MCG

Title	Improving Diffusion Models for Inverse Problems using Manifold Constraints
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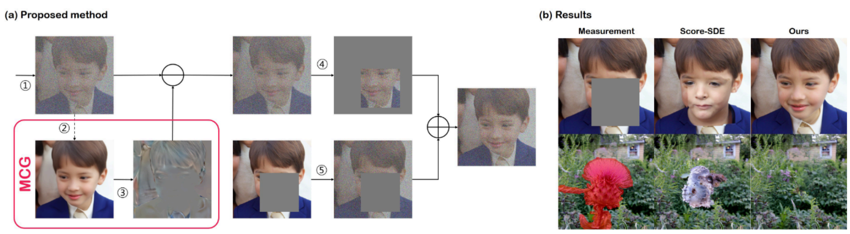
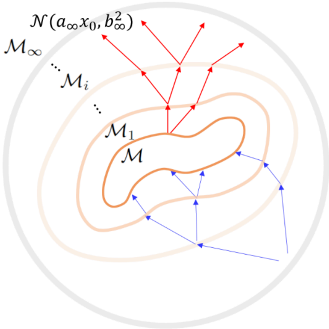
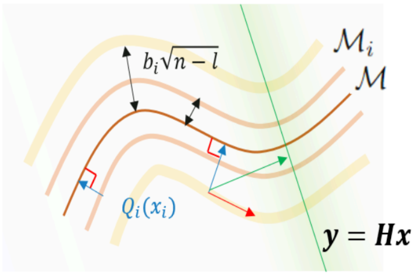


Figure 1: Visual schematic of the MCG correction step. (a) ① Unconditional reverse diffusion generates $\boldsymbol{x}_i$; ② Q_i maps the noisy $\boldsymbol{x}_i$ to generate $\hat{\boldsymbol{x}}_0$; ③ Manifold Constrained Gradient (MCG) $\frac{\partial}{\partial \boldsymbol{x}_i}\|\boldsymbol{W}(\boldsymbol{y}-\boldsymbol{H}\hat{\boldsymbol{x}}_0)\|_2^2$ is applied to fix the iteration on manifold; ④ Takes the orthogonal complement; ⑤ Samples from $p(\boldsymbol{y}_i|\boldsymbol{y})$, then combines $\boldsymbol{A}\boldsymbol{x}'_{i-1}$ and $\boldsymbol{y}_i$. (b) Representative results of inpainting, compared with score-SDE [41]. Reconstructions with score-SDE produce incoherent results, while our method produces high fidelity solutions.



(a) Geometry of diffusion model



(b) MCG correction

Figure 2: In both (a) and (b), the central manifolds represent the data manifold $\mathcal{M}$, encircled by manifolds of noisy data $\mathcal{M}_i$. The concentration on the manifold of noisy data and the distance from the clean data manifold are prescribed by Proposition 1. In (a), the backward (resp. forward) step depicted by blue (resp. red) arrows can be considered as transitions from $\mathcal{M}_i$ to $\mathcal{M}_{i-1}$ (resp. $\mathcal{M}_{i-1}$ to $\mathcal{M}_i$). In (b), arrows refer to the directions of conventional projection onto convex sets (POCS) step (green arrow) and MCG step (red arrow) which can be predicted by Theorem 1.

BACKGROUND

Discrete Form of Diffusion

- Forward Process

$$x_i = a_i x_0 + b_i z, z \sim \mathcal{N}(0, \mathbf{I})$$

- Inverse Process

$$x_{i-1} = f(x_i, s_{\theta^*}) + g(x_i)z, z \sim \mathcal{N}(0, \mathbf{I})$$

Conditional Generative models for Inverse problems

目标：从measurement y中采样x，也就是从$p(x|y)$中采样

$$y = Hx + \epsilon$$

方法之一就是先利用Unconditional Score更新一步，再用Projection-based Measurement Constraint来Impose the Conditions

$$\begin{aligned} x'_{i-1} &= f(x_i, s_\theta) + g(x_i)z, z \sim \mathcal{N}(0, \mathbf{I}) \\ x_{i-1} &= Ax'_{i-1} + b_i \end{aligned}$$

