

# On some modern developments in generative modelling

ISA Oberseminar

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Lukas Trottnner

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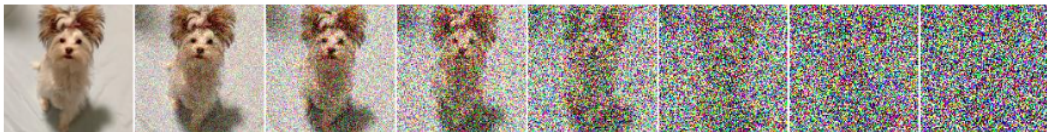
University of Stuttgart



**University of Stuttgart**  
Germany

## Motivation:

*“Creating noise from data is easy; creating data from noise is **generative modeling**.”*



Source: Song et al. (2021). Score based generative modeling through stochastic differential equations. *ICLR*.

# Generative modelling

**Setup:** identically distributed samples  $X_1, \dots, X_n$  with **unknown distribution**  $P$  are given

**Goal:** develop sampling algorithms that do not rely on structural assumptions on  $P$

- ~> involves (implicitly) **learning the underlying distribution** of a dataset to generate new samples that
  - a) follow approximately the same distribution as the training data;
  - b) should not be drawn from the training data set
- ~> essential in applications like image synthesis, text generation, data augmentation ...

## Noise transformation

**Inverse transform sampling:** for an  $\mathbb{R}$ -valued random variable  $X$  with cdf  $F$  and  $U \sim \mathcal{U}((0, 1))$ , we have  $F^{-1}(U) \stackrel{d}{=} X$  for the left-inverse  $F^{-1}$  of  $F$

- we don't know  $F$ , but are only given samples  $X_1, \dots, X_n \stackrel{d}{=} X$
  - naïve approach: replace  $F$  by empirical cdf  $\hat{F}(x) = \frac{\#\{X_i: X_i \leq x\}}{n}$  and set  $\hat{X} = \hat{F}^{-1}(U)$  for an independent  $U \sim \mathcal{U}((0, 1))$
  - if  $X_{(1)}, \dots, X_{(n)}$  is an increasing ordering of the data set and  $U \in [k/n, (k+1)/n)$ , then  $\hat{X} = X_{(k)}$
- $\rightsquigarrow$  algorithm learns the empirical distribution  $\mathbb{P}_n = \frac{1}{n} \sum_{i=1}^n \delta_{X_i} \rightsquigarrow$  **overfitting**/"no creativity"

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To evaluate the performance of an algorithm that outputs  $\hat{X} = \hat{T}(U)$ , for some  $\hat{T} \in \sigma(X_1, \dots, X_n)$  and independent noise  $U$  we can

- analyse the rate of convergence of

$$\mathbb{E}\left[d(\hat{T}_{\#}\mathbb{P}_U, \mathbb{P}_X)\right], \quad d \text{ some probability distance or divergence}$$

- study distance of generated distribution to empirical distribution  $\mathbb{P}_n$
- inspect samples visually

# Generative Adversarial Networks (GANs)

**Key idea:** GANs use a game-theoretic setup:

- **Generator  $G$ :** maps random, easy to-sample-from noise  $U$  to data space to generate samples
- **Discriminator  $D$ :** distinguishes between real samples  $X$  and generated samples  $G(U)$

**Objective:** A minimax game is played:

$$\inf_{G \in \mathcal{G}} \sup_{D \in \mathcal{D}} |\mathbb{E}[D(X)] - \mathbb{E}[D(G(U))]|$$

