Geometric Neural Diffusion Processes

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Papers of Reference and Collaborators

Neural Diffusion Processes. ICML 2023.

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Alan Saul

Zoubin Ghahramani

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Geometric Neural Diffusion Processes. Under submission.

Émile Mathieu[*]

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Michael Hutchinson[*]

Valentin De Bortoli

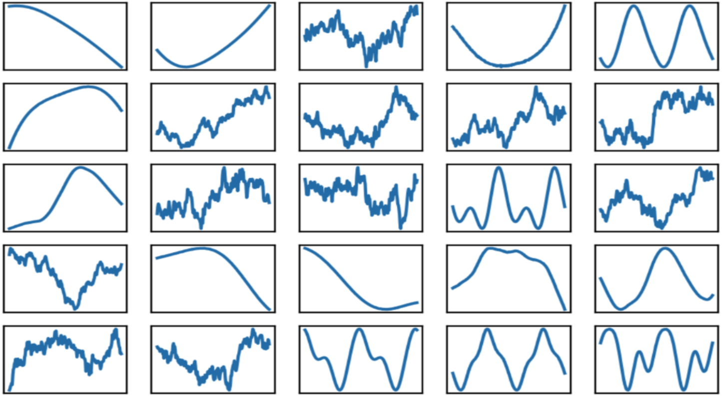
Yee Whye Teh

Richard E. Turner

Rise of Diffusion Models

Figure 1: Samples from stable diffusion

Goal



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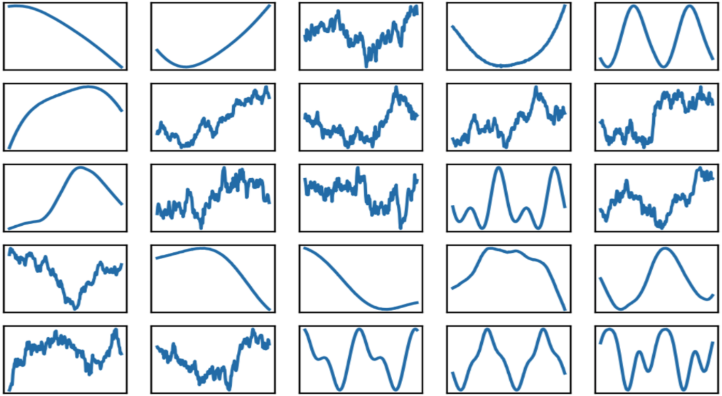
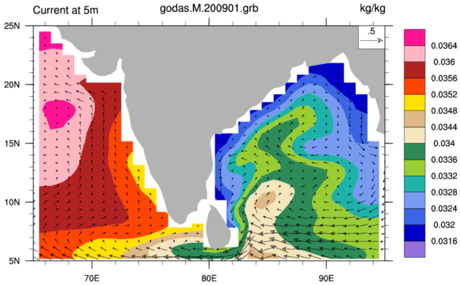


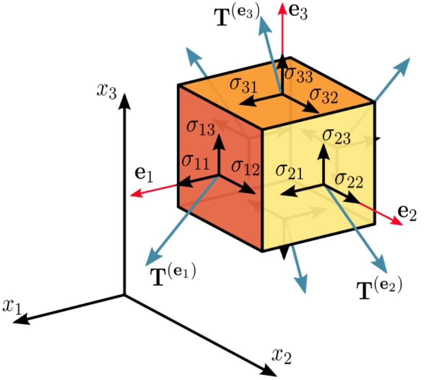
Why

- Many physical and natural phenomena are better characterised as functions.
- Meta-learn and treat limited data as originating from a function.

- Mathematical framework for modelling natural phenomena.
- Examples: Temperature $f : \mathcal{X} \to \mathbb{R}$, and wind direction on globe $f : \mathcal{S}^2 \to T\mathcal{S}^2$.



(a) Temperature map and wind vector fields.



(b) 3D stress tensor (type-2) diagram.

