

Unlocking Dis^{con}tinuities in Flow Models: Jumps, Control Flow, Insertions, Deletions, etc



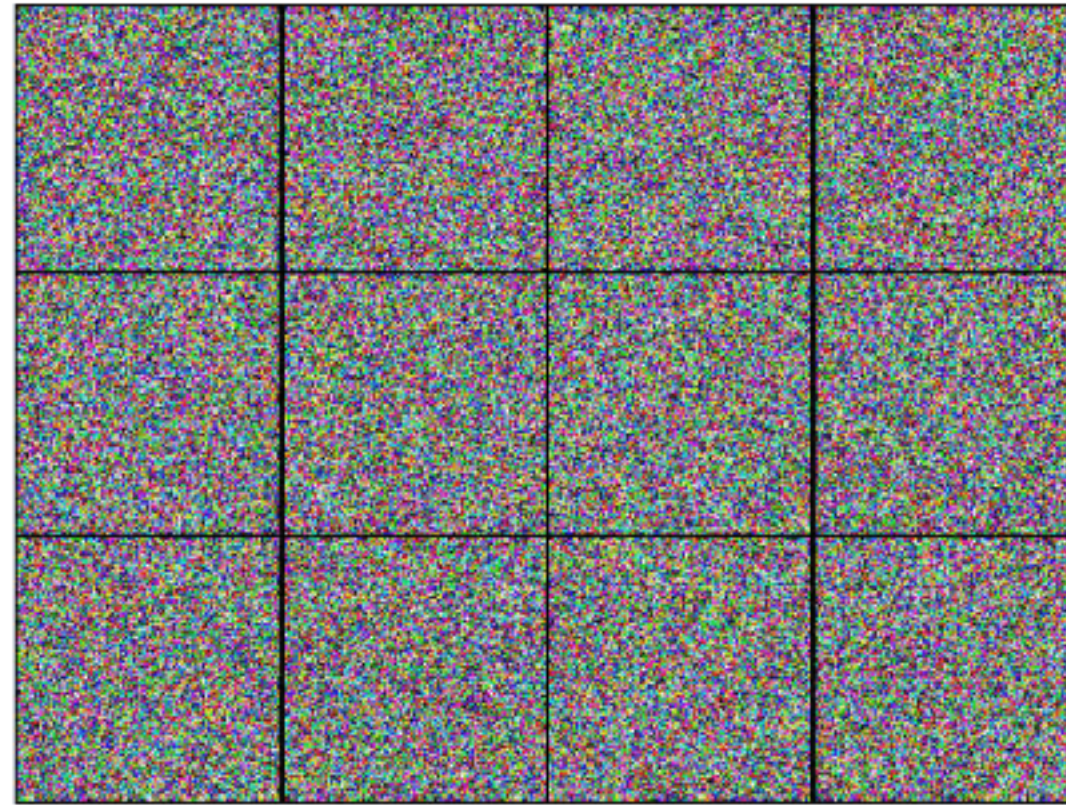
Ricky T. Q. Chen



About me and this talk

Data-driven

- fit to data
- simple & scalable



Flow Matching

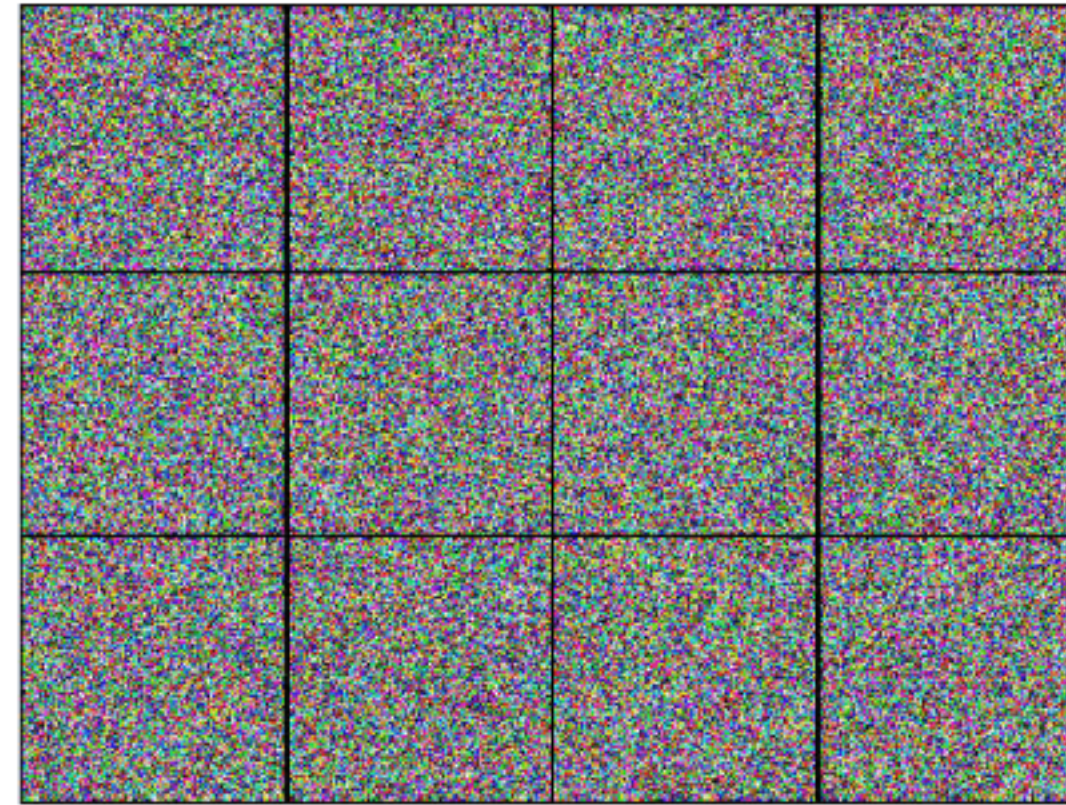


Meta MovieGen

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- fit to data
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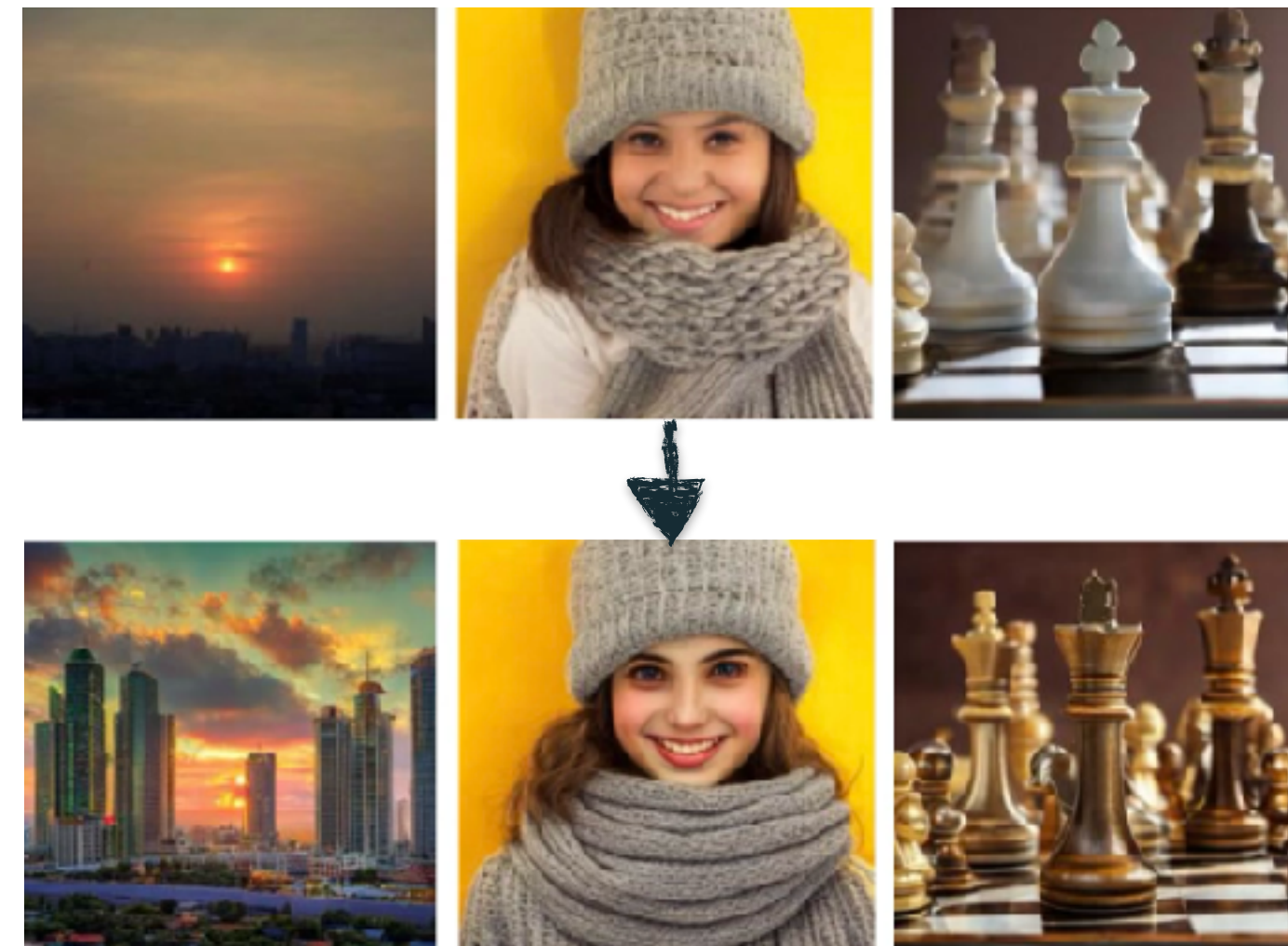
Flow Matching



Meta MovieGen

Reward-driven

- maximize reward
- no data available



Adjoint Matching

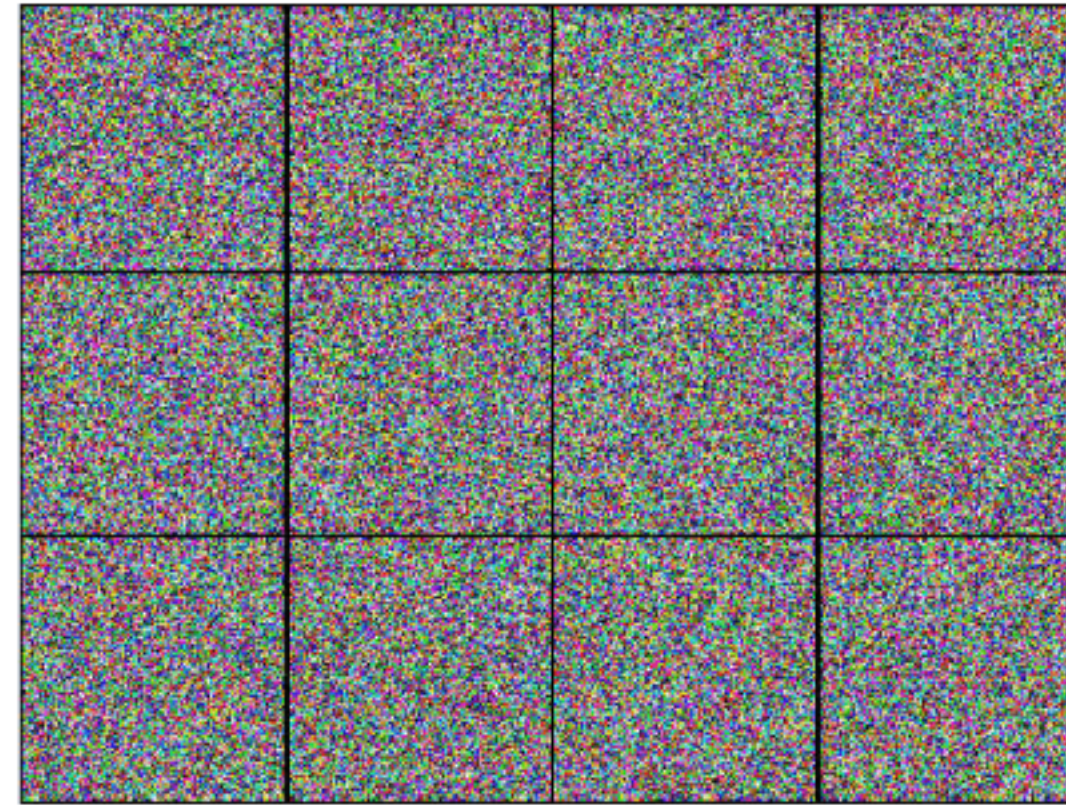


Adjoint Sampling

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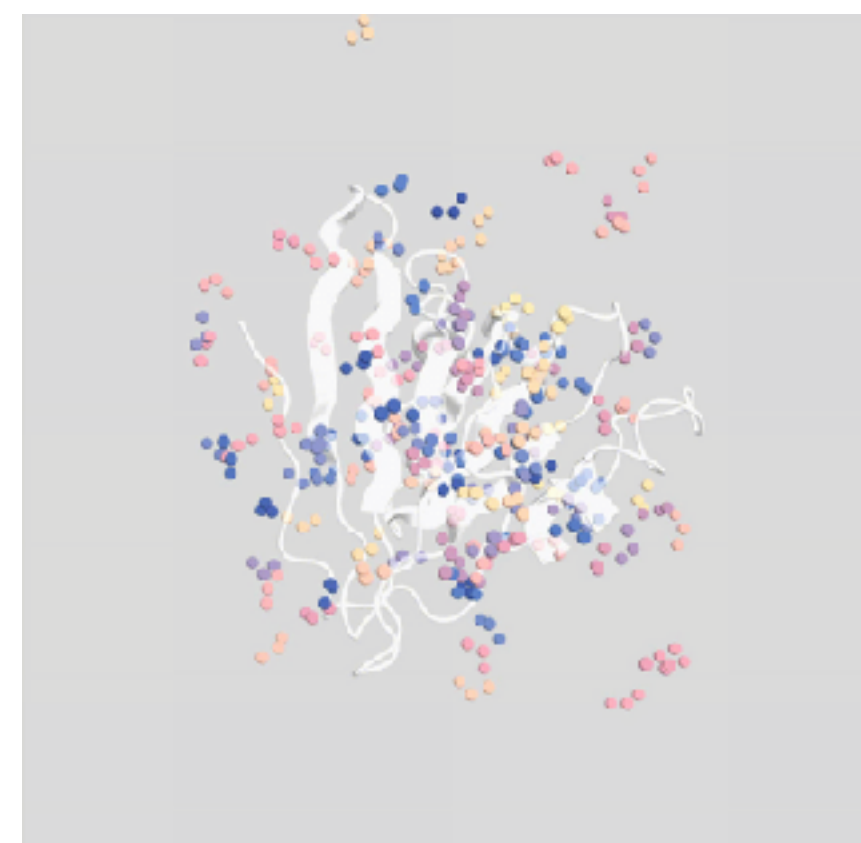
Flow Matching



Meta MovieGen

This Talk

- Generator Matching
- Discrete Flow Matching
- Edit Flows



```
def is_prime(n: int) -> bool:
```

Generator Matching

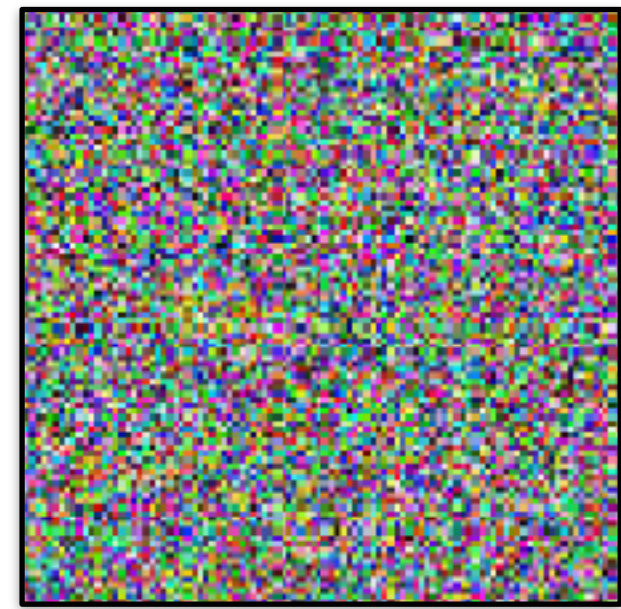
Extending the Flow Matching recipe to jump Markov processes

The Generative Modeling problem

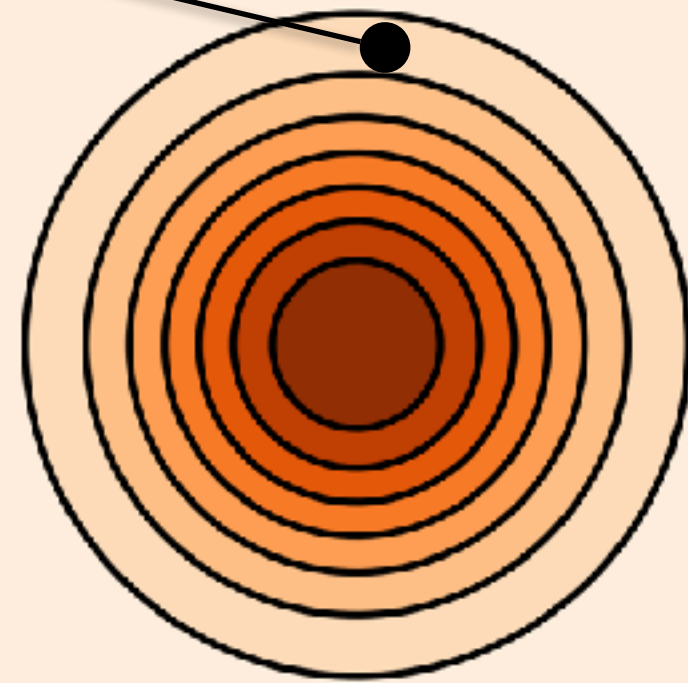
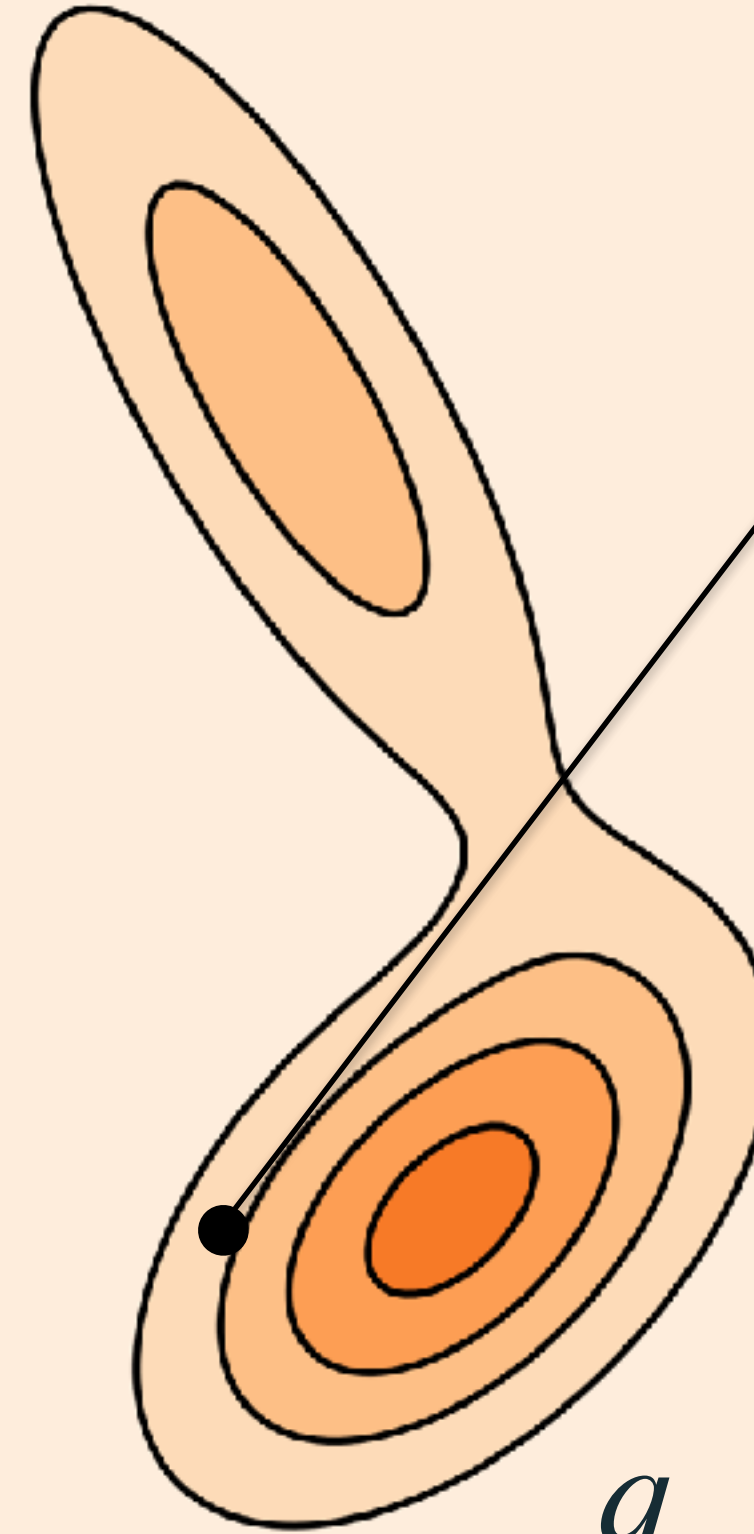
$\mathbb{R}^d$

A large, solid orange rectangle occupies the lower two-thirds of the slide. It represents the latent space $\mathbb{R}^d$ in the context of generative modeling.

