

Beyond conventional text generation

Aman @ Yiming Yang Lab seminar, 4/5/2022

LM-based generation models

- Typically involve a transformer-based language model + large parallel corpus

- **Established**

- Pre-train —> Fine-tune —> test

- **Popular setups**

- Unsupervised
 - GANs
 - Few-shot
 - Retrieval-augmented
 - Plan-based
 - Structured-generation
 - VAE/De-noising objectives
 - Structure-guided generation *
 - Memory-guided generation *

- **Today**

- Few things not on the list
 - Text generation as optimization (aka Gradient-based approaches)
 - Stochastic processes

Outline

- Part A:
 - Text generation as optimization
- Part B
 - Modeling dynamics of text using stochastic processes
- Part C
 - Fast-slow graph generation

Text generation as optimization

Text generation as optimization

- **Given**

- A large pre-trained language model p_θ
- A set of constraints, specified as functions $f_1, f_2, \dots, f_m, g_1, g_2, \dots, g_n$
 - $g : X \times Y \rightarrow R$
 - Constraints on inputs x and output y (e.g., semantic similarity)
 - $f : Y \rightarrow R$
 - Constraints on just the output (e.g., fluency)
 - Constraints \Leftrightarrow Desired attributes

- **Generate**

- samples (text) from p_θ **without re-training** that satisfy the constraints
- Admits several popular controllable text generation problems:
 - Make text polite
 - Include certain words in the output
 - Condition output on certain keywords

Text generation as optimization: y as a parameter

- $\mathcal{L}(x, y) = f_1(y) + g_1(x, y) + p_\theta(y \mid x)$
- Given an initial y^0
 - $y^{t+1} \leftarrow y^t - \eta \nabla_y(L)$
 - But y is discrete...
- Formality transfer:
 - Given $y = “give\ me\ the\ data”$ generate $“please\ share\ the\ data”$
 - A formality constraint (e.g., $f_1(y)$ measures how polite the sentence y is)
 - What is $\nabla_y L??$
 - The intuition is well-motivated (how to change $“give\ me\ the\ data”$ so that loss is lower), but not differentiable

Recurring theme: y as a parameter

- Instead, y_i is treated as a simplex ($0 \leq y_{il} \leq 1$, $\sum_{l=1}^{|V|} y_{il} = 1$, $|V|$ is the vocabulary size)
 - In short, maintain a continuous representation of y so that it can be back propagated
 - y a tensor like any other parameter, can be attached to the computation graph and backpropagated through
 - Other solutions like Gumbel-softmax

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Towards Decoding as Continuous Optimisation in Neural Machine Translation

Published as a conference paper at ICLR 2017

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CATEGORICAL REPARAMETERIZATION WITH GUMBEL-SOFTMAX

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Controlled Text Generation as Continuous Optimization with Multiple Constraints

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Neurips 2021

Formulation

- Decoding as an optimization problem:
 - The language model will give some distribution over the input $p_\theta(y \mid x)$
 - Improve samples drawn from $p_\theta(y \mid x)$ without changing θ

$$\mathbf{y}^* = \arg \min_{\mathbf{y} \in \mathcal{Y}} (-\log p(\mathbf{y}|\mathbf{x}), f_1(\mathbf{y}), \dots, f_u(\mathbf{y}), g_1(\mathbf{x}, \mathbf{y}), \dots, g_v(\mathbf{x}, \mathbf{y}))$$

- **Initial attempt:** Treat constraints and likelihood as a function of \mathbf{y} , and perform gradient descent on \mathbf{y}
- Optimization problem with constraints
 -

$$\arg \min_y -\alpha \log p(\mathbf{y}|\mathbf{x}) + \sum_{i=1}^u \lambda_i f_i(\mathbf{y}) + \sum_{j=1}^v \mu_j g_j(\mathbf{x}, \mathbf{y}),$$

