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Data Science in Hamburg
HELMHOLTZ Graduate School
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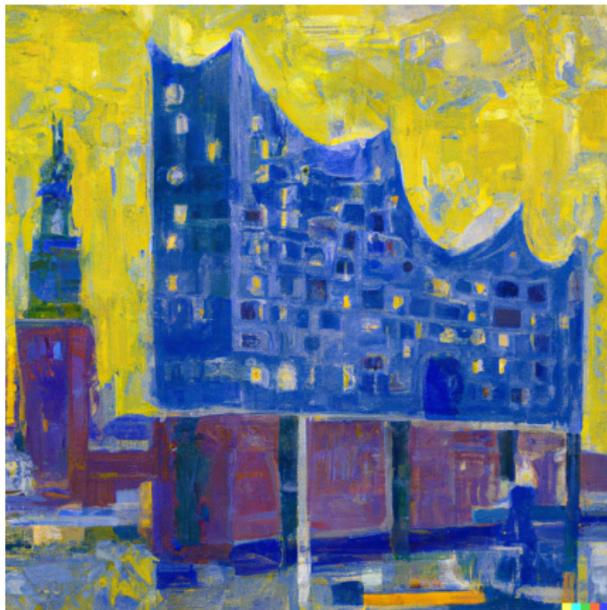
Blind Drifting: Diffusion models with a linear SDE drift term for blind image restoration tasks

The Symbiosis of Deep Learning and Differential Equations II

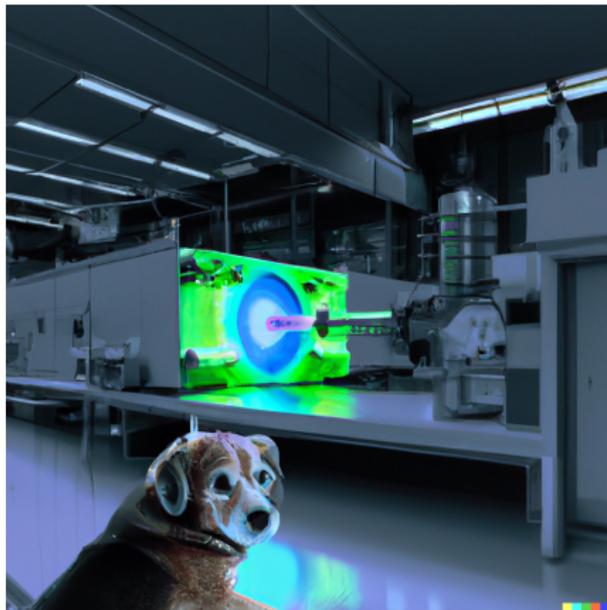
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“Elbphilharmonie, Hamburg, by
Vincent van Gogh”



“Dog who has no idea what he’s
doing at an international Free
Electron Laser research facility”

Score-based generative models (SGMs) consist of two processes:^[1,2]

- *Forward process*, gradually adds noise to the input
- *Reverse process*, generates data by gradual denoising

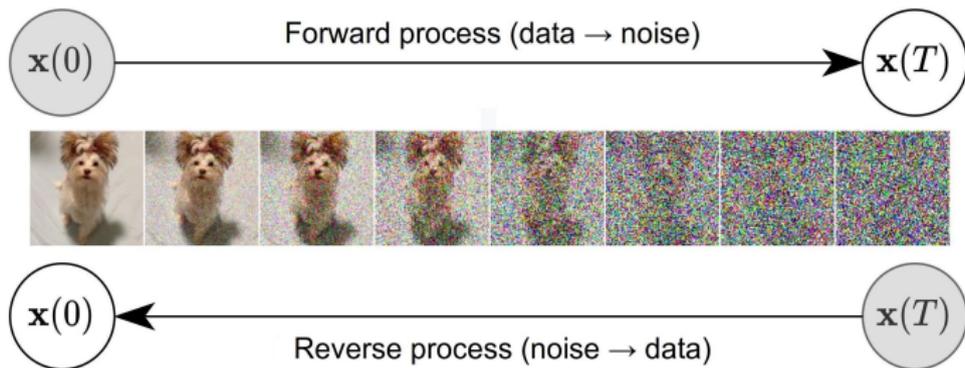


Figure: Graphic by Song et al. [2]

[1] J. Sohl-Dickstein, E. Weiss, N. Maheswaranathan, and S. Ganguli, "Deep unsupervised learning using nonequilibrium thermodynamics," in *International Conference on Machine Learning*, 2015, pp. 2256–2265.

[2] Y. Song, J. Sohl-Dickstein, D. P. Kingma, A. Kumar, S. Ermon, and B. Poole, "Score-based generative modeling through stochastic differential equations," *Int. Conf. on Learning Representations (ICLR)*, 2021.