The Generative Modeling problem

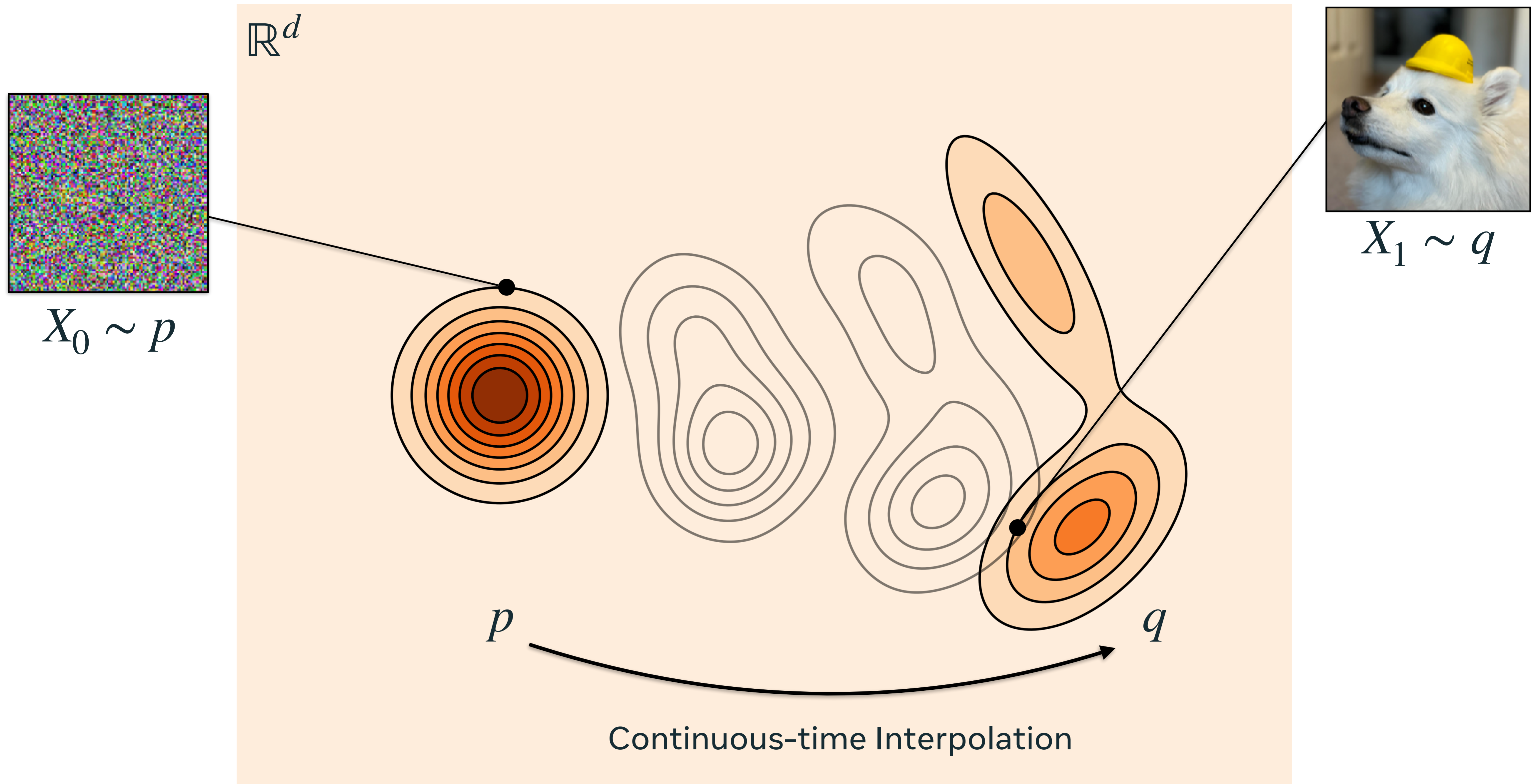


$$X_0 \sim p$$

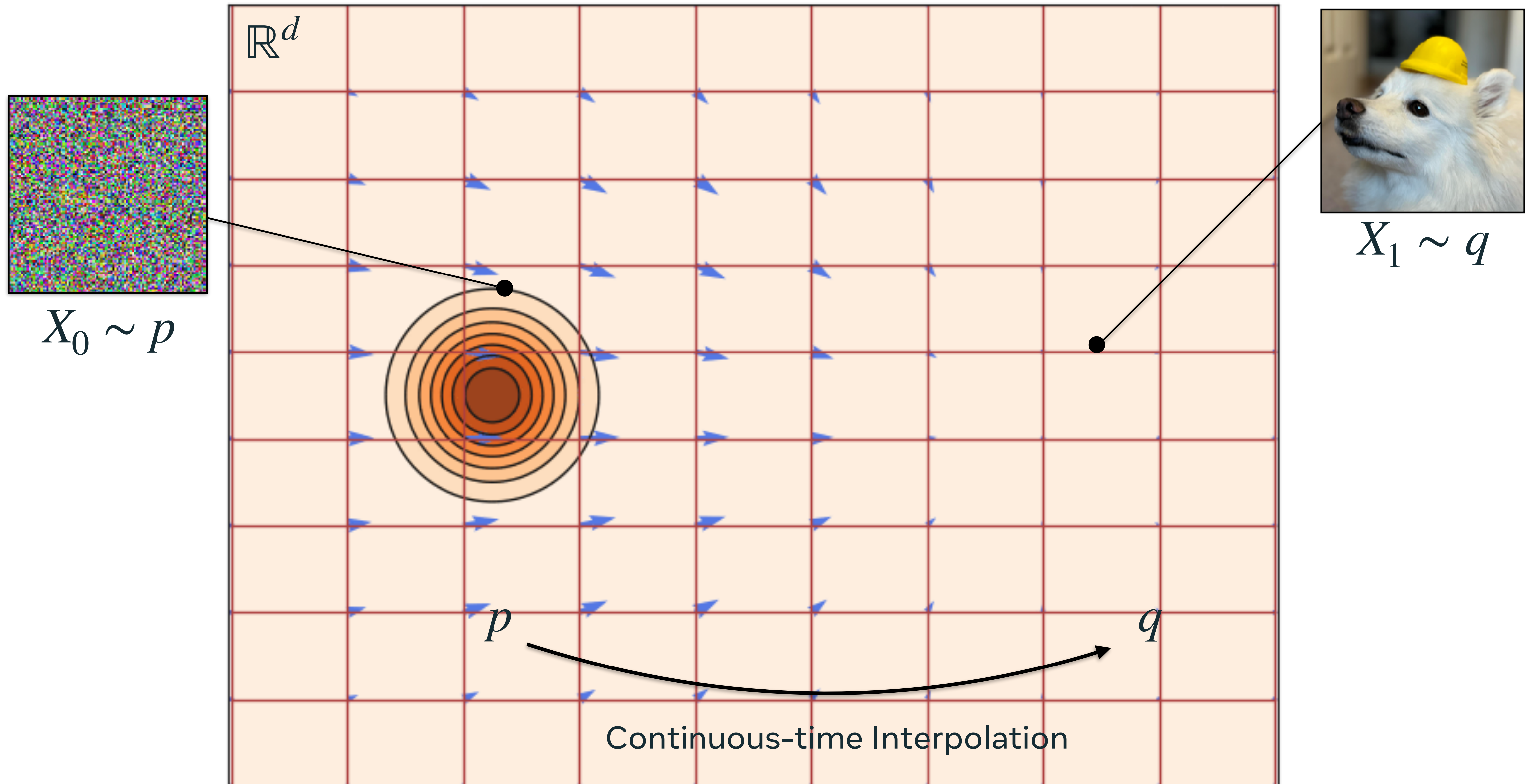
 $\mathbb{R}^d$  p  q 

$$X_1 \sim q$$

The Generative Modeling problem



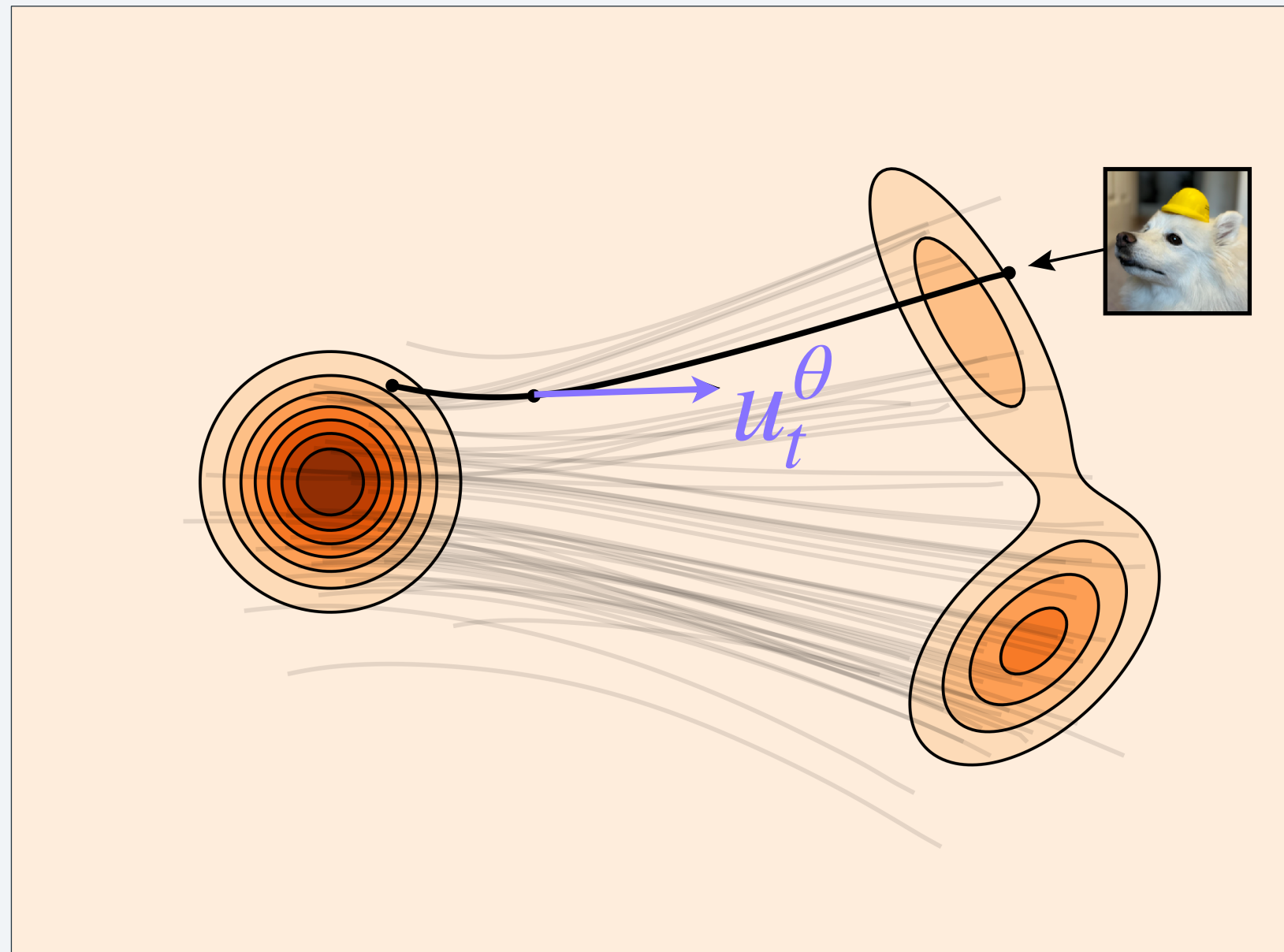
The Generative Modeling problem



Continuous-time Markov Processes

Parameterization

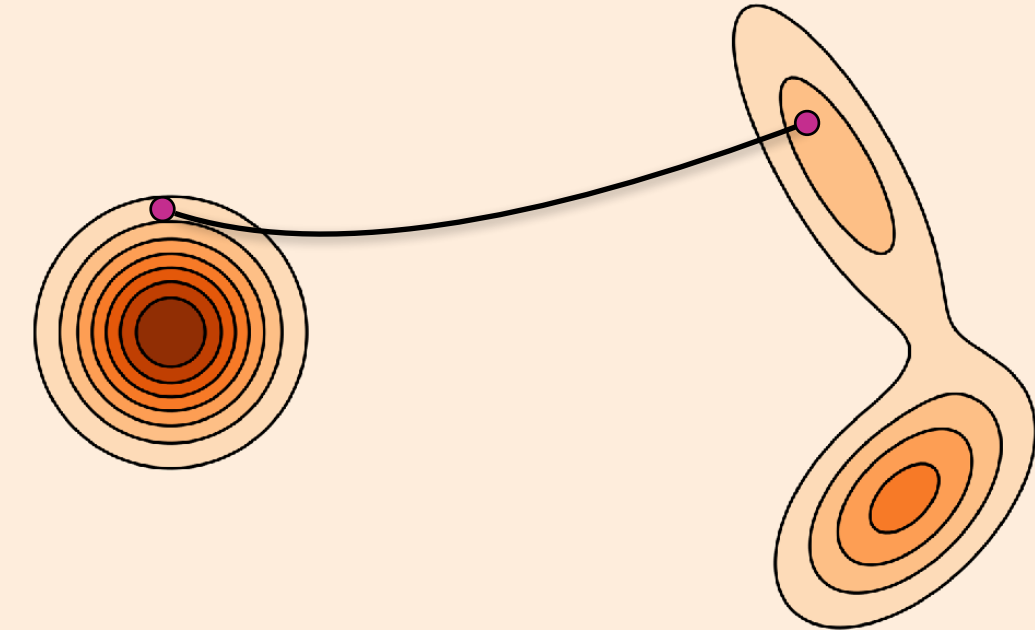
A **vector field** u_t^θ that points towards the data



Sampling

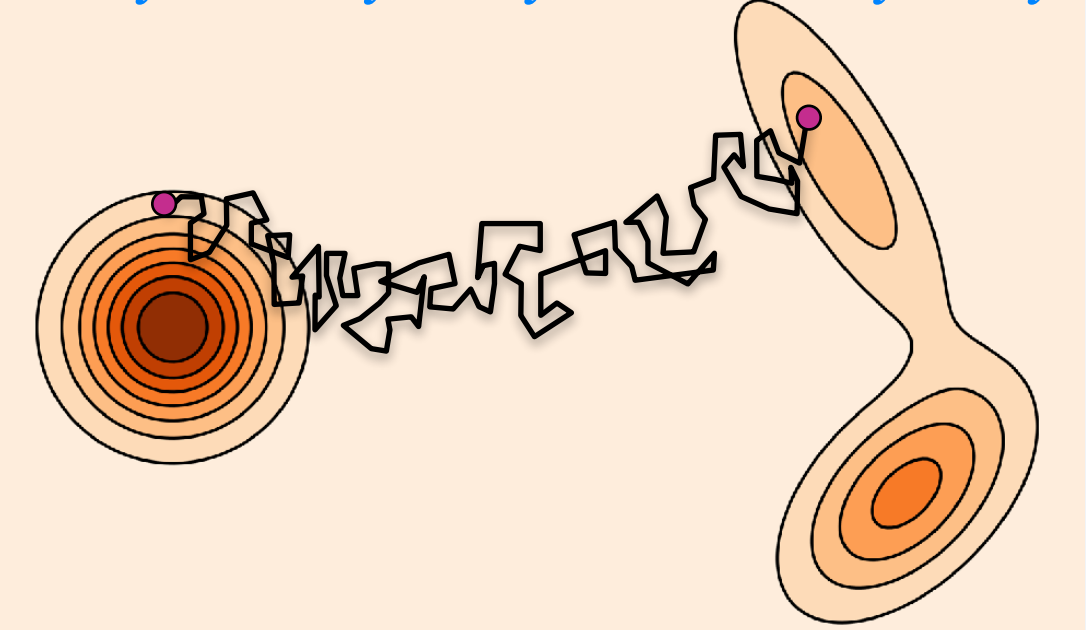
A **diffusion process** X_t with (optional) diffusion coefficient σ_t

