



Fast Samplers for Inverse Problems in Iterative Refinement Models

Kushagra Pandey*, Ruihan Yang*, Stephan Mandt (Slide Made By: Kushagra Pandey, Poster Presenter: Ruihan Yang)







Background - Inverse Problems



Source: Palette: Image to Image Diffusion Models, Saharia et al.



Background - Inverse Problems





Main Idea: Given a degradation model h(.) and observations $oldsymbol{y}$ infer $oldsymbol{x}_0$

$$y = h(x_0) + n$$



Main Idea: Given a degradation model h(.) and observations ${m y}$ infer ${m x}_0$

$$egin{aligned} y &= h(x_0) + n \ & lackslash \ & lackslash \ & p(x_0|y) \propto p(y|x_0) p(x_0) \ & p(y|x_0) = \mathcal{N}(h(x_0), \sigma_y^2) \end{aligned}$$



Main Idea: Given a degradation model h(.) and observations ${m y}$ infer ${m x}_0$

$$y = h(x_0) + n$$

 $p(x_0|y) \propto p(y|x_0)p(x_0) \longrightarrow ext{ Idea: Use pretrained generative models}}$
 $p(y|x_0) = \mathcal{N}(h(x_0), \sigma_y^2)$



Main Idea: Condition the reverse diffusion process on the degradations $oldsymbol{y}$

$$rac{dx_t}{dt} = F_t x_t - rac{1}{2} G_t G_t^ op
abla_{x_t} \log p(x_t) \, ,$$



Main Idea: Condition the reverse diffusion process on the degradations $oldsymbol{y}$

$$egin{aligned} rac{dx_t}{dt} &= F_t x_t - rac{1}{2}G_t G_t^ op
abla_{x_t} \log p(x_t) \ &igcup_{x_t} \log p(x_t) \ &igcup_{x_t} \log p(x_t) \ &igcup_{x_t} \log p(x_t|y) \end{aligned}$$



Main Idea: Condition the reverse diffusion process on the degradations $oldsymbol{y}$

$$egin{aligned} rac{dx_t}{dt} &= F_t x_t - rac{1}{2} G_t G_t^ op
abla_t \nabla_{x_t} \log p(x_t) \ &lackslash \ &lac$$



Main Idea: Condition the reverse diffusion process on the degradations $oldsymbol{\mathcal{Y}}$

$$egin{aligned} rac{dx_t}{dt} &= F_t x_t - rac{1}{2}G_t G_t^ op \nabla_{x_t} \log p(x_t) \ &lackslash \ &lackslash \ &rac{dx_t}{dt} &= F_t x_t - rac{1}{2}G_t G_t^ op \nabla_{x_t} \log p(x_t|y) \ &lackslash \ &lackslash$$



$$rac{dx_t}{dt} = F_t - rac{1}{2}G_tG_t^ op \left[s_ heta(x_t,t) + w_t
abla_{x_t} \log p(y|x_t)
ight]$$

Caveat 1: Can use a pretrained score model $s_{ heta}(x_t,t)$



$$rac{dx_t}{dt} = F_t - rac{1}{2}G_tG_t^ op \left[s_ heta(x_t,t) + w_t
abla_{x_t} \log p(y|x_t)
ight]$$

Caveat 1: Can use a pretrained score model $s_{ heta}(x_t,t)$ Caveat 2: Need to approximate $abla_{x_t} \log p(y|x_t)$



$$rac{dx_t}{dt} = F_t - rac{1}{2}G_tG_t^ op \left[s_ heta(x_t,t) + w_t
abla_{x_t} \log p(y|x_t)
ight]$$

Caveat 1: Can use a pretrained score model $s_{ heta}(x_t,t)$ Caveat 2: Need to approximate $abla_{x_t} \log p(y|x_t)$

$$p(y|x_t) = \int p(y|x_0) p(x_0|x_t) dx_0$$
 $lacksquare$
Degradation Model
 $\mathcal{N}(h(x_0), \sigma_y^2)$



$$rac{dx_t}{dt} = F_t - rac{1}{2}G_tG_t^ op \left[s_ heta(x_t,t) + w_t
abla_{x_t} \log p(y|x_t)
ight]$$