Issues with vanilla formulation

$$\arg \min_{\mathbf{y}} -\alpha \log p(\mathbf{y}|\mathbf{x}) + \sum_{i=1}^u \lambda_i f_i(\mathbf{y}) + \sum_{j=1}^v \mu_j g_j(\mathbf{x}, \mathbf{y}),$$

- Who decides weights over the constraints? different constraints may have different scales, some might be objective
- Non-convex “Pareto-front”, hard to achieve
- Reformulate again as a Lagrangian optimization problem:

$$\begin{aligned} & \arg \min_{\mathbf{y}} -\log P(\mathbf{y}|\mathbf{x}) \text{ subject to} \\ & f_i(\mathbf{y}) \leq \epsilon_i, i \in \{1, \dots, u\} \\ & g_j(\mathbf{x}, \mathbf{y}) \leq \xi_j, j \in \{1, \dots, v\}. \end{aligned}$$

- Upper limits are easy to manually specify (e.g. probability of formality > 0.5) than weights



Lagrangian formulation

- Lagrangian formulation

$$\mathcal{L}(y, \lambda_1, \dots, \lambda_u, \mu_1, \dots, \mu_v) = -\log p(\mathbf{y}|\mathbf{x}) - \sum_{i=1}^u \lambda_i (\epsilon_i - f_i(y)) - \sum_{j=1}^v \mu_j (\xi_j - g_j(x, y))$$

$$\begin{aligned} & \arg \min_{\mathbf{y}} -\log P(\mathbf{y}|\mathbf{x}) \text{ subject to} \\ & f_i(\mathbf{y}) \leq \epsilon_i, i \in \{1, \dots, u\} \\ & g_j(\mathbf{x}, \mathbf{y}) \leq \xi_j, j \in \{1, \dots, v\}. \end{aligned}$$

- Typical solution:

- $\arg \min_{\mathbf{y}} \max_{\lambda_i \geq 0, \mu_i \geq 0} \mathcal{L}(\mathbf{y}, \lambda_i, \mu_i)$
- First solve the dual function to find Lagrangians, then plug Lagrangians to minimize
- Similar issue as the previous formulation: first clipping the constraints *is not working*
- Final approach:
 - Method of multipliers: jointly optimize for both
 - $\mathbf{y}^{(t)} = \mathbf{y}^{(t-1)} - \eta_1 \nabla_{\mathbf{y}} \mathcal{L}, \lambda_i^t = \lambda_i^{t-1} + \eta_2 \nabla_{\lambda_i} \mathcal{L}, \mu_i^t = \mu_i^{t-1} + \eta_2 \nabla_{\mu_i} \mathcal{L}$
 - Increase the value of the multiplier with each gradient step as long as the constraint is violated (make the optimization process take constraints more seriously)

Algorithm 1: MuCoCo: detailed decoding algorithm

Input: input sequence \mathbf{x} , output length L , base model \mathcal{G} , attribute functions f_i and g_j and their respective initial and final thresholds, threshold update schedule, step sizes η_1, η_2 ;

Result: output sequence \mathbf{y}

For all $k \in \{1, \dots, L\}$, initialize $\tilde{\mathbf{y}}_k^0$ uniformly over Δ_V ;

For all $i \in \{1, \dots, u\}$ and $j \in \{1, \dots, v\}$, initialize λ_i^0, μ_i^0 as 0 and the thresholds ϵ_i^0, ξ_j^0 with the given values ;

for $t = 1, \dots, \text{MAXSTEPS}$ **do**

 // forward pass

 for all k , compute $\hat{y}_k = \text{one-hot}(\arg \max \tilde{y}_k)$ and compute the loss \mathcal{L} (using (5));

 // backward pass

 for all k, i and j , compute $\nabla_{\tilde{y}_k}^{t-1} = \frac{\partial \mathcal{L}}{\partial \tilde{y}_k}, \nabla_{\lambda_i}^{t-1} = \frac{\partial \mathcal{L}}{\partial \lambda_i}, \nabla_{\mu_j}^{t-1} = \frac{\partial \mathcal{L}}{\partial \mu_j}$;