$$dX_t = u_t^\theta(X_t)dt$$



Ordinary Differential Equation

$$dX_t = u_t^\theta(X_t)dt + \sigma_t dB_t$$

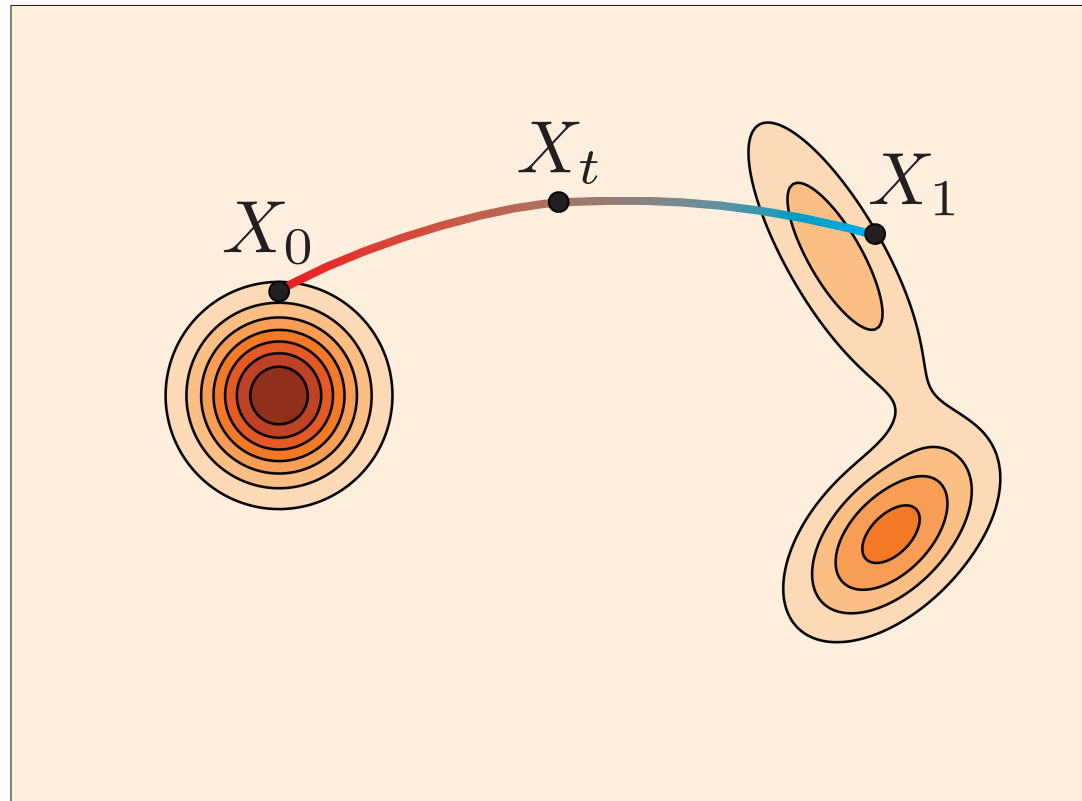


Stochastic Differential Equation

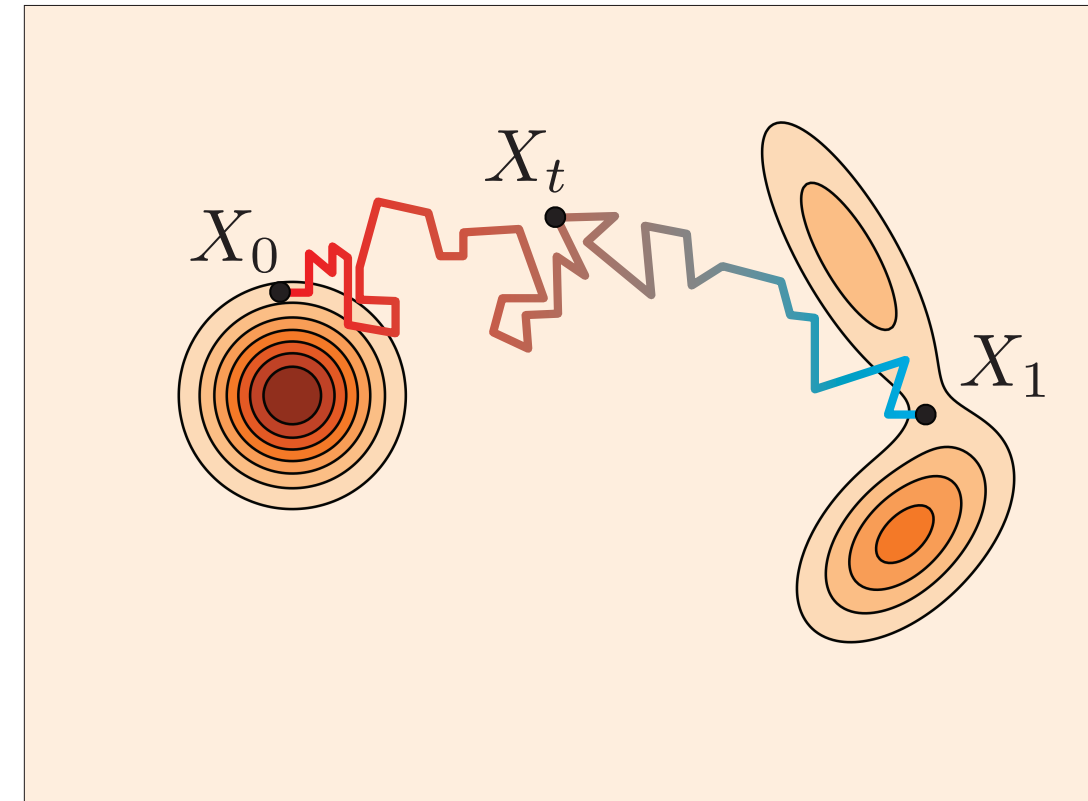
Continuous-time Markov Processes

Local perturbations only

Flow



Diffusion



Transition kernel

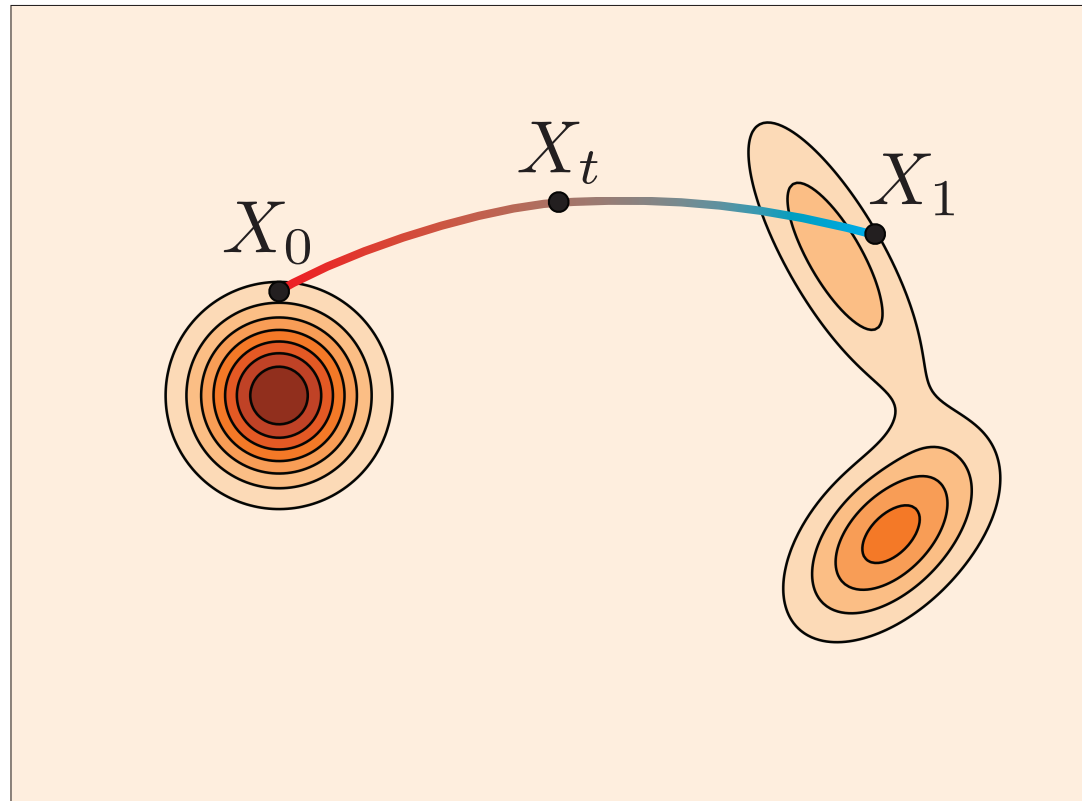
$$X_{t+h} \sim p_{t+h|t}(\cdot, X_t)$$

$$X_0 \sim p$$

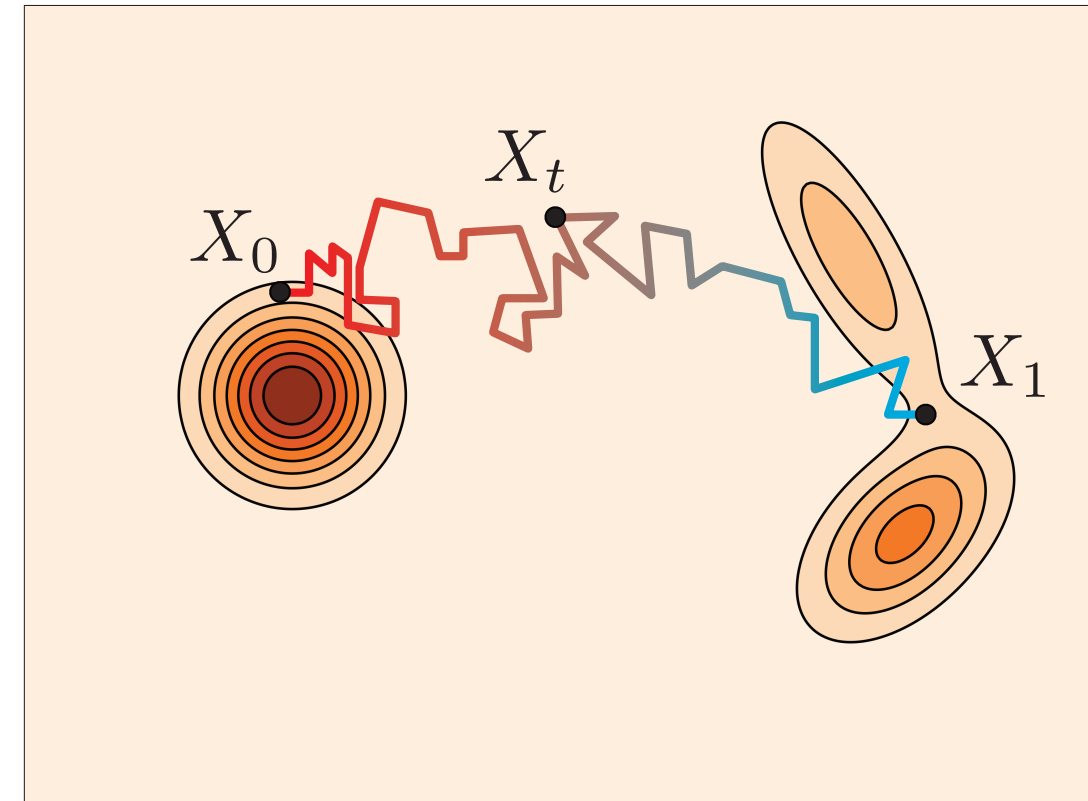
Generalizing beyond local perturbations

Local perturbations only

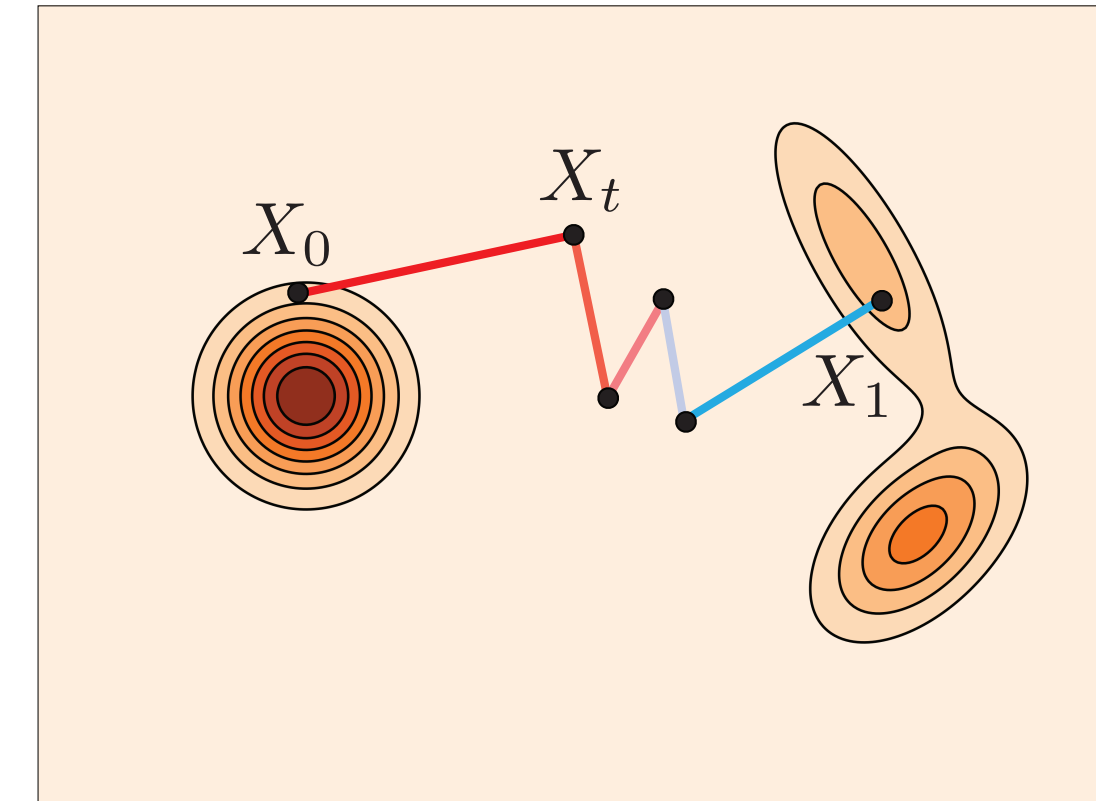
Flow



Diffusion



Jump



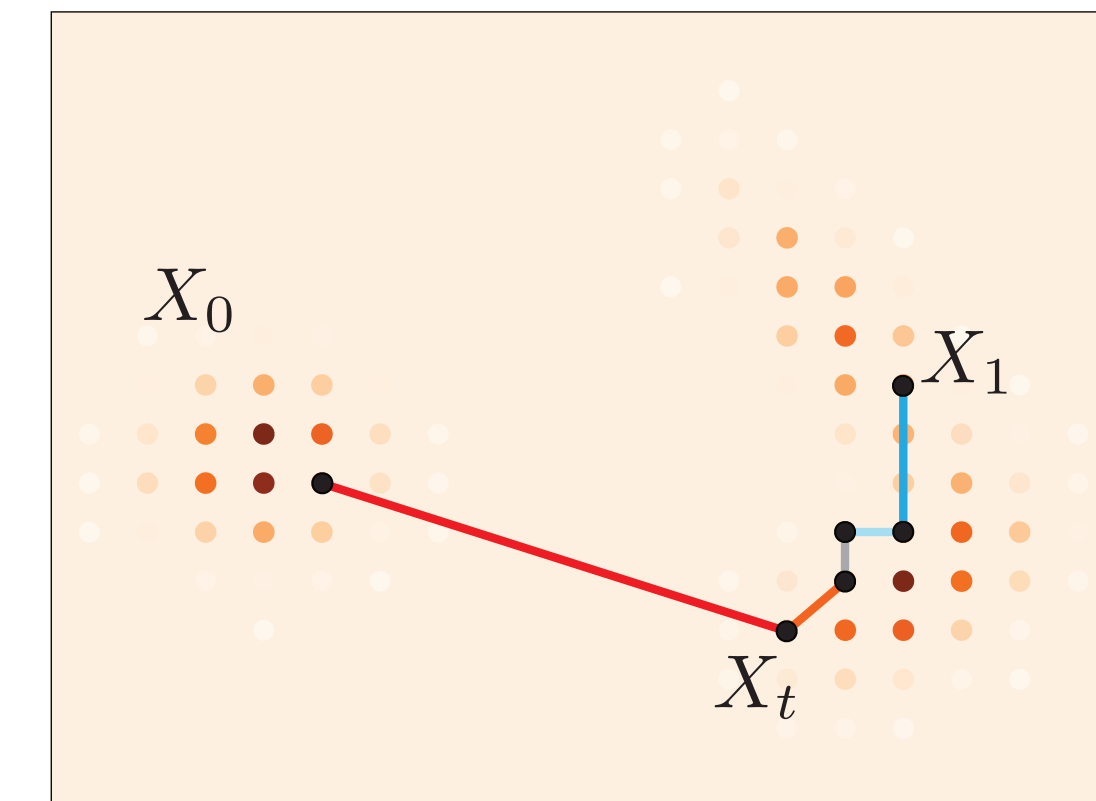
$$\mathcal{S} = \mathbb{R}^d$$

Transition kernel

$$X_{t+h} \sim p_{t+h|t}(\cdot, X_t)$$

$$X_0 \sim p$$

CTMC



$$\mathcal{S} = \mathcal{D}$$

Infinitesimal Generator

Generalize the notion of **first-order characterization**

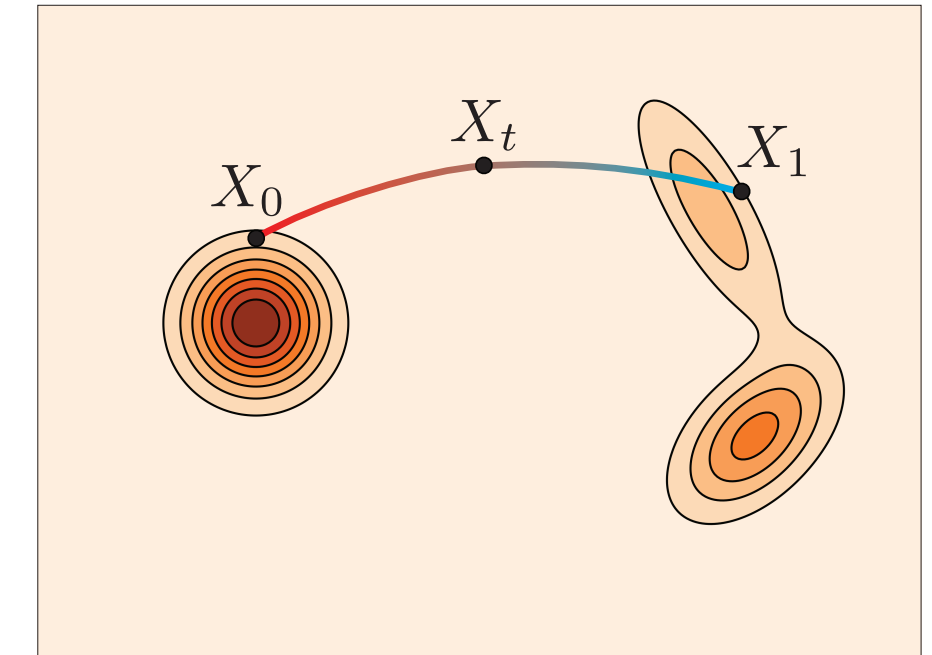
Generator

$$p_{t+h|t}(\cdot, X_t) = \underbrace{\delta_{X_t}}_{0^{\text{th}} \text{ order}} + h \underbrace{\left. \frac{d}{dh} p_{t+h|t}(\cdot, X_t) \right|_{h=0}}_{1^{\text{st}} \text{ order}} + \underbrace{o(h)}_{\text{error}}$$

First-order characterizations

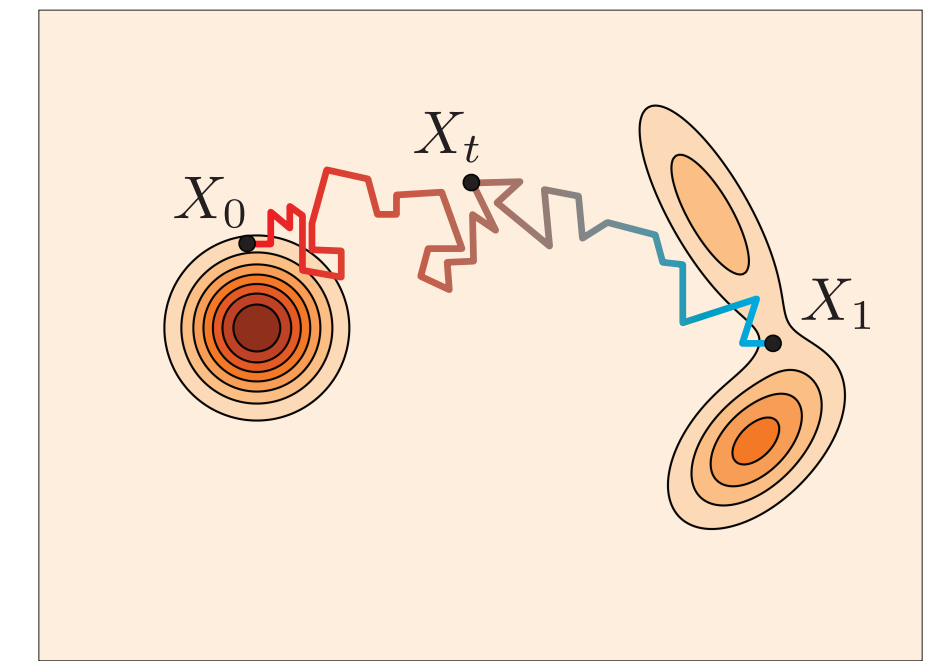
ODE:

$$X_{t+h} = \underbrace{X_t}_{0^{\text{th}} \text{ order}} + \underbrace{hu_t(X_t)}_{1^{\text{st}} \text{ order}} + \underbrace{o(h)}_{\text{error}}$$



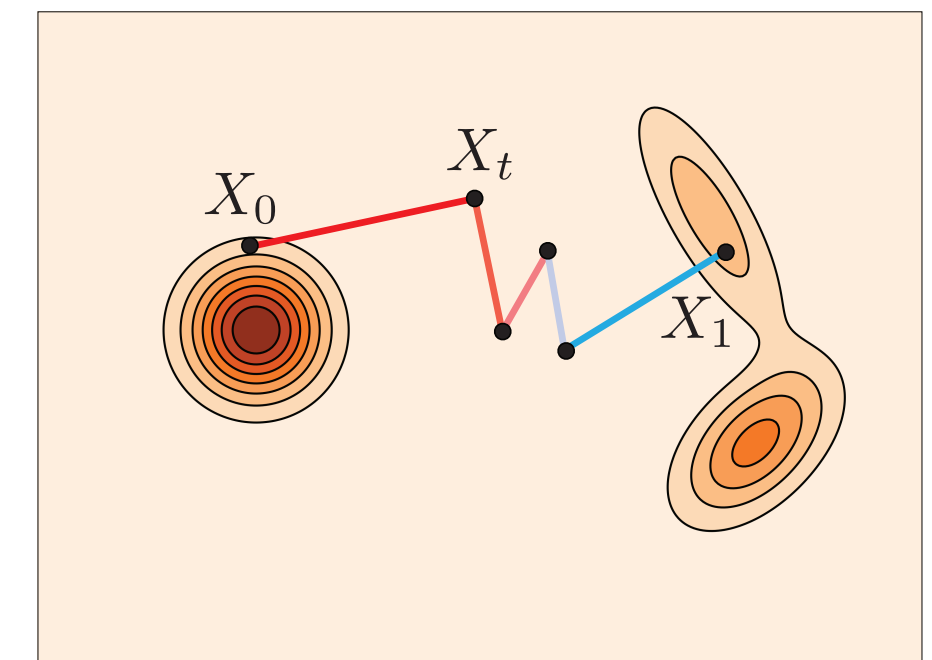
SDE:

$$X_{t+h} = \underbrace{X_t}_{0^{\text{th}} \text{ order}} + \underbrace{hu_t(X_t)}_{1^{\text{st}} \text{ order}} + \underbrace{\sqrt{h}\sigma_t\varepsilon + o(h)}_{\text{error}}$$



Jump &
CTMC:

$$X_{t+h} \sim \underbrace{\delta_{X_t}(\cdot)}_{0^{\text{th}} \text{ order}} + \underbrace{hu_t(\cdot | X_t)}_{1^{\text{st}} \text{ order}} + \underbrace{o(h)}_{\text{error}}$$



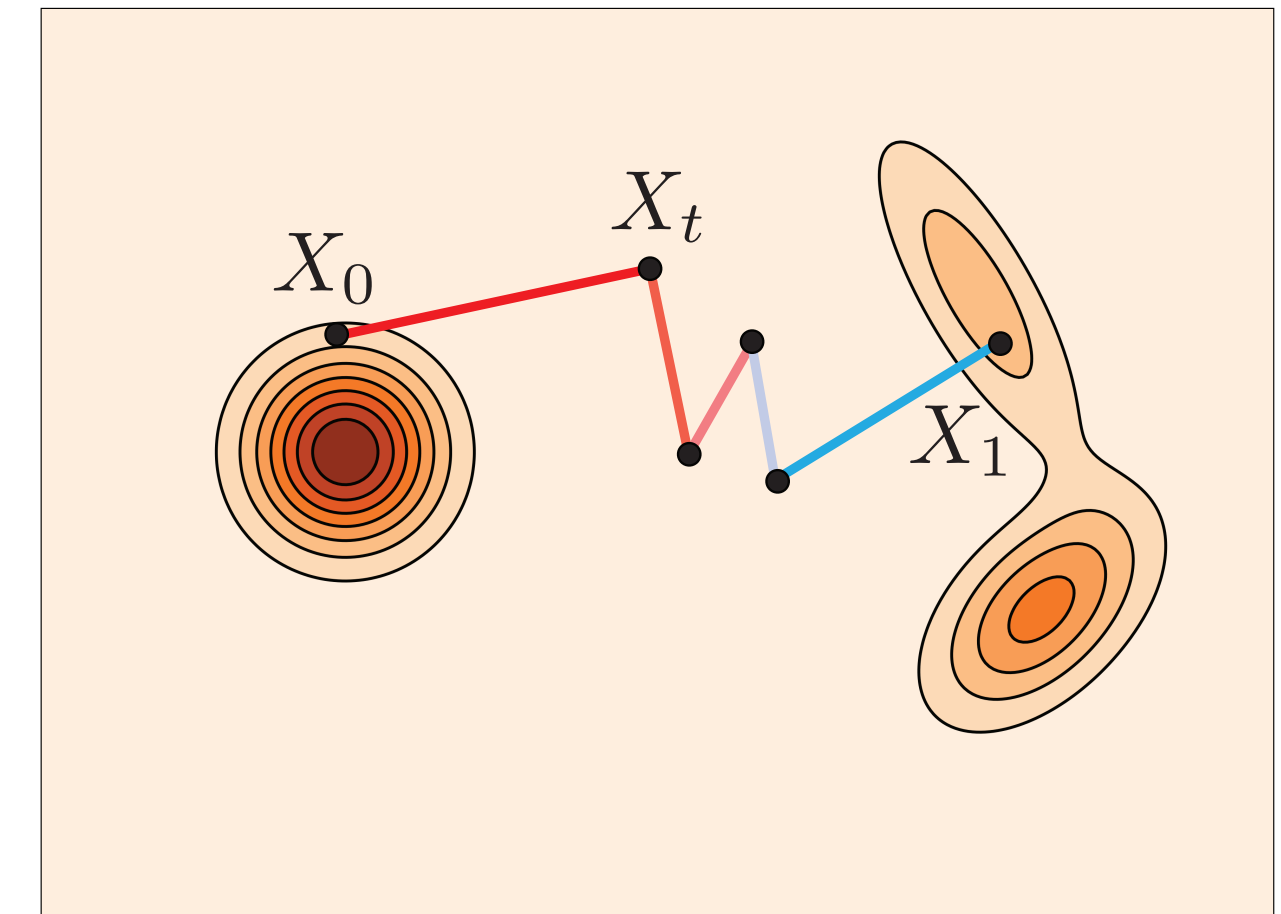
Jump Markov process

$$X_{t+h} \sim \delta_{X_t}(\cdot) + h \boxed{u_t(\cdot | X_t)}$$

Unnormalized distribution

Interpret $u_t(\cdot | X_t) = \boxed{\lambda_t(X_t)} \boxed{Q_t(\cdot | X_t)}$

Jump rate Normalized



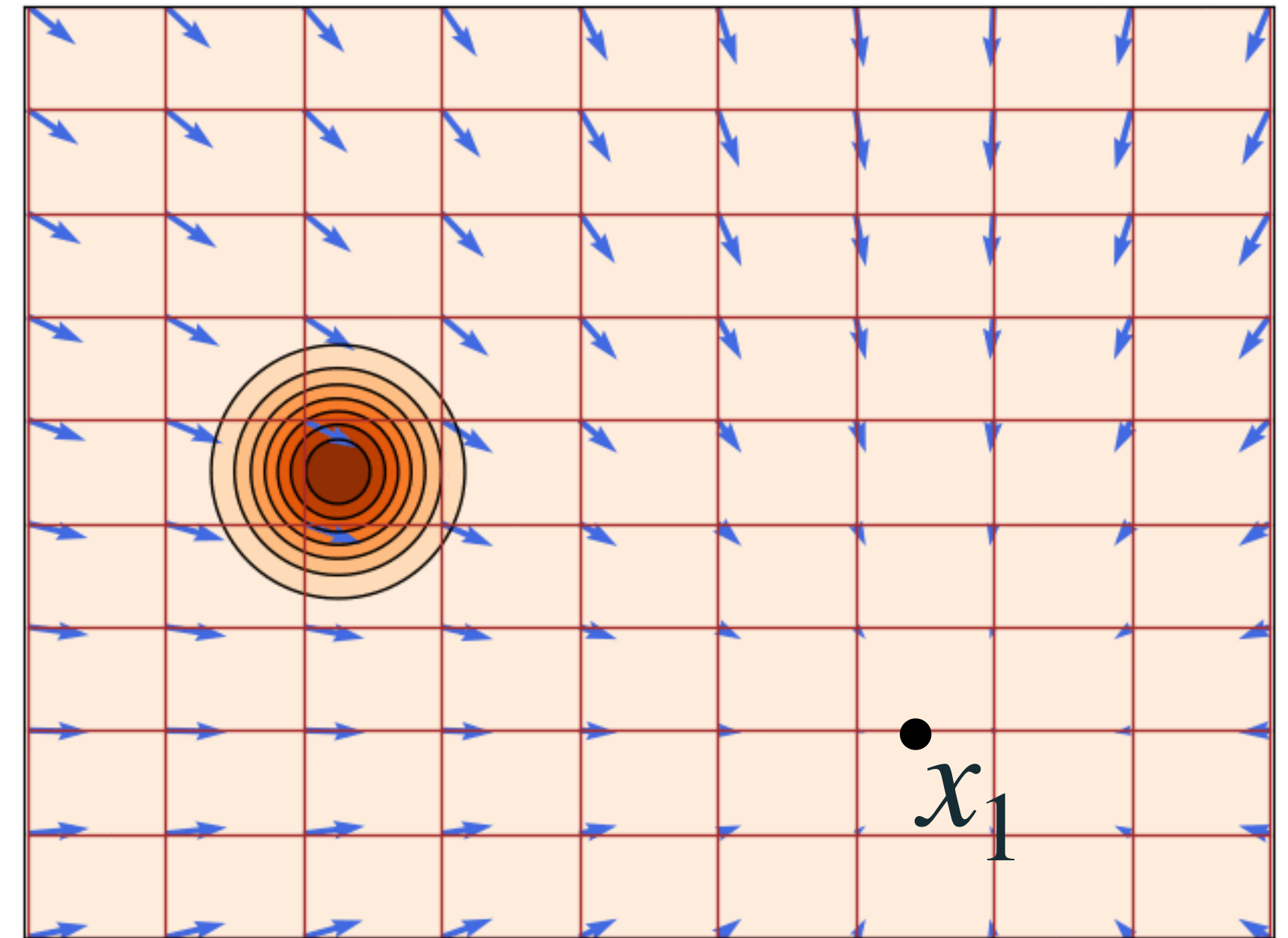
Jump process (sampling)