Prior invariances

Encode invariances w.r.t. group transformations. For a group G, we want $\forall g \in G$

$$p(f) = p(g \cdot f) \quad \text{with} \quad g \cdot f = \rho(g) f(g^{-1}x).$$

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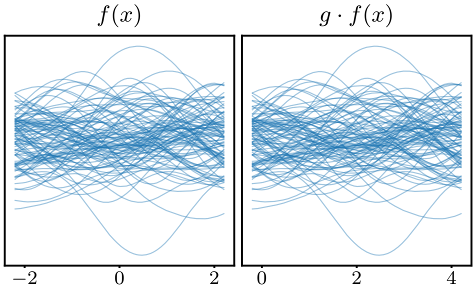
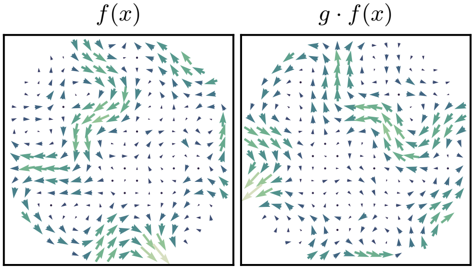
Examples translation invariance (stationarity) and rotational invariance.

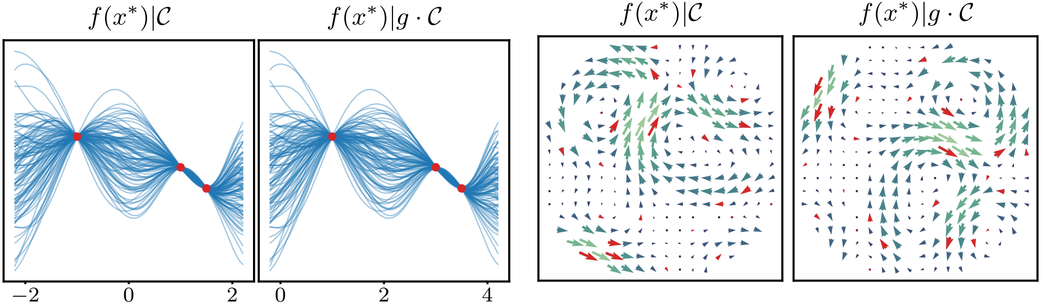




Conditional process

- Interested in the conditional process given a set of observations $\mathcal{C} = \{(x_n, y_n)\}_{n=1}$.
- If the prior is G-invariant, then the conditional is G-equivariant:

$$p(f \mid \mathcal{C}) = p(g \cdot f | g \cdot \mathcal{C}) \quad \text{where} \quad g \cdot \mathcal{C} = \{(g \cdot x_n, \rho(g) y_n)\}.$$



Continuous diffusion models

Principles of continuous diffusion models

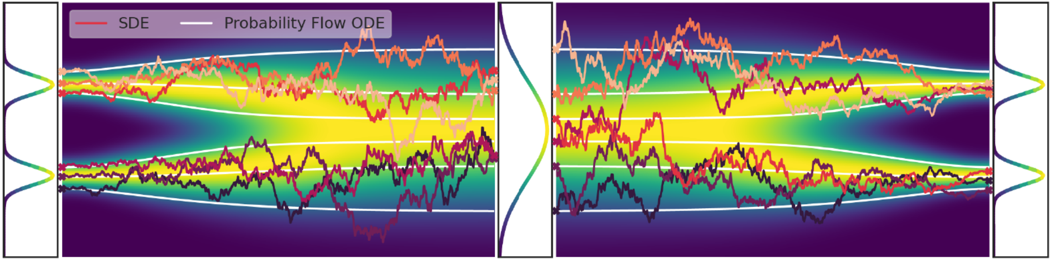


Figure 5: (Song et al., 2021)

- Idea: Destruct data with *continuous* series of noise.
- Do this by constructing an **SDE** forward noising process $(\mathbf{Y}_t)_{t\in[0,T]}$.
- Have this noising converge to a **known distribution**.
- **Invert** this SDE noising process to get **denoising** process.

Continuous noising processes

The **Forward process** progressively perturbs the data following a SDE

$$\mathrm{d}\mathbf{Y}_t = -\mathbf{Y}_t \,\mathrm{d}t + \sqrt{2}\,\mathrm{d}\mathbf{B}_t, \tag{1}$$

where $\mathbf{B}_t$ is Brownian motion (think of it conceptually as $\mathrm{d}\mathbf{B}_t/\mathrm{d}t \sim \mathcal{N}(0, \mathrm{d}t)$).

