An alternative view of denoising diffusion models

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Problem set-up
Sampling with iterative algorithms

- **Sampling from probability distribution** $p(x) \propto \exp(-f(x))$
  - high-dimensional and "complex"
  - f given or f estimated from i.i.d. data

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  - Discretization of diffusion $dX_t = -\nabla f(X_t)dt + \sqrt{2}dB_t$:

$$x_{k+1} = -\gamma \nabla f(x_k) + \sqrt{2\gamma} \cdot \mathcal{N}(0, I)$$

  - (slow) convergence (see, e.g., Bakry et al., 2008)
  - fast for smooth log-concave distributions
    (Dalalyan, 2017, Durmus and Moulines, 2017, Chewi, 2022, etc.)

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- **Going beyond log-concave distributions**

A short introduction to denoising diffusion models (Song and Ermon, 2019, Song et al., 2019)

[following expositions from Bortoli (2023) and Peyré (2023)]

- **Forward flow**
  - Ornstein-Uhlenbeck process $dX_t = -X_t dt + \sqrt{2} dB_t$
  - started from $p(x) \propto \exp(-f(x))$ at time $t = 0$
  - marginal distribution: $X_t = e^{-t} X_0 + \sqrt{1 - e^{-2t}} \cdot \mathcal{N}(0, I)$

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- **Backward flow**
  - For T large, $X_T \approx \mathcal{N}(0, I) \quad \Rightarrow \quad$ backward simulations
  - $Y_t = X_{T-t}$ follows $dY_t = [Y_t + 2\nabla \log r_{T-t}(Y_t)]dt + \sqrt{2} dB_t$
    with r_t the density of X_t
  - Simulate the backward SDE using "only" the densities of X_t

$$y_{k+1} = y_k + \gamma y_k + 2\gamma \nabla r_{T-\gamma k}(y_k) + \sqrt{2\gamma} \cdot \mathcal{N}(0, I)$$

Denoising score matching

- **Score functions after adding noise** $\nabla \log q_t(x) = \frac{\nabla q_t}{q_t}(x)$
  - with q_t density of $X_t = e^{-t} X_0 + \sqrt{1 - e^{-2t}} \cdot \mathcal{N}(0, I)$
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- **Empirical Bayes** (Robbins, 1956, Miyasawa, 1961)
  - Notation: q_σ density of $Y = X + \sigma \cdot \mathcal{N}(0, I)$
  - Key result: $\mathbb{E}\big[X|Y\big] = Y + \sigma^2 \nabla \log q_\sigma(Y)$
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- **Denoising score matching** (Hyvärinen, 2005, Vincent, 2011)
  - Estimate the density of the noisy variable y by minimizing

$$\frac{1}{n} \sum_{i=1}^{n} \big\| x_i - y_i - \sigma^2 \nabla \log q_\sigma(y_i) \big\|^2$$

A short introduction to denoising diffusion models (Song and Ermon, 2019, Song et al., 2019)

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- **Learning score functions of noisy samples at various scales**
  - Denoising score matching

- **Denoising diffusion models**
  - Start from T large, $y_0 = X_T$, and discretize the backward SDE

$$y_{k+1} = y_k + \gamma y_k + 2\gamma e^{t_k} \nabla \log q_{\sigma_k}(y_k e^{t_k}) + \sqrt{2\gamma} \cdot \mathcal{N}(0, I)$$

  - with $t_k = T - \gamma k$, and $\sigma_k = e^{T - \gamma k} \sqrt{1 - e^{-2T + 2\gamma k}}$

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- **Alternative view** (Saremi, Park, B., 2023)