$$X_{t+h} \sim Q_t(\cdot | X_t) \quad \text{if } h\lambda_t(X_t) \geq U[0,1]$$

$$X_{t+h} = X_t \quad \text{otherwise}$$

Build flow from conditional flows

Generate a single target point

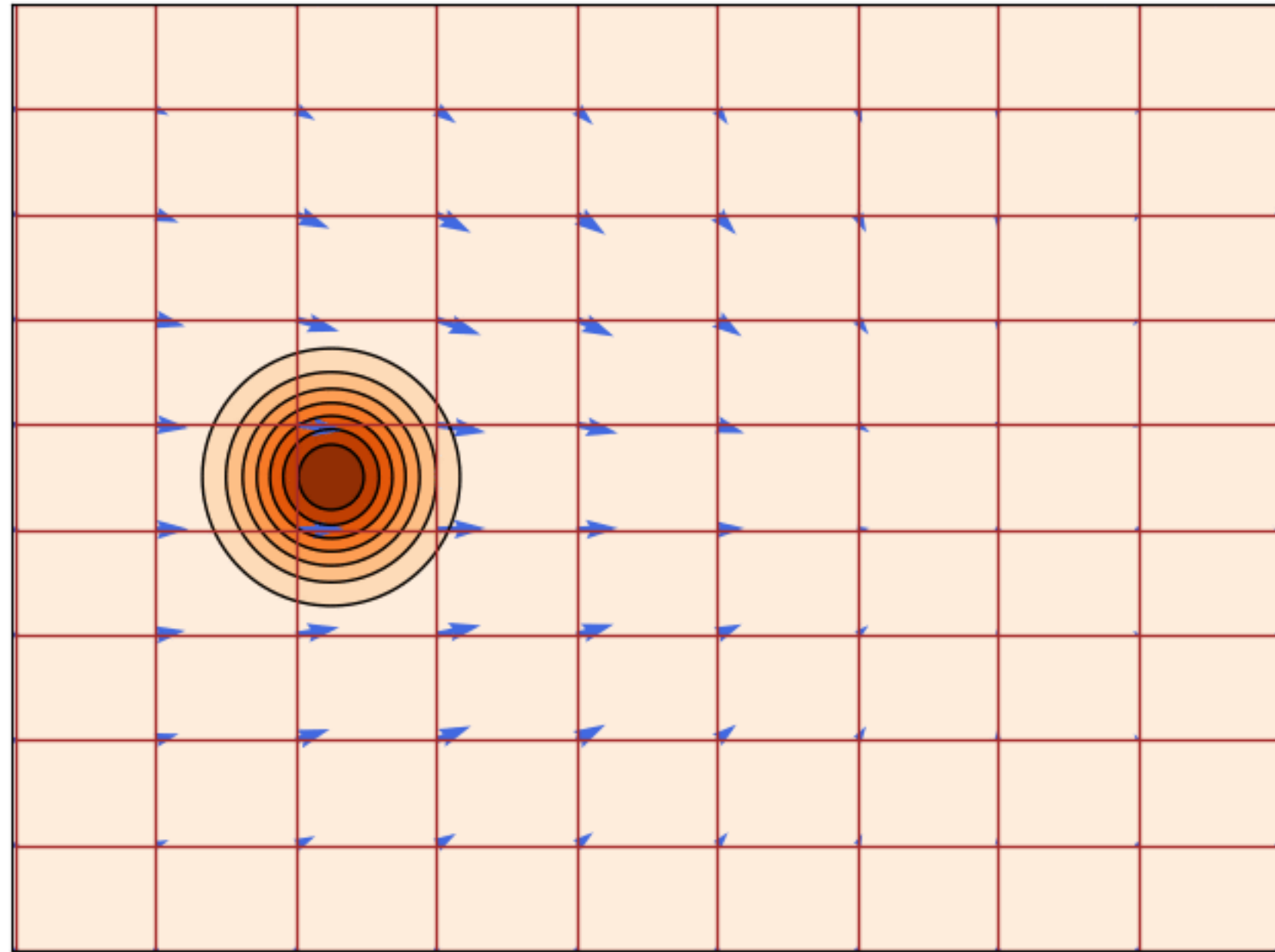


$$X_t = (1 - t)X_0 + tX_1$$

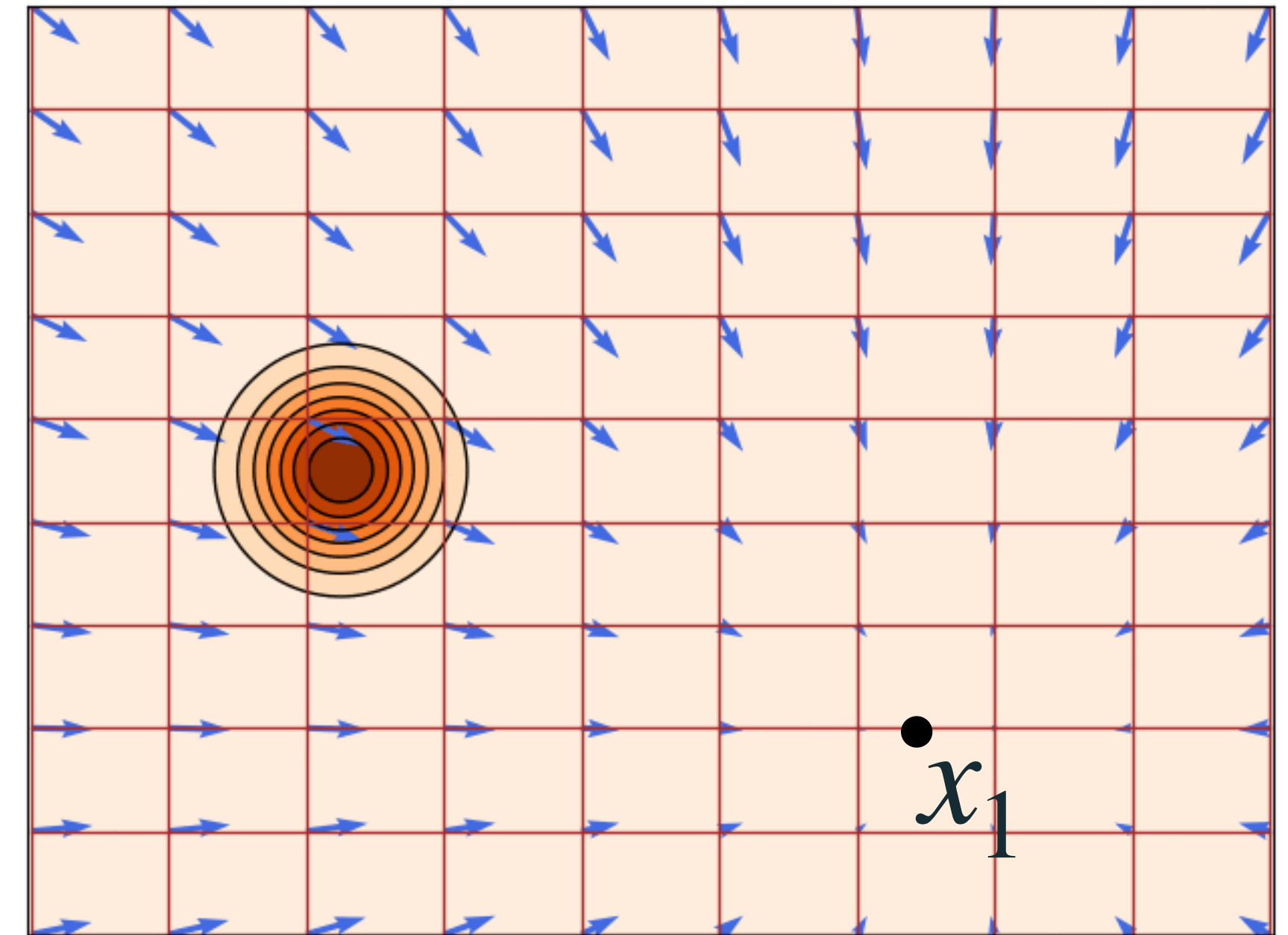
$p_{t|1}(x | x_1)$ conditional probability

$u_t(x | x_1)$ conditional velocity

Build flow from conditional flows



Generate a single target point



$$X_t = (1 - t)X_0 + tX_1$$

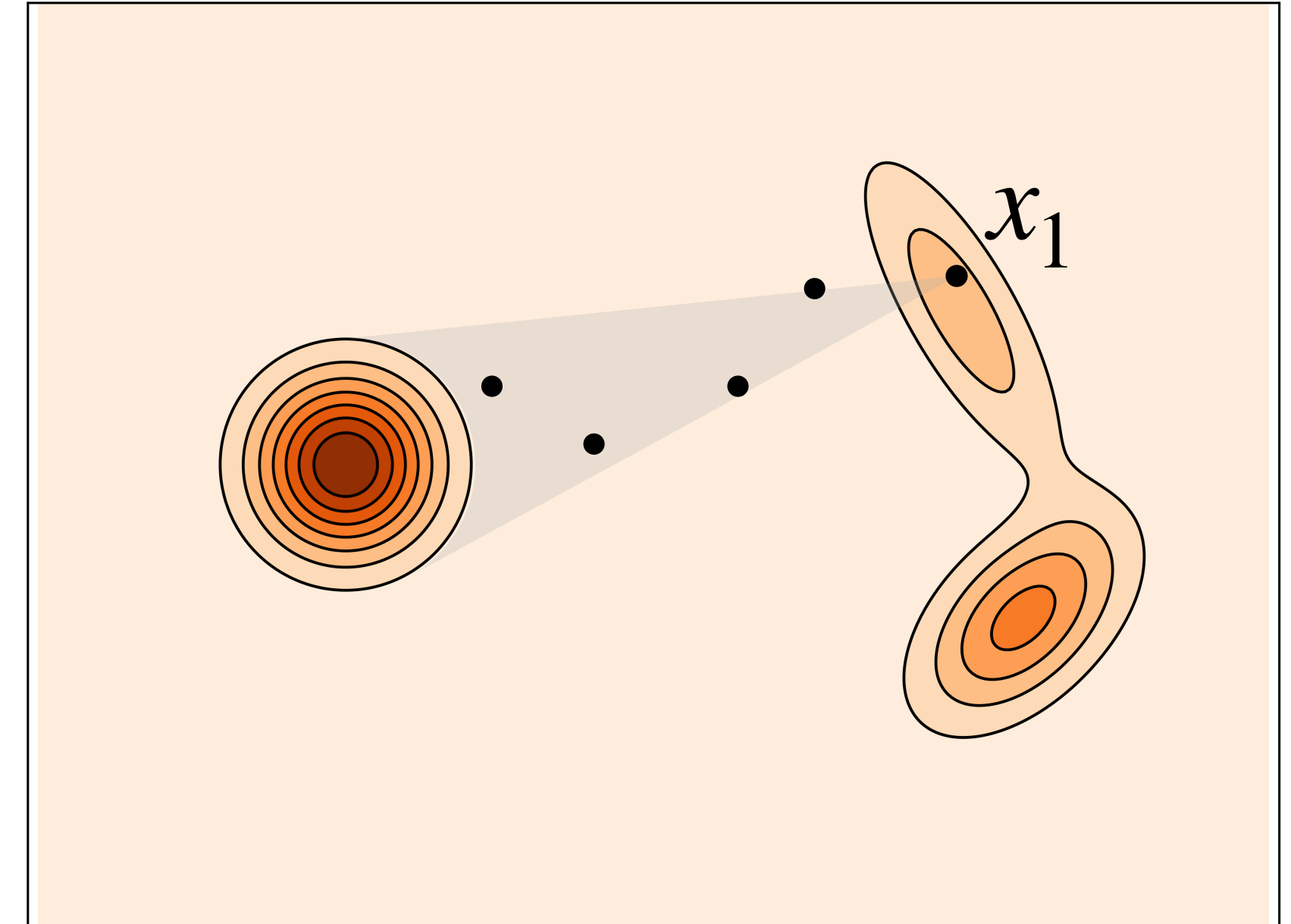
$$p_t(x) = \mathbb{E}_{X_1} p_{t|1}(x | X_1) \longleftarrow p_{t|1}(x | x_1) \text{ conditional probability}$$

average

$$u_t(x) = \mathbb{E} [u_t(X_t | X_1) \mid X_t = x] \longleftarrow u_t(x | x_1) \text{ conditional velocity}$$

Building generator from conditional generators

Identical recipe as the flow case...

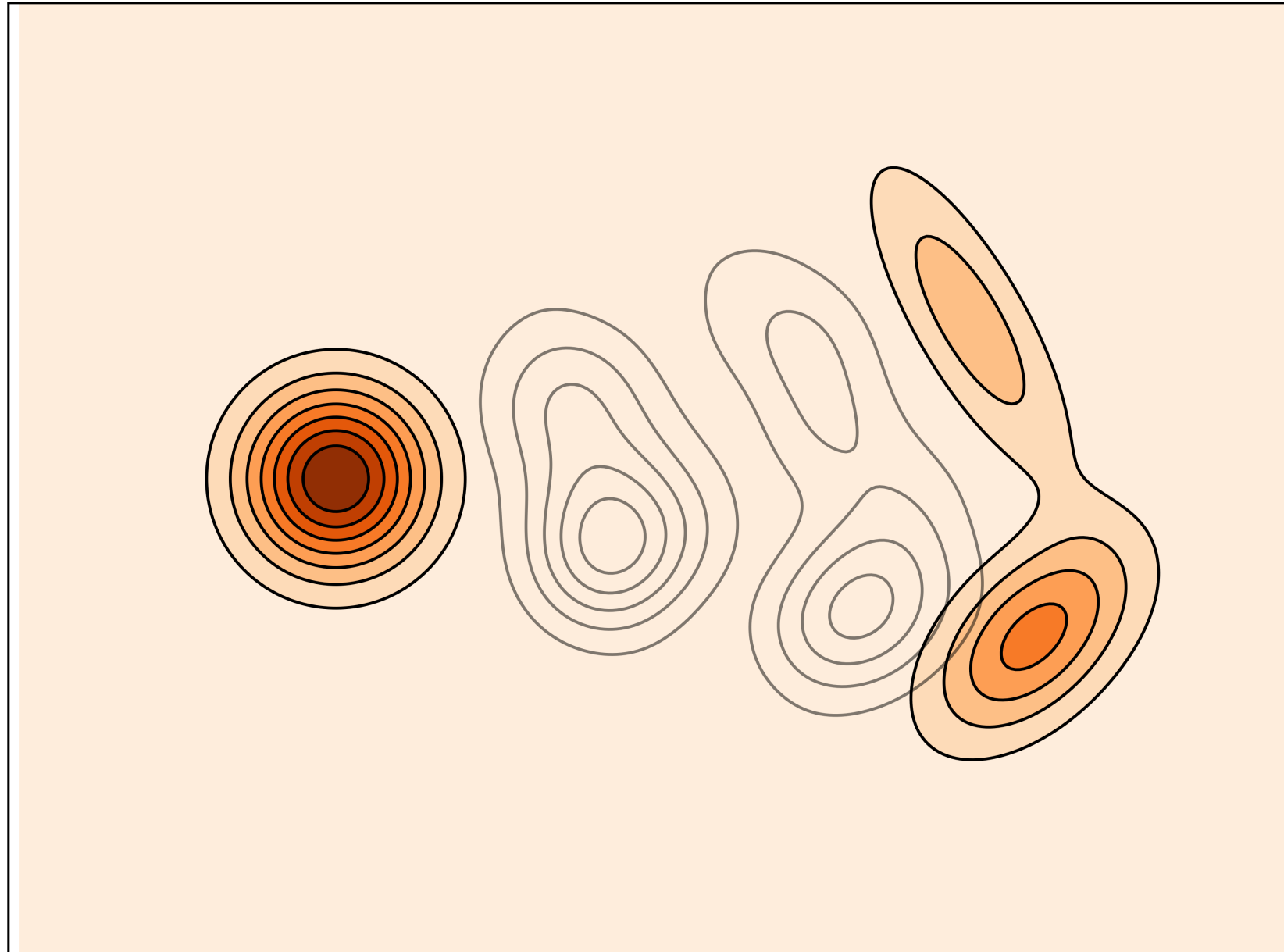


$p_{t|1}(x | x_1)$ conditional probability

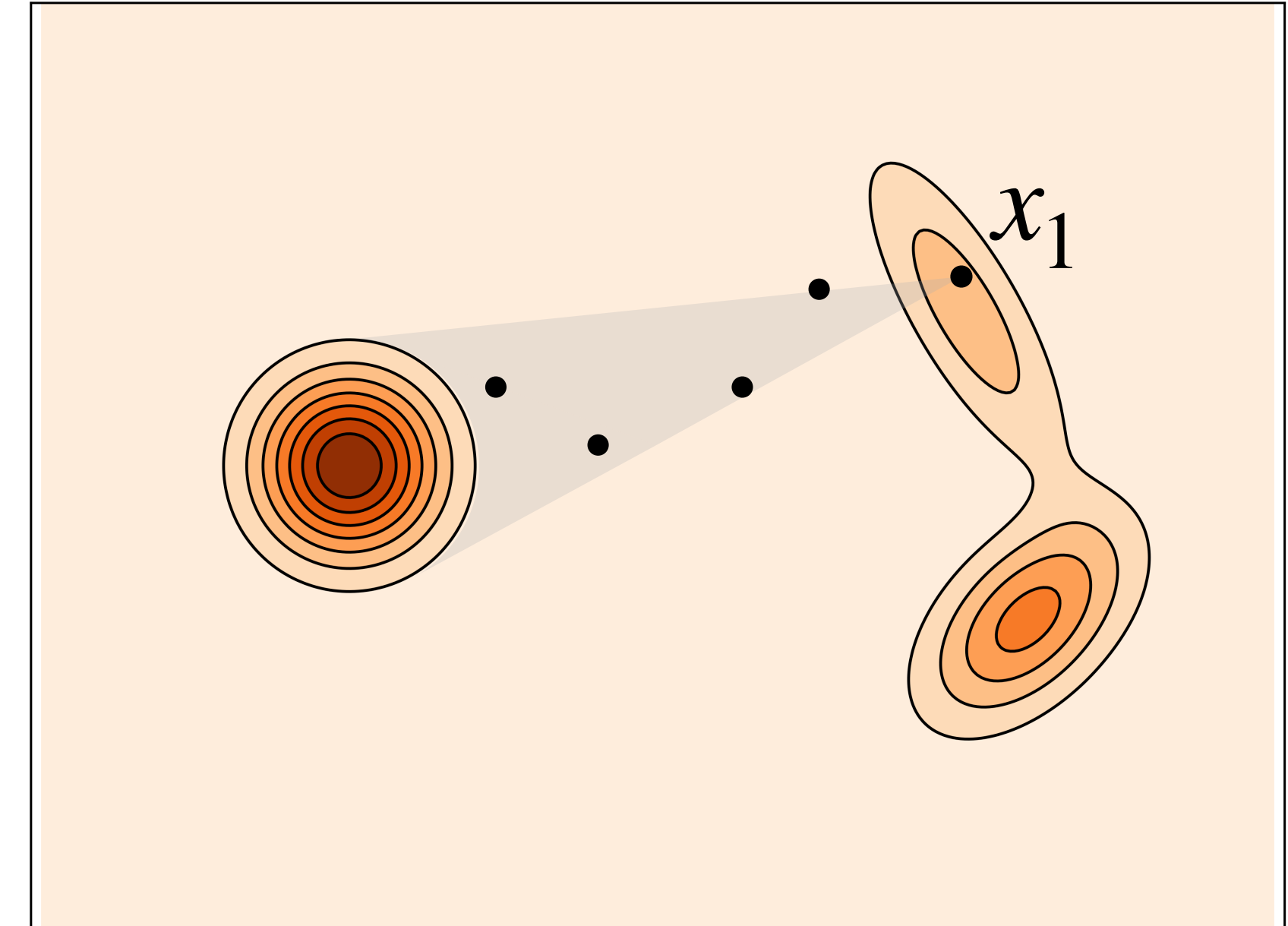
$u_t(\cdot | x, x_1)$ conditional **generator**

Building generator from conditional generators

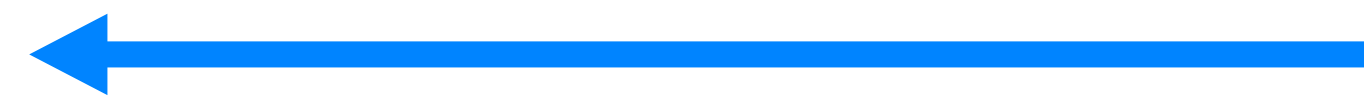
Identical recipe as the flow case...



Generate a single target point

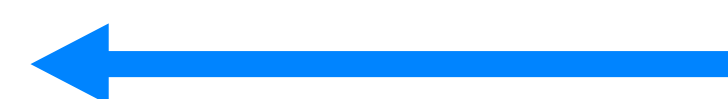


$$p_t(x) = \mathbb{E}_{X_1} p_{t|1}(x | X_1)$$



$$p_{t|1}(x | x_1) \text{ conditional probability}$$

average



$$u_t(\cdot | x) = \mathbb{E} \left[u_t(\cdot | X_t, X_1) \mid X_t = x \right]$$

$$u_t(\cdot | x, x_1) \text{ conditional generator}$$

The Marginalization Trick

Theorem: The **marginal generator** generates the **marginal probability** path.