A, b_i取决于H, ϵ, x_0

Tweedie's formula for denoising

- Tweedie’s formula
  设
  $\tilde{x} \sim \mathcal{N}(x, \mathbf{I})$，则有后验期望

$$\mathbb{E}[x|\tilde{x}] = \tilde{x} + \sigma^2 \nabla_{\tilde{x}} \log p(\tilde{x})$$

于是，对前向过程$x_i \sim \mathcal{N}(a_i x_0, b_i^2 \mathbf{I})$，有

$$\mathbb{E}[x_0|x_i] = [x_i + b_i^2 \nabla_{x_i} \log p(x_i)]/a_i$$

Conditional Diffusion using Manifold Constraints

由于

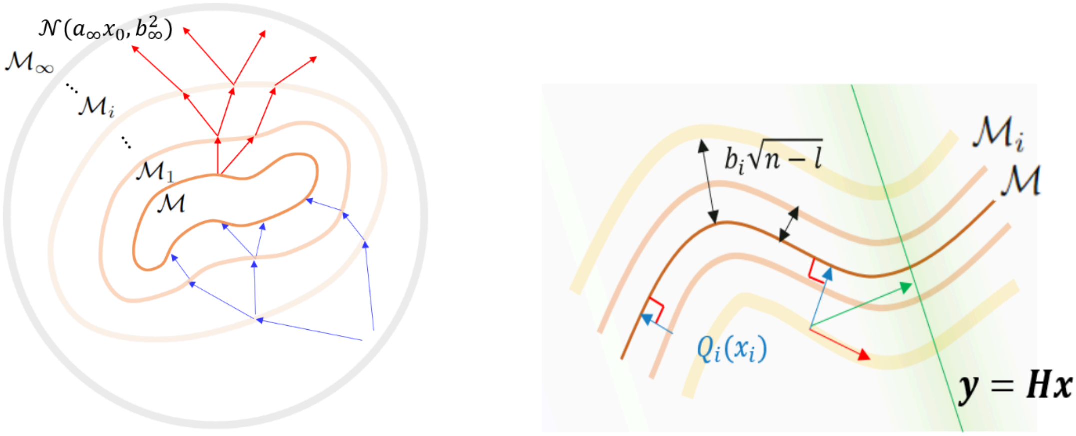
$$\nabla_x \log p(x|y) = \nabla_x \log p(x) + \nabla_x \log p(y|x)$$

于是，将采样过程修改为

$$\begin{aligned}
&x'_{i-1} = f(x_i, s_\theta) - \alpha \frac{\partial}{\partial x_i} \|W(y - H\hat{x}_0(x_i))\|_2^2 + g(x_i)z, \quad z \sim \mathcal{N}(0, \mathbf{I}), \\
&x_{i-1} = Ax'_{i-1} + b.
\end{aligned}$$

其中$\alpha \frac{\partial}{\partial x_i} \|W(y - H\hat{x}_0(x_i))\|_2^2$可以理解为对后验对数梯度$\nabla_x \log p(y|x)$的估计，$\alpha, W$取决于噪声的协方差矩阵

后面的定理证明，$\alpha \frac{\partial}{\partial x_i} \|W(y - H\hat{x}_0(x_i))\|$_2^2为数据流形$\mathcal{M}_i$上的切矢量，其在一定程度上修正了由Projection-based Measurement Constraint带来的偏离流形的问题



(a) Geometry of diffusion model (b) MCG correction

Figure 2: In both (a) and (b), the central manifolds represent the data manifold $\mathcal{M}$, encircled by manifolds of noisy data $\mathcal{M}_i$. The concentration on the manifold of noisy data and the distance from the clean data manifold are prescribed by Proposition 1. In (a), the backward (resp. forward) step depicted by blue (resp. red) arrows can be considered as transitions from $\mathcal{M}_i$ to $\mathcal{M}_{i-1}$ (resp. $\mathcal{M}_{i-1}$ to $\mathcal{M}_i$). In (b), arrows refer to the directions of conventional projection onto convex sets (POCS) step (green arrow) and MCG step (red arrow) which can be predicted by Theorem 1.

