ell=0}^{L} \sqrt{V_\ell C_\ell} \right)^2 \\ &\lesssim \begin{cases} \varepsilon^{-2} V_0 C_0 & V_\ell C_\ell \to 0 \\ \varepsilon^{-2} L^2 & V_\ell C_\ell \approx \mathrm{const} \\ \varepsilon^{-2} V_L C_L & V_\ell C_\ell \to \infty \end{cases} \end{aligned}$$

- Compare with standard MC at finest level:

$$C_{\mathrm{MC}} \lesssim \quad \varepsilon^{-2} V_0 C_L \quad \Rightarrow \text{MLMC much cheaper if } V_\ell C_\ell \downarrow$$

Need for Exponential Integrators

- Diffusion models discretise stiff SDEs in reverse:

$$dX_t = \left(A_t X_t - B_t^2 \nabla \log K_{t;0}(x_t|x_0)\right) dt + B_t dW_t$$

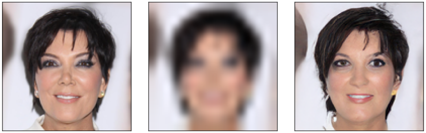
- As $t \to T$, we have $\gamma_t \to 0$, hence A_t becomes unbounded, leading to instability.
- Exponential integrators mitigate instability due to the linear terms:

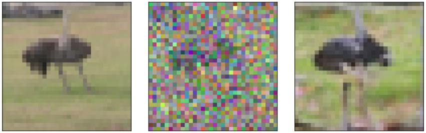
$$\begin{aligned} x^r_{t-M} = \quad & e^{-\int_t^{t-M} A_\tau d\tau} x_t \\ & - s_\theta(x_t, y, t) \int_t^{t-M} e^{\int_s^{t-M} A_\tau d\tau} B_s^2 \, \mathrm{d}s \\ & + \int_t^{t-M} e^{\int_s^{t-M} A_\tau d\tau} B_s \, \mathrm{d}W_s \end{aligned}$$

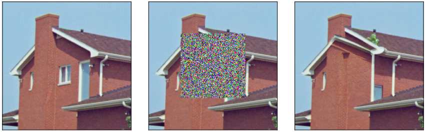
- Crucially, correlating the fine and coarse paths needs to take into account previous variance coefficient.

Three Imaging Inverse Problems

left to right: truth x; observation y; posterior sample from a DM.







1. Super-resolution: $y = Ax$, A downsampling, ill-posed
2. Denoising: $y = x + \eta$, high noise
3. Inpainting: $y = Mx$, partial masking

Use $f(x) = x^2$ to estimate marginal second moment (modelling pixel-wise uncertainty).

Convergence Rates

- Empirically fit α and β:

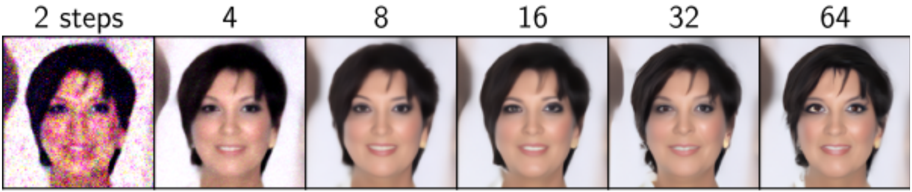
$$\left| \mathrm{E}[\, f(X) - f(\widehat{X}_\ell)\,] \right| \sim M^{-\alpha\ell}$$

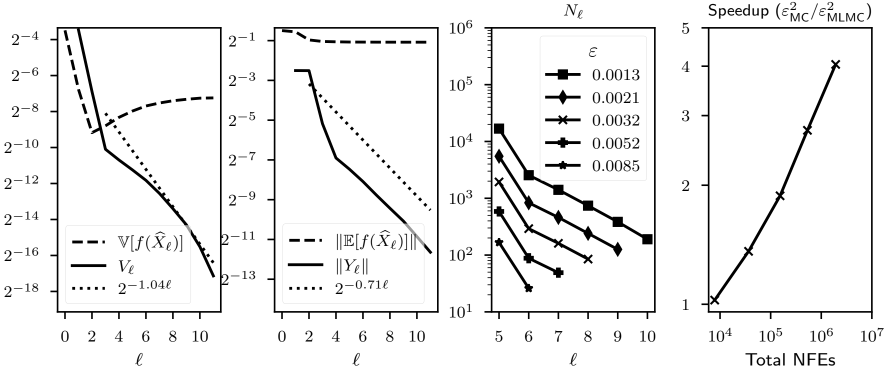
and

$$\mathrm{Var}[\, f(\widehat{X}_\ell) - f(\widehat{X}_{\ell-1})\,] \sim M^{-\beta\ell}$$

