Emergent structure of the learned action functional landscape from data

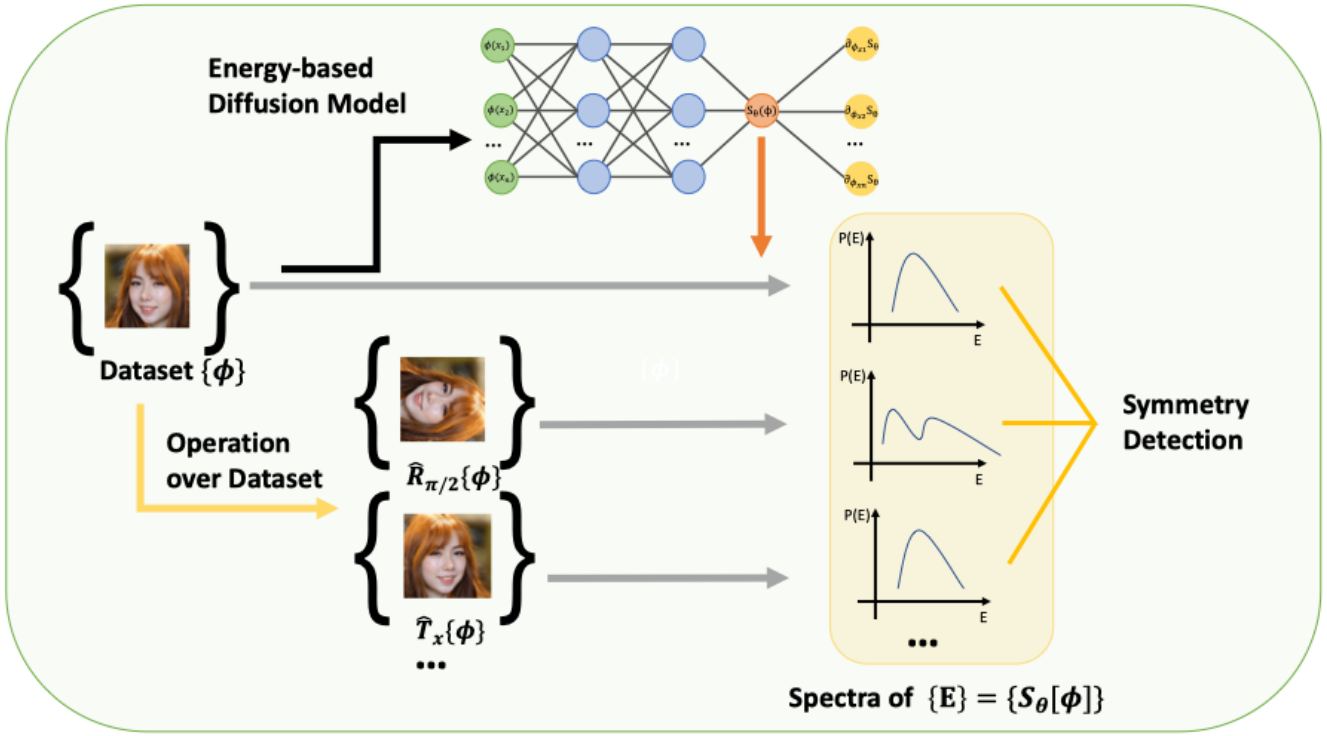
Jinyang Li

Collaborating with: Lingxiao Wang ,Yangyang Tan and Satoshi Iso

1. Overview

Diffusion Model: $\{\phi(x)\} \sim P[\phi] = \lim_{t\to 0} \frac{1}{Z_t} e^{-S_\theta[\phi(x),t]}$ ⟺ **Field theory explanation**

- Symmetry
- Local minima (1st order derivative)
- Hessian structure (2nd order derivative)
- Landscape (Data encoding structure)
- Topology extraction
- Effective interpretations ……

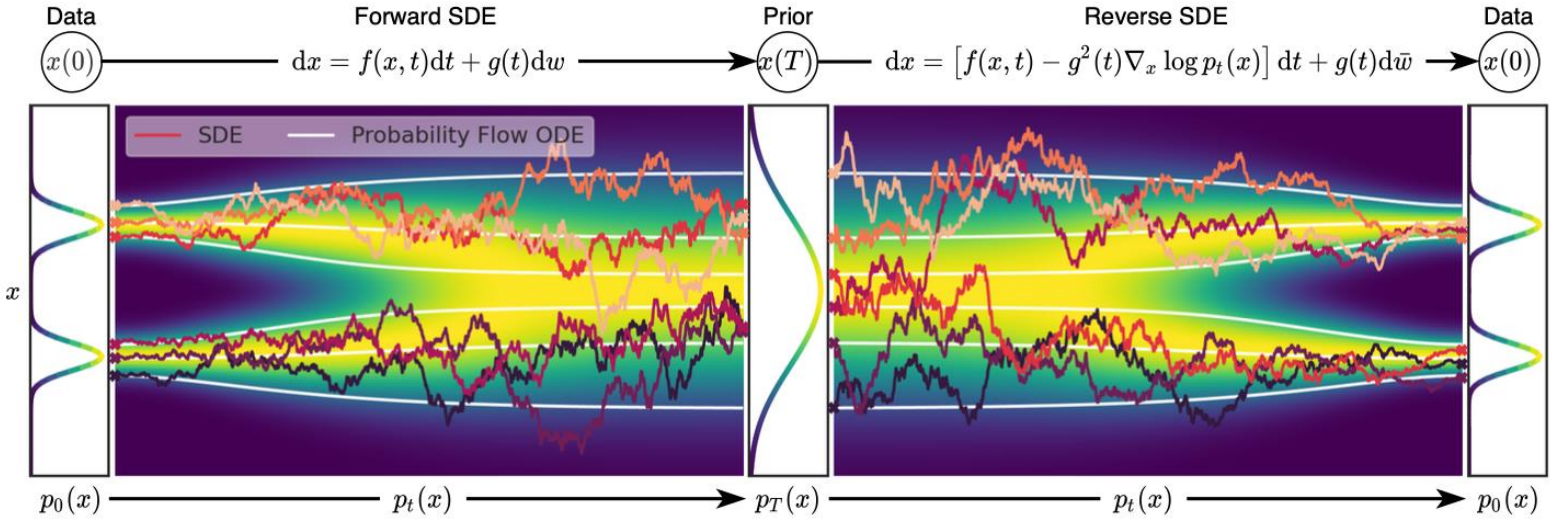


2. Diffusion model and Energy-based Diffusion Model

Diffusion model in equations

arXiv:2011.13456v2

Noise (Trivial Distribution)



Dataset ≈ Nontrivial Distribution

Rebuilt Nontrivial Distribution

Stochastic Differential Equation (SDE)

$$\mathrm{d}\vec{x} = \vec{f}(\vec{x}, t)\,\mathrm{d}t + \mathbf{G}(\vec{x}, t)\,\mathrm{d}\vec{w}$$

Fokker-Planck Equation

$$\partial_t p(\vec{x}, t) = -\nabla \cdot \vec{j}(\vec{x}, t)$$

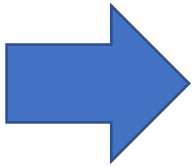
where

$$\begin{cases} \vec{j} = \tilde{\vec{f}}\, p, \\ \tilde{\vec{f}}(\vec{x}, t) := \vec{f}(\vec{x}, t) - \frac{1}{2}\nabla \cdot \left[\mathbf{G}(\vec{x}, t)\mathbf{G}(\vec{x}, t)^{\mathsf{T}}\right] - \frac{1}{2}\mathbf{G}(\vec{x}, t)\mathbf{G}(\vec{x}, t)^{\mathsf{T}}\nabla_{\vec{x}} \log p_t(\vec{x}). \end{cases}$$

For reverse process

$$\mathrm{d}x = \left[f(x,t) - g^2(t)\nabla_x \log p_t(x)\right]\mathrm{d}t + g(t)\mathrm{d}\bar{w}$$

$$\mathcal{L} = \int dt\mathcal{L}_{SM} = \int dt E_{x_t \sim p_t}\left[\|s_\theta(x,t) - \nabla_x \log p(x,t)\|^2\right] = \int dt \int dx q(x,t)\,\|s_\theta(x,t) - \nabla_x \log p(x,t)\|^2$$



$$s_\theta(x,t) \approx \nabla_x \log p(x,t) \qquad \forall x,t$$

Energy-based Diffusion Model

arXiv:2510.01328v1 [hep-lat]