Example: 2D Gaussian data

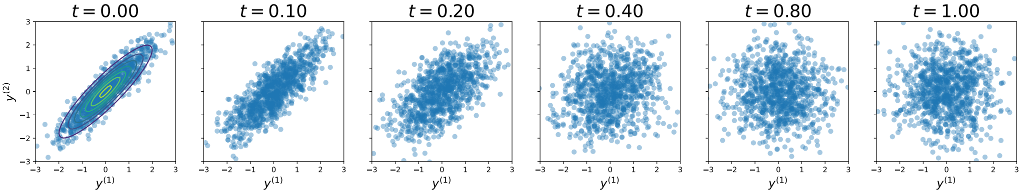


Figure 6: Forward process

Continuous score-based models: Time reversal process

Theorem 1: (Cattiaux et al., 2021; Haussmann and Pardoux, 1986)

The time-reversed process $(\bar{\mathbf{Y}}_t)_{t\geq 0} = (\mathbf{Y}_{T-t})_{t\in[0,T]}$, with forward process $\mathrm{d}\mathbf{Y}_t = -\mathbf{Y}_t \mathrm{d}t + \sqrt{2}\mathrm{d}\mathbf{B}_t$, also satisfies an SDE given by

$$\mathrm{d}\bar{\mathbf{Y}}_t = \left[-\bar{\mathbf{Y}}_t + 2\,\nabla \log p_t(\bar{\mathbf{Y}}_t)\right]\mathrm{d}t + \sqrt{2}\mathrm{d}\mathbf{B}_t,$$

assuming $\bar{\mathbf{Y}}_0$ is distributed the same as $\mathbf{Y}_T$.

Continuous score-based models: Time reversal process

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assuming $\bar{\mathbf{Y}}_0$ is distributed the same as $\mathbf{Y}_T$.

Problem The Stein score $\nabla \log p_t$ $= \nabla \log \int p_{data}(\mathbf{Y}_0) p_{t|0}(\mathbf{Y}_t \mid \mathbf{Y}_0) \mathrm{d}\mathbf{Y}_0$ is intractable.

Denoising Score Matching

Parameterise score using neural network $\mathbf{s}_\theta : [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$ and learn score using the Denoising Score Matching objective

$$\mathcal{L}(\theta) = \mathbb{E}[\| \mathrm{s}_\theta(t, \mathbf{Y}_t) - \nabla \log p_t(\mathbf{Y}_t|\mathbf{Y}_0)\|^2]. \tag{2}$$

Example

$$\mathrm{d}\bar{\mathbf{Y}}_t = \left[-\bar{\mathbf{Y}}_t + 2\, s_\theta(t, \bar{\mathbf{Y}}_t)\right] \mathrm{d}t + \sqrt{2}\mathrm{d}\mathbf{B}_t,$$

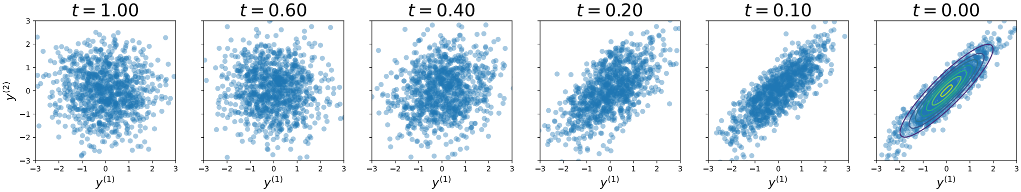
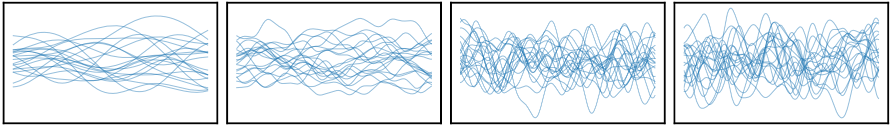