Flow and diffusion:

$$u_t(x) = \mathbb{E} \left[u_t(X_t | X_1) \mid X_t = x \right]$$

$$p_t(x) = \mathbb{E}_{X_1} p_{t|1}(x | X_1)$$

Jump and CTMC:

$$u_t(\cdot | x) = \mathbb{E} \left[u_t(\cdot | X_t, X_1) \mid X_t = x \right]$$

Flow Matching Loss

- Flow Matching loss:

$$\mathcal{L}_{\text{FM}}(\theta) = \mathbb{E}_{t, X_t} \left\| u_t^\theta(X_t) - u_t(X_t) \right\|^2$$

- Conditional Flow Matching loss:

$$\mathcal{L}_{\text{CFM}}(\theta) = \mathbb{E}_{t, X_1, X_t} \left\| u_t^\theta(X_t) - u_t(X_t | X_1) \right\|^2$$

Theorem: Losses are equivalent,

$$\nabla_{\theta} \mathcal{L}_{\text{FM}}(\theta) = \nabla_{\theta} \mathcal{L}_{\text{CFM}}(\theta)$$

Generalized Flow Matching Loss

- **Flow Matching loss:**

$$\mathcal{L}_{\text{FM}}(\theta) = \mathbb{E}_{t, X_t} \boxed{D} \left(u_t(X_t), u_t^\theta(X_t) \right)$$

- **Conditional Flow Matching loss:**

$$\mathcal{L}_{\text{CFM}}(\theta) = \mathbb{E}_{t, X_1, X_t} \boxed{D} \left(u_t(X_t | X_1), u_t^\theta(X_t) \right)$$

Theorem: Losses are equivalent if and only if D is a **Bregman divergence**.

$$\nabla_{\theta} \mathcal{L}_{\text{FM}}(\theta) = \nabla_{\theta} \mathcal{L}_{\text{CFM}}(\theta)$$

Generalized Flow Matching Loss

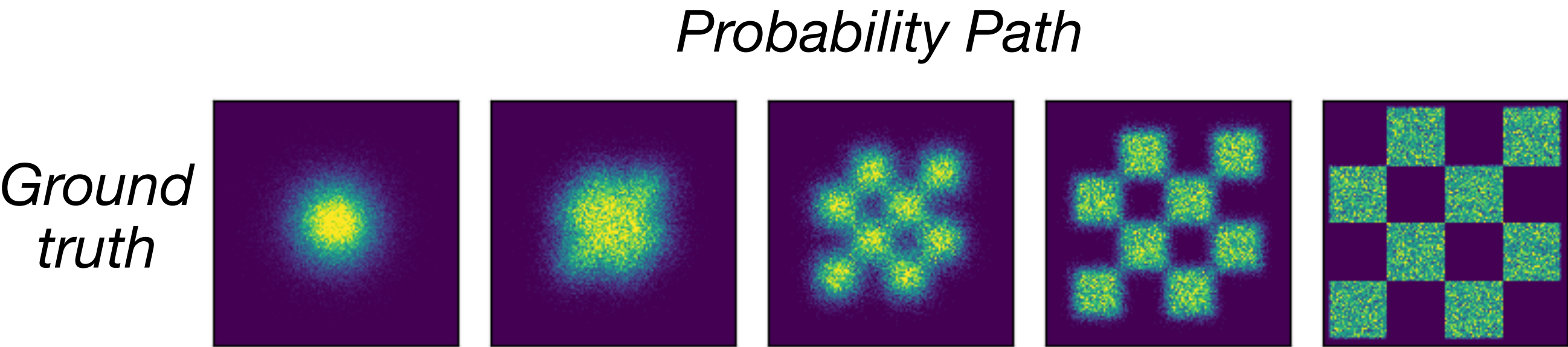
Theorem: Losses are equivalent iff D is a Bregman divergence.

$$\nabla_{\theta} \mathbb{E}_{X,Y} D(\textcolor{blue}{Y}, g^{\theta}(X)) = \nabla_{\theta} \mathbb{E}_X D(\mathbb{E}[\textcolor{blue}{Y} | \textcolor{blue}{X}], g^{\theta}(X))$$

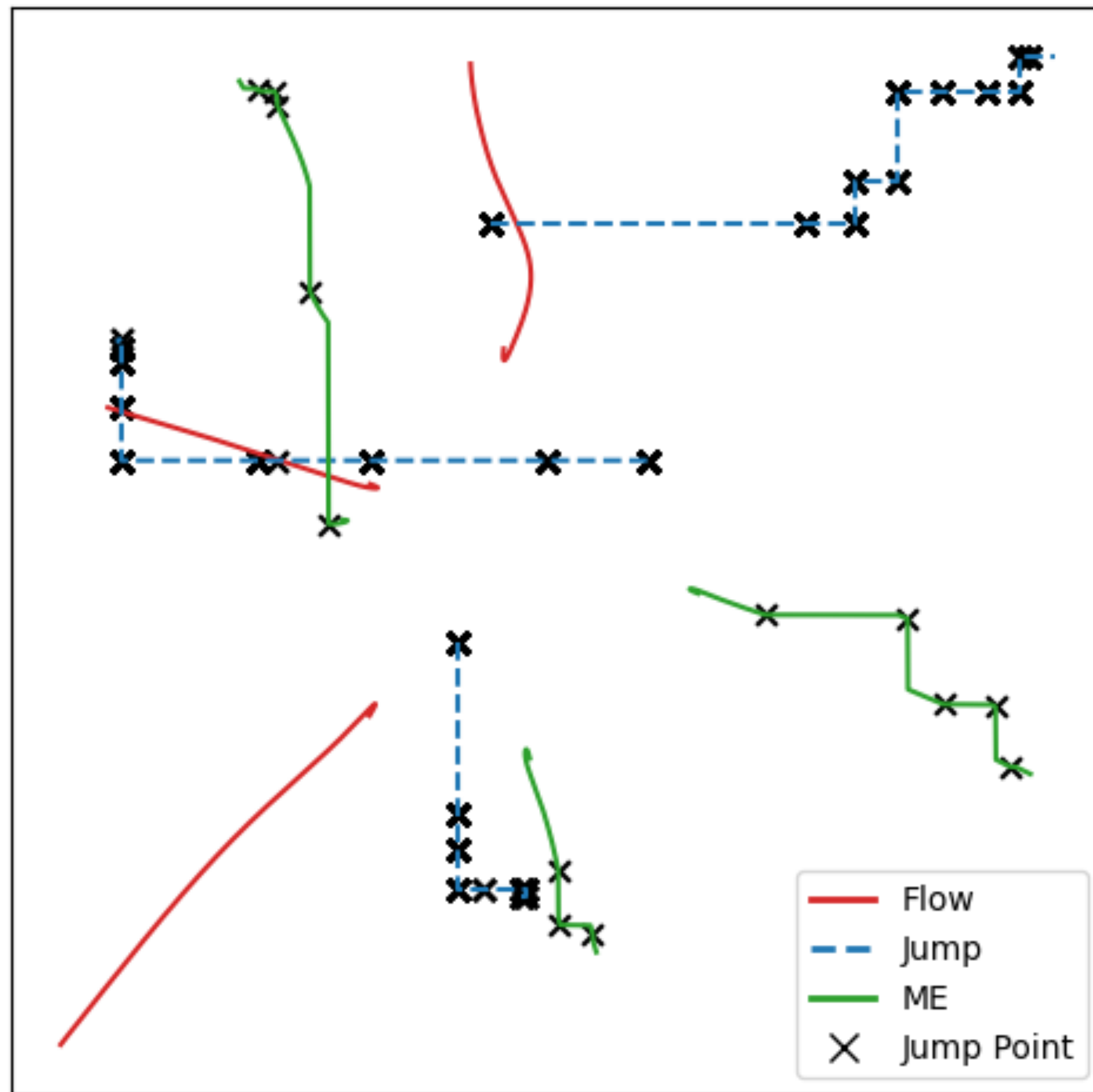
$$D(a, b) = \phi(a) - [\phi(b) + \langle a - b, \nabla \phi(b) \rangle]$$

- Includes MSE, ELBO, many many possible instantiations ...

Toy problem illustration



Toy problem illustration



Different sample paths

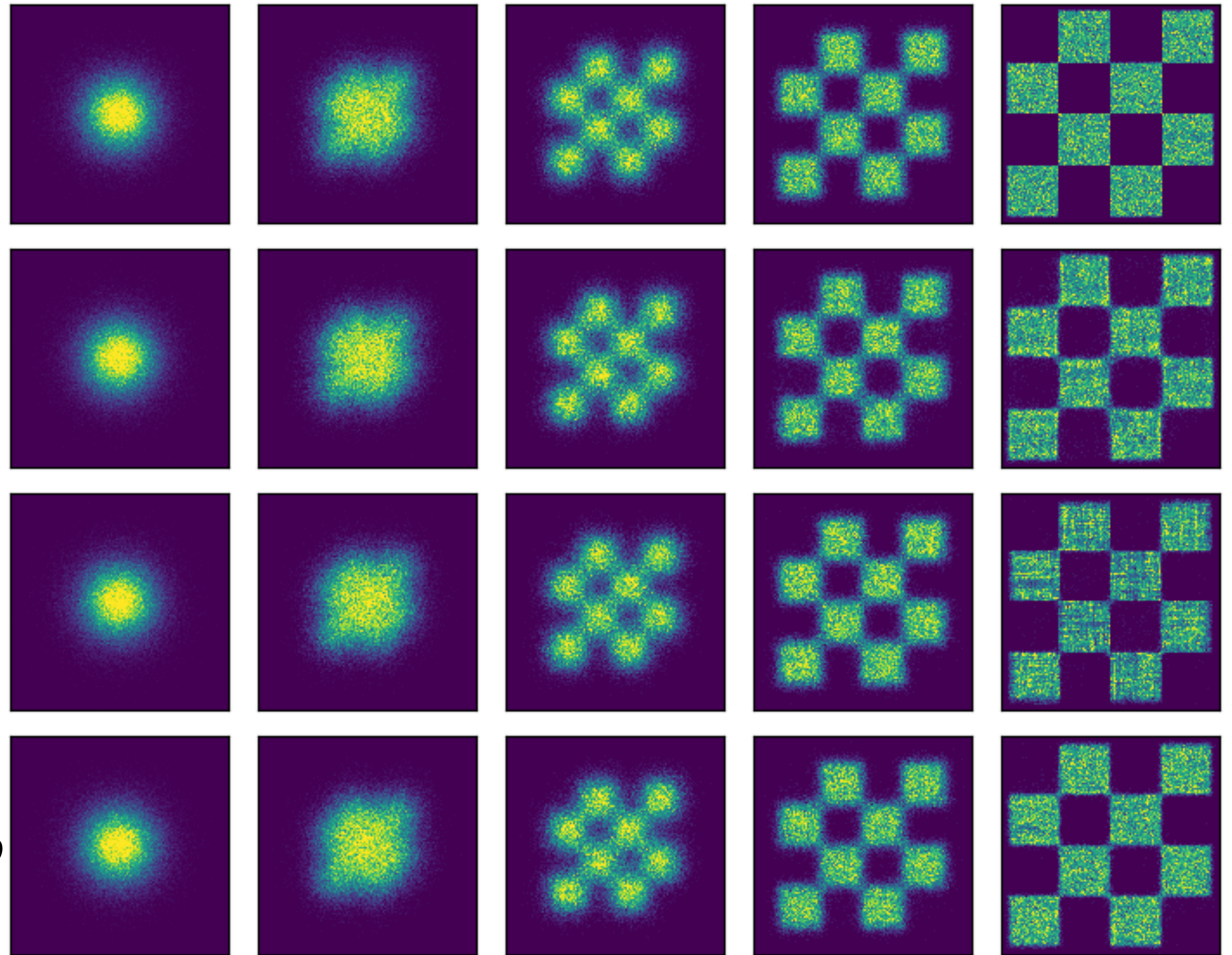
Probability Path

Ground truth

Flow

Jump

Flow + Jump



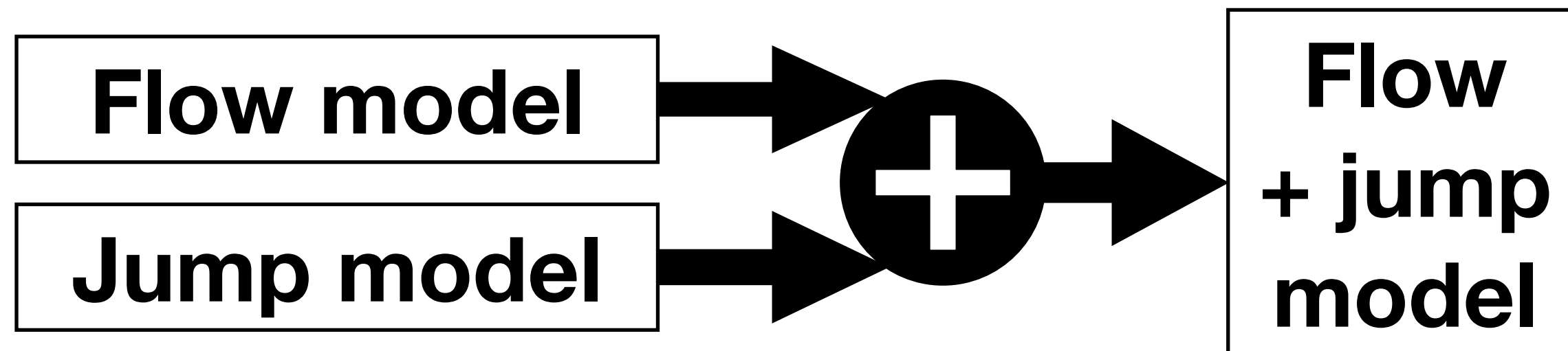
Same probability path

Image Generation

Markov jump model

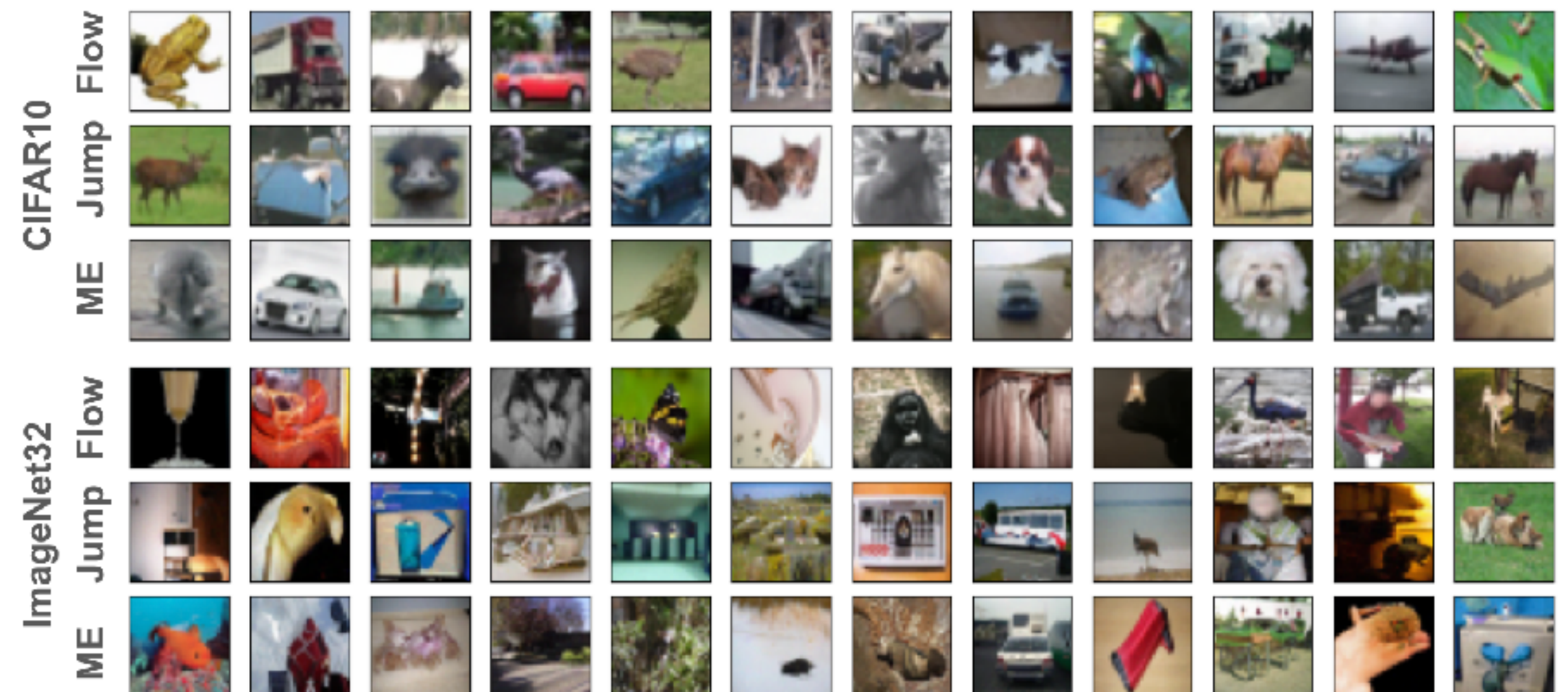
Large unexplored design space!

Markov superposition



Markov superpositions show synergistic effects of two models!

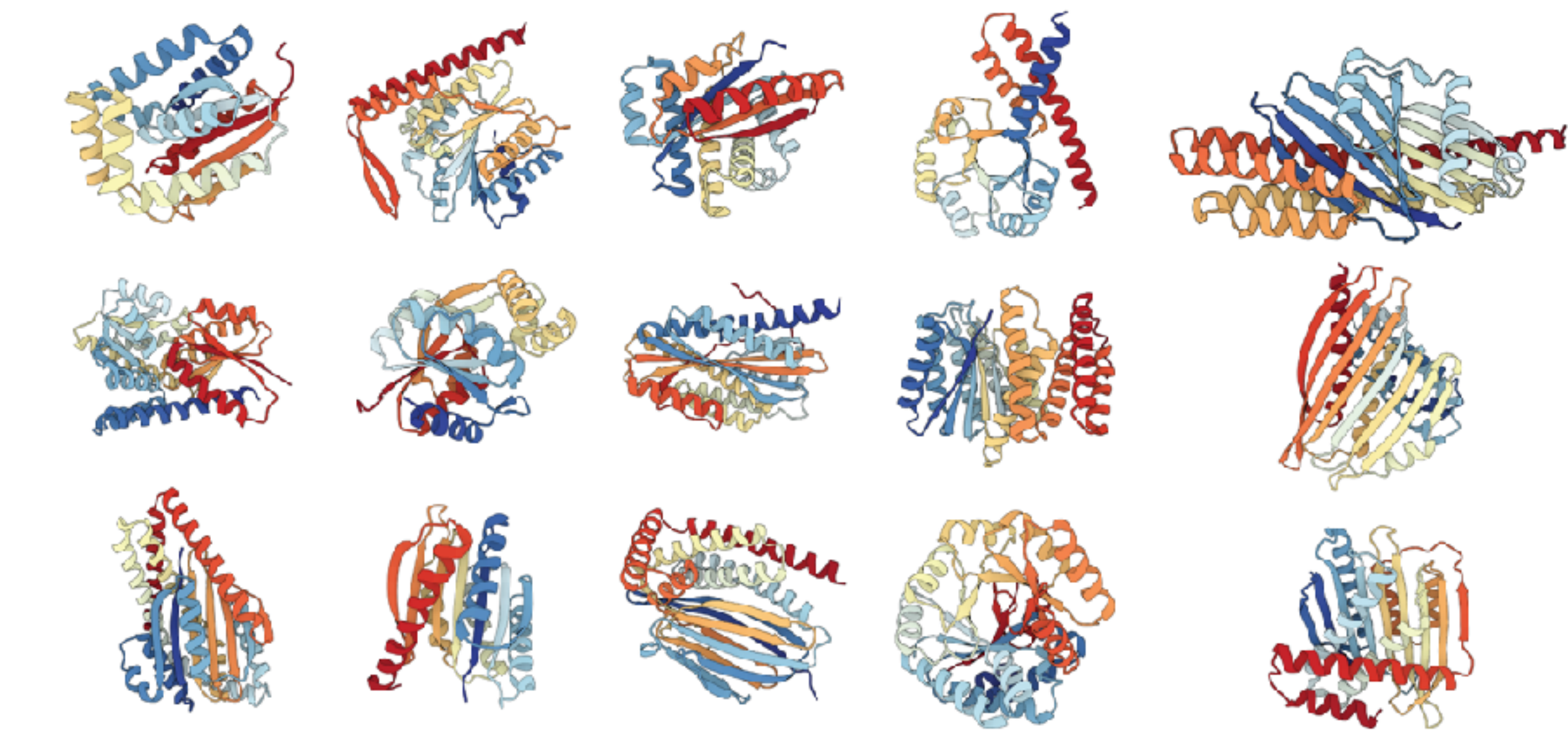
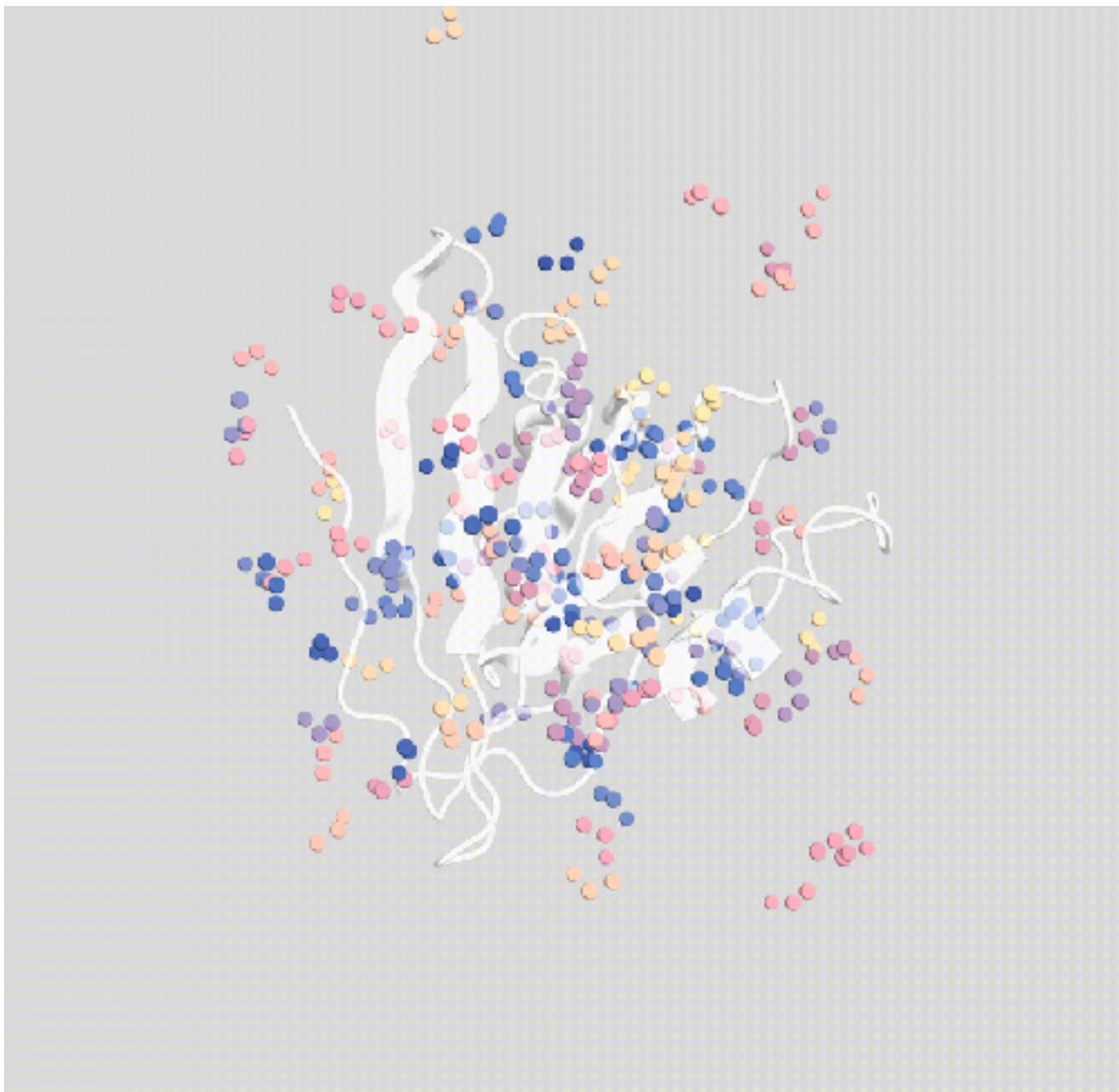
Method	CIFAR10	ImageNet
DDPM (Ho et al., 2020)	3.17	6.99
VP-SDE (Song et al., 2020)	3.01	6.84
EDM (Karras et al., 2022)	1.98	—
Flow model (Euler)	2.94	4.58
Jump model (Euler)	4.23	7.66
Jump + Flow MS (Euler)	2.49	3.47
Flow model (2nd order)	2.48	3.59
Jump + Flow MS (mixed)	2.36	3.33



FrameJump : Protein Generation

Manifold jump model on $SO(3)$.