Caveat 1: Can use a pretrained score model $s_{ heta}(x_t,t)$ Caveat 2: Need to approximate $abla_{x_t} \log p(y|x_t)$

p

$$egin{aligned} (y|x_t) &= \int p(y|x_0) p(x_0|x_t) dx_0 \ & egin{aligned} & egin{aligned}$$



Degradation Model (Linear):

$$y=Hx_0+\sigma_y z, \qquad p(y|x_0)=\mathcal{N}(Hx_0,\sigma_y^2 I_d)$$



Degradation Model (Linear):

Posterior Approximation(π GDM)

$$egin{aligned} y &= Hx_0 + \sigma_y z, \qquad p(y|x_0) = \mathcal{N}(Hx_0, \sigma_y^2 I_d) \ p(x_0|x_t) &pprox \mathcal{N}(ar{x}_t, r_t^2 I_d) \ ar{x}_t &= \mathbb{E}[x_0|x_t] = x_t + \sigma_t^2 s_ heta(x_t, t) \end{aligned}$$



Degradation Model (Linear):

Posterior Approximation(π GDM)

$$egin{aligned} y &= Hx_0 + \sigma_y z, \qquad p(y|x_0) = \mathcal{N}(Hx_0, \sigma_y^2 I_d) \ p(x_0|x_t) &pprox \mathcal{N}(ar{x}_t, r_t^2 I_d) \ ar{x}_t &= \mathbb{E}[x_0|x_t] = x_t + \sigma_t^2 s_ heta(x_t, t) \ p(y|x_t) &= \int p(x_0|x_t) p(y|x_0) dx_0 \ &= \mathcal{N}(Har{x}_t, r_t^2 H H^ op + \sigma_y^2 I_d) \end{aligned}$$



Degradation Model (Linear):

Posterior Approximation(ΠGDM)

Noisy Likelihood Score $abla_{x_t}\log p(y|x_t)$

$$egin{aligned} y &= Hx_0 + \sigma_y z, \qquad p(y|x_0) = \mathcal{N}(Hx_0,\sigma_y^2 I_d) \ p(x_0|x_t) &pprox \mathcal{N}(ar{x}_t,r_t^2 I_d) \ ar{x}_t &= \mathbb{E}[x_0|x_t] = x_t + \sigma_t^2 s_ heta(x_t,t) \ (y - Har{x}_t)^ op (r_t^2 H H^ op + \sigma_y^2 I_d)^{-1} H rac{\partial ar{x}_t}{\partial x_t} \ oldsymbol{\psi} \ \sigma_y &= 0 \quad ext{[Noiseless inverse problems]} \ r_t^{-2} \left[H^\dagger (y - Har{x}_t) rac{\partial ar{x}_t}{\partial x_t}
ight] \end{aligned}$$



Degradation Model (Linear):

Posterior Approximation(π GDM)

$$egin{aligned} y &= Hx_0 + \sigma_y z, \qquad p(y|x_0) = \mathcal{N}(Hx_0, \sigma_y^2 I_d) \ p(x_0|x_t) &pprox \mathcal{N}(ar{x}_t, r_t^2 I_d) \ ar{x}_t &= \mathbb{E}[x_0|x_t] = x_t + \sigma_t^2 s_ heta(x_t, t) \ r_t^{-2} \left[H^\dagger(y - Har{x}_t) rac{\partialar{x}_t}{\partial x_t}
ight] \ & ext{ [Noiseless inverse problems]} \end{aligned}$$

Noisy Likelihood Score $abla_{x_t}\log p(y|x_t)$

$$r_t^{-2}ig[H^\dagger(y-Har{x}_t)rac{\partialar{x}_t}{\partial x_t}ig] ~~$$
 [Noiseless inverse problems] $\sigma_y=0$



Degradation Model (Linear):