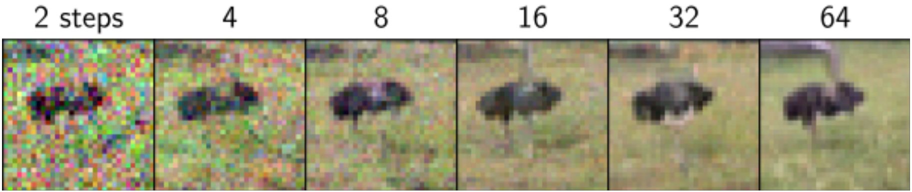
- Expected: $\alpha = 1$ and $\beta = 2$; corresponding to rates from Milstein scheme.

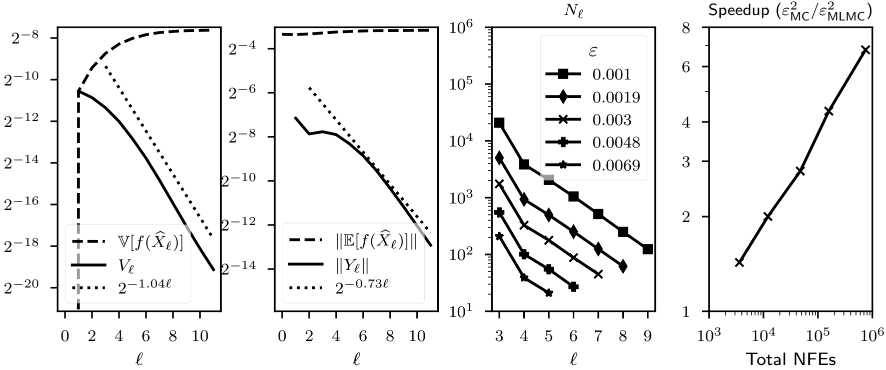
Results: Super-resolution



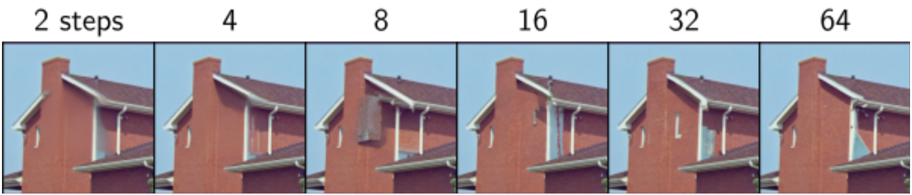


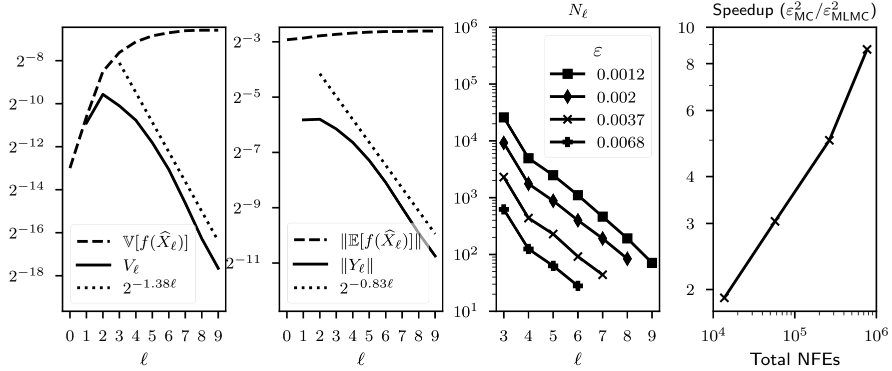
Results: Denoising





Results: Inpainting





Concluding Remarks

A.-L. Haji-Ali, M. Pereyra, L. Shaw, and K. Zygalakis. "Bayesian computation with generative diffusion models by Multilevel Monte Carlo". In: *Philosophical Transactions A* (2024). accepted. DOI: 10.48550/arxiv.2409.15511. arXiv: 2409.15511 [stat.CO]

- MLMC is a powerful variance reduction tool – for diffusion-based Bayesian inference, MLMC reduces NFEs by 4–9 times for fixed accuracy.
- Requires careful time discretisation and coupling.
- Need better analysis of the approximation of the score function to understand degradation of convergence rates.
- Future work
  - Combine with distillation and quantisation.
  - Multilevel training of DMs.
  - Tackle cost associated to other approximations parameters (model, finite-time and truncation errors).