Make **multimodal**: Combine continuous and discrete models



Method	Multimodal		Unimodal	
	Div.	Nov.	Div.	Nov.
RFdiffusion (Watson et al., 2023)	N/A		0.4	0.37
FrameFlow (Yim et al., 2024)	N/A		0.39	0.39
FoldFlow (Bose et al., 2023)	N/A		0.24	0.32
Protpardelle (Chu et al., 2024)	0.1	0.4	0.12	0.41
ProteinGenerator (Lisanza et al., 2023)	0.09	0.31	0.19	0.35
MultiFlow (Campbell et al., 2024b)	0.38	0.39	0.52	0.39
w/ $SO(3)$ jumps (ours)	0.48	0.41	0.63	0.41
w/ $SO(3)$ jumps + flow (ours)	0.47	0.4	0.59	0.40

Discrete Flow Matching

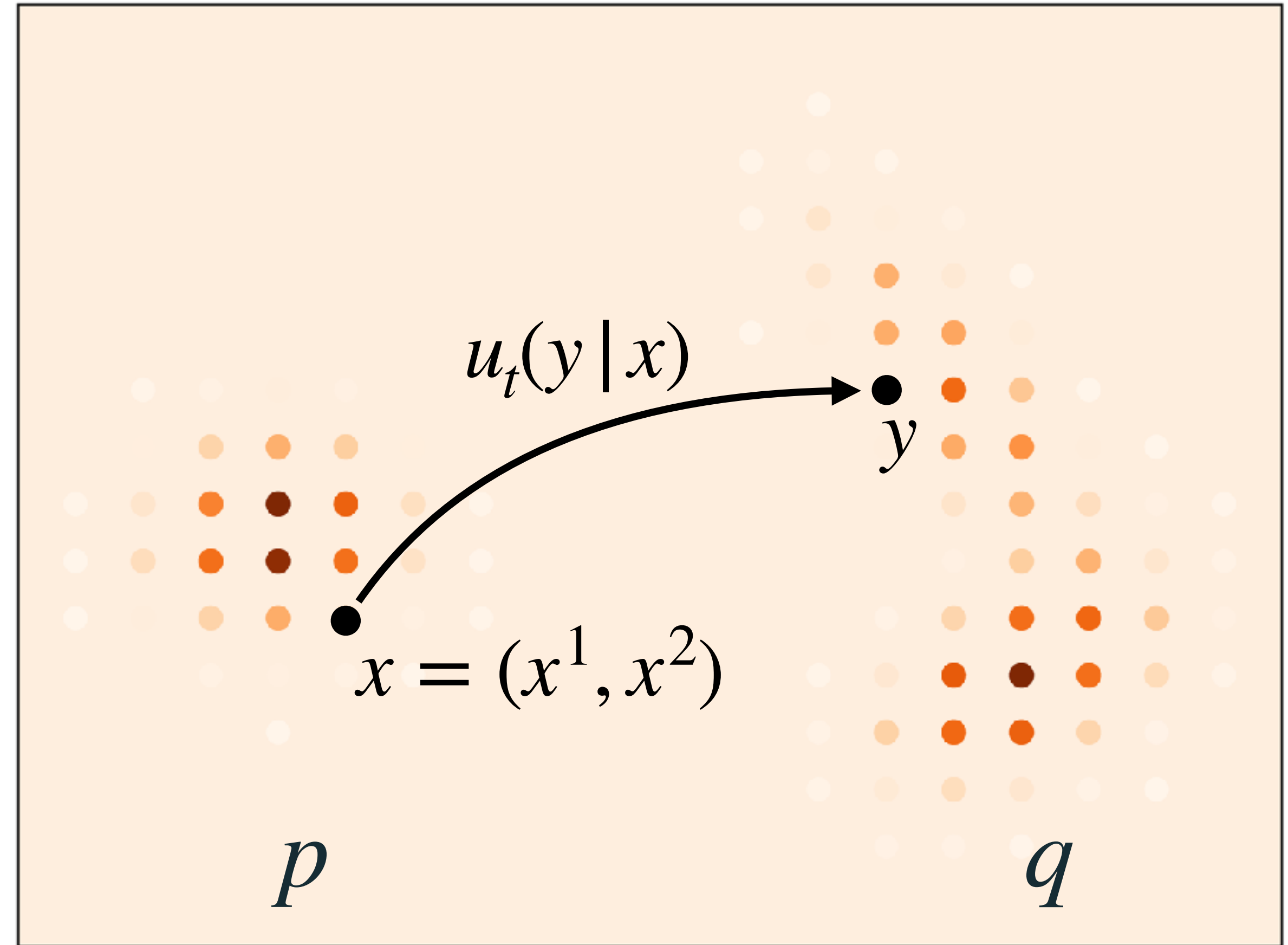
Discrete space diffusion, general corruption processes

Continuous-time Markov Chains (CTMC)

- State space $\mathcal{X} = \mathcal{T}^d$: **sequences of tokens**
- $x = (x^1, x^2, \dots, x^d) \in \mathcal{X}$

$$p_{t+h|t}(\cdot, X_t) = \delta_{X_t}(\cdot) + h \boxed{u_t(\cdot | X_t)} + o(h)$$

**Unnormalized
distribution over $\mathcal{X}$**



Factorized velocity

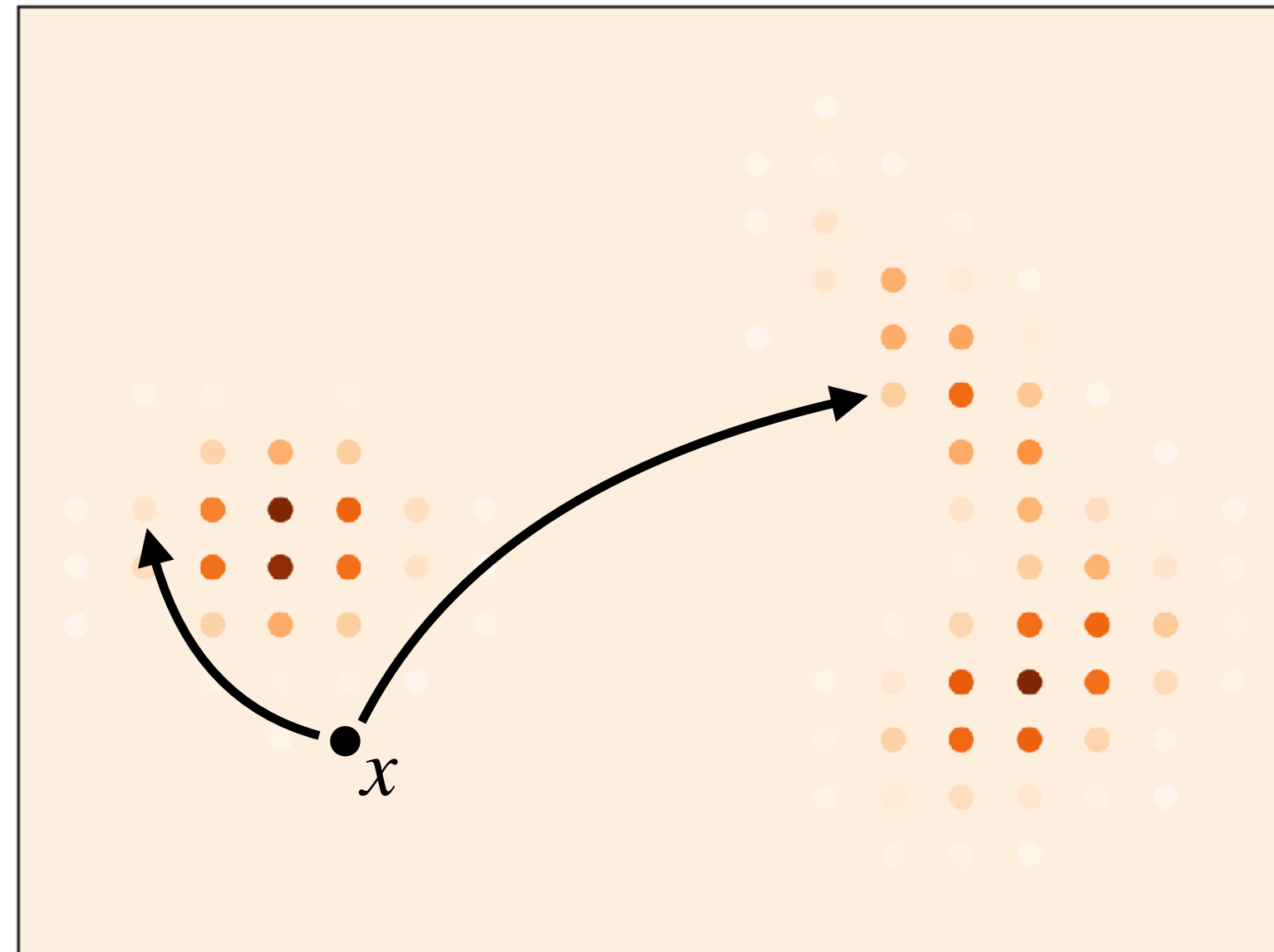
Similar to continuous case $\mathcal{S} = \mathbb{R}^d$:
 $u_t(x) = [u_t^1(x), \dots, u_t^d(x)]$

Example:

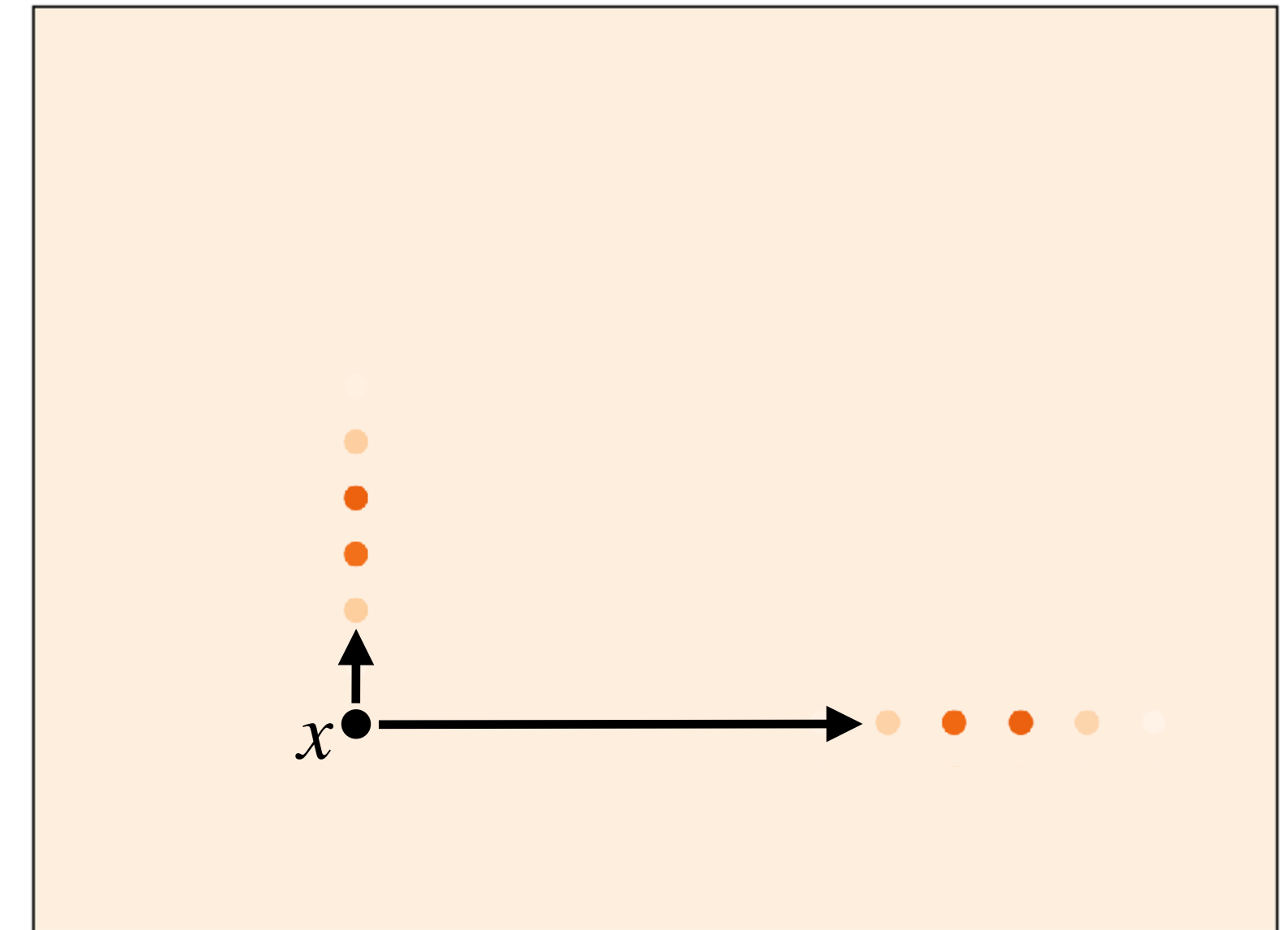
$d \approx 1000, |\mathcal{T}| \approx 50000$

```
def fib(n: int):  
    """Return n-th Fibonacci  
    number.  
    >>> fib(10)  
    55  
    >>> fib(1)  
    1  
    >>> fib(8)  
    21  
    """  
    if n < 1: return 0  
    if n < 2: return 1  
    return fib(n-1) + fib(n-2)
```

$$u_t(\cdot | x) \in \mathbb{R}^{\mathcal{T}^d}$$



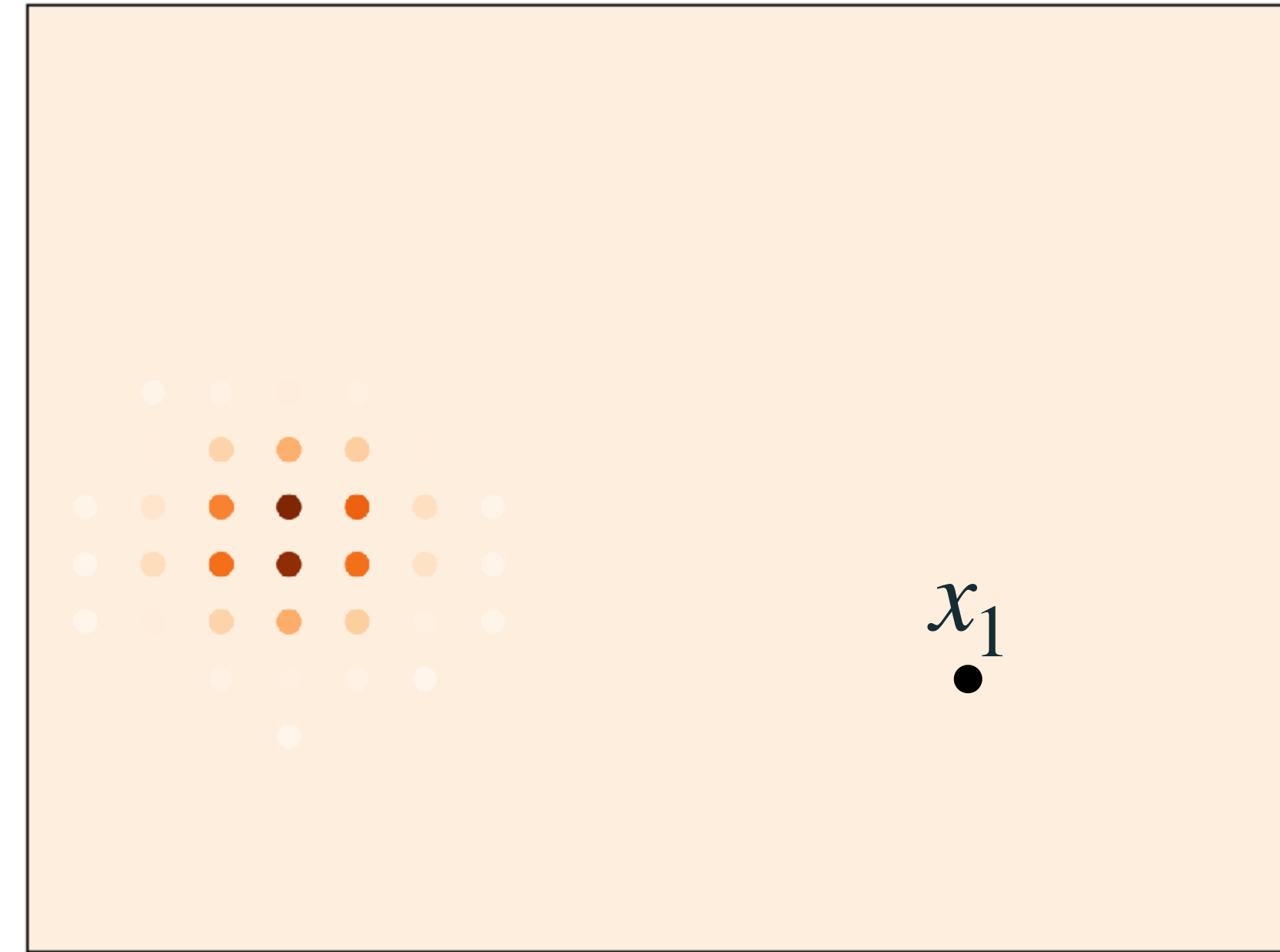
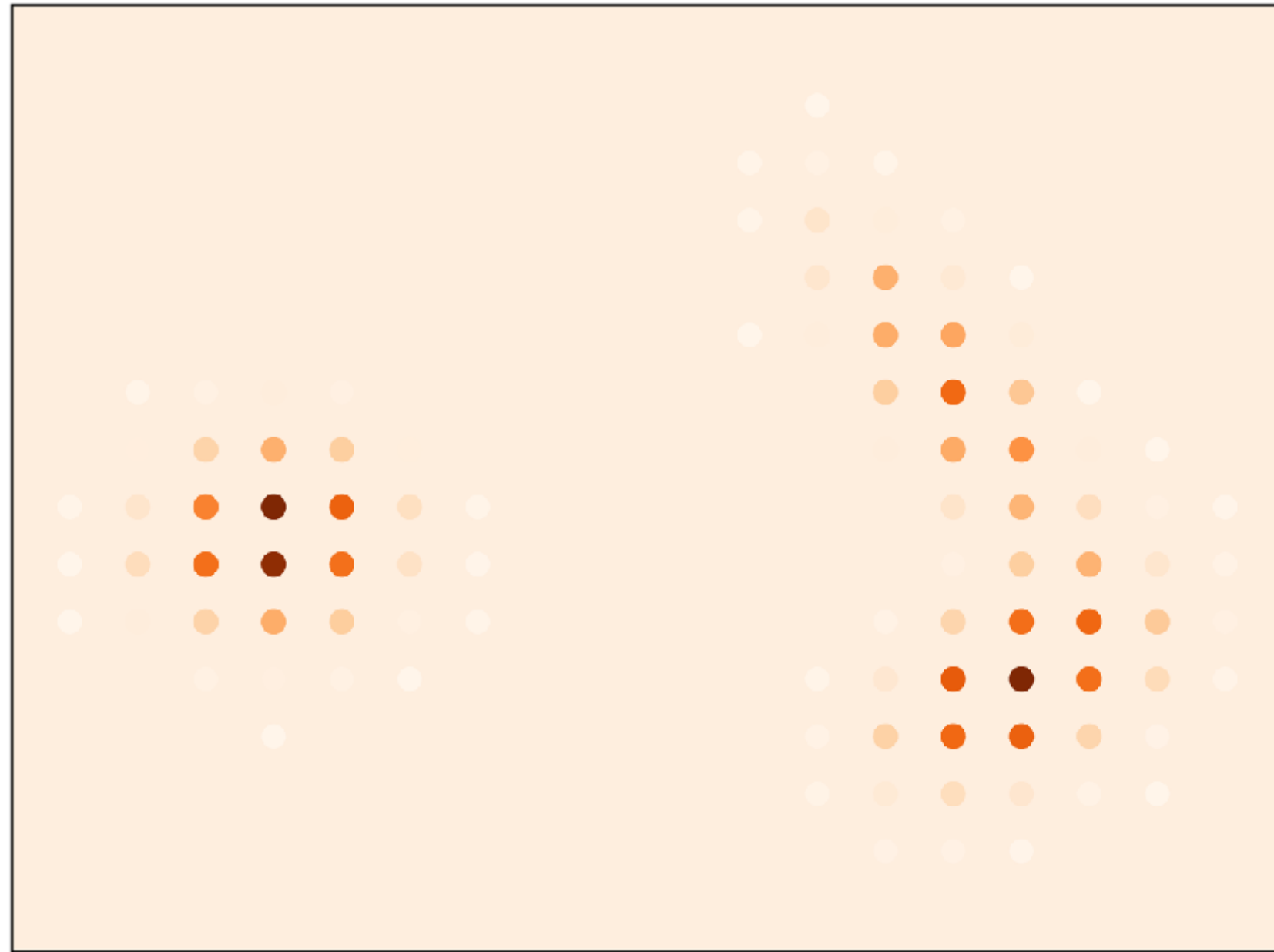
$$u_t(\cdot | x) \in \mathbb{R}^{d|\mathcal{T}|}$$