Posterior Approximation(ΠGDM)

$$egin{aligned} y &= Hx_0 + \sigma_y z, \qquad p(y|x_0) = \mathcal{N}(Hx_0,\sigma_y^2 I_d) \ p(x_0|x_t) &pprox \mathcal{N}(ar{x}_t,r_t^2 I_d) \ ar{x}_t &= \mathbb{E}[x_0|x_t] = x_t + \sigma_t^2 s_ heta(x_t,t) \ r_t^{-2} \Big[H^\dagger (y - Har{x}_t) rac{\partial ar{x}_t}{\partial x_t} \Big] & ext{[Noiseless inverse problems]} \ \sigma_t &= 0 \end{aligned}$$

Noisy Likelihood Score $abla_{x_t}\log p(y|x_t)$

 $H^{\dagger} = H^{\top} (HH^{\top})^{-1}$ denotes the "Pseudo-Inverse" of the degradation operator H



Degradation Model (Linear):

Noisy Likelihood Score

 $abla_{x_t}\log p(y|x_t)$

Posterior Approximation(Π GDM)

$$egin{aligned} y &= Hx_0 + \sigma_y z, \qquad p(y|x_0) = \mathcal{N}(Hx_0, \sigma_y^2 I_d) \ p(x_0|x_t) &pprox \mathcal{N}(ar{x}_t, r_t^2 I_d) \ ar{x}_t &= \mathbb{E}[x_0|x_t] = x_t + \sigma_t^2 s_ heta(x_t, t) \ r_t^{-2} \Big[H^\dagger (y - Har{x}_t) rac{\partial ar{x}_t}{\partial x_t} \Big] & ext{[Noiseless inverse problems]} \ \sigma_y &= 0 \end{aligned}$$

$$rac{dx_t}{dt} = F_t - rac{1}{2}G_tG_t^ op \left[s_ heta(x_t,t) + w_t
abla_{x_t} \log p(y|x_t)
ight]$$



Motivation

Noisy Likelihood Score $abla_{x_t}\log p(y|x_t)$





Motivation

Noisy Likelihood Score

$$\nabla_{x_t} \log p(y|x_t)$$

$$r_t^{-2} \left[H^{\dagger}(y - H\hat{x}_t) \right]_{\partial x_t}^{\partial x_t} \right]^{\top}$$

$$\frac{dx_t}{dt} = F_t - \frac{1}{2} G_t G_t^{\top} \left[s_{\theta}(x_t, t) + w_t \nabla_{x_t} \log p(y|x_t) \right]_{\theta}$$
Score Function
Evaluation
$$I = \int_{\Gamma} \int_{\Gamma} \int_{\Gamma} g_{\theta}(x_t, t) dx_t$$

Solving Inverse Problems with pretrained models is very slow!



Conditional Conjugate Integrators - Overview





Conditional Conjugate Integrators - Overview





Conditional Conjugate Integrators - Overview





Conditional Conjugate Integrators - Formulation

Original Space: $\frac{dx_t}{dt} = F_t - \frac{1}{2}G_tG_t^{ op}\left[s_{ heta}(x_t,t) + w_t
abla_{x_t} \log p(y|x_t)
ight]$ $\downarrow \hat{x}_t = A_t x_t$

Projected Space:

$$rac{d\hat{x}_t}{dt} = A_t B_t A_t^{-1} \hat{x}_t + d\Phi_t \epsilon_ heta(x_t,t) + d\Phi_y oldsymbol{y} + d\Phi_j \Big[oldsymbol{\partial}_{x_t} \epsilon_ heta(x_t,t) (H^\dagger y - P \hat{x}_0) \Big]$$

$$A_t = \exp\left[\int_0^t B_s - \left(F_s + rac{w_s r_s^{-2}}{2\mu_s^2}G_s G_s^ op P
ight)
ight]$$