Geometry of Diffusion Models and Manifold Constrained Gradient

假设原始数据流形$\mathcal{M}$局部线性

Assumption 1 (Strong manifold assumption: linear structure)**.** *Suppose $\mathcal{M} \subset \mathbb{R}^n$ is the set of all data points, here we call the data manifold. Then, the manifold coincides with the tangent space with dimension $l \ll n$.*

$$\mathcal{M} \cap B_R(\boldsymbol{x}_0) = T_{\boldsymbol{x}_0}\mathcal{M} \cap B_R(x_0) \text{ and } T_{\boldsymbol{x}_0}\mathcal{M} \cong \mathbb{R}^l.$$

Moreover, the data distribution p_0 is the uniform distribution on the data manifold $\mathcal{M}$.

Proposition 1 (Concentration of noisy data)**.** *Consider the distribution of noisy data $p_i(\boldsymbol{x}_i) = \int p(\boldsymbol{x}_i|\boldsymbol{x})p_0(\boldsymbol{x})d\boldsymbol{x}, p(\boldsymbol{x}_i|\boldsymbol{x}) \sim \mathcal{N}(a_i\boldsymbol{x}, b_i^2\boldsymbol{I})$. Then $p_i(\boldsymbol{x}_i)$ is concentrated on $(n-1)$-dim manifold $\mathcal{M}_i := \{\boldsymbol{y} \in \mathbb{R}^n : d(\boldsymbol{y}, a_i\mathcal{M}) = r_i := b_i\sqrt{n-l}\}$. Rigorously, $p_i(B_{\epsilon r_i}(\mathcal{M}_i)) > 1-\delta$, for some small $\epsilon, \delta > 0$.*

Proposition 2 (score function)**.** *Suppose s_θ is the minimizer of the denoising score matching loss in* (3)*. Let Q_i be the function that maps $\boldsymbol{x}_i$ to $\hat{\boldsymbol{x}}_0$ for each i,*

$$Q_i : \mathbb{R}^d \to \mathbb{R}^d, \boldsymbol{x}_i \mapsto \hat{\boldsymbol{x}}_0 := \frac{1}{a_i}(\boldsymbol{x}_i + b_i^2 s_\theta(\boldsymbol{x}_i, i)).$$

Then, $Q_i(\boldsymbol{x}_i) \in \mathcal{M}$ and $\boldsymbol{J}_{Q_i}^2 = \boldsymbol{J}_{Q_i} = \boldsymbol{J}_{Q_i}^T : \mathbb{R}^d \to T_{Q_i(\boldsymbol{x}_i)}\mathcal{M}$. Intuitively, Q_i is locally an orthogonal projection onto $\mathcal{M}$.

最后，有如下定理

Theorem 1 (Manifold constrained gradient)**.** *A correction by the manifold constrained gradient does not leave the data manifold. Formally,*

$$\frac{\partial}{\partial \boldsymbol{x}_i}\|\boldsymbol{W}(\boldsymbol{y} - \boldsymbol{H}\hat{\boldsymbol{x}}_0)\|_2^2 = -2\boldsymbol{J}_{Q_i}^T \boldsymbol{H}^T \boldsymbol{W}^T \boldsymbol{W}(\boldsymbol{y} - \boldsymbol{H}\hat{\boldsymbol{x}}_0) \in T_{\hat{\boldsymbol{x}}_0}\mathcal{M},$$

the gradient is the projection of the data fidelity term onto $T_{\hat{\boldsymbol{x}}_0}\mathcal{M}$,