Intractable

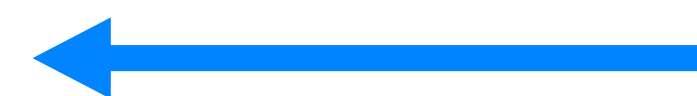
$$u_t^i(y^i | x)$$

Build (factorized) velocities



Mixture path

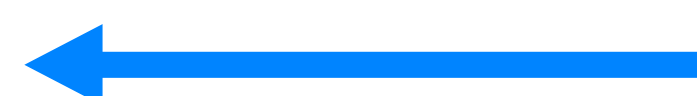
$$p_t(x) = \dots$$



average

$$p_{t|1}^i(x^i | x_1) = (1 - t)p(x^i) + t\delta(x^i, x_1^i)$$

$$u_t^i(y^i | x) = \dots$$

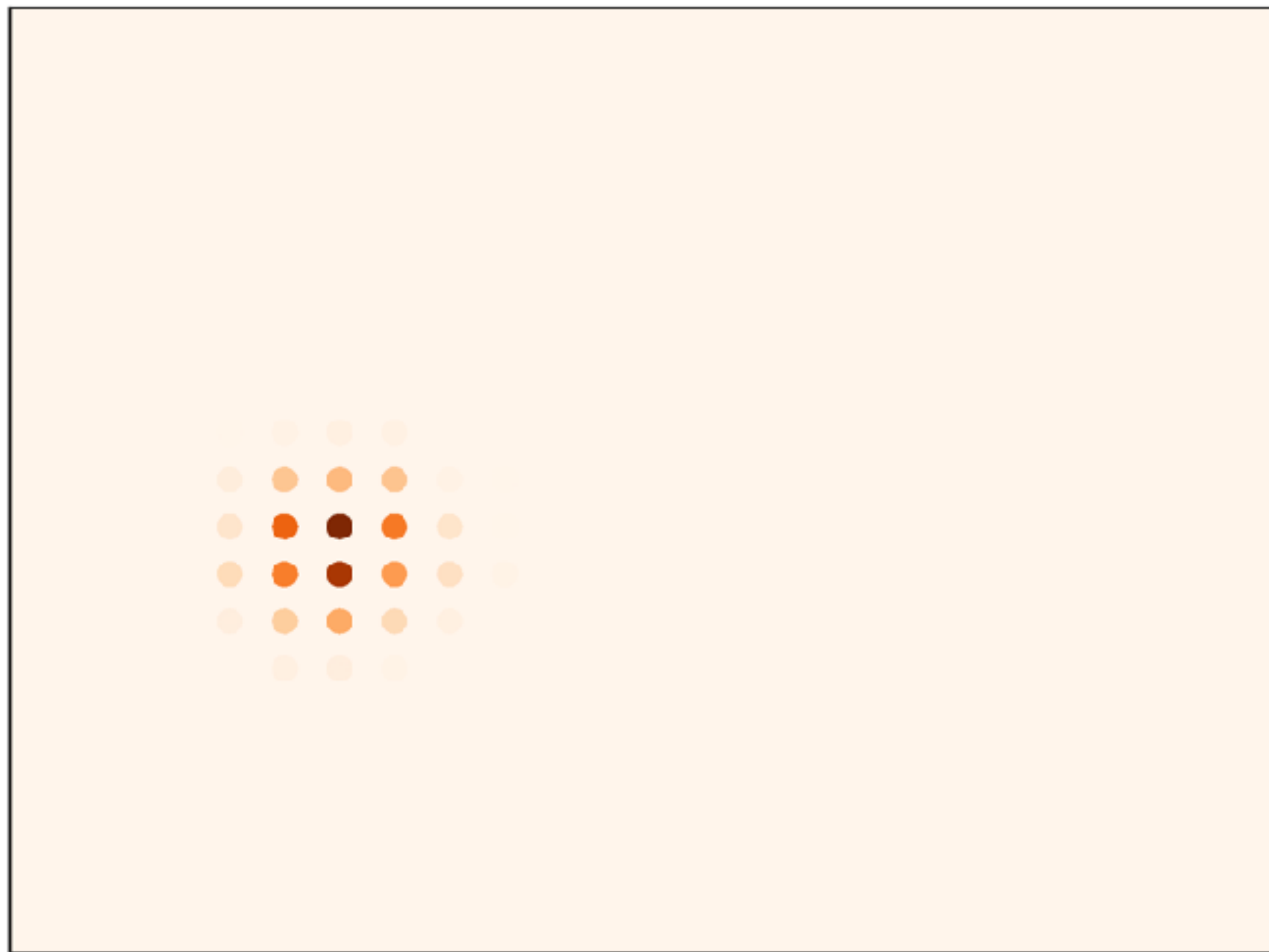


$$u_t^i(y^i | x^i, x_1) = \frac{1}{1 - t} \delta_{x_1^i}(y^i) \quad y^i \neq x^i$$

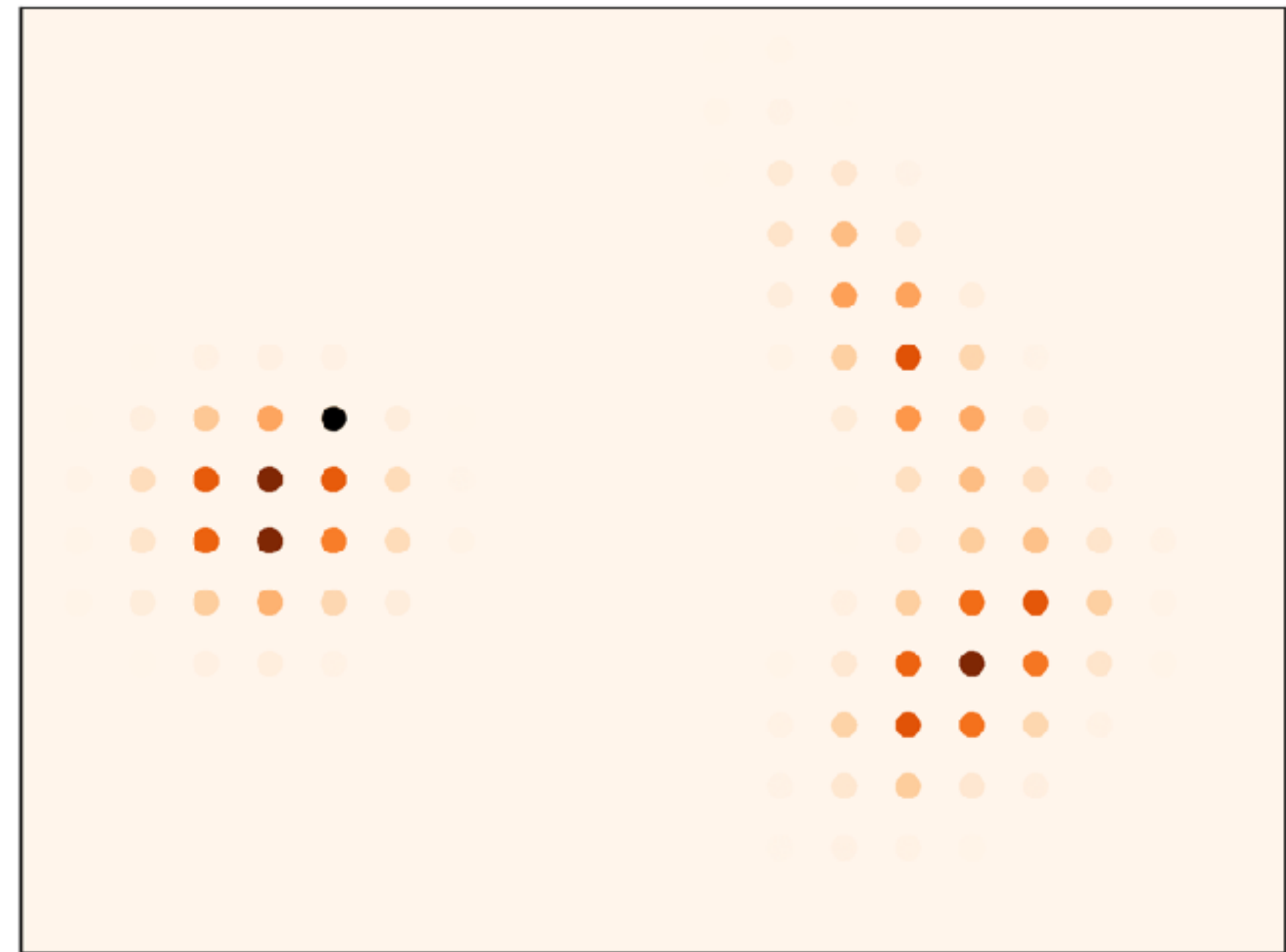
jump rate

where to jump

Discrete Flow Matching



$$p_t(x)$$



$$(X_t)_{0 \leq t \leq 1}$$

“Discrete Flow Matching” Gat et al. (2024)

“Flow Matching with General Discrete Paths: A Kinetic-Optimal Perspective” Shaul et al. (2024)

“Discrete Diffusion Modeling by Estimating the Ratios of the Data Distribution” Lou et al. (2024)

Example: code generation mask model (1.7B)

```
def binary_search(arr, x):
```

```
    # If x is greater
```

```
    # If x is smaller
```

```
else:
```

"Simple and Effective Masked Diffusion Language Models" Sahoo et al. (2024)

"Simplified and Generalized Masked Diffusion for Discrete Data" Shi et al. (2024)

"Discrete Flow Matching" Gat et al. (2024)

General Discrete Probability Paths

Given any (conditional) probability path $p_t(x)$,
a **kinetic optimal** (conditional) velocity is:

$$u_t(y | x) = \frac{\text{ReLU}(p_t(x)\dot{p}_t(y) - \dot{p}_t(x)p_t(y))}{p_t(x)}$$

E.g. Metric paths:

$$p_{t|1}(x | x_1) = \text{softmax}(-\beta_t d(x, x_1))$$

$$u_t(y | x, x_1) = p_{t|1}(x | x_1) \dot{\beta}_t \text{ReLU}(d(x, x_1) - d(y, x_1))$$

CIFAR10

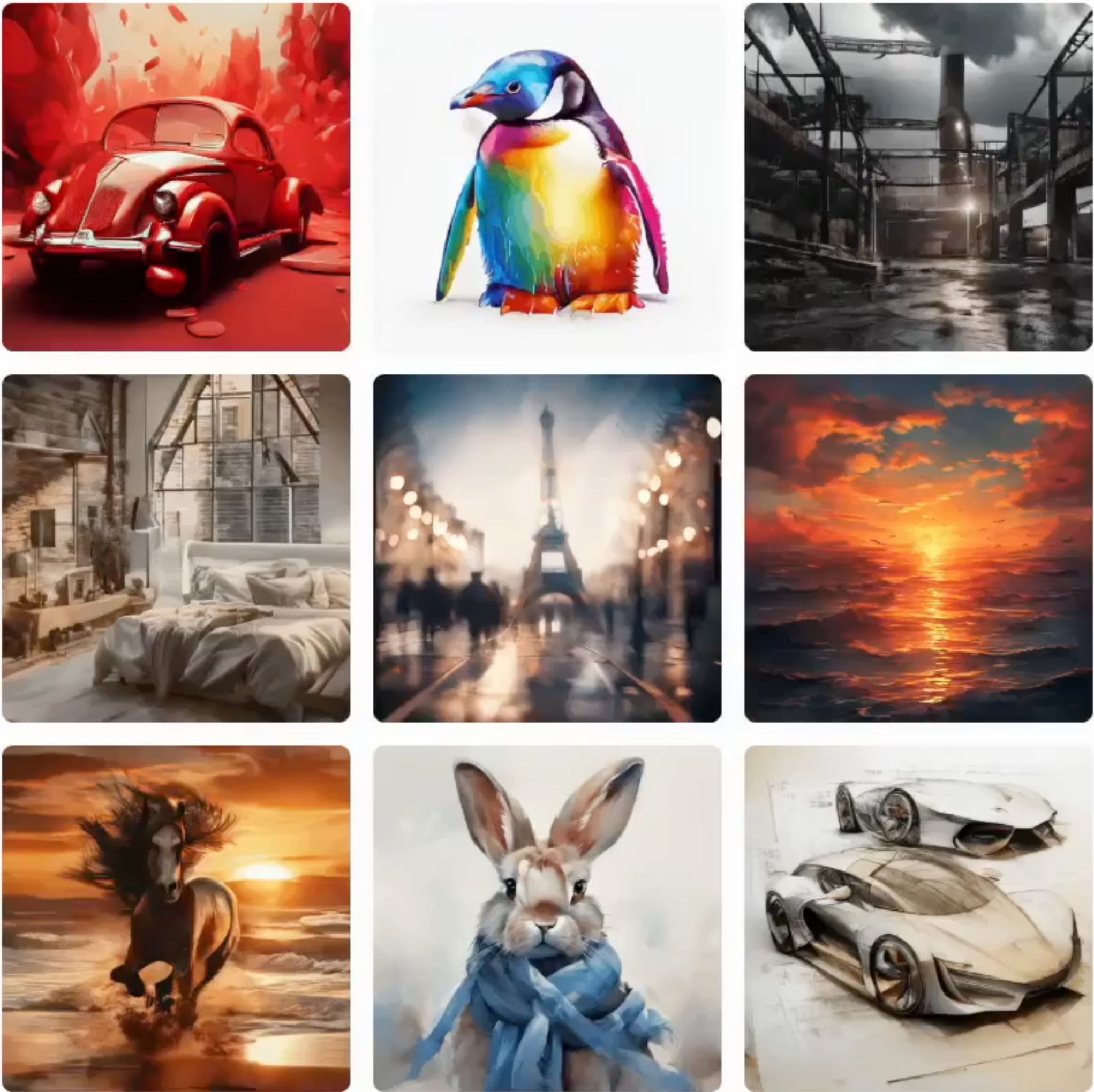
Method	FID ↓
D3PM (Austin et al., 2021)	7.34
CTDD (Nisonoff et al., 2024)	7.86
τ LDR-10 (Campbell et al., 2022)	3.74
DFM w/ mask (Gat et al., 2024)	3.63
DFM w/ metric (Ours)	3.43

ImageNet 256x256

Method	NFE	FID
LlamaGen (AR) (Sun et al., 2024)	256	5.46
LlamaGen (AR)* (Sun et al., 2024)	256	4.81
DFM - Mask* (Gat et al., 2024)	100	5.72
DFM - Metric (Ours)	100	4.50

FUDOKI: Multimodal w/ General Discrete Paths

 Image Generation



Discrete flow matching denoises step by step, transforming noise into vivid images.

 Image Understanding



Where is the group of people playing music positioned on the stage?
A. Left side of the stage
B. Right side of the stage
[C]. Center of the stage ✓
D. They are sitting in front of the stage

Text Generation Progress:

The	group	of	people	playing	music
is	positioned	in	the	center	of
the	stage	.	<eos>	<pad>	<pad>
<pad>	<pad>	<pad>	<pad>	<pad>	<pad>
<pad>	<pad>	<pad>	<pad>	<pad>	<pad>

100%

Edit Flows

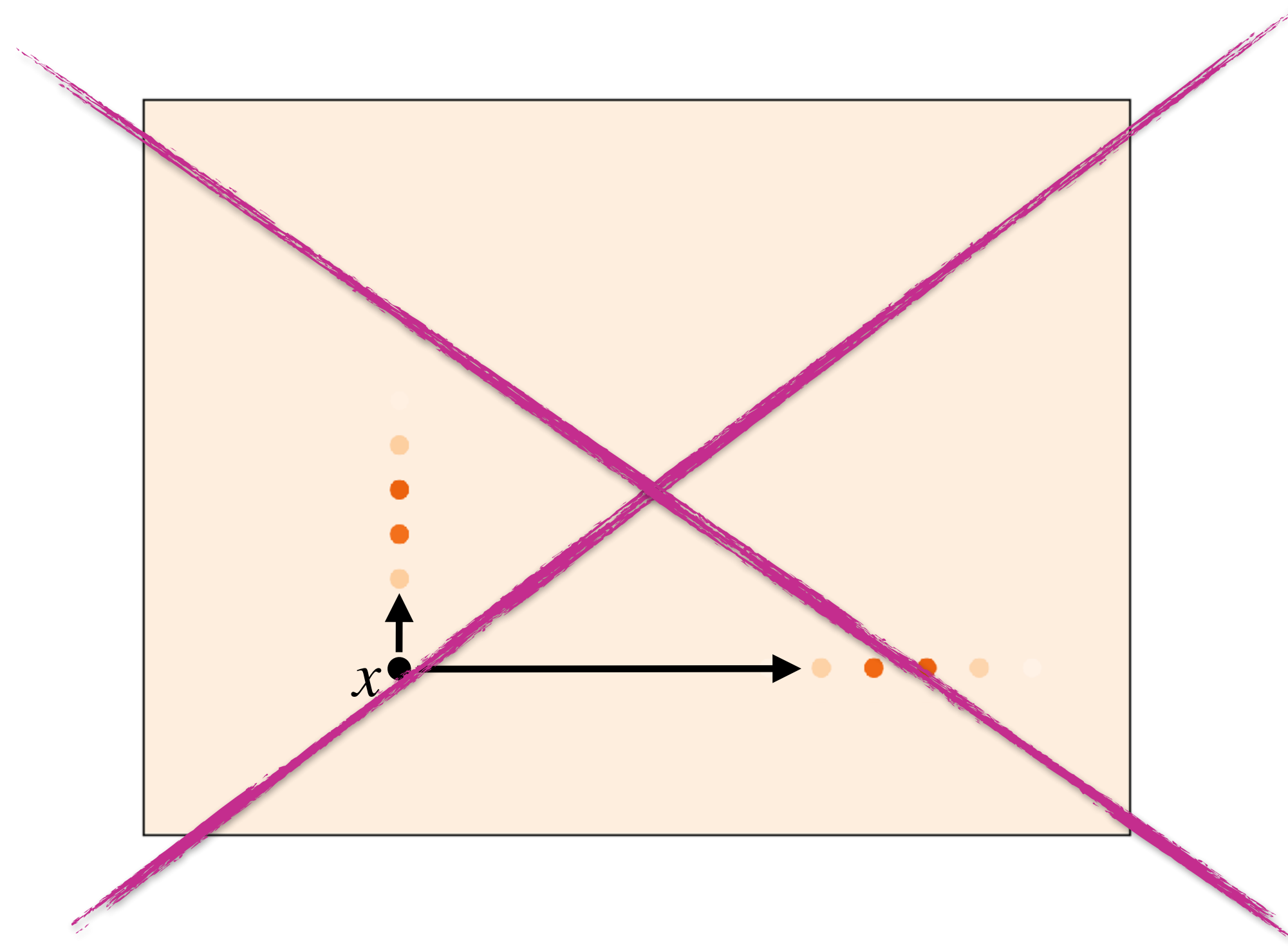
Imbuing diffusion with dimensional changes

Designing a model for variable length sequences

State space

$$X \in \bigcup_{n=0}^N \mathcal{T}^n$$

Data contains
variable length
sequences



Forcefully aligning tokens doesn't make sense for sequence generation

- Requires padding with <EOS> to handle variable length generation
- Makes the model over-confident in predicting <EOS>

Designing a model for variable length sequences

State space

$$X \in \bigcup_{n=0}^N \mathcal{T}^n$$

Data contains
variable length
sequences

VERY rough description of some prior works:

- Train on an (ordered) sequence of edit operations
- 2-stage model to predict # edits, use causal mask model to predict tokens

Insertion Transformer: Flexible Sequence Generation via Insertion Operations

Mitchell Stern^{1,2} William Chan¹ Jamie Kiros¹ Jakob Uszkoreit¹

Levenshtein Transformer

Jiatao Gu[†], Changhan Wang[†], and Jake Zhao (Junbo)^{‡,§}

[†]Facebook AI Research

[‡]New York University [§]Tigerobo Inc.

[†]{jgu, changhan}@fb.com [‡]jakezhao@cs.nyu.edu

Preprint

DIFFUSER: DISCRETE DIFFUSION VIA EDIT-BASED RECONSTRUCTION

Machel Reid
Google Research*
machelreid@google.com

Vincent J. Hellendoorn
Software and Societal Systems Department
Carnegie Mellon University
vhellendoorn@cmu.edu

Graham Neubig
Language Technologies Institute,
Carnegie Mellon University
Inspired Cognition
gneubig@cs.cmu.edu

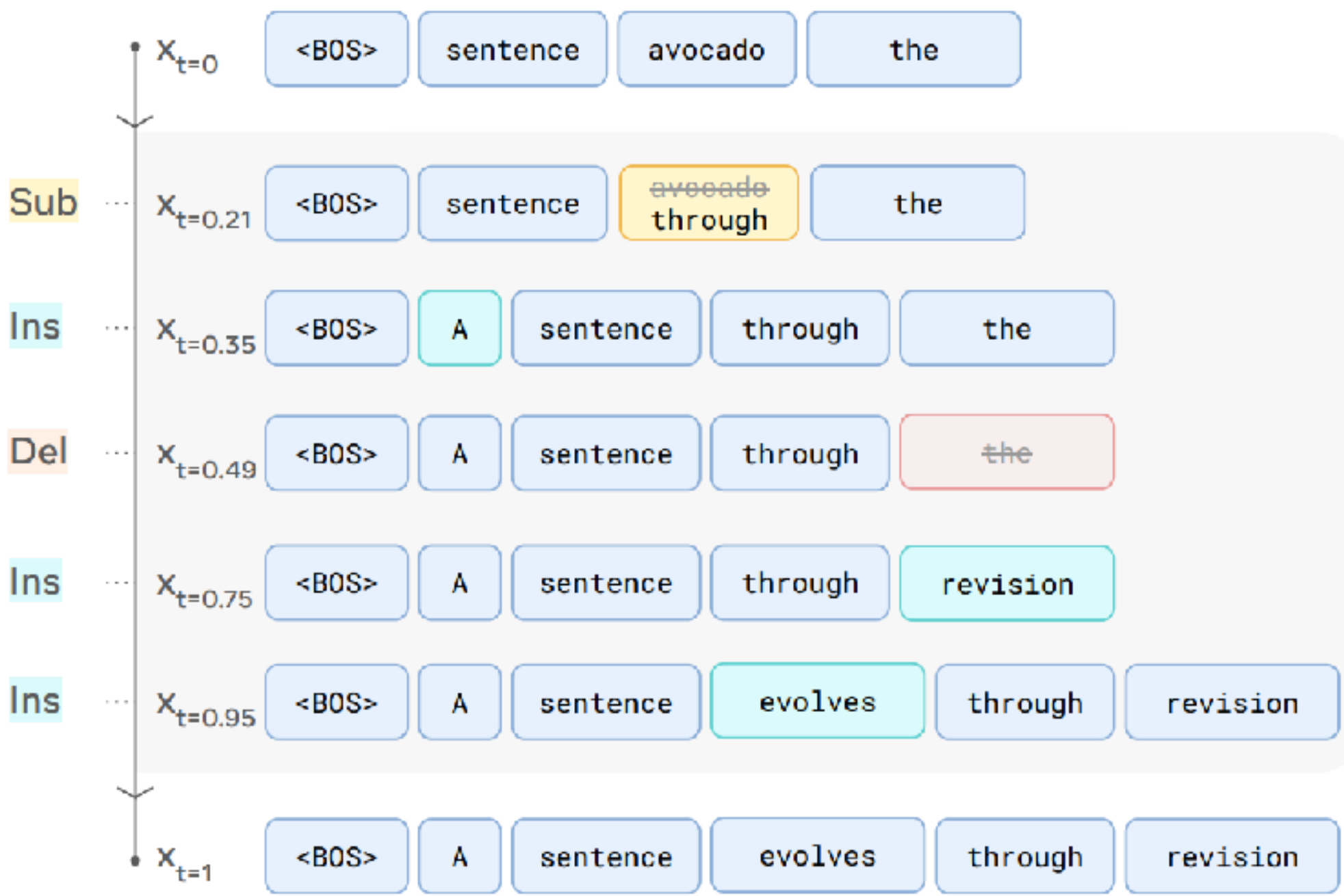
Designing a model for variable length sequences