Figure 7: Reverse process

Diffusion on Function Spaces

Continuous noising process

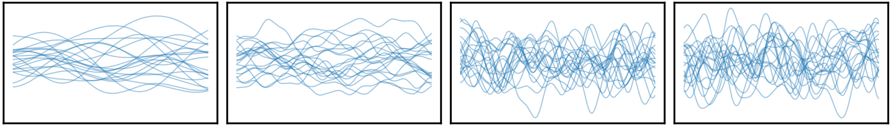


We construct the forward **noising process** $(\mathbf{Y}_t(x))_{t\geq 0} \triangleq (\mathbf{Y}_t(x^1), \ldots, \mathbf{Y}_t(x^n))_{t\geq 0}$ defined by the multivariate SDE (multivariate Ornstein-Uhlenbeck process)

$$\mathrm{d}\mathbf{Y}_t(x) = \tfrac{1}{2}\left\{m(x) - \mathbf{Y}_t(x)\right\}\beta_t \,\mathrm{d}t + \beta_t^{1/2}\mathrm{K}(x,x)^{1/2}\,\mathrm{d}\mathbf{B}_t, \tag{3}$$

where $\mathrm{K}(x,x)_{i,j} = k(x^i, x^j)$ with $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ a kernel and $m : \mathcal{X} \to \mathcal{Y}$.

Continuous noising process



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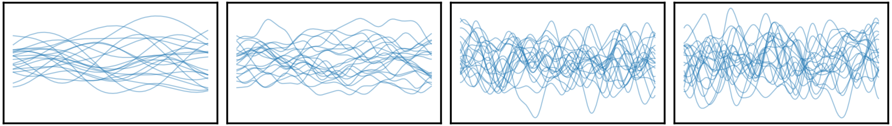
- $\mathbf{Y}_t(x) \to \mathrm{N}(m(x), \mathrm{K}(x,x))$ with geometric rate, for any $x \in \mathcal{X}^n$.
- $\mathbf{Y}_t \to \mathrm{GP}(m,k) \triangleq \mathbf{Y}_\infty$ (Phillips et al., 2022).

Continuous noising process



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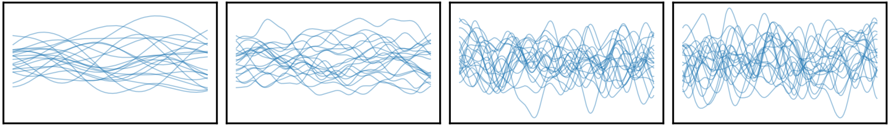
- $\mathbf{Y}_t(x) \to \mathrm{N}(m(x), \mathrm{K}(x,x))$ with geometric rate, for any $x \in \mathcal{X}^n$.
- $\mathbf{Y}_t \to \mathrm{GP}(m,k) \triangleq \mathbf{Y}_\infty$ (Phillips et al., 2022).
- $\mathbf{Y}_t$ interpolates between $\mathbf{Y}_0$ and $\mathbf{Y}_\infty$.

Continuous noising process

$$k(x, x') = k_{\mathrm{rbf}}(x, x') = \sigma^2 \exp\left(\frac{\|x - x'\|^2}{2l^2}\right), \text{ with } l = 1.$$



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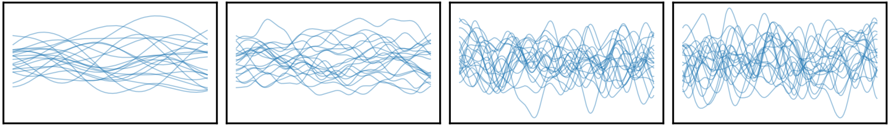
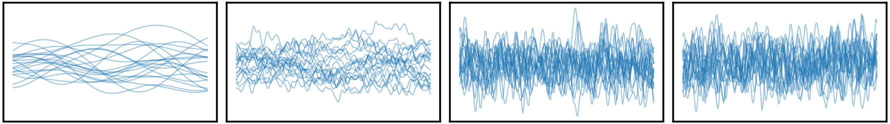


$$k(x, x') = k_{\mathrm{rbf}}(x, x'),$$ with $l = 0.2$.