 // Update the parameters

 update $\tilde{y}_k^{(t+1)} \propto \tilde{y}_k^{(t)} \exp(1 - \eta_1 \nabla_{\tilde{y}_k} \mathcal{L})$;

 update $\lambda_i^t = \max(0, \lambda_i^{t-1} + \eta_2 \nabla_{\lambda_i} \mathcal{L})$, and $\mu_i^t = \max(0, \mu_i^{t-1} + \eta_2 \nabla_{\mu_i} \mathcal{L})$;

 update ϵ_i^t, ξ_j^t following the threshold update schedule

end

return $\arg \min_t \{-\log p(\tilde{\mathbf{y}}^{(t)} | \mathbf{x}) : \forall i, f_i(\tilde{\mathbf{y}}^{(t)}) \leq \epsilon_i, \forall j, g_j(\mathbf{x}, \tilde{\mathbf{y}}^{(t)}) \leq \xi_j\}$;

Can select one of
“Pareto-optimal solutions”

Experiments

- Style transfer: make a given sentence more formal (*give me that data* → *please share the data*)
- Task requirements:
 - Attribute transfer: the transferred sentence should be formal
 - Content preservation: the transferred sentence should not lose the original meaning
- Constraints, one per requirement:
 - $-\log(p_{formal}(\mathbf{y})) < -\log(0.5) = 0.3$
 - Force $p_{formal}(\mathbf{y})$ to be greater than 0.5
 - $p_{formal}(\mathbf{y})$ using a classifier \mathbf{y}
 - Start with $-\log(p_{formal}(\mathbf{y})) < 10$ and slowly anneal
- Cosine similarity: $USIM(x, y)$
 - $-USIM(x, y) < -0.15$

Results

Method	Constraint	Fluency	Transfer	Content Preservation (w.r.t. input)		Content Preservation (w.r.t. ref)	
				WSIM	USIM	WSIM	USIM
STRAP	None	91%	78%	0.69	0.77	0.72	0.80
FUDGE	FORMAL(y)	90%	85%	0.71	0.77	0.73	0.81
MuCoCo	FORMAL(y)	89%	93%	0.67	0.75	0.72	0.78
MuCoCo	USIM(x, y)	92%	85%	0.71	0.78	0.74	0.81
MuCoCo	USIM(x, y), WMD(x, y)	92%	87%	0.73	0.79	0.77	0.86
MuCoCo	SIM(x, y), WMD(x, y), FORMAL(y)	93%	92%	0.71	0.79	0.75	0.84

Table 1: Automatic evaluation of fluency, formality transfer, and content preservation for informal-to-formal style transfer models.

COLD Decoding: Energy-based Constrained Text Generation with Langevin Dynamics

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Introduction

- *COLD decoding is a flexible framework that can be applied directly to off-the-shelf left-to-right language models without the need for any task-specific fine-tuning*
- Setup:
 - Given
 - A language model
 - A set of constraints specified as differentiable functions of output
 - Generate samples that satisfy the constraint

Background Energy distribution

- Energy-based distribution

$$\bullet \quad p(y) = \frac{\exp^{-E(y)}}{\sum_y \exp^{-E(y)}}$$

- $E(y)$ is the “energy function”
 - Lower (more negative) energy states are more likely
 - Terminology from physics, low-value energy states are preferable (second-law of thermodynamics)
 - $E(y)$ can be arbitrary in principle
- We don’t care about the actual distribution typically, only the samples

Encoding constraints in energy function

- Let $f_i(y)$ be a constraint function, which is high if constraint is better satisfied

$$\bullet p(y) = \frac{\exp \sum_i \lambda_i f_i(y)}{Z}$$

- E.g., number of tokens in y that are one of {cat, dog, elephant}, more the better