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- for  $\mathcal{D} = \{D : D \text{ is 1-Lipschitz}\}$  this is equivalent to

$$\inf_{G \in \mathcal{G}} W_1(\mathbb{P}_X, G_{\#}\mathbb{P}_U) = \inf_{G \in \mathcal{G}} \inf_{\gamma \in \Gamma(\mathbb{P}_X, G_{\#}\mathbb{P}_U)} \int \|x - y\| \gamma(dx, dy), \quad (\text{Wasserstein-GAN})$$

where  $\gamma \in \Gamma(\mathbb{P}_X, G_{\#}\mathbb{P}_U)$  iff  $\gamma(dx \times \mathbb{R}^d) = \mathbb{P}_X(dx)$  and  $\gamma(\mathbb{R}^d \times dy) = \mathbb{P}(G(U) \in dy)$

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- in practice,  $\mathcal{D}$  and  $\mathcal{G}$  are chosen as **parameterised neural network classes** and **expectations are replaced by empirical means**:

$$\text{ERM: } \hat{G} \in \arg \min_{G \in \mathcal{G}} \underbrace{\sup_{D \in \mathcal{D}} |\mathbb{E}_n D - \mathbb{E}[D(G(U))]|}_{\approx W_1(\mathbb{P}_n, G_{\#}\mathbb{P}_U)}$$



## Langevin diffusion models

Langevin MCMC algorithm: given target density  $p_0$  simulate diffusion

$$dZ_t = \nabla \log p_0(Z_t) dt + \sqrt{2} dW_t$$

and output  $Z_T$  for  $T$  “sufficiently large”: if  $p_0$  is sufficiently nice, then  $Z_t \xrightarrow{d} p_0$

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- denoising score matching: let  $X \sim p_0$ ,  $X_\sigma^2 = X + \sigma \varepsilon \sim p_0 * \phi_{0,\sigma^2}$ , for indep. noise  $\varepsilon \sim \mathcal{N}(0, \mathbb{I}_d)$

$$\begin{aligned} \nabla \log p_{0,\sigma^2}(x) &= \frac{\int \nabla_x \phi_{0,\sigma^2}(x-y) p_0(dy)}{p_{0,\sigma^2}(x)} = \int \nabla_x \log \phi_{0,\sigma^2}(x-y) \underbrace{\frac{\phi_{0,\sigma^2}(x-y) p_0(dy)}{p_{0,\sigma^2}(x)}}_{=P(X \in dy | X_{\sigma^2}=x)} \\ &= \mathbb{E}[\nabla \log \phi_{X,\sigma^2}(X_{\sigma^2}) \mid X_{\sigma^2} = x] \end{aligned}$$

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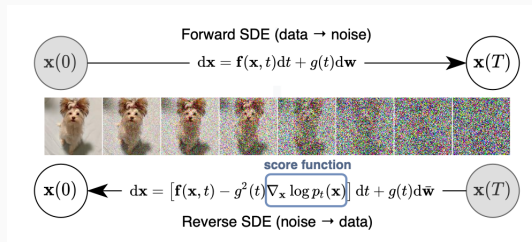
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$$\text{ERM: } \hat{s} \in \arg \min_{s \in \mathcal{S}} \frac{1}{M} \sum_{j=1}^M \|s(X_{i_j,\sigma^2}) - \nabla \log \phi_{X_{i_j,\sigma^2}}(X_{i_j,\sigma^2})\|^2 = \arg \min_{s \in \mathcal{S}} \frac{1}{M} \sum_{j=1}^M \|s(X_{i_j,\sigma^2}) + \frac{1}{\sigma} \varepsilon_{i_j}\|^2,$$

where the  $X_{i_j}$  are uniformly sampled from  $X_1, \dots, X_n$  and  $X_{i_j,\sigma^2} = X_{i_j} + \sigma \varepsilon_{i_j}$

# Denoising diffusion models

- provide an **iterative generative algorithm** to create new samples that approximately match the target distribution  $p_0$ , given a finite number of samples corresponding to an unknown  $p_0$
- general idea: find a **stochastic process** that perturbs  $p_0$  to a new distribution  $p_T$  such that
  - 1)  $p_T$  or a good approximation thereof is **easy to sample from**, and
  - 2) the perturbation is **reversible** in the sense that we know how to **simulate the time-reversed process**