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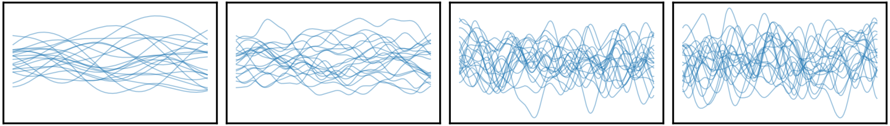

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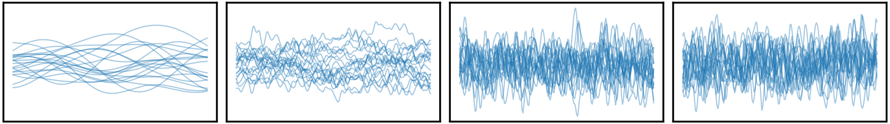
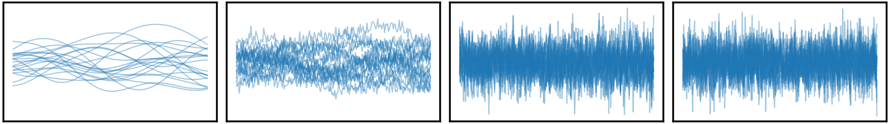
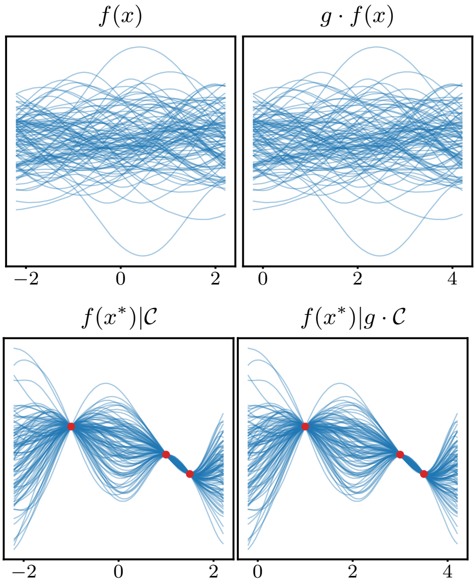


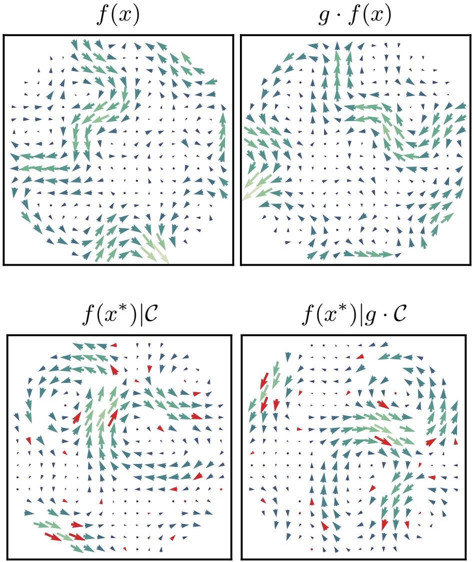
$k(x, x') = \delta_x(x')$ (The tranditional DDPM settings).



Encoding Invariances

Prior and Conditional Symmetries





Invariant neural diffusion processes

Proposition 1: Invariant Neural Diffusion Processes

The denoising process on functions as defined above and with initial sample given by $p(\bar{\mathbf{Y}}_0) = \mathrm{GP}(m, k)$ is G-invariant if

1. m and k are both G-equivariant (i.e. G-invariant Gaussian process), i.e.

$$m(g \cdot x) = \rho(g) m(x) \quad \text{and} \quad k(g \cdot x, g \cdot x') = \rho(g) k(x, x') \rho(g)^\top,$$

2. the score network is G-equivariant vector field, i.e.

$$\mathbf{s}_\theta(t, g \cdot x, \rho(g) y) = \rho(g) \mathbf{s}_\theta(t, x, y),$$

for all $x \in \mathcal{X}, g \in G$.

Conditional Process

Conditional sampling in diffusion models

Goal: Sample from $y \sim p(\cdot \mid \mathcal{C})$ given a condition $\mathcal{C}$.

Conditional sampling in diffusion models

Goal: Sample from $y \sim p(\cdot \mid \mathcal{C})$ given a condition $\mathcal{C}$.

"a hedgehog using a calculator" | "a corgi wearing a red bowtie and a purple party hat" | "robots meditating in a vipassana retreat" | "a fall landscape with a small cottage next to a lake"

Figure 10: $p(image \mid text)$

Often the condition is a property (e.g., caption).