- *Song et al.*^[2]: Model forward process as a stochastic differential equation (SDE)

$$d\mathbf{x} = \underbrace{\mathbf{f}(\mathbf{x}, t)}_{\text{Drift}} dt + \underbrace{g(\mathbf{x}, t)}_{\text{Diffusion}} d\mathbf{w}, \quad t \in [0, 1] \quad (1)$$

which has an associated *Reverse SDE*:

$$d\mathbf{x} = \left[-\mathbf{f}(\mathbf{x}, t) + g(\mathbf{x}, t)^2 \underbrace{\nabla_{\mathbf{x}} \log p(\mathbf{x})}_{\text{Score of } p(\mathbf{x})} \right] dt + g(\mathbf{x}, t) d\bar{\mathbf{w}} \quad (2)$$

- Learn *score network* $s_{\theta}(\mathbf{x}, t) \approx \text{score } \nabla_{\mathbf{x}} \log p_t(\mathbf{x})$, plug s_{θ} into (2) to create a **Reverse Neural SDE**
 - **As initial value**: $t = 1$, $x_{t=1} =$ pure Gaussian noise
- Numerically solving this initial value problem **generates** new samples!

[2] Y. Song, J. Sohl-Dickstein, D. P. Kingma, A. Kumar, S. Ermon, and B. Poole, "Score-based generative modeling through stochastic differential equations," *Int. Conf. on Learning Representations (ICLR)*, 2021.

Score-based generative models (SGMs) for inverse problems?

- **Motivation:** SGMs exhibit strong modeling of data distributions
→ make inverse problems easier
- Some inverse problems have been tackled^[3,4], but approaches typically assume **known and/or linear** forward operators T
- No such luxuries for blind inverse problems:
 - Blind deconvolution
 - Non-uniform deblurring
 - Artifact removal
 - Background removal
 - ...

[3] B. Kawar, M. Elad, S. Ermon, and J. Song, "Denoising diffusion restoration models," in *ICLR Workshop on Deep Generative Models for Highly Structured Data*, 2022. [Online]. Available: <https://openreview.net/forum?id=BExXihV0vWq>.

[4] H. Chung, J. Kim, M. T. Mccann, M. L. Klasky, and J. C. Ye, "Diffusion posterior sampling for general noisy inverse problems," *arXiv preprint arXiv:2209.14687*, 2022.

- Many SGMs use something like the Variance Exploding SDE:

$$\mathbf{f}(\mathbf{x}, t) = 0, \quad g(t) = \left[\sigma_{\min} \left(\frac{\sigma_{\max}}{\sigma_{\min}} \right)^t \right] \quad (3)$$

- Much exploration of the diffusion term g in the literature
- But very little of the **drift** \mathbf{f}
- Our idea: **Utilize the drift term** for our blind problems

- Let ($\mathbf{x}_0 =$ clean image, $\mathbf{y} =$ corrupted image) **from a paired dataset**
- Idea:** Realize increasing corruption of image via new forward SDE

Variance Exploding SDE

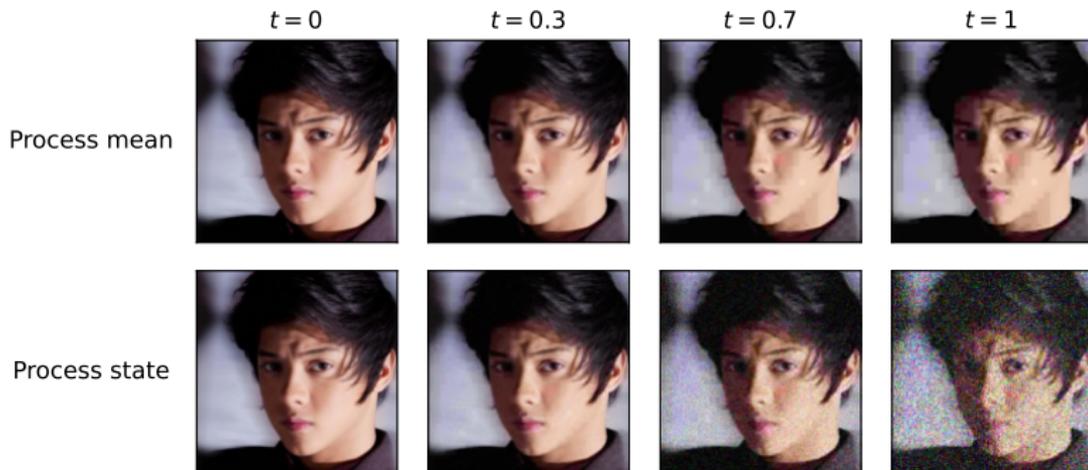
$$d\mathbf{x}_t = \underbrace{\left[\sigma_{\min} \left(\frac{\sigma_{\max}}{\sigma_{\min}} \right)^t \right]}_{\text{Diffusion } g} d\mathbf{w}$$

Our proposal: Add a drift term

$$d\mathbf{x}_t = \underbrace{\gamma F(t)(\mathbf{y} - \mathbf{x}_t)}_{\text{Drift } \mathbf{f}} dt + \underbrace{\left[\sigma_{\min} \left(\frac{\sigma_{\max}}{\sigma_{\min}} \right)^t \right]}_{\text{Diffusion } g} d\mathbf{w}$$