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# Denoising Diffusion Models

- for some fixed time  $T > 0$  consider the forward model

$$dX_t = b(t, X_t) dt + \sigma(t, X_t) dW_t, \quad t \in [0, T], X_0 \sim p_0$$

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- letting  $p_t(x) = \int p_{0,t}(y, x) p_0(dy)$  be the marginal densities of  $(X_t)$ , the **time reversal**  $\tilde{X}_t = X_{T-t}$  solves

$$d\tilde{X}_t = -\bar{b}(T-t, \tilde{X}_t) dt + \sigma(T-t, \tilde{X}_t) d\bar{W}_t, \quad t \in [0, T], \tilde{X}_0 \sim p_T,$$

where

$$\begin{aligned} \bar{b}_i(t, x) &= b_i(t, x) - \frac{1}{p_t(x)} \sum_{j,k=1}^d \frac{\partial}{\partial x_j} (p_t(x) \sigma_{ik}(t, x) \sigma_{jk}(t, x)) \\ &= b_i(t, x) - (\nabla \cdot \Sigma(t, x))_i - (\nabla \log p_t(x))_i, \quad i = 1, \dots, d, \Sigma = \sigma \sigma^\top \end{aligned}$$



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~> time-reversed process solves a **time-inhomogeneous SDE**, now with drift  $-\bar{b}(T - \cdot, \cdot)$  involving the **score**  $\nabla \log p_t$ , which depends on the **unknown** data distribution  $p_0$

~> score needs to be estimated from the data

# Denoising score matching

- denoising score matching:

$$\begin{aligned}\nabla \log p_t(x) &= \frac{\int \nabla_x p_{0,t}(y, x) p_0(dy)}{p_t(x)} = \int \nabla_x \log p_{0,t}(y, x) \underbrace{\frac{p_{0,t}(y, x) p_0(dy)}{p_t(x)}}_{=P(X_0 \in dy | X_t=x)} \\ &= \mathbb{E}[\nabla_2 \log p_{0,t}(X_0, X_t) \mid X_t = x]\end{aligned}$$

and thus

$$\mathfrak{s} := \nabla \log p_t \in \arg \min_{s \text{ meas.}} \mathbb{E}[\|s(X_t) - \nabla_2 \log p_{0,t}(X_0, X_t)\|^2]$$

$\leadsto$  given data  $(X_0^i)_{i \in [n]} \stackrel{\text{iid}}{\sim} p_0$  define the **denoising score estimator**

$$\hat{\mathfrak{s}} \in \arg \min_{s \in \mathcal{S}} \frac{1}{n} \sum_{i=1}^n \mathbb{E}_{X_0^i} \left[ \int_{\underline{I}}^T \|s(t, X_t) - \nabla_2 \log p_{0,t}(X_0, X_t)\|^2 dt \right],$$

where  $0 < \underline{I} \ll T$  and  $\mathcal{S}$  is an approximating function class, e.g. **space-time neural networks**

## Generative process

On  $[0, T - \underline{T}]$ , simulate

$$dY_t = \left( -b(T-t, Y_t) + \nabla \cdot \Sigma(T-t, Y_t) + \Sigma(T-t, Y_t) \hat{\mathfrak{z}}(T-t, Y_t) \right) dt + \sigma(T-t, Y_t) dW_t, \quad \mathbb{P}^{Y_0}(dy) \approx p_T(y) dy$$

Output:

$$Y_{T-\underline{T}} \stackrel{d}{\approx} \tilde{X}_{T-\underline{T}} = X_{\underline{T}} \stackrel{d}{\approx} X_0$$

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### Minimax optimality of diffusion models

Assumptions on data distribution  $p_0$  with support  $\mathcal{M}$ :