Empirical Bayes with multiple measurements

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- **Multiple measurements:** $Y_i = X + \varepsilon_i$, $i = 1, \ldots, m$
  - Posterior mean: $\mathbb{E}\big[X|Y_1, \ldots, Y_m\big] = \bar{Y}_{1:m} + \frac{\sigma^2}{m} \nabla \log q_{\sigma/\sqrt{m}}(\bar{Y}_{1:m})$ with $\bar{Y}_{1:m} = \frac{1}{m}\sum_{i=1}^m Y_i$
  - Increased concentration around the mean (S., P. and B., 2023)

$$W_2\big(\text{ law of } X, \text{ law of } \mathbb{E}[X|Y_1, \ldots, Y_m]\big)^2 \leqslant \frac{\sigma^2 d}{m}$$

  - Improved results with "strong" priors

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- **Idea #1** (Saremi and Srivastava, 2022)
  - Sampling X by sampling $Y_1, \dots, Y_m$ and then Empirical Bayes

Multimeasurement generative models (Saremi and Srivastava, 2022)

x $\quad$ y_1 $\quad$ y_2 $\quad$ y_3 $\quad$ y_4 $\quad$ $\bar{y}_{1:m}$

$\mathbb{E}[x|y_1, \ldots, y_m]$

- **Still hard to sample from** $(y_1, \ldots, y_m)$

Idea #2: Sequential denoising (S., P. and B., 2023)

- **Multiple measurements:** $Y_i = X + \varepsilon_i$, $i = 1, \ldots, m$

- **Algorithm**
  - Sample y_1 from Y_1
  - Iteratively sample y_i from $Y_i | y_1, \ldots, y_{i-1}$, for $i = 1, \ldots, m$

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- **Sampling steps using Langevin algorithms**
  - Overall non-Markovian
  - Each sampling step Markovian

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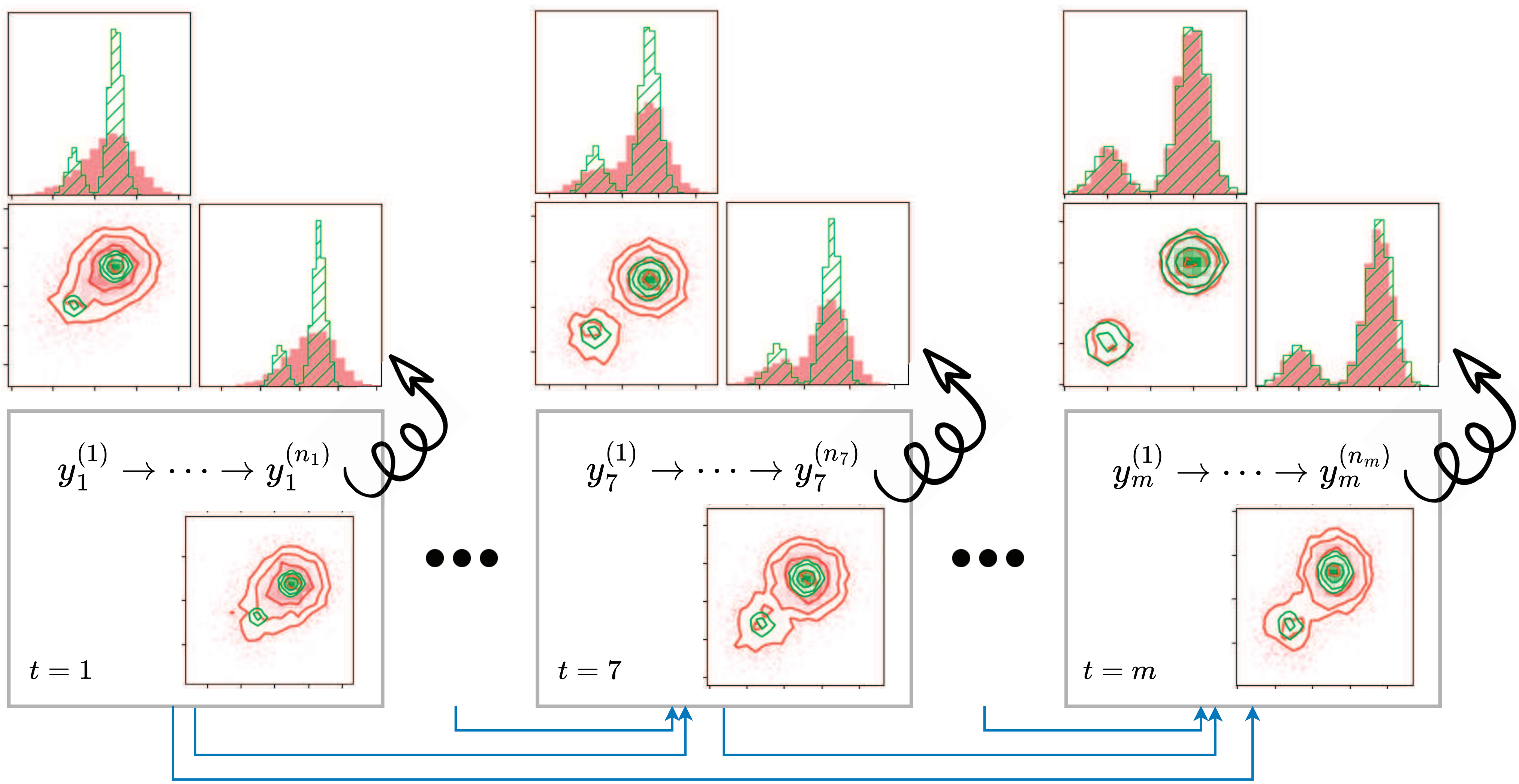