- Drift $\mathbf{f} = \gamma F(t)(\mathbf{y} - \mathbf{x}_t)$** pulls \mathbf{x}_t towards \mathbf{y}
 - adds the corruption in \mathbf{y} over increasing process time t
 - \mathbf{f} affine in $\mathbf{x}_t \Rightarrow$ closed-form mean and variance
- **Solving the Reverse SDE removes the corruption**

Forward process, illustrated



- Adds relatively little noise even at $t = 1.0$
- Diffuses within a much smaller region than classic SGMs

- Task: JPEG Artifact Removal
 - Example task with nonlinear forward operator
 - We **do not** inform models about quality factor or how JPEG works
- Train NCSN++ network^[2] on *CelebA-HQ 256x256*
 - Random JPEG quality factors 0–30%
 - **Proposed:** Train as task-adapted score model
 - **Baseline:** Train via simple L_2 regression
- Forward SDE drift term: $\mathbf{f} = \gamma(\mathbf{y} - \mathbf{x}_t)$
 - {Ornstein-Uhlenbeck + Variance Exploding} (OUVE) SDE
- Solve Reverse SDE with Euler-Maruyama, $N = 100$ steps

[2] Y. Song, J. Sohl-Dickstein, D. P. Kingma, A. Kumar, S. Ermon, and B. Poole, “Score-based generative modeling through stochastic differential equations,” *Int. Conf. on Learning Representations (ICLR)*, 2021.

- Input JPEG quality level 10%:



- ✓ Outperforms regression baseline with same network architecture
- ✓ Much better at fine details & modeling the clean image distribution

	KID↓	FID↓	LPIPS↓	SSIM↑
Corrupted	22.53	36.26	0.20	0.82
Baseline	38.18	45.92	0.13	0.90
Ours (OUVE)	2.37	15.69	0.08	0.83

Table: Metrics for JPEG quality factor 10%

- ✓ Our SGM beats the L_2 baseline perceptually and in terms of distribution metrics

Conclusion

- Power of the SDE formalism for SGMs should be explored further
 - Drift term \mathbf{f} is often ignored
- A simple affine drift term can **adapt SGMs to image-to-image tasks**
 - Qualitatively different outputs than regression baseline even with
 - the same training dataset
 - the same DNN architecture
 - no loss engineering or feature engineering
 - ✓ Training: similarly simple as supervised regression
 - ✓ Needs relatively few steps even with basic solvers
 - ✓ No intricate knowledge of corruption needed

- [1] J. Sohl-Dickstein, E. Weiss, N. Maheswaranathan, and S. Ganguli, “Deep unsupervised learning using nonequilibrium thermodynamics,” in *International Conference on Machine Learning*, 2015, pp. 2256–2265.
- [2] Y. Song, J. Sohl-Dickstein, D. P. Kingma, A. Kumar, S. Ermon, and B. Poole, “Score-based generative modeling through stochastic differential equations,” *Int. Conf. on Learning Representations (ICLR)*, 2021.
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- [4] H. Chung, J. Kim, M. T. Mccann, M. L. Klasky, and J. C. Ye, “Diffusion posterior sampling for general noisy inverse problems,” *arXiv preprint arXiv:2209.14687*, 2022.
- [5] M. Ehrlich, L. Davis, S.-N. Lim, and A. Shrivastava, “Quantization guided JPEG artifact correction,” in *Eur. Conf. Comput. Vis.*, Springer, 2020, pp. 293–309.

Training objective: Minimize L^2 loss between **model output** and the **score**

$$\|s_\theta(\mathbf{x}, \mathbf{y}, t) - \nabla_{\mathbf{x}} \log p_{0t}(\mathbf{x}|\mathbf{x}_0, \mathbf{y})\|_2^2. \quad (4)$$

When p_{0t} is Gaussian, its score equals

$$\nabla_{\mathbf{x}} \log p_{0t}(\mathbf{x}|\mathbf{x}_0, \mathbf{y}) = -\frac{\mathbf{x} - \boldsymbol{\mu}(\mathbf{x}_0, \mathbf{y}, t)}{\sigma(t)^2} = \frac{-\mathbf{z}}{\sigma(t)}, \quad (5)$$

where $\mathbf{x} = \boldsymbol{\mu}(\mathbf{x}_0, \mathbf{y}, t) + \sigma(t)\mathbf{z}$, $\mathbf{z} \sim \mathcal{N}_{\mathbb{C}}(0, \mathbf{I})$.

- s_θ is trained as a task-adapted Gaussian denoiser, able to deal with multiple noise scales

- QGAC^[5] is a SotA method for JPEG artifact removal
- TSDVE: $\mathbf{f} = \gamma t(\mathbf{y} - \mathbf{x}_t)$

	KID ↓	FID ↓	LPIPS ↓	SSIM ↑
Corrupted	22.53	36.26	0.20	0.82
QGAC	46.89	53.97	0.14	0.90
Baseline	38.18	45.92	0.13	0.90
Ours (TSDVE)	2.32	15.72	0.08	0.83
Ours (OUVE)	2.37	15.69	0.08	0.83

Table: Metrics for JPEG quality factor 10%

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