Score as derivative of scalar $s_\theta(x,t) = -\nabla_x S_\theta(x,t) = -\nabla_x |v_\theta(x,t)|^2$

remind $s_\theta(x,t) \approx \nabla_x \log p(x,t) \quad \forall x,t$

Diffusion model describes any given dataset as analog-action

Dataset ≈ Nontrivial Distribution

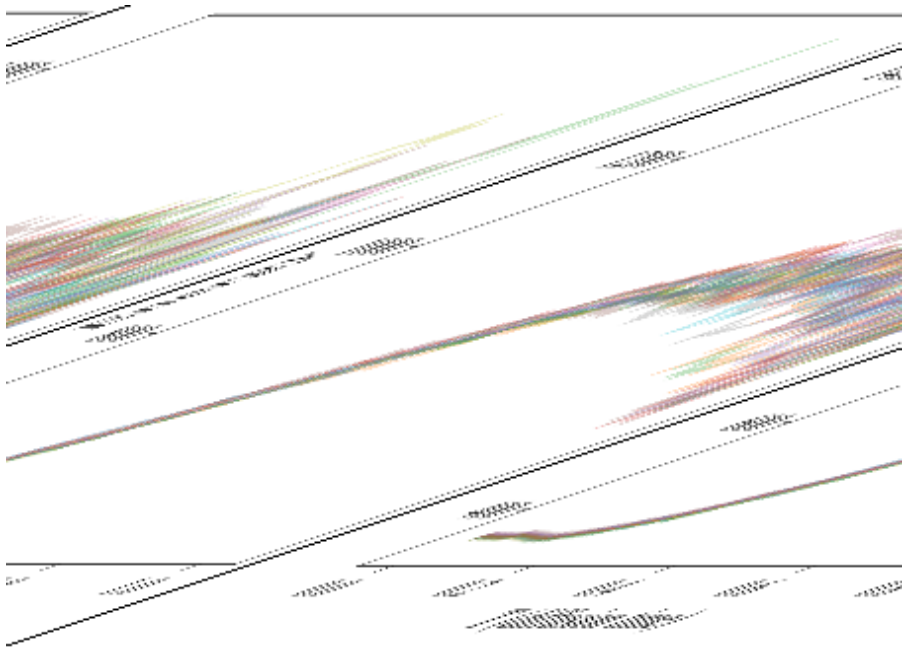


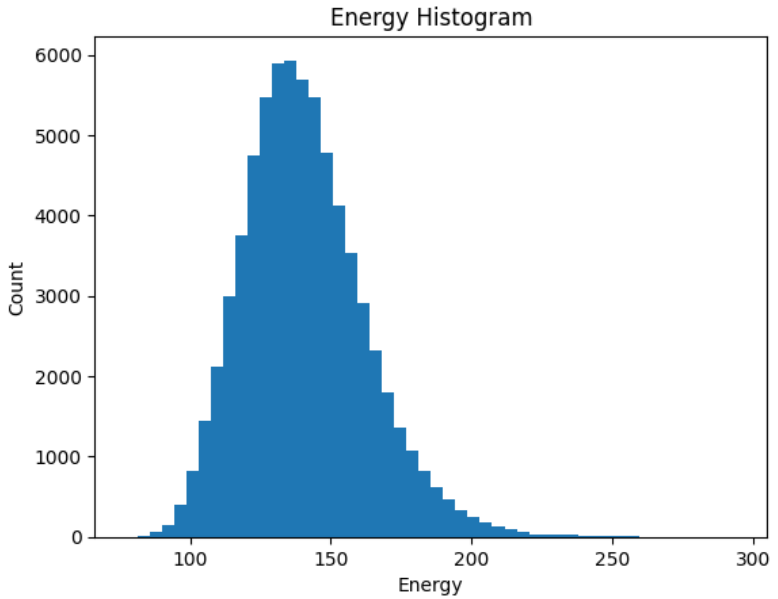
$$Z = \int Dx\, e^{-S_\theta(x,t)}$$



2501.09064v1







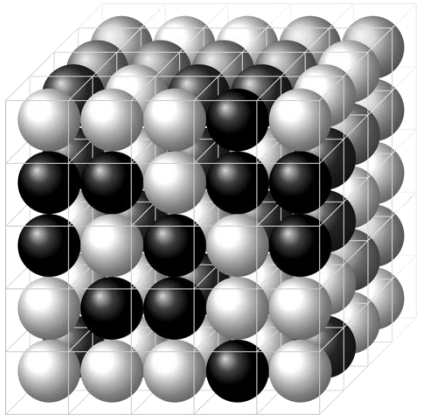
Energy spectrum at T=0 for whole dataset

3. Symmetry

What is Symmetry?

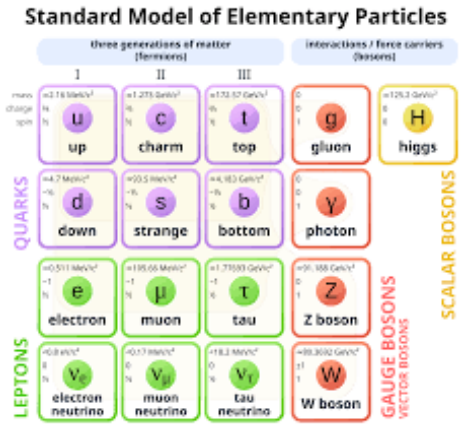
The **symmetry** of a physical system is a physical or mathematical feature of the system (observed or intrinsic) that is preserved or remains unchanged under some transformation.
——From Wiki (https://en.wikipedia.org/wiki/Symmetry_(physics))

Observed (Data point level)





Intrinsic (Action level)



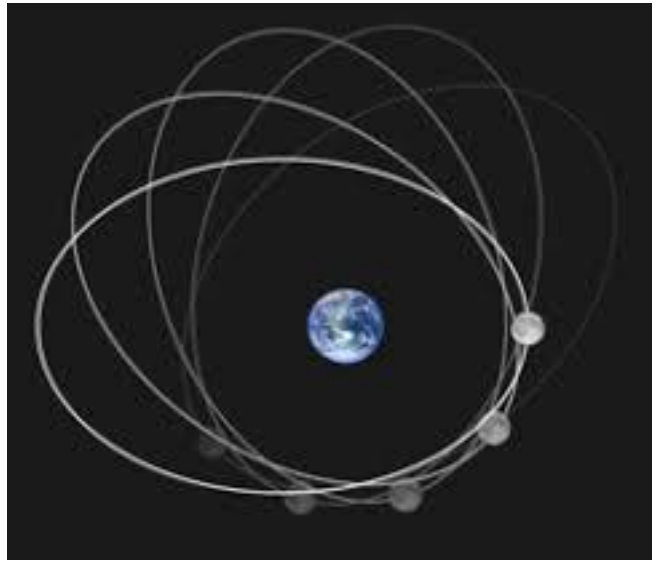
$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R + \Lambda g_{\mu\nu} = 8\pi G T_{\mu\nu}.$$

Diffeomorphism

$$U(1) \times SU(2)_w \times SU(3)_c$$

Symmetry in Action level usually doesn't mean symmetry at Data point level

$$L = \frac{1}{2} m_E \dot{\mathbf{r}}_E^2 + \frac{1}{2} m_M \dot{\mathbf{r}}_M^2 + \frac{G m_E m_M}{r}$$



Action level:

$$t \to t + \varepsilon$$

Time translation

$$\mathbf{r} \to \mathcal{R}\mathbf{r} \quad (\mathcal{R} \in SO(3))$$

Spacial Rotation

$$\mathbf{r}_E \to \mathbf{r}_E + \mathbf{a}, \quad \mathbf{r}_M \to \mathbf{r}_M + \mathbf{a}$$

Spacial translation

Data point level:

Periodicity

4. Discovering Symmetry from Energy-Based Diffusion Models

What Symmetry means now

Rephrase into field theory language

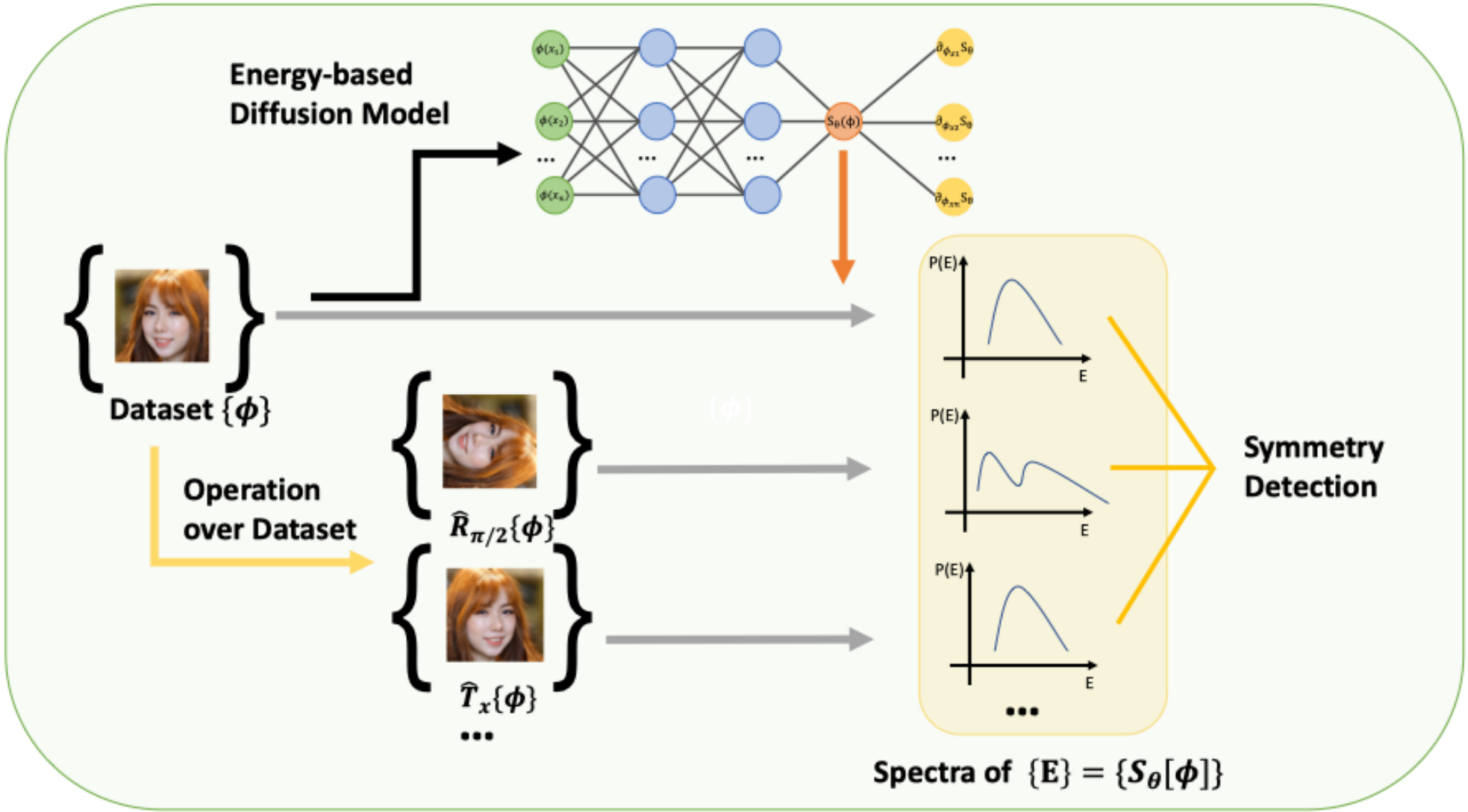
$$\vec{x} \rightarrow \phi(x) \qquad Z = \int D\phi(x)\, e^{-S_\theta[\phi(x),t]}$$

Symmetry in action level means:

$$S'(\phi'(x)) = S_\theta(\phi'(x))$$

$$\phi'(x) = \hat{T}\phi(x)$$

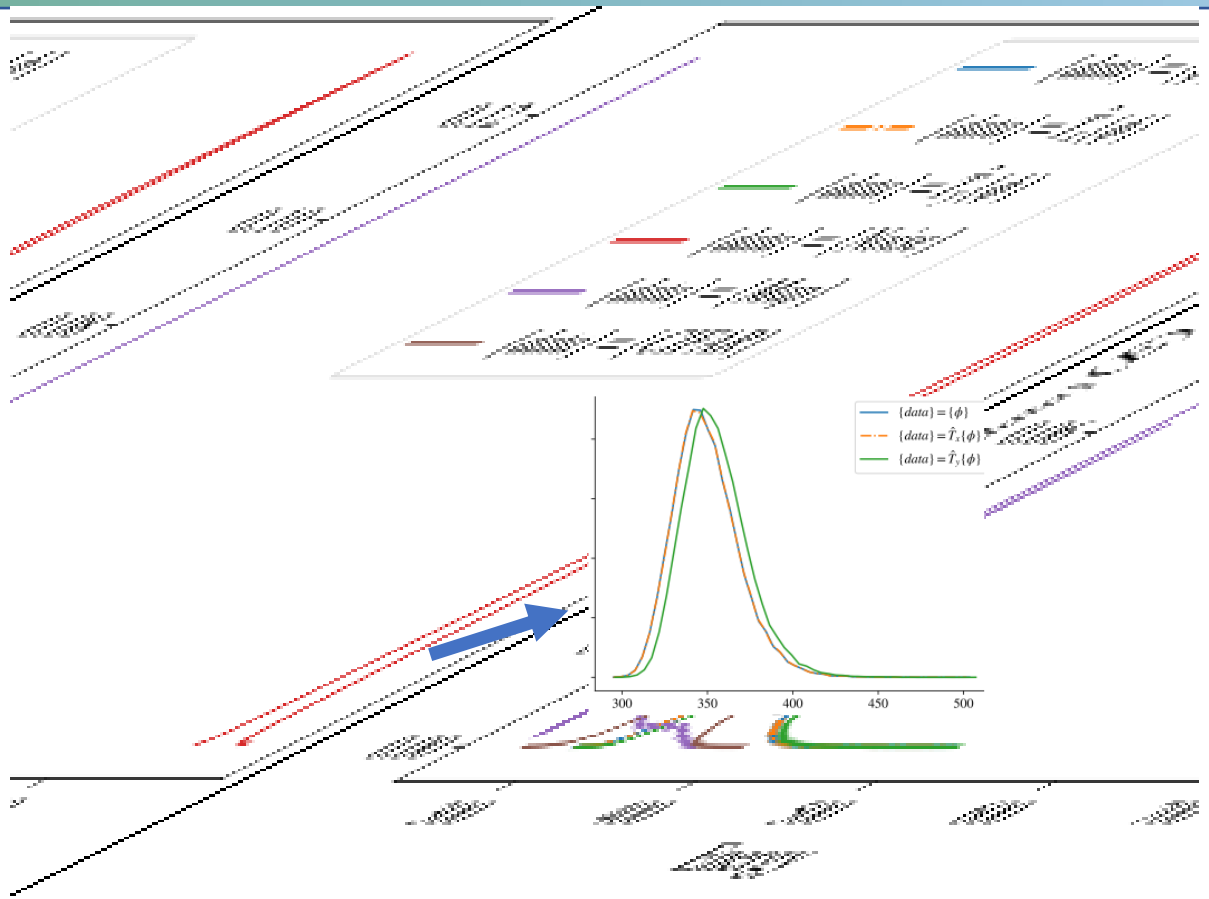
T stands for any possible (**group) operation**,


Energy-based
Diffusion Model
Dataset $\{\phi\}$
Operation
over Dataset
$\hat{R}_{\pi/2}\{\phi\}$
$\hat{T}_x\{\phi\}$
P(E)
E
Symmetry
Detection
Spectra of $\{\mathbf{E}\} = \{S_\theta[\phi]\}$

On FFHQ dataset

https://github.com/NVlabs/ffhq-dataset





Energy distribution of whole dataset (w/o flip)

Symmetry Operation	$D_{\mathrm{SKL}}/10^{-2}$	$D_{\mathrm{L2}}/10^{-2}$
Reflection (x-direction)	0.1265	0.0017
Reflection (y-direction)	4.9047	1.3607

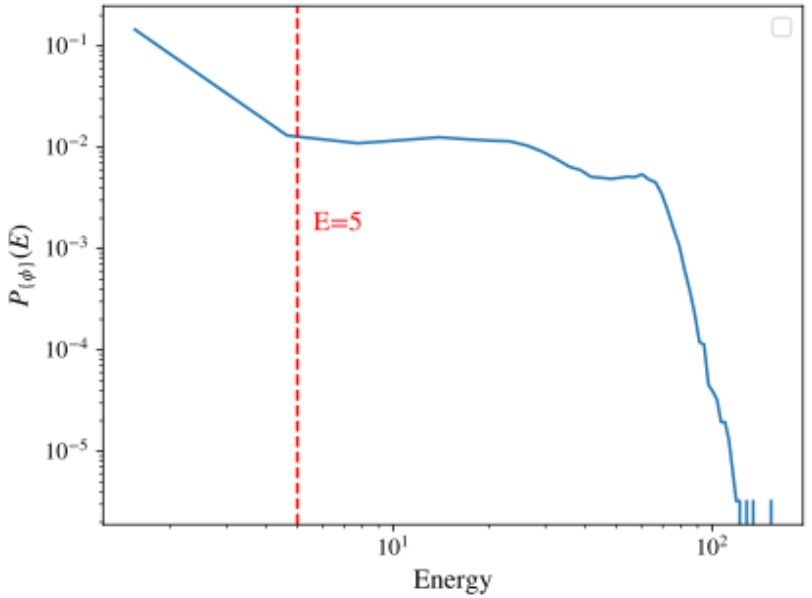
$$D_{\mathrm{SKL}}(P \,\|\, Q) = \frac{1}{2} \int \mathrm{d}x \, \left[P(x) \log \frac{P(x)}{Q(x)} + Q(x) \log \frac{Q(x)}{P(x)} \right]$$

$$D_{\mathrm{L2}}(P \,\|\, Q) = \int \mathrm{d}x \, \left[P(x) - Q(x) \right]^2$$