Conditional sampling in Neural Diffusion Processes

Condition is a subspace of the state space: $\mathbf{Y}^{\mathcal{C}} = (y^{(1)}, \ldots, y^{(m)})$.

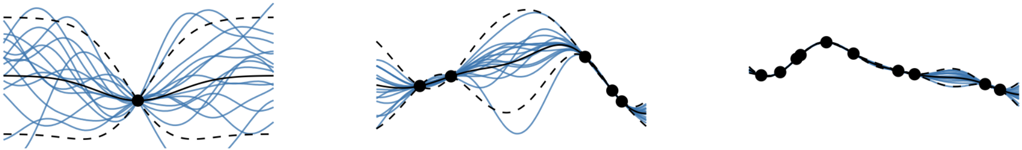


Figure 11: Conditional samples $p(\cdot \mid \mathbf{Y}^{\mathcal{C}})$.

Conditional sampling in Neural Diffusion Processes

- We need the **conditional score** $\nabla \log p_t(\mathbf{Y}_t) \implies \nabla \log p_t(\mathbf{Y}_t \mid \mathbf{Y}^{\mathcal{C}})$
- Applying Bayes rule to the conditional score

$$\nabla_{\mathbf{Y}_t} \log p_t(\mathbf{Y}_t \mid \mathbf{Y}^{\mathcal{C}}) = \nabla_{\mathbf{Y}_t} \log p_t(\mathbf{Y}_t, \mathbf{Y}^{\mathcal{C}}) - \nabla_{\mathbf{Y}_t} \log p_t(\mathbf{Y}^{\mathcal{C}}) = \nabla_{\mathbf{Y}_t} \log p_t(\mathbf{Y}_t, \mathbf{Y}^{\mathcal{C}})$$

- Use standard reverse process with score $s_\theta(t, [\mathbf{Y}_t, \mathbf{Y}^{\mathcal{C}}])$.

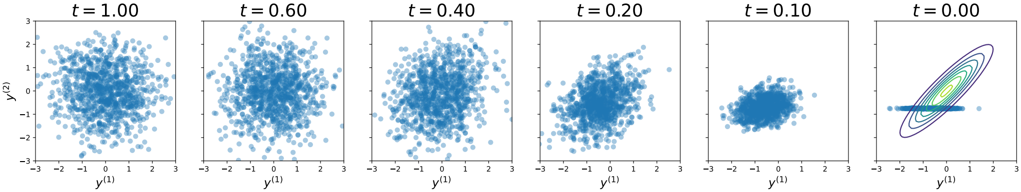
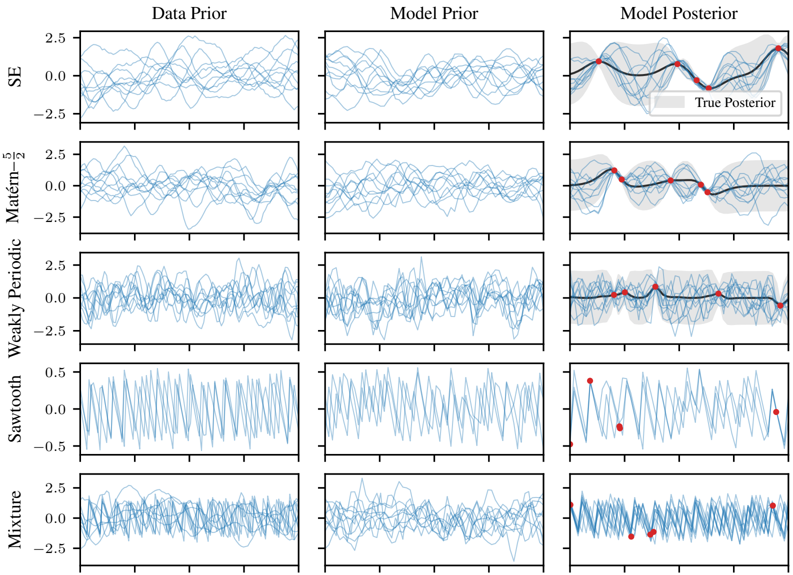


Figure 12: Conditional reverse process $p(\mathbf{Y}_0 \mid y^{(2)} = -1)$

Experimental results

1D regression: Datasets



1D regression: Predictive log-likelihood (Cont'd)