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  - Feasibility:

$$\nabla_{y_m} \log p(y_m | y_1, \ldots, y_{m-1}) = \frac{1}{\sigma^2}\Big[\bar{y}_{1:m} - y_m + \frac{\sigma^2}{m} \nabla \log q_{\sigma/\sqrt{m}}(\bar{y}_{1:m})\Big]$$

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- **Main benefit**
  - If σ large enough, only log-concave distributions to sample from
  - If m large enough, $\frac{\sigma}{\sqrt{m}}$ is small enough to obtain clean samples

More and more log-concave

- **Single measurement:** $Y = X + \sigma \cdot \mathcal{N}(0, I)$
  - Enough Gaussian blurring leads to unimodality (Loog et al., 2001)
  - Enough Gaussian blurring leads to log-concavity
  - "Proof" (see paper for quantitative statements)

$$\nabla^2 \log q(y) = -\frac{1}{\sigma^2}\Big[I - \frac{1}{\sigma^2}\mathrm{cov}(X|Y = y)\Big]$$

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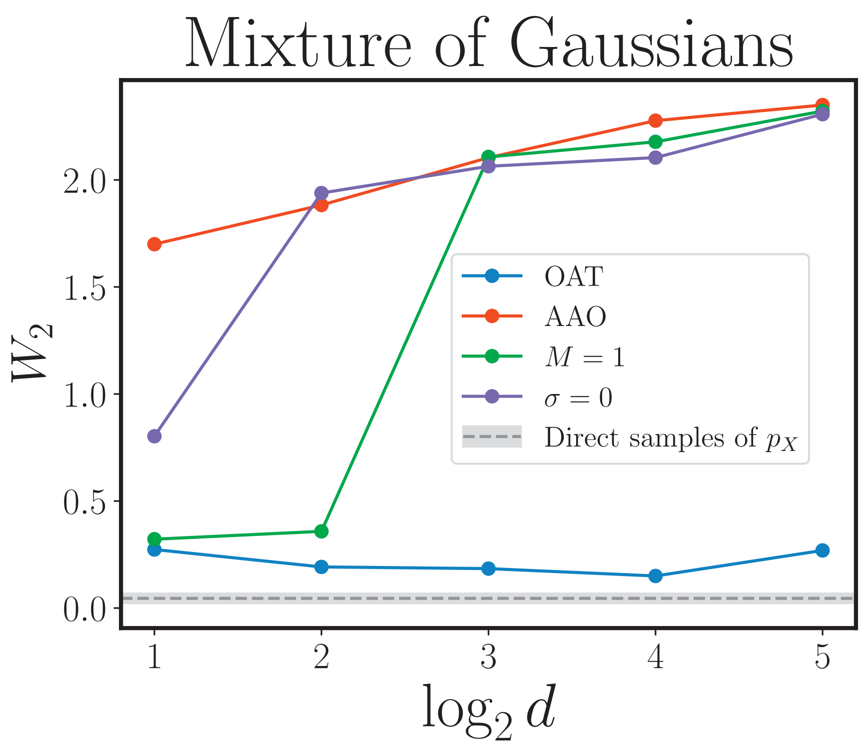