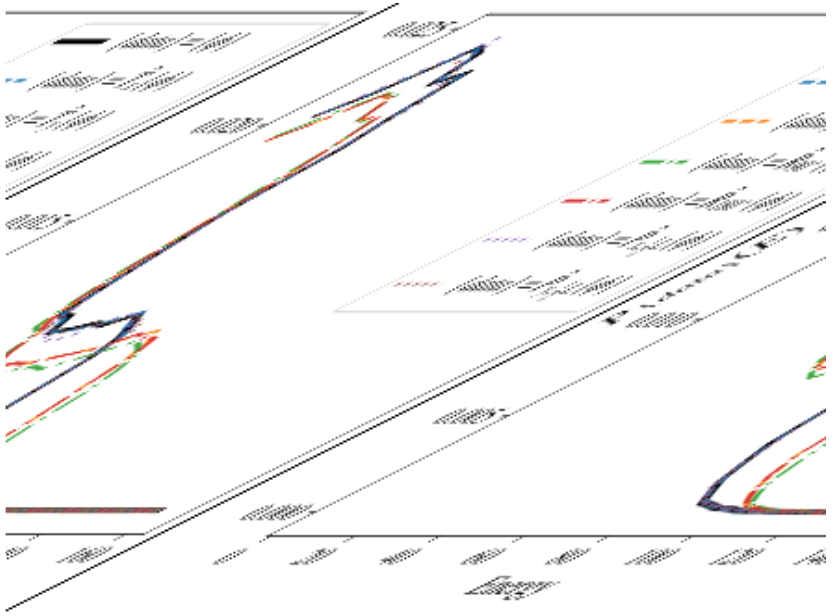
On Tokyo area dataset

Tokyo area W*H=46848*57344

16 examples W*H=128*128



Energy distribution



Energy distribution with operations

Symmetry Operation	$D_{SKL}/10^{-2}$	$D_{L2}/10^{-4}$
Reflection (x-direction)	0.1768	0.0146
Reflection (y-direction)	5.9895	5.0851
Translation (x-direction, $L/2$)	0.3021	0.1257
Translation (y-direction, $L/2$)	0.2202	0.1220
Rotation (90°)	8.1004	6.4320
Rotation (180°)	5.9172	5.1434

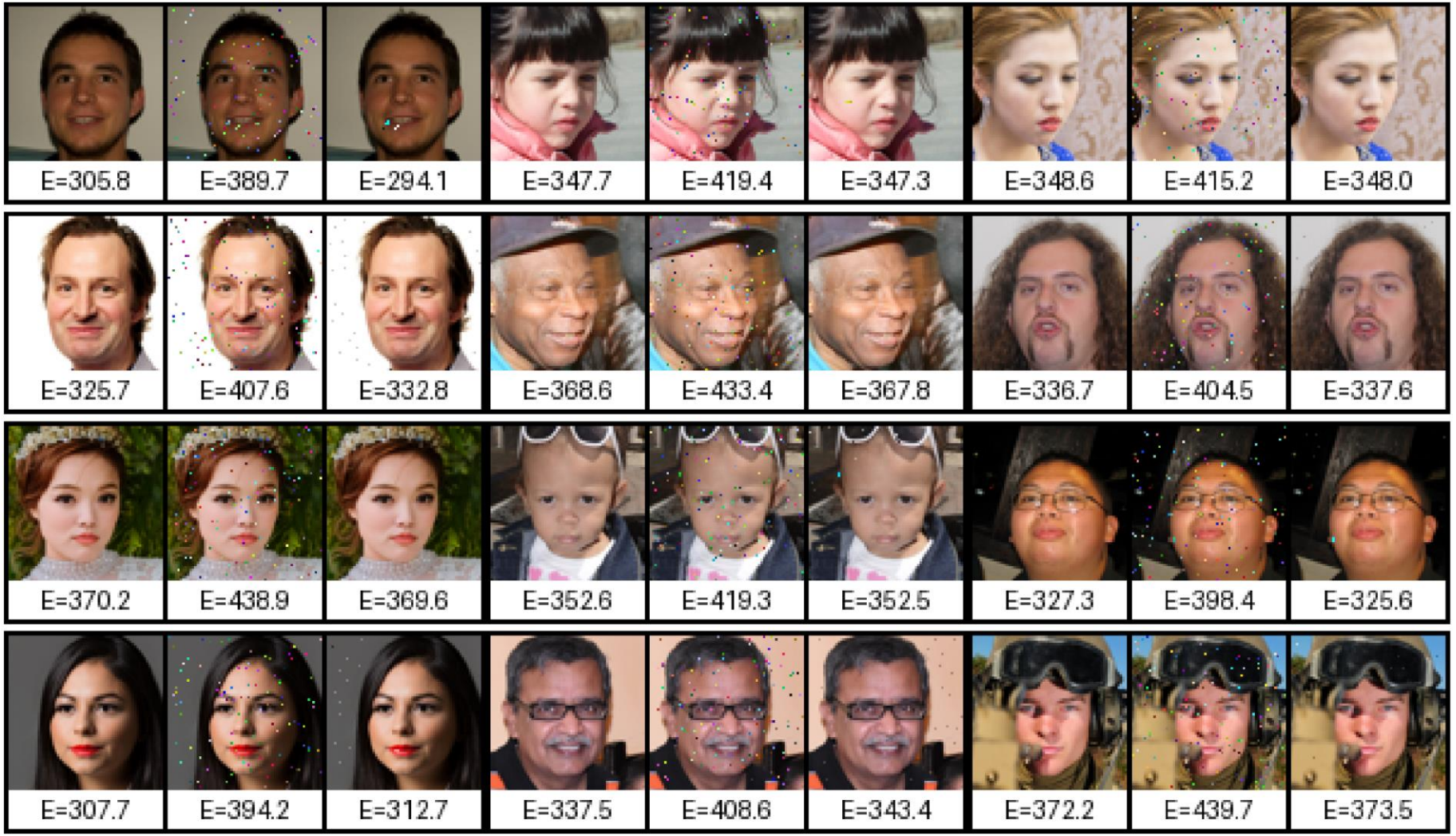
5. Emergent structures

Data-points are Local minima

Remind: $P[\phi] \sim e^{-S_\theta[\phi]}$

$$\frac{\delta S_\theta[\phi_i]}{\delta \phi} \approx 0$$

where ϕ_i corresponds to different data points in training data



Experimentally, we added perturbation over the data points and minimize the analogy action

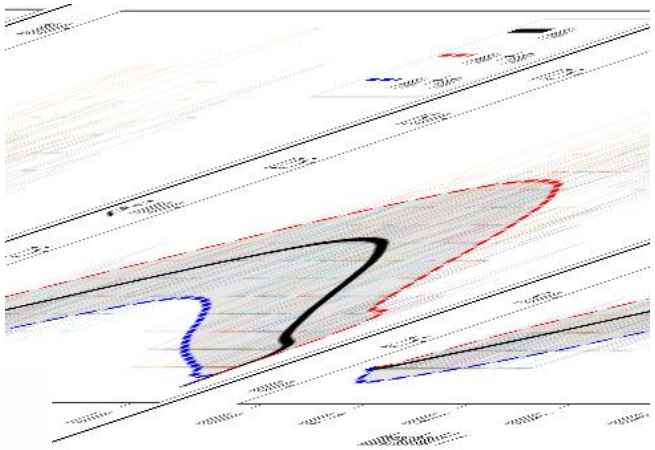
Hessian structure

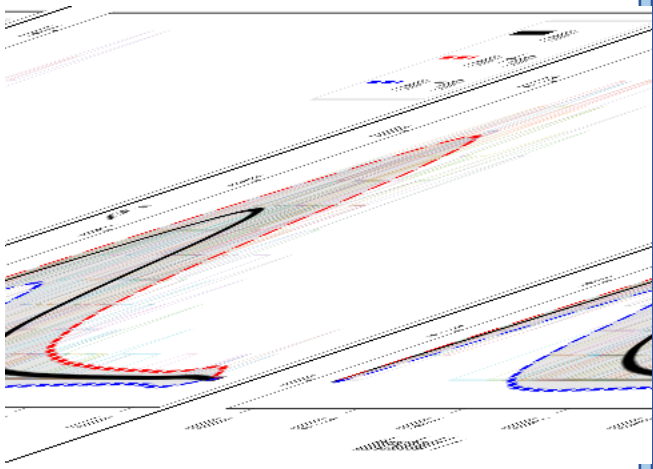
$$H_i(x,y) = \frac{\delta^2 S_\theta[\phi_i]}{\delta\vec{\phi}_c(x)\,\delta\vec{\phi}_c(y)}$$