- $\text{Leb}(\mathcal{M}) > 0$ ,  $\mathcal{M}$  bounded,  $p_0|_{\mathcal{M}} \geq m > 0$  and  $\beta$ -smooth: [Oko, Akiyama, Suzuki \(ICML '23\)](#), [Dou, Kotekal, Xu and Zhou \('24+\)](#) [ $d = 1$ , no log-factors], [Holk, Strauch, LT \('25+\)](#) [reflected models]
- $d = 1$ ,  $\mathcal{M} = \mathbb{R}$ ,  $p_0$  not lower bounded: [Zhang et al. \('25, ICML\)](#)
- $\mathcal{M}$  bounded and  $\subset$  linear subspace: [Oko, Akiyama, Suzuki \(ICML '23\)](#), [Chen et al. \(ICML '23\)](#)
- $\mathcal{M}$  is a  $d^*$ -dimensional submanifold: [Tang and Yang \(AISTATS '24\)](#), [Azangulov, Delegiannidis and Rousseau \('24+\)](#) [rates adapt to intrinsic dimension  $d^*$ ]
- $\log p_0(x) = \sum_{J \subset [d], |J| \leq d^*} f_J(x_J)$ , for  $f_J$   $\beta$ -Hölder: [Kwon et. al \('25+\)](#), [Fan, Gu and Li \('25+\)](#)
- ... [?]

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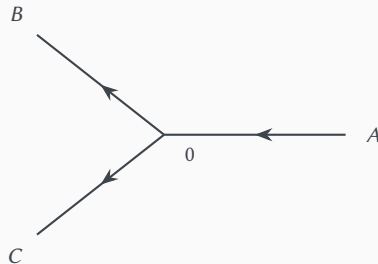
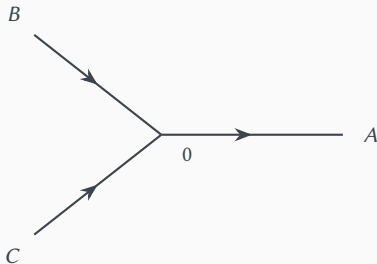
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## Some fundamental observations

- time reversal at **deterministic** time  $T$  forces the backward process to be time-inhomogeneous
- if  $p_0$  has **low-dimensional support**  $\mathcal{M}$ , for small  $t$  and  $x$  close to  $\mathcal{M}$ ,  $\nabla \log p_t(x)$  is approximately **orthogonal** to  $\mathcal{M}$  (Stanczuk et al., ICML '24)
- initialising the generative process in a distribution that is not close to  $\mathbb{P}^{X_T}$  and simulating for  $T - \underline{T}$  time units will not give useful results  $\leadsto$  algorithm is **not adaptive** to the noise level in the data

# Homogeneous time reversal

- Markov property: “the past and future of a Markov process are conditionally independent given the present”  $\leadsto$  time-reversed Markov processes are Markov
- to ensure that a **homogeneous Markov process** remains homogeneous under time reversal, we need to reverse at a suitable **random (life)time  $\zeta$** . This can be
  - a randomised stopping time such as an **independent exponential time**;
  - a **last exit time**;
  - a **first hitting time**;
  - any **terminal time**, that is, any stopping time  $T$  such that  $T = t + T \circ \theta_t$  on  $\{T > t\}$
- retaining the strong Markov property under time reversal is a bit more tricky:



## $h$ -transforms and time reversal

### $h$ -transform

For a possibly killed, homogeneous strong Markov process  $X$  with state space  $S$ , let  $h$  be an excessive function, that is

$$\mathbb{E}_x[h(X_t)] \leq h(x) \quad \text{and} \quad \lim_{t \rightarrow 0} \mathbb{E}_x[h(X_t)] = h(x).$$

Then,

$$p_t^h f(x) = \mathbb{E}_x \left[ \frac{h(X_t)}{h(x)} f(X_t) \mathbf{1}_{\{X_t \in S\}} \right] \mathbf{1}_{(0, \infty)}(h(x)), \quad f \in \mathcal{B}_b(\mathbb{R}^d),$$

defines a sub-Markov semigroup. The corresponding Markov process  $X^h$  is strong Markov and is called  $h$ -transform of  $X$ .