Table 1: Mean test log-likelihood (TLL) (higher is better)

		SE	Matérn($\frac{5}{2}$)	Weakly Per.	Sawtooth	Mixture
Interpolat.	GP (optimum)	0.70 ± 0.00	0.31 ± 0.00	-0.32 ± 0.00	-	-
	T(1)−GeomNDP	$\mathbf{0.72} \pm 0.03$	$\mathbf{0.32} \pm 0.03$	$\mathbf{-0.38} \pm 0.03$	$\mathbf{3.39} \pm 0.04$	$\mathbf{0.64} \pm 0.08$
	NDP*	$\mathbf{0.71} \pm 0.03$	$\mathbf{0.30} \pm 0.03$	$\mathbf{-0.37} \pm 0.03$	$\mathbf{3.39} \pm 0.04$	$\mathbf{0.64} \pm 0.08$
	GNP	$\mathbf{0.70} \pm 0.01$	$\mathbf{0.30} \pm 0.01$	-0.47 ± 0.01	0.42 ± 0.01	0.10 ± 0.02
	ConvNP	-0.46 ± 0.01	-0.67 ± 0.01	-1.02 ± 0.01	1.20 ± 0.01	-0.50 ± 0.02

1D regression: Predictive log-likelihood (Cont'd)

Table 2: Mean test log-likelihood (TLL) (higher is better)

		SE	Matérn($\frac{5}{2}$)	Weakly Per.	Sawtooth	Mixture
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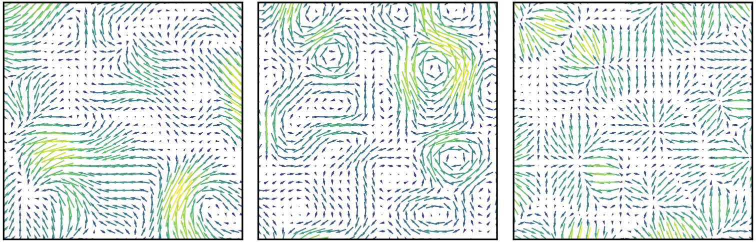
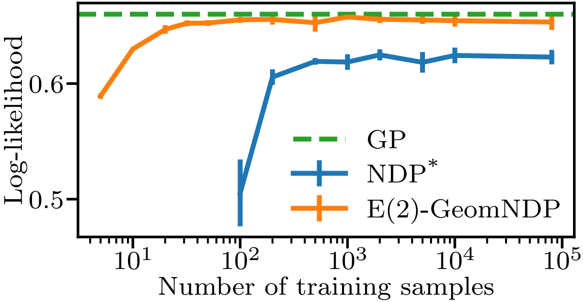
Generalisat.	GP (optimum)	0.70 ± 0.00	0.31 ± 0.00	-0.32 ± 0.00	-	-
	T(1)−GeomNDP	$\mathbf{0.70} \pm 0.02$	$\mathbf{0.31} \pm 0.02$	$\mathbf{-0.38} \pm 0.03$	$\mathbf{3.39} \pm 0.03$	$\mathbf{0.62} \pm 0.02$
	NDP*	*	*	*	*	*
	GNP	$\mathbf{0.69} \pm 0.01$	$\mathbf{0.30} \pm 0.01$	-0.47 ± 0.01	0.42 ± 0.01	0.10 ± 0.02
	ConvNP	-0.46 ± 0.01	-0.67 ± 0.01	-1.02 ± 0.01	1.19 ± 0.01	-0.53 ± 0.02

2D invariant Gaussian vector fields



Model	SE	Curl-free	Div-free
GP	$0.56_{\pm 0.00}$	$0.66_{\pm 0.00}$	$0.66_{\pm 0.00}$
NDP	$0.55_{\pm 0.00}$	$0.62_{\pm 0.01}$	$0.62_{\pm 0.01}$
E(2)-GeomNDP	$\mathbf{0.56_{\pm 0.01}}$	$\mathbf{0.65_{\pm 0.01}}$	$\mathbf{0.66_{\pm 0.01}}$

2D invariant Gaussian vector fields (Cont'd)



Global tropical cyclone trajectory prediction

Learn $f : \mathbb{R} \to \mathcal{S}^2$ from hurricane trajectory data (Knapp et al., 2018).