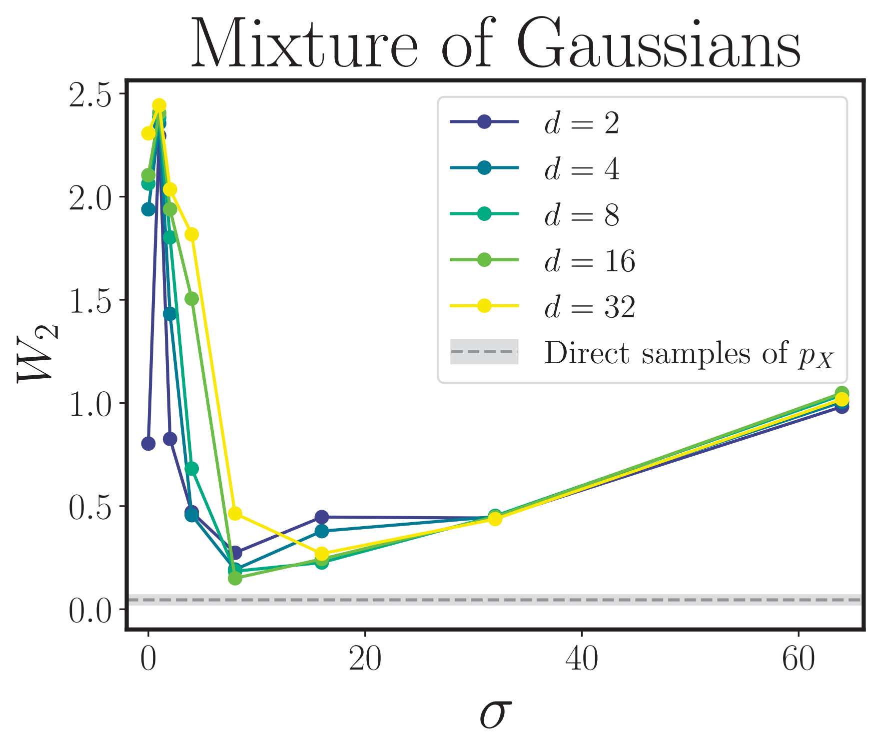
  - Conditioning reduces uncertainty (on average)
  - See precise statements in paper

Synthetic experiments

- **Mixtures of two Gaussians**
  - covariance matrices $\sigma^2 I$, $\Delta\mu = 6 \cdot (1, \dots, 1) \in \mathbb{R}^d$





Discussion

- **Sampling from score functions of smoothed densities**
  - Similar steps to denoising diffusion models
  - Clear initialization: σ large enough to obtain log-concavity
  - m large enough to obtain good quality samples
  - Only two hyperparameters: noise level σ and number of measurements m

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- **Extensions**
  - Application to image generation
  - Theoretical analysis (see Conforti et al., 2023)
- **Preprint**
  - Saeed Saremi, Ji Won Park, Francis Bach. Chain of Log-Concave Markov Chains. arXiv:2305.19473, 2023.

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