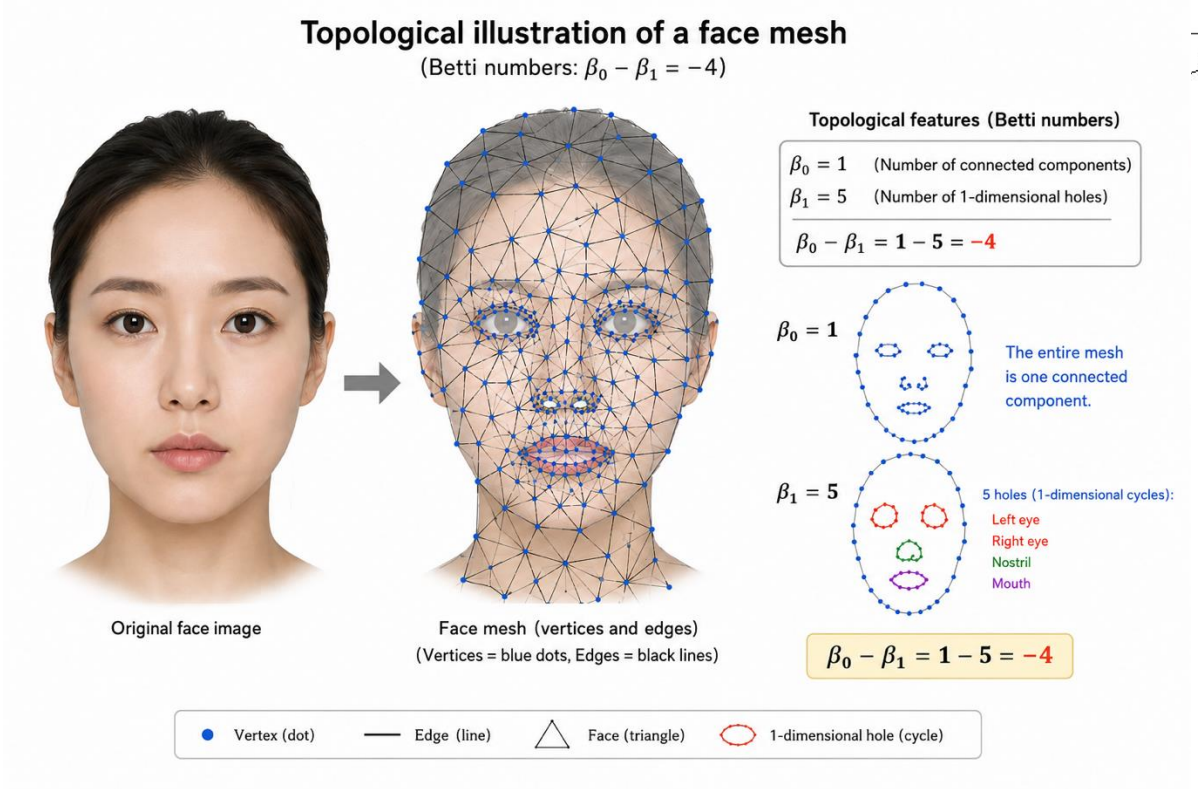


Several examples of diagonal component of $H_{\mathrm{i}}(x,x)$

Euler characteristic over $H_i(x, x)$







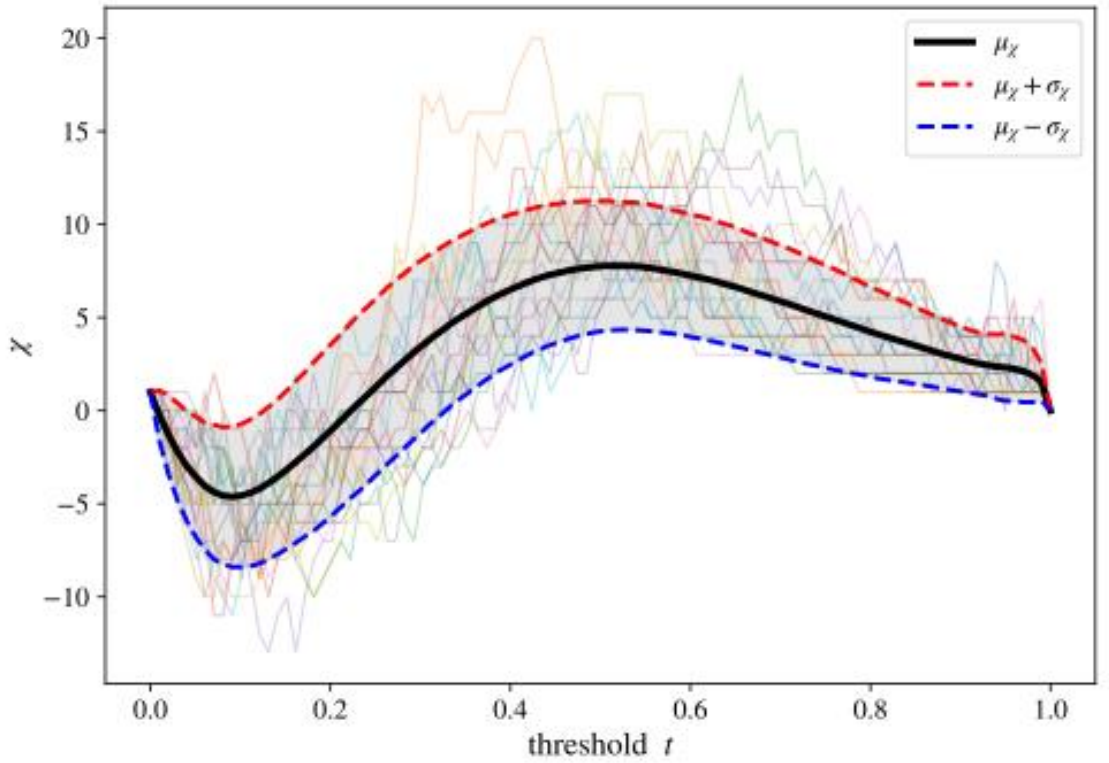
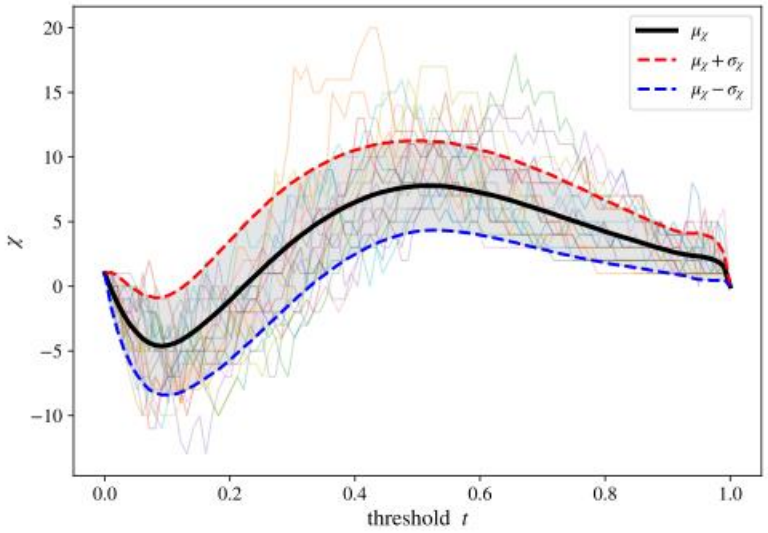