State space

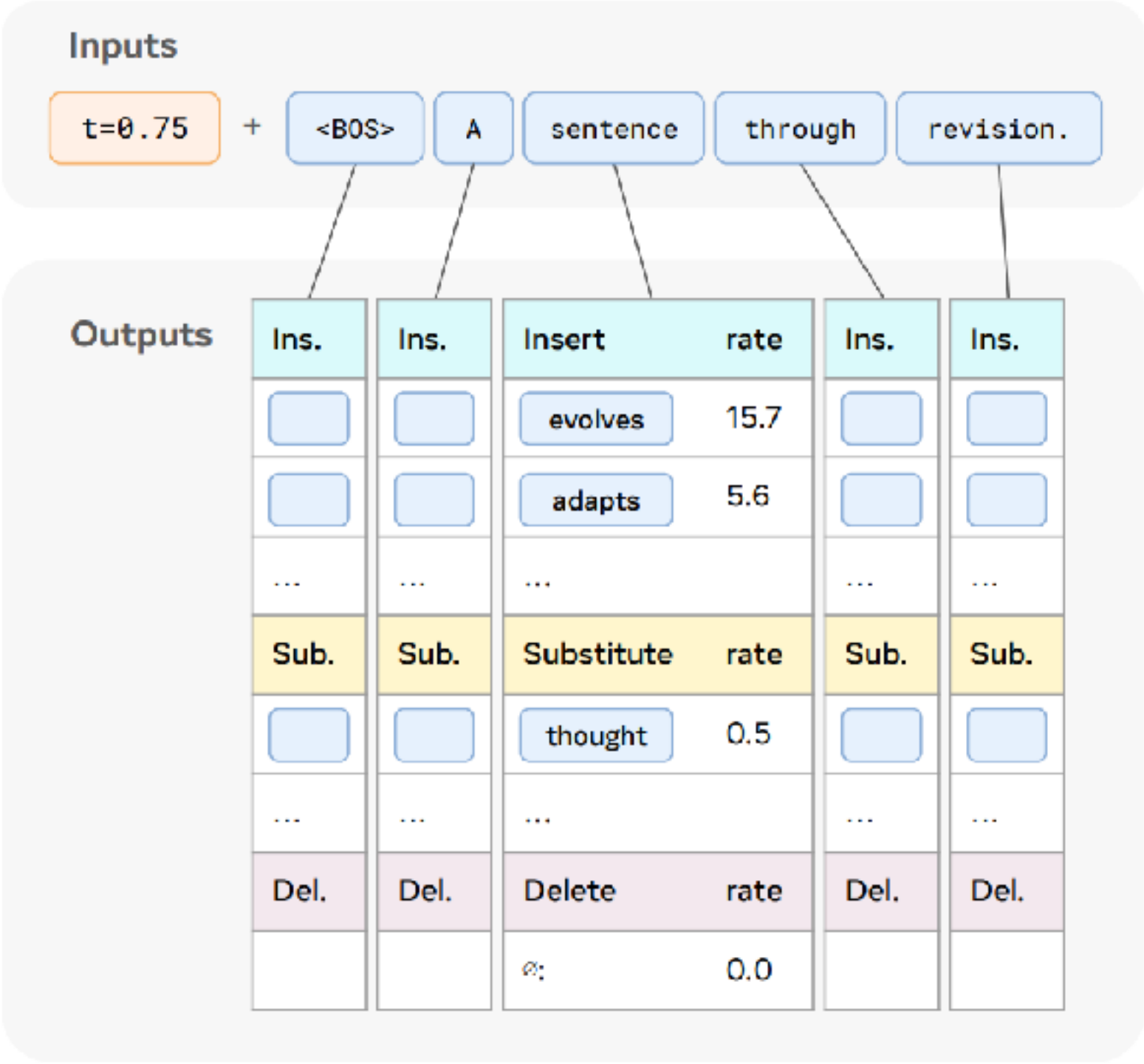
$$X \in \bigcup_{n=0}^N \mathcal{T}^n$$

Data contains
variable length
sequences

Sampling process



Inputs / Outputs



CTMC Model

$$\begin{aligned}
 u_t^\theta(\text{ins}(x, i, a)|x) &= \lambda_{t,i}^{\text{ins}}(x) Q_{t,i}^{\text{ins}}(a|x) && \text{for } i \in \{1, \dots, n(x)\} \\
 u_t^\theta(\text{del}(x, i)|x) &= \lambda_{t,i}^{\text{del}}(x) && \text{for } i \in \{1, \dots, n(x)\} \\
 u_t^\theta(\text{sub}(x, i, a)|x) &= \lambda_{t,i}^{\text{sub}}(x) Q_{t,i}^{\text{sub}}(a|x) && \text{for } i \in \{1, \dots, n(x)\}
 \end{aligned}$$

Define unique set of edits via alignments

Multiple ways to map X_t to X_1 $\longrightarrow$ Intractable to construct $u_t(x | X_t, X_1)$

Alignments

$$Z \in \mathcal{T}^N$$

Fixed-length (padded) sequences

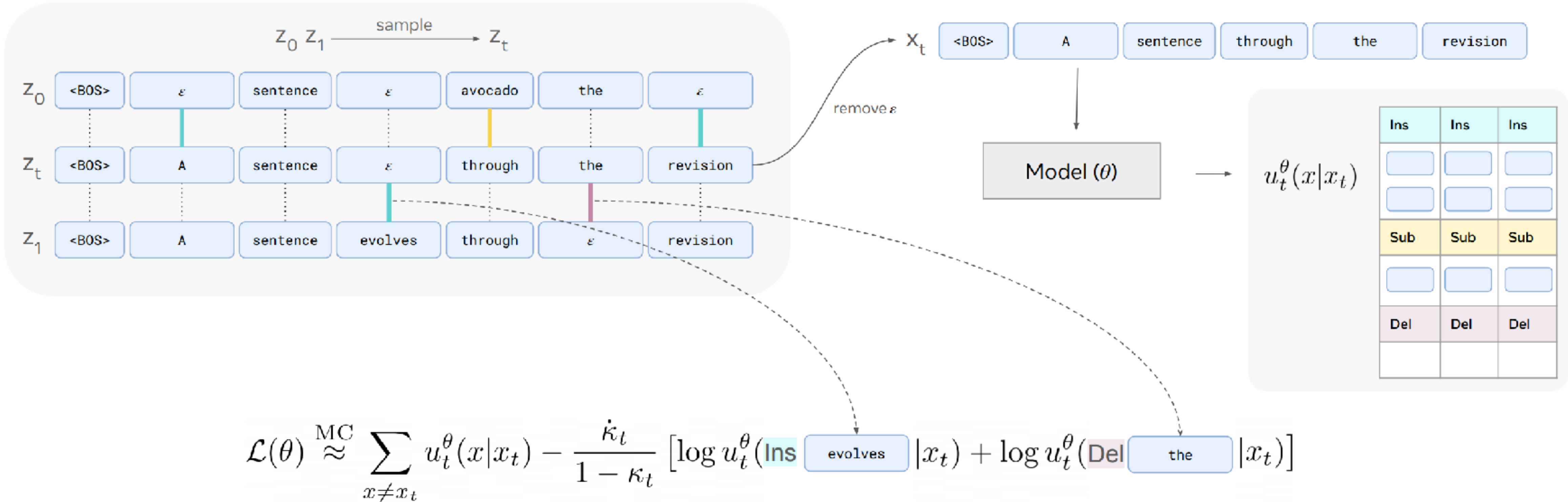
K	ε	I	T	T	E	N
↓	↓					
S	M	I	T	T	E	N

K	I	T	T	E	N	ε	ε	ε	ε	ε	ε
↓	↓	↓		↓	↓	↓					
S	M	I	T	T	E	N	ε	ε	ε	ε	ε

K	I	T	T	E	N	ε	ε	ε	ε	ε	ε	
↓	↓	↓	↓	↓	↓	↓	↓	↓	↓	↓	↓	
ε	ε	ε	ε	ε	ε	S	M	I	T	T	E	N

(Z_0, Z_1) defines a **unique set of edit operations** to map X_0 to X_1

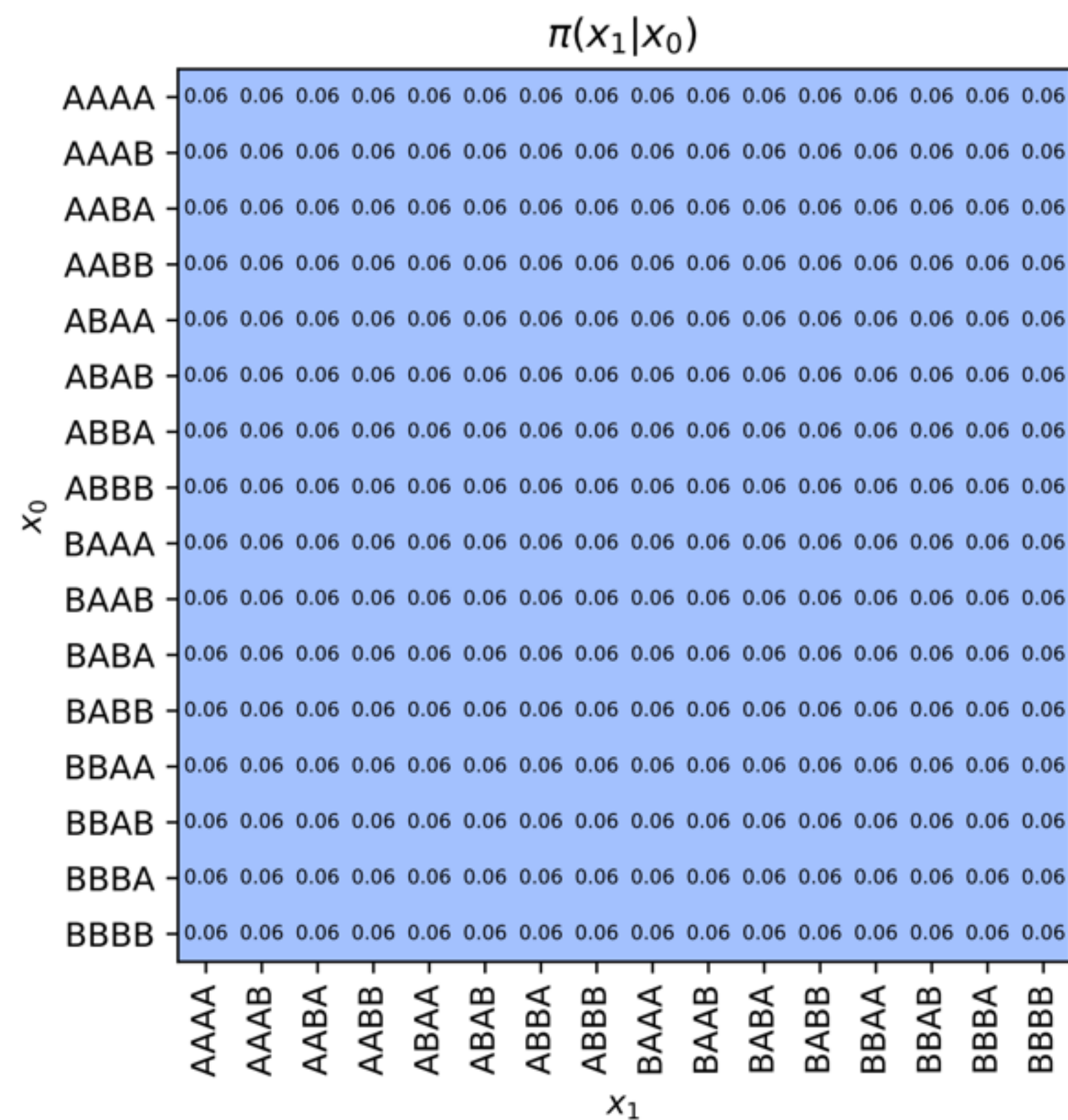
Discrete Flow Matching with auxiliary variables



Inherits similar optimality as continuous space

Learned model will try to **minimize the number of edits!** Maps nearby (X_0, X_1) .

Training (X_0, X_1) pairs



Generated (X_0, X_1) pairs

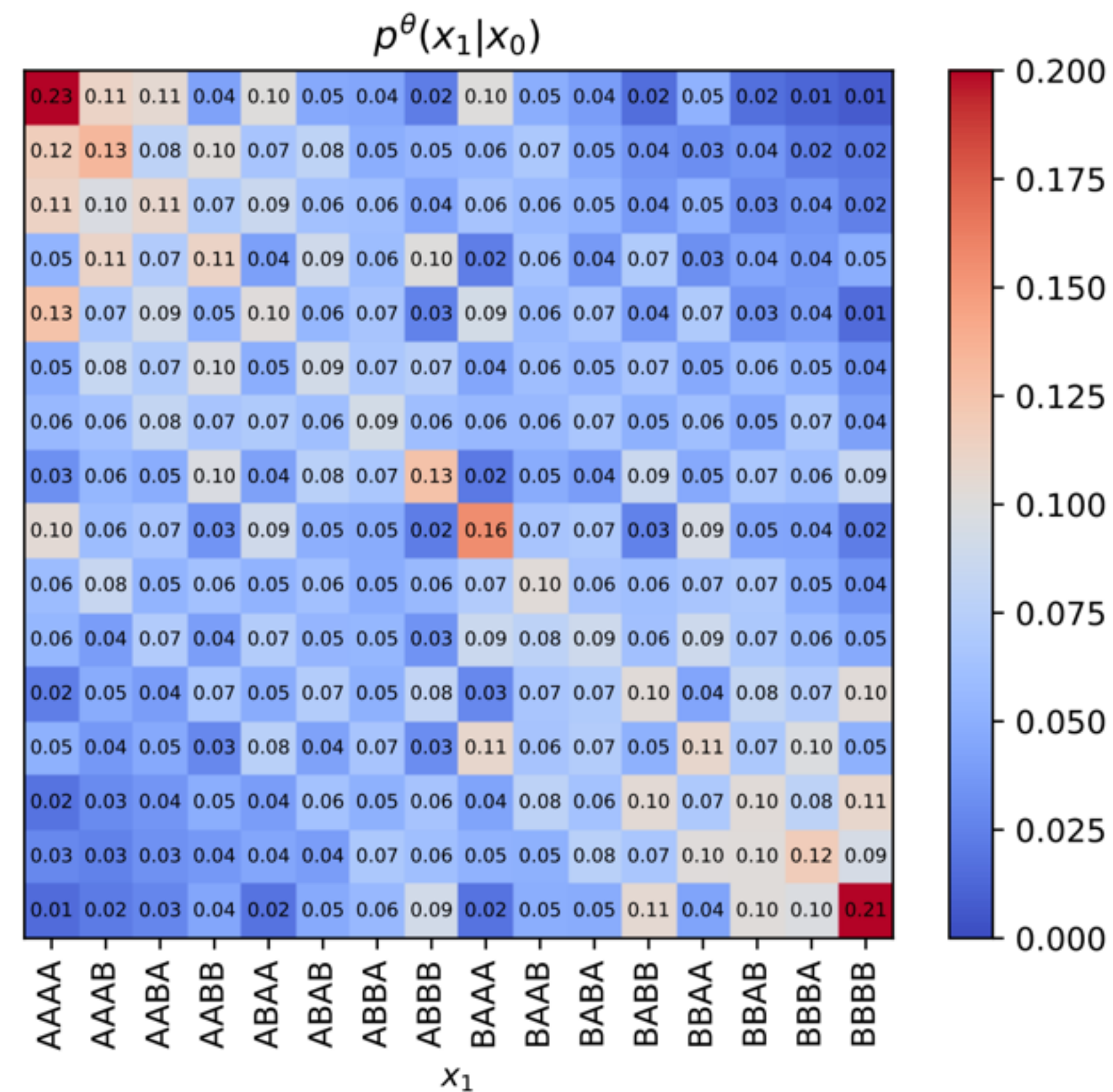


Image Captioning

Method	MS COCO			Image Captioning 3M		
	METEOR	CIDEr	SPICE	ROUGE-L	CIDEr	SPICE
VLP [†] (Zhou et al., 2020)	28.4	117.7	21.3	24.3	77.5	16.5
ClipCap [†] (Mokady et al., 2021)	27.1	108.3	20.1	26.7	87.2	18.5
Autoregressive	25.7	95.5	19.6	25.2	85.8	17.8
Mask DFM	25.3	95.6	19.2	27.4	96.2	20.3
Edit Flow (Ours)	27.4	108.1	21.1	29.0	101.9	21.7
Localized Edit Flow (Ours)	27.4	105.1	22.1	28.3	99.7	20.8



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floor



tree



www.shutterstock.com · 695915347

camera

Text & Code Generation (1.3B)

Insert-only

```
def is_prime(n: int) -> bool:
```

Insert + Delete + Substitute

```
def is_prime(n: int) -> bool:
    if n <= 1:
        return True
    for i in range(2, n):
        if i % n == 0:
            return True
    return False
```

Method	HellaSwag	ARC-E	ARC-C	PIQA	OBQA	WinoGrande
Autoregressive	49.5	71.0	36.3	76.0	30.4	62.1
Mask DFM	38.3	55.4	27.8	65.3	22.6	52.3
Edit Flow (CFG applied to u_t) (Ours)	49.0	63.1	33.0	68.8	28.6	53.6
Edit Flow (CFG applied to $\mathcal{L}$) (Ours)	54.5	61.0	34.0	65.0	37.2	54.3

Table 2 Zero-shot text benchmarks using 1.3B parameter models trained on DCLM-baseline 1.0 (Li et al., 2024). Colors show the best and second best among each metric.

Method	HumanEval		HumanEval+		MBPP	
	Pass@1	Pass@10	Pass@1	Pass@10	Pass@1	Pass@10
Autoregressive (Gat et al., 2024)	14.3	21.3			17.0	34.3
Autoregressive [†]	17.0	34.7	14.0	28.6	25.6	45.4
Mask DFM (Gat et al., 2024)	6.7	13.4			6.7	20.6
Mask DFM (Oracle Length) (Gat et al., 2024)	11.6	18.3			13.1	28.4
Mask DFM [†]	9.1	17.6	7.9	13.4	6.2	25.0
Uniform X_0 + Edit Flow (Ours)	9.7	24.3	9.7	19.5	9.4	33.4
Edit Flow (Ours)	12.8	24.3	10.4	20.7	10.0	36.4
Localized Edit Flow (Ours)	14.0	22.6	10.4	18.9	14.8	34.0

Table 3 Code generation benchmarks using 1.3B parameter models trained on the CodeLlama (Roziere et al., 2023) datamix. [†]Superscript denotes our own implementation. We highlight the best non-autoregressive models, where colors show the best and second best among each metric.

Summary: Jumps with the Flow Matching recipe!

$$X_{t+h} \sim \delta_{X_t}(\cdot) + h u_t(\cdot | X_t)$$

Unnormalized distribution

$$u_t(\cdot | X_t) = \lambda_t(X_t) \mathcal{Q}_t(\cdot | X_t)$$

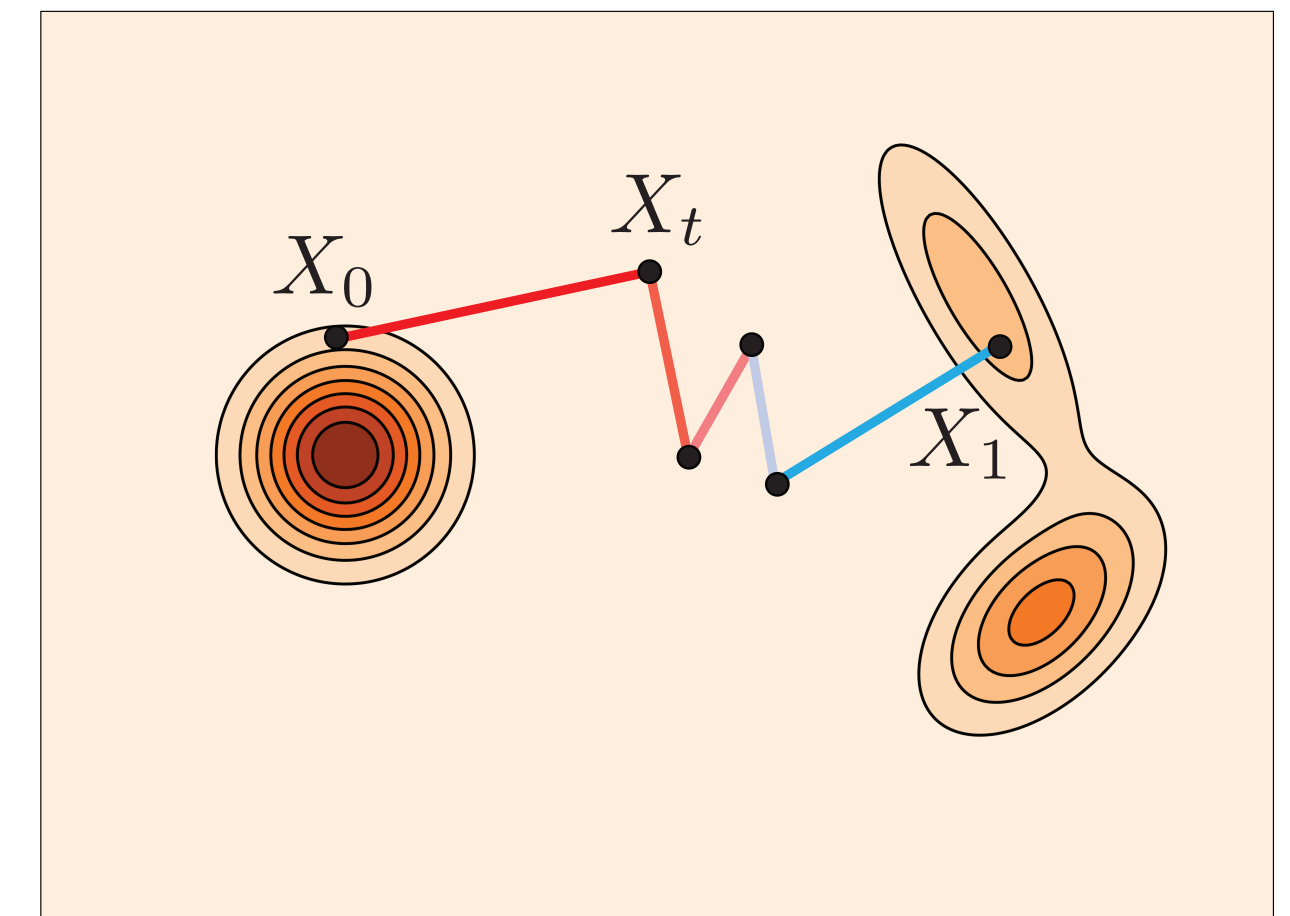
Jump rate

Normalized

Jump process (sampling)

$$X_{t+h} \sim \mathcal{Q}_t(\cdot | X_t) \quad \text{if } h\lambda_t(X_t) \leq U[0,1]$$

$$X_{t+h} = X_t \quad \text{otherwise}$$



Learn conditional expectation

$$u_t(\cdot | x) = \mathbb{E}[u_t(\cdot | X_t, X_1) | X_t = x]$$

Collaborators



Marton Havasi



Itai Gat



Peter Holderrieth



Neta Shaul



Brian Karrer



Yaron Lipman



Tal Remez



Felix Kreuk



Gabriel Synnaeve



Daniel Severo



Anuroop Sriram



Ricky Chen