- suppose that  $X$  is a continuous and **self-dual** Feller process (i.e., its generator satisfies  $A = A^*$ )
- if  $X^h$  has a finite killing time  $\zeta$ , then the time-reversed process  $X_t^{\leftarrow h} = X_{\zeta-t}^h$  is **homogeneous, strong Markov** and is a  $\tilde{h}$ -transform of  $X$ .

## $h$ -transforming a killed diffusion

- consider a **symmetric** diffusion process

$$dX_t = b(X_t) dt + \sigma(X_t) dW_t$$

with invariant measure  $m$  and let  $Z$  be its version **killed at an independent exponential time** with parameter  $r > 0$

- as an excessive function for  $Z$  use

$$h(x) = \int G_r(x, y) \kappa(dy)$$

for the **Green kernel**  $G_r(x, y) = \int_0^\infty e^{-rt} p_t(x, y) dy$  and a **representing measure**  $\kappa$

- $\kappa(dy) = r dy \rightsquigarrow h = 1$  and  $Z^h = Z$
- $\kappa(dy) = \frac{1}{G_r(x_0, y)} \beta(dy) \rightsquigarrow Z$  conditioned to have distribution  $\beta$  before killing if started in  $x_0$
- $Z$  is a killed Brownian motion and  $\kappa(dy) = \sigma_R(dy)$  for the surface measure  $\sigma_R$  of an  $R$ -sphere  $\mathbb{S}^{d-1}(R) \rightsquigarrow Z^h$  is killed at last exit from  $\mathbb{S}^{d-1}(R)$



# A time-homogeneous generative process

**Proposition** (Christensen, Strauch and LT (2025+))

1.  $Z^h$  is an Itô-diffusion with dynamics

$$dZ_t^h = (b(Z_t^h) + \Sigma(X_t) \nabla \log h(X_t)) dt + \sigma(Z_t^h) dW_t$$

outside  $\text{supp } \kappa$  and its distribution at the lifetime is given by

$$\mathbb{P}_x(Z_{\zeta-}^h \in dy) = \frac{G_r(x, y)}{h(x)} \kappa(dy)$$

2. Let  $\alpha = \mathbb{P}^{Z_0^h}$ . Then  $\tilde{Z}_t^h$  is an  $\tilde{h}$ -transform of  $Z$  with initial distribution  $\mathbb{P}_\alpha(Z_{\zeta-}^h \in dy)$  and

$$\tilde{h}(x) := \int \frac{G_r(x, y)}{h(y)} \alpha(dy).$$

In particular,  $\tilde{Z}^h$  has dynamics

$$d\tilde{Z}_t^h = (b(\tilde{Z}_t^h) + \Sigma(\tilde{Z}_t^h) \nabla \log \tilde{h}(\tilde{Z}_t^h)) dt + \sigma(\tilde{Z}_t^h) d\bar{W}_t,$$

outside  $\text{supp } \alpha =: \mathcal{M}$  and  $\mathbb{P}_\alpha(\tilde{Z}_{\zeta-}^h \in dy \mid Z_0^h = x) = \frac{G_r(x, y)}{\tilde{h}(x)h(y)} \alpha(dy)$  for  $\mathbb{P}_\alpha(Z_{\zeta-}^h \in \cdot)$ -a.e.  $x$ .

# A time-homogeneous generative process

Idealised algorithm:

1. Initialise  $Z_0^{\tilde{h}} \sim \tilde{\beta} \approx \mathbb{P}_\alpha(Z_{\zeta-}^h)$ 
  - for ergodic forward process with stationary distribution  $\mu$  and small exponential killing rate  $r > 0$ , choose  $\tilde{\beta} = \mu$  [ $\leftrightarrow$  [ergodic diffusion model](#)]
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  - for  $\kappa(dy) = \frac{1}{G_r(x_0, y)} \delta_z$ , choose  $\tilde{\beta} = \delta_z$
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# A time-homogeneous generative process

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# Learning to kill

## Polarity hypothesis

Assume that  $\mathcal{M} = \text{supp } \alpha$  is **polar** for  $X$ , i.e., for any  $x \in \mathbb{R}^d$ ,  $\mathbb{P}_x(\inf\{t > 0 : X_t \in \mathcal{M}\} < \infty) = 0$ .