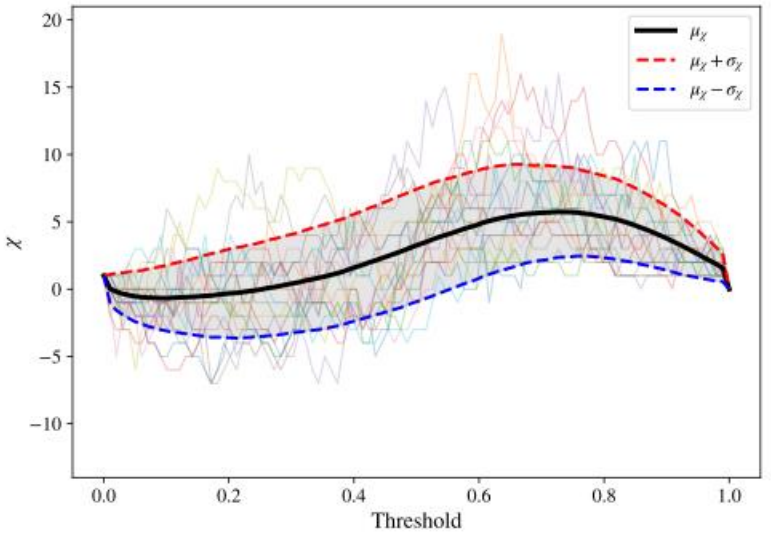
Illustration generated by ChatGPT5.5

Compared with Grayscale

Hessian



Grayscale

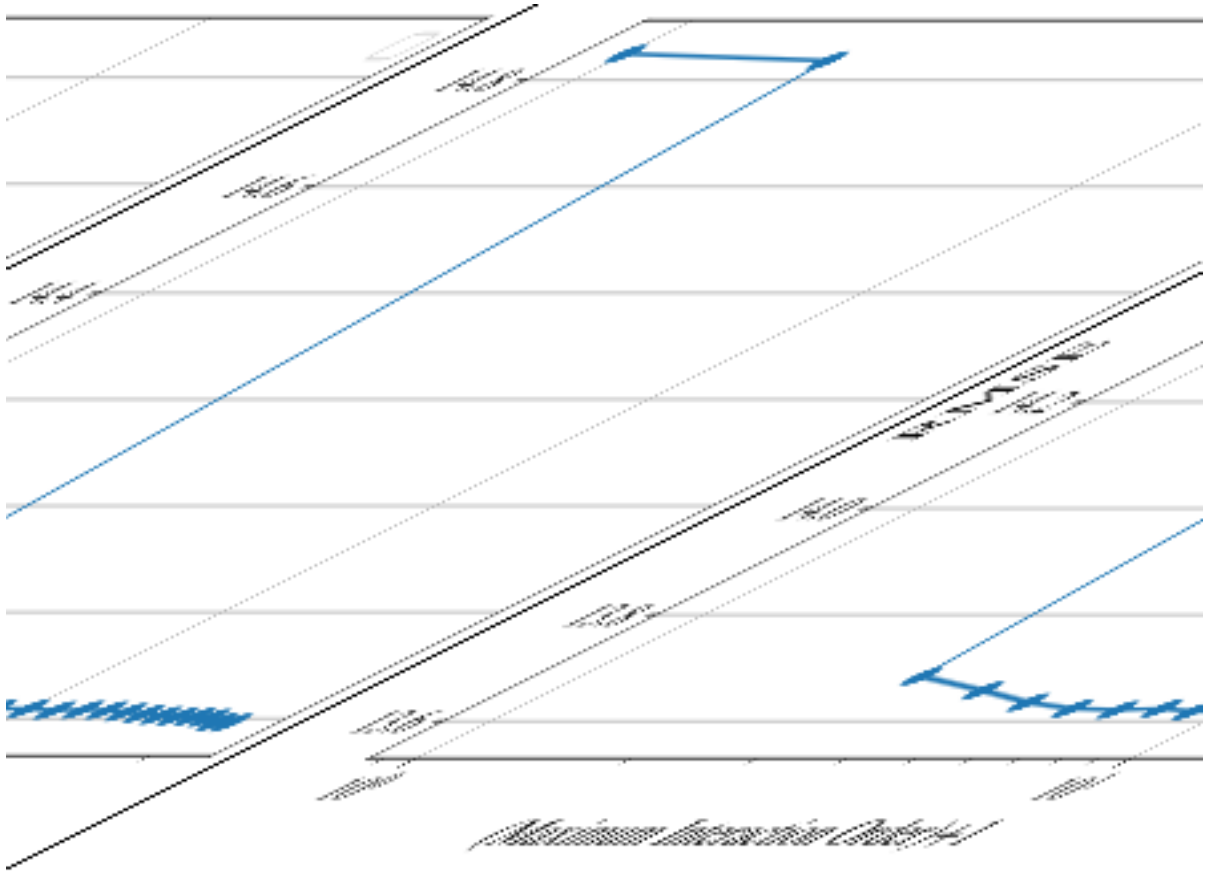




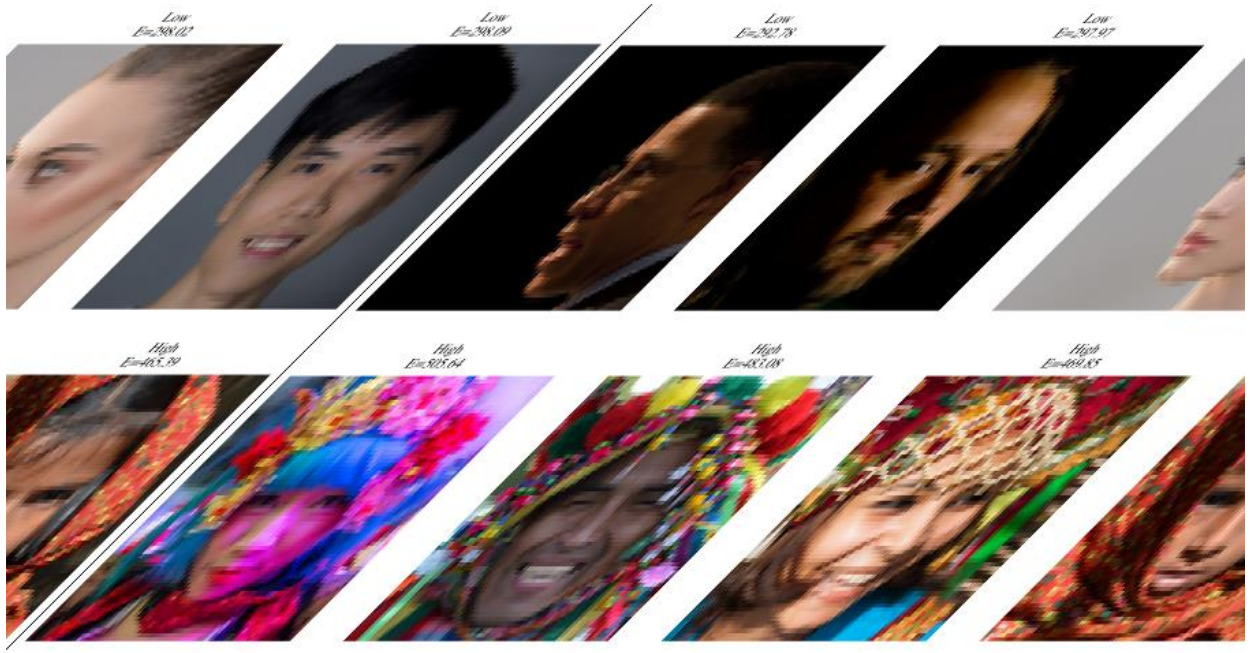
Effective interpretation with finite order field theory

$$S_{\text{eff}}[\phi] = \int dx \sum_c \left[\alpha_1 (\partial_x \phi_c)^2 + \alpha_2 (\partial_y \phi_c)^2 + \sum_{n=1}^{N} \lambda_n \phi_c^n \right] + C$$

with $$\text{RMSE}(N) = \sqrt{\frac{1}{M} \sum_{i=1}^{M} \left(S_\theta[\phi_i] - S_{\text{eff}}^{(N)}[\phi_i] \right)^2}$$



Highest and Lowest energy points in the dataset





THANK YOU

6. Renormalization Group Diffusion Models (RGDM)

For Gaussian noise

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I}) \quad q(\mathbf{x}_{1:T}|\mathbf{x}_0) = \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1})$$

$$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$$

where $\alpha_t = 1 - \beta_t$ and $\bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i$

After a bit of math: $$\mathcal{L}_{SM} = \int \mathrm{d}x_0\, \mathrm{d}x_t\; q(x_t, x_0)\; \|s_\theta(x_t) - \nabla_{x_t} \log q(x_t \mid x_0)\|^2 + C_2.$$

Renormalization Group in short

2202.11737v3

$$Z_\Lambda[J] := \int [d\phi]\, e^{-\frac{1}{2}\int \frac{d^d p}{(2\pi)^d}\left(\phi(p)\phi(-p)(p^2+m^2)K_\Lambda^{-1}(p^2)+J(p)\phi(-p)\right)-S_{\mathrm{int},\Lambda}[\phi]}$$

RG means: $$-\Lambda\frac{d}{d\Lambda}Z_\Lambda[J] = C_\Lambda\, Z_\Lambda[J]$$

(Any correlation functions below the changed scale stays the same.)

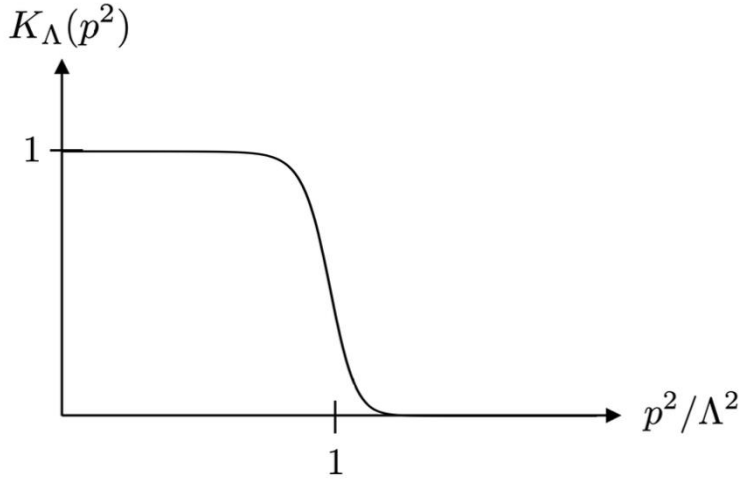


Figure 1: Depiction of a smooth cutoff function $K_\Lambda(p^2)$.