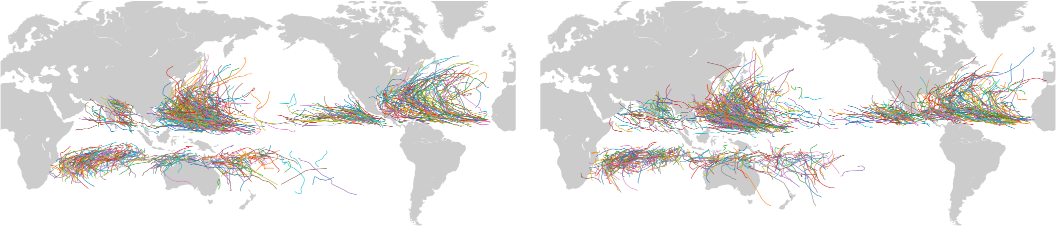
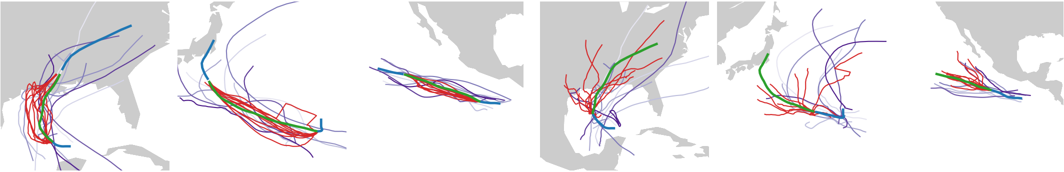


Figure 13: *Left:* 1000 samples from the training data. *Right:* 1000 samples from trained model.

Global tropical cyclone trajectory prediction (Cont'd)



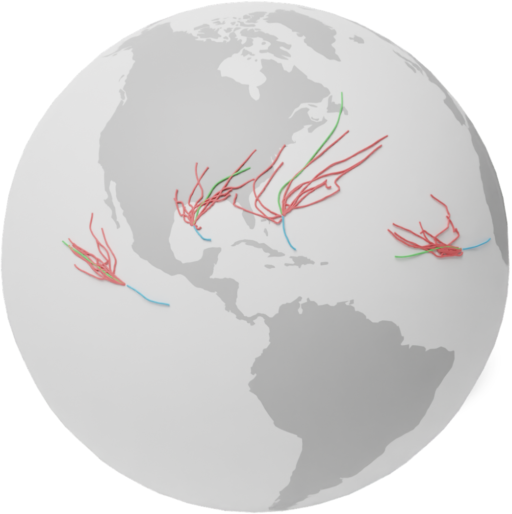
(a) Interpolation **(b)** Extrapolation

Model	Test data	Interpolation		Extrapolation	
	Likelihood	Likelihood	MSE (km)	Likelihood	MSE (km)
GeomNDP($\mathbb{R} \to \mathcal{S}^2$)	$\mathbf{802}_{\pm 5}$	$\mathbf{535}_{\pm 4}$	$\mathbf{162}_{\pm 6}$	$\mathbf{536}_{\pm 4}$	$\mathbf{496}_{\pm 14}$
Stereo GP ($\mathbb{R} \to \mathbb{R}^2/\{0\}$)	$393_{\pm 3}$	$266_{\pm 3}$	$2619_{\pm 13}$	$245_{\pm 2}$	$6587_{\pm 55}$
NDP ($\mathbb{R} \to \mathbb{R}^2$)	-	-	$166_{\pm 22}$	-	$769_{\pm 48}$
GP ($\mathbb{R} \to \mathbb{R}^2$)	-	-	$6852_{\pm 41}$	-	$8138_{\pm 87}$

Recap: Geometric diffusion neural processes

- Aim: probabilistic model over features fields.
- Constructed diffusion models over function space by correlating finite marginals
- Incorporating group invariance by
  - targetting invariant Gaussian processes and
  - parameterising the score with an equivariant neural network
- Sampling from the conditional process
- Empirically demonstrated modelling capacity on scalar and vector fields, with Euclidean and spherical output space

Thank you for your attention. Questions?



Credits to Michael Hutchinson for this 3D render.

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