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Possible strategies to estimate a  $\delta$ -fattening  $\mathcal{M}_\delta = \{x : \text{dist}(x, \mathcal{M}) \leq \delta\}$  given data  $X^1, \dots, X^n \stackrel{\text{iid}}{\sim} \alpha$  and an estimator  $\hat{\mathfrak{z}}$  of  $\mathfrak{z} := \nabla \log h$ :

- **explicit** plug-in approach: estimate  $\mathcal{M}_\delta$  directly or indirectly by setting  $\widehat{\mathcal{M}}_\delta = (\widehat{\mathcal{M}})_\delta$ ; then set  $\hat{\zeta} := \inf\{t \geq 0 : Z_t^{\hat{\mathfrak{z}}} \in \widehat{\mathcal{M}}_\delta\}$
- **implicit approach**: use explosive behaviour of  $\mathfrak{z}$  as  $x \rightarrow \mathcal{M}$

## Theorem (Christensen, Kallsen, Strauch and LT (2025+))

Suppose that  $\mathcal{M}$  is polar for  $X$  and  $Y$  solving  $dY_t = \sigma(Y_t) dB_t$ . Then, it a.s. holds that

$$\zeta = \inf\left\{t \geq 0 : \sup_{s \leq t} |\mathfrak{z}(Z_s^{\leftarrow h})| = \infty\right\} = \inf\left\{t \geq 0 : \|\mathfrak{z}(Z^{\leftarrow h})\|_{L^2([0, t])} = \infty\right\}.$$

## Denoising score matching

- for  $\mathbb{P}_\alpha(Z_{\zeta_-}^h \in \cdot)$ -a.e.  $x$

$$\begin{aligned}\mathfrak{s}(x) &= \nabla \log \tilde{h}(x) = \frac{1}{\tilde{h}(x)} \int \nabla_x G_r(x, y) \frac{1}{\tilde{h}(y)} \alpha(dy) = \int \nabla_x \log G_r(x, y) \frac{G_r(x, y)}{\tilde{h}(x)h(y)} \alpha(dy) \\ &= \mathbb{E}[\nabla_x \log G_r(x, Z_{\zeta_-}^h) \mid Z_0^h = x] \\ &= \mathbb{E}_\alpha[\nabla_x \log G_r(x, Z_0^h) \mid Z_{\zeta_-}^h = x]\end{aligned}$$

- this implies that on  $\mathbb{R}^d \setminus \mathcal{M}_\delta$ ,  $\mathfrak{s}$  agrees  $\mathbb{P}_\alpha(Z_{\zeta_-}^h \in \cdot)$ -a.e. with the minimiser of

$$\mathcal{B}(\mathbb{R}^d; \mathbb{R}^d) \ni s \mapsto \mathbb{E}_\alpha \left[ \|s(Z_{\zeta_-}^h) - \nabla \log G_r(Z_0^h, Z_{\zeta_-}^h)\|^2 \mathbf{1}_{\{\|Z_{\zeta_-}^h - Z_0^h\| > \delta\}} \right]$$

- note that if  $Z^h = Z$ , then  $\zeta \sim \text{Exp}(r)$  independent of  $X$ ,  $Z_{\zeta_-} = X_\zeta$  has full support and we have

$$\mathbb{E}_\alpha \left[ \|s(Z_{\zeta_-}^h) - \nabla \log G_r(Z_0^h, Z_{\zeta_-}^h)\|^2 \mathbf{1}_{\{\|Z_{\zeta_-}^h - Z_0^h\| > \delta\}} \right] = r \mathbb{E}_\alpha \left[ \int_0^\zeta \|s(Z_t^h) - \nabla \log G_r(Z_0^h, Z_t^h)\|^2 \mathbf{1}_{\{\|Z_t^h - Z_0^h\| > \delta\}} dt \right]$$