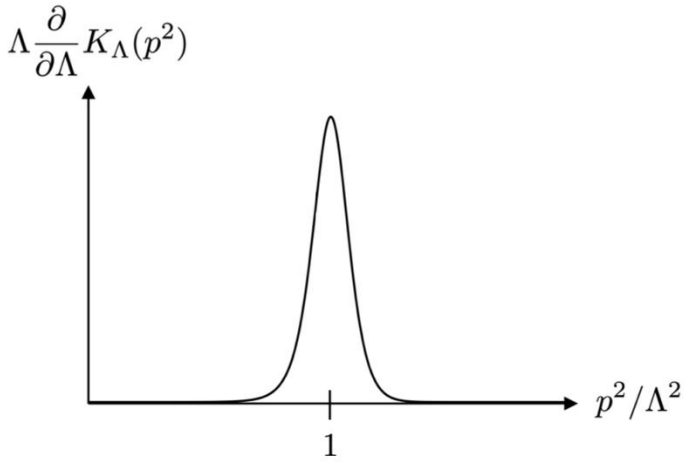


Figure 2: The derivative $\Lambda\frac{\partial}{\partial\Lambda}K_\Lambda(p^2)$ of the smooth cutoff function.

Polchinki's answer:

$$-\Lambda\frac{\partial S_{\mathrm{int},\Lambda}[\phi]}{\partial\Lambda} = \frac{1}{2}\int d^dp\,(2\pi)^d(p^2+m^2)^{-1}\,\Lambda\frac{\partial K_\Lambda(p^2)}{\partial\Lambda}\left\{\frac{\delta^2 S_{\mathrm{int},\Lambda}}{\delta\phi(p)\delta\phi(-p)} - \frac{\delta S_{\mathrm{int},\Lambda}}{\delta\phi(p)}\frac{\delta S_{\mathrm{int},\Lambda}}{\delta\phi(-p)}\right\}.$$

$$-\Lambda\frac{d}{d\Lambda}Z_\Lambda[J] = \left(-\frac{1}{2}\int d^dp\,\Lambda\frac{\partial\log K_\Lambda(p^2)}{\partial\Lambda}\,\delta^d(0)\right)\,Z_\Lambda[J]$$

$$-\Lambda\frac{d}{d\Lambda}\,P_\Lambda[\phi] = \frac{1}{2}\int d^dp\,(2\pi)^d(p^2+m^2)^{-1}\,\Lambda\frac{\partial K_\Lambda(p^2)}{\partial\Lambda}\,\frac{\delta^2}{\delta\phi(p)\delta\phi(-p)}\,P_\Lambda[\phi]$$
$$+\int d^dp\,\Lambda\frac{\partial\log K_\Lambda(p^2)}{\partial\Lambda}\,\frac{\delta}{\delta\phi(p)}\,(\phi(p)\,P_\Lambda[\phi])$$

where $P_\Lambda[\phi] = e^{-S_\Lambda[\phi]}/Z_\Lambda$

More general answer (Wegner-Morris):

$$-\Lambda\frac{d}{d\Lambda}\,P_\Lambda[\phi] = \int d^dx\,\frac{\delta}{\delta\phi(x)}\,(\Psi_\Lambda[\phi,x]\,P_\Lambda[\phi])$$

$$\Psi_\Lambda[\phi,x] = -\int d^dy\,\frac{1}{2}\,\dot{C}_\Lambda(x-y)\,\frac{\delta\Sigma_\Lambda[\phi]}{\delta\phi(y)}\,,$$

Renormalization Group Diffusion Models (RGDM)

2308.12355v2
2501.09064v1

On discrete basis

$$\partial_t p_t(\phi) = -\frac{1}{2}\sum_k \frac{v}{k^2}\frac{\partial_t K_t(k)}{K_t(k)}\frac{\partial^2 p_t(\phi)}{\partial^2 \phi_k} - \sum_k \frac{\partial}{\partial \phi_k}\left(\frac{1}{2}\frac{\partial_t K_t}{K_t}\phi_k p_t(\phi)\right)$$

Realize by SDE

$$\text{forward}: \phi_{tk} = \sqrt{\bar{\alpha}_{tk}}\phi_{0k} + \sqrt{\bar{\beta}_{tk}}\epsilon_k,$$

$$\text{backward}: \phi_{t-1k} = \frac{1}{\sqrt{\alpha_{tk}}}\left(\phi_{tk} - \frac{\beta_{tk}}{\bar{\beta}_{tk}}\xi_{\theta k}(\phi_t, t)\right) + \sqrt{\beta_{tk}}\epsilon_k,$$

where

$$\bar{\alpha}_{tk} = K_t(k), \quad \alpha_{tk} = \begin{cases} K_t(k) & (t=1) \\ K_t(k)/K_{t-1}(k) & (t=2,\ldots,T) \end{cases},$$

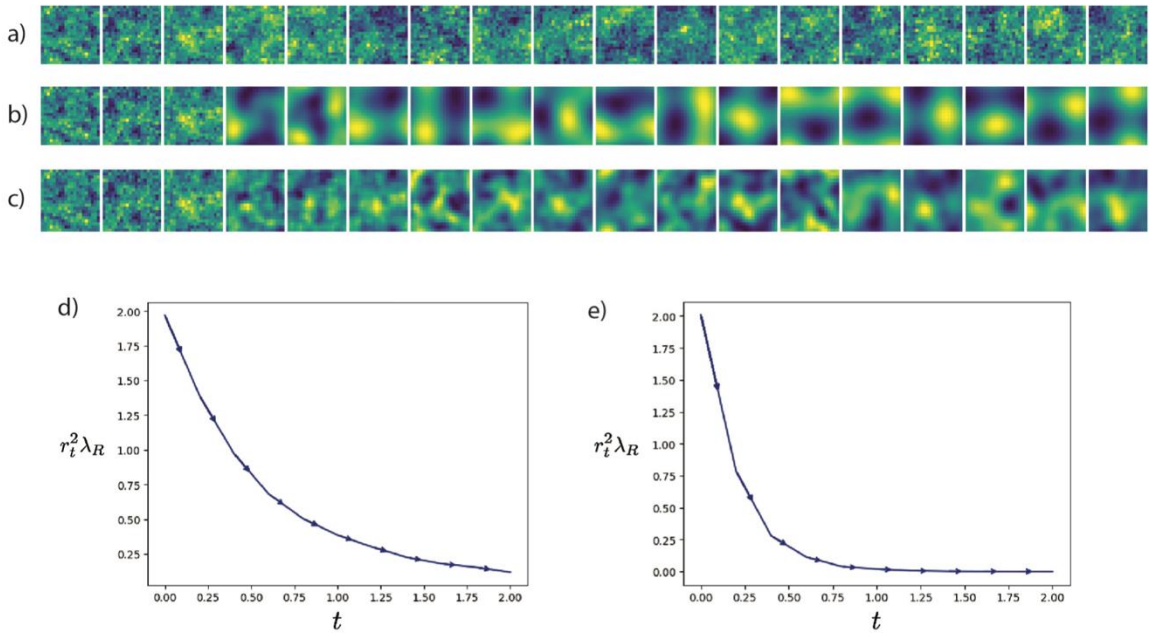
$$\bar{\beta}_{tk} = \frac{v}{k^2+m^2}(1-\bar{\alpha}_{tk}), \quad \beta_{tk} = \frac{v}{k^2+m^2}(1-\alpha_{tk}),$$

$$K_t(k) = \frac{r_{tk}}{1+r_{tk}}, \quad r_{tk} = r\left(k^2/\Lambda_t^2\right), \quad \Lambda_t = \Lambda_0 e^{-t/\tau}.$$

Renormalizing Diffusion Models

Jordan Cotler[1,a] **and Semon Rezchikov**[2,3,b]