Conditional Conjugate Integrators - Formulation

Original Space: $\frac{dx_t}{dt} = F_t - \frac{1}{2}G_tG_t^{\top} \left[s_{\theta}(x_t, t) + w_t \nabla_{x_t} \log p(y|x_t) \right]$ $\downarrow \hat{x}_t = A_t x_t$ Projected Space: $\frac{d\hat{x}_t}{dt} = A_t B_t A_t^{-1} \hat{x}_t + d\Phi_t \epsilon_{\theta}(x_t, t) + d\Phi_y y + d\Phi_j \left[\partial_{x_t} \epsilon_{\theta}(x_t, t) (H^{\dagger}y - P\hat{x}_0) \right]$ $A_t = \exp \left[\int_0^t B_s - \left(F_s + \frac{w_s r_s^{-2}}{2\mu_s^2} G_s G_s^{\top} P \right) \right]$

 $P = H^{\dagger}H$ denotes the Orthogonal Projector operator



Conditional Conjugate Integrators - Design Space

Choice of Diffusion (VP-SDE): $F_t = -\frac{1}{2}\beta_t I_d$ $G_t = \sqrt{\beta_t} I_d$

Score Parameterization:

$$C_{ ext{skip}}(t) = 0$$
 $s_{ heta}(x_t,t) = C_{ ext{out}}(t)\epsilon_{ heta}(x_t,t)$



Conditional Conjugate Integrators - Design Space

Choice of Diffusion (VP-SDE):
$$F_t = -\frac{1}{2}\beta_t I_d$$
 $G_t = \sqrt{\beta_t} I_d$ Score Parameterization: $C_{skip}(t) = 0$ $s_{\theta}(x_t, t) = C_{out}(t)\epsilon_{\theta}(x_t, t)$ Projection: $\hat{x}_t = A_t x_t$ Design Choice: $B_t = \lambda I_d$



Conditional Conjugate Integrators - Design Space

Choice of Diffusion (VP-SDE):
$$F_t = -\frac{1}{2}\beta_t I_d$$
 $G_t = \sqrt{\beta_t} I_d$ Score Parameterization: $C_{skip}(t) = 0$ $s_{\theta}(x_t, t) = C_{out}(t)\epsilon_{\theta}(x_t, t)$ Projection: $\hat{x}_t = A_t x_t$ Design Choice: $B_t = \lambda I_d$

$$egin{aligned} A_t &= \exp\left[\int_0^t B_s - \left(F_s + rac{w_s r_s^{-2}}{2\mu_s^2}G_sG_s^ op P
ight)
ight] \ & igstarrow \ & A_t &= \kappa_t^1(\lambda,w_t)\Big[I_d + \kappa_t^2(\lambda,w_t)P\Big] \end{aligned}$$



Conditional Conjugate Integrators - Results (4x SR)

Degraded Input







Conditional Conjugate Integrators - Results (4x SR)

| Diffusion Results | | C-ПGDM | ПGDM | DPS | DDRM | C-ПGDM | ПGDM | DPS | DDRM | С-ПGDM | ПGDM | DPS | DDRM |
|-------------------|---------------|-------------------------|--------------------------------|-------|-------|--------------------|--------------------|------|------|-------------------------|-------------------------|--------|-------|
| Super-Resolution | 5 10 20 | 0.220 0.206 0.207 | 0.306 0.252 0.222 | 0.252 | 0.318 | 2.7 1.6 1.7 | 6.3 4.8 2.5 | 5.8 | 14.1 | 37.31 34.22 34.28 | 49.06 44.30 37.36 | 38.18 | 51.64 |
| Deblurring | 5 10 20 | 0.272 0.272 0.268 | 0.349 0.294 0.259 | 0.619 | 0.336 | 3.89 3.6 3.5 | 14.1 5.3 4.2 | 59.5 | 12.3 | 44.42 43.37 43.70 | 63.94 47.80 44.20 | 139.58 | 62.53 |

4x improvement in Speed-vs-Quality Tradeoffs over vanilla Π GDM



Conditional Conjugate Integrators - Results (Noisy 4xSR)

Degraded Input









Reference



$$\sigma_y=0.05$$

Extends to Non-linear inverse problems as well

$$A_t^{\sigma_y} = A_t + \kappa_t H^\dagger (H^\dagger)^ op + \mathcal{O}(\sigma_y^4)$$



TLDR