## Projection learning

- we don't have to start the backward process approximately in  $\mathbb{P}_\alpha(Z_{\zeta_-}^h \in dy)$ : it will always be killed on the data support  $\mathcal{M}$  and different initialisations will yield different output distributions supported on  $\mathcal{M}$   $\rightsquigarrow$  **natural conditioning**
- a natural question is therefore what happens if we don't start the generative process from pure noise but something more informative, say a **masked** or **moderately noised** picture



- it turns out that the natural conditioning aspect entails a **blessing of dimensionality**

## Projection learning

Let  $Z$  be an **exponentially killed Brownian motion**. Then,

$$\tilde{h}(x) = \int G_r(x, y) \alpha(dy), \quad G_r(x, y) = 2(2\pi)^{-d/2} r \left( \frac{\sqrt{2}r}{|x - y|} \right)^{\frac{d-2}{2}} K_{\frac{d-2}{2}} \left( \frac{\sqrt{2}r}{|x - y|} \right).$$

For large  $d$ ,

$$\nabla \log \tilde{h}(x) \approx d \frac{\int \frac{x-y}{|x-y|^d} \alpha(dy)}{\int |x-y|^{2-d} \alpha(dy)}$$

and thus, if there is a unique projection  $x^* \in \arg \min_{y \in \mathcal{M}} |x - y|$  of  $x$  onto  $\mathcal{M}$ , then

$$\nabla \log \tilde{h}(x) \approx d \frac{x^* - x}{|x^* - x|^2} = d \frac{\text{sign}(x^* - x)}{|x^* - x|}$$

**Theorem** (Christensen, Kallsen, Strauch and LT (2025+))

Let  $\delta, \varepsilon > 0$  and fix an observation  $x \in \mathbb{R}^d$ . If  $\alpha(B(x, r)) > \varepsilon$  for some ball  $B(x, r)$  with radius  $r > 0$  around  $y$ , then

$$\mathbb{P}\left(Z_{\zeta-}^{\tilde{h}} \in \mathcal{M} \cap B(x, (1+\delta)r) \mid Z_0^{\tilde{h}} = x\right) \geq 1 - \frac{1}{\varepsilon} (1+\delta)^{2-d}.$$

## Projection learning

Consider now estimators  $\hat{\mathfrak{s}}_n$ , an independent Brownian motion  $W$  and let  $\widehat{Z}^{\hat{\mathfrak{s}}_n}$  be the process solving

$$d\widehat{Z}_t^{\hat{\mathfrak{s}}_n} = \hat{\mathfrak{s}}_n(\widehat{Z}_t^{\hat{\mathfrak{s}}_n}) \mathbf{1}_{\{t \leq \hat{\zeta}\}} dt + \mathbf{1}_{\{t \leq \tilde{\zeta}\}} dW_t, \quad \hat{\zeta} := \inf \left\{ t \geq 0 : \|\widehat{Z}^{\hat{\mathfrak{s}}_n}\|_{L^2[0,t]} > M \right\}.$$

**Theorem** (Christensen, Kallsen, Strauch and LT (2025+))

Fix an observation  $x \in \mathbb{R}^d$ . Suppose that

- for any  $\tilde{\delta}, \delta, \varepsilon > 0$  it holds for sufficiently large  $n$  that

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- for any  $n \in \mathbb{N}$  and  $\tilde{\delta} > 0$ , the function  $\hat{\mathfrak{s}}_n$  is  $L_{\tilde{\delta}}$ -Lipschitz on  $\mathcal{M}_{\tilde{\delta}}^c$

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Thank you for your attention!