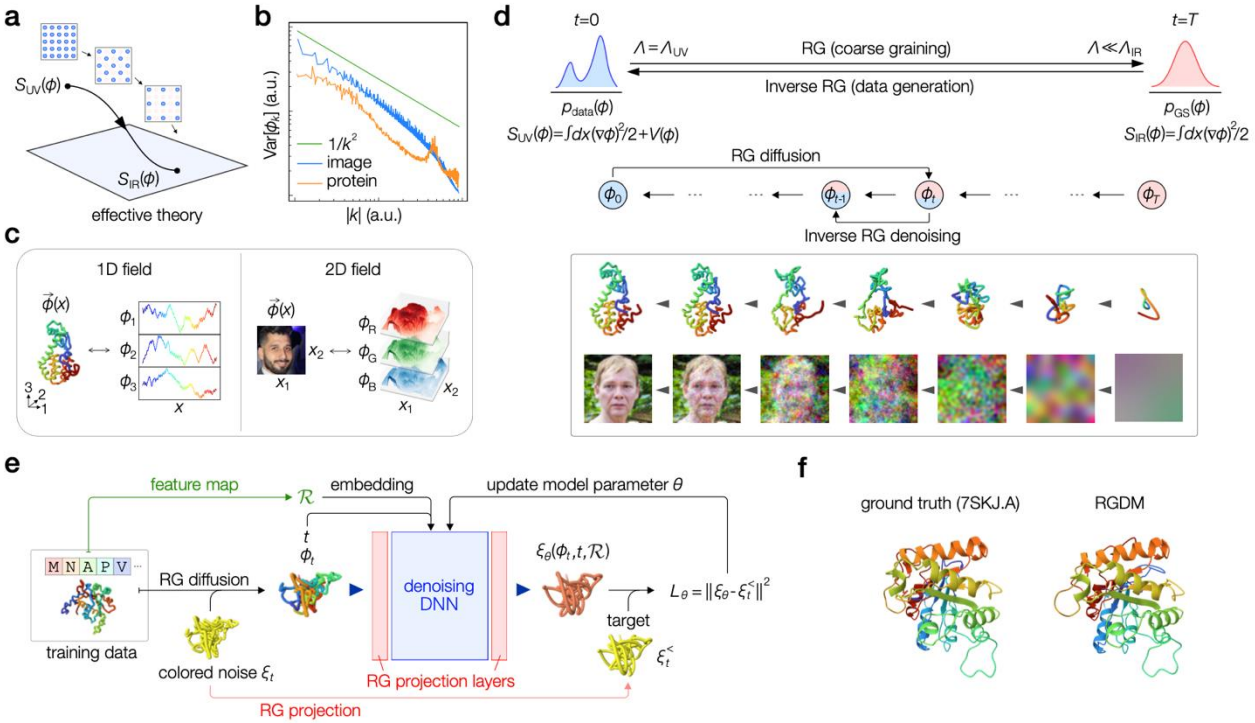
[1] *Society of Fellows, Harvard University, Cambridge, MA 02138, USA*
[2] *Department of Mathematics, Princeton University, Princeton, NJ 08544, USA*
[3] *Institute for Advanced Study, Princeton, NJ 08540, USA*



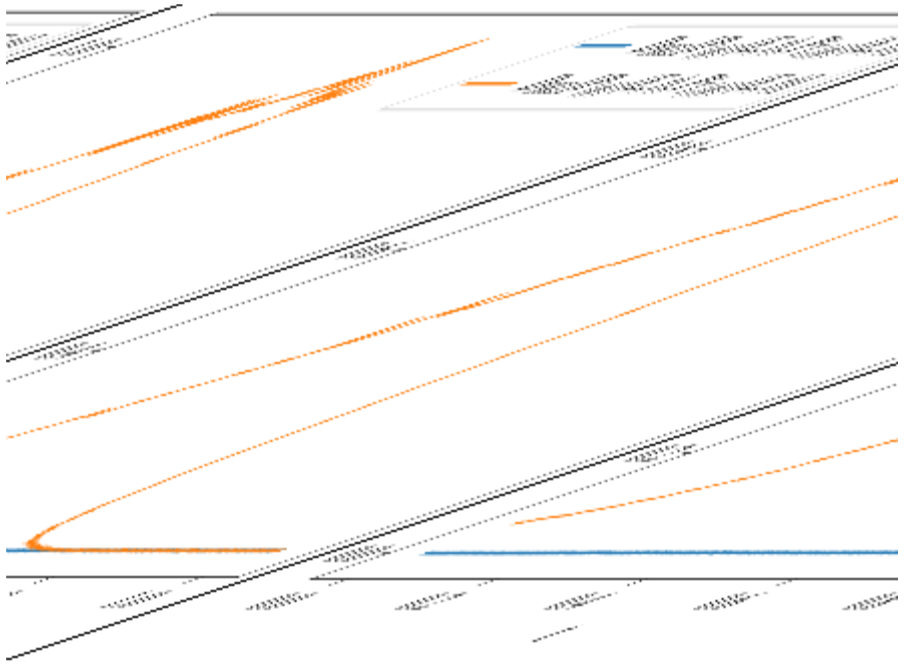
Generative diffusion model with inverse renormalization group flows

Kanta Masuki[1,*] and Yuto Ashida[1,2,†]

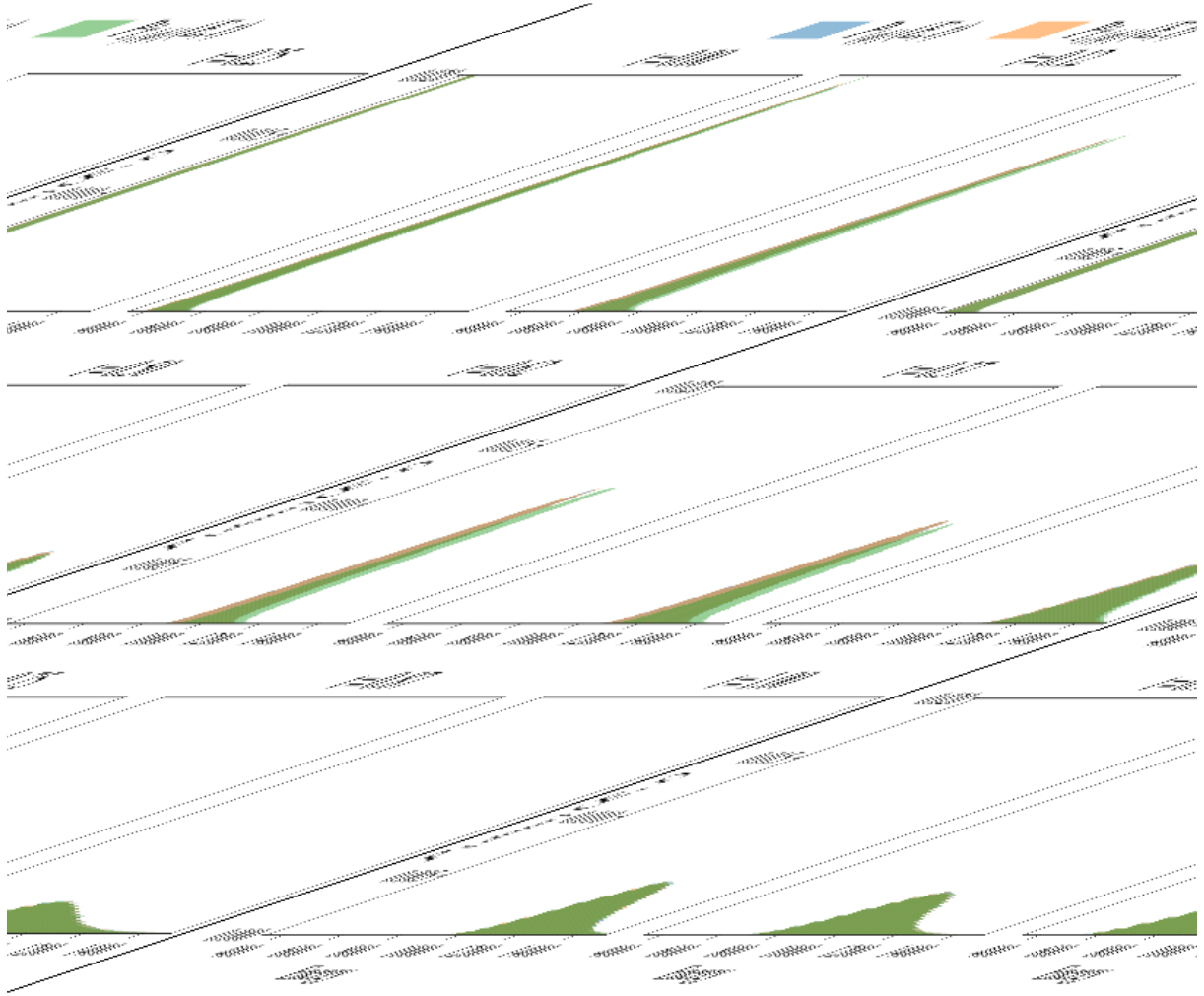
[1] *Department of Physics, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan*
[2] *Institute for Physics of Intelligence, The University of Tokyo, 7-3-1 Hongo, Tokyo 113-0033, Japan*



Energy-based RGDM



KL divergence over diffusion process in FFHQ experiment



Distributions at different snapshots