- **Desired:**

- A way to draw samples from the energy function

- **Langevin dynamics**

- MCMC method, used for sampling from energy functions

- Langevin dynamics is motivated and originally derived as a discretization of a stochastic differential equation whose equilibrium distribution is the posterior distribution

- $y^{n+1} \leftarrow y^n - \eta \nabla_y E(y^n) + \epsilon^n$

- η : step size, $\epsilon \sim \mathcal{N}(0, \sigma)$

- Welling & Teh 2011 prove that $\lim_{n \rightarrow \infty} y^n \sim p$

- Problem as usual:

- $\nabla_y E(y)$

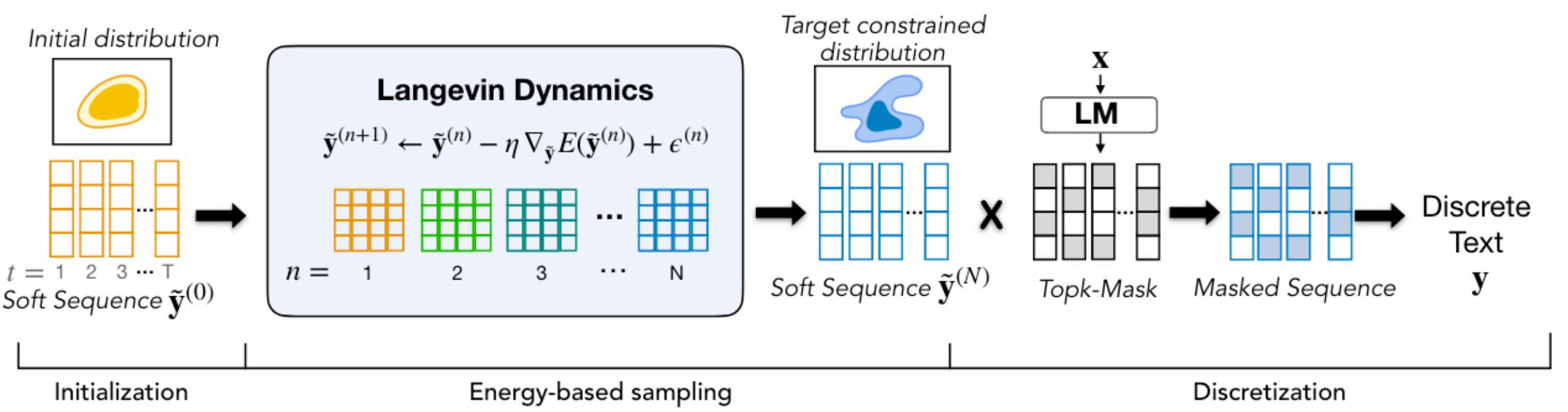
- Differentiate w.r.t. concrete text

- Same solution as used by Kumar 2021 \rightarrow soft tokens

- Same constraint: the constraint functions need to be differentiable



COLD decoding overview



Algorithm 1 Constrained Decoding w/ Langevin Dynamics.

```

input Constraints  $\{f_i\}$ , length  $T$ , iterations  $N$ .
output Sample sequence  $\mathbf{y}$ .
 $\tilde{\mathbf{y}}_t^{(0)} \leftarrow \text{init}()$  for all position  $t$  // init soft-tokens
for  $n \in \{1, \dots, N\}$  do
     $E^{(n)} \leftarrow E(\tilde{\mathbf{y}}^{(n)}; \{f_i\})$  // compute energy (§3.2)
     $\tilde{\mathbf{y}}_t^{(n+1)} \leftarrow \tilde{\mathbf{y}}_t^{(n)} - \eta \nabla_{\tilde{\mathbf{y}}_t} E^{(n)} + \epsilon_t^{(n)}$  for all  $t$  // update
        soft tokens (Eq.2)
end for
 $y_t = \arg \max_v \text{topk-filter}(\tilde{\mathbf{y}}_t^{(N)}(v))$  for all  $t$  // discretize (Eq.6)
return:  $\mathbf{y} = (y_1, \dots, y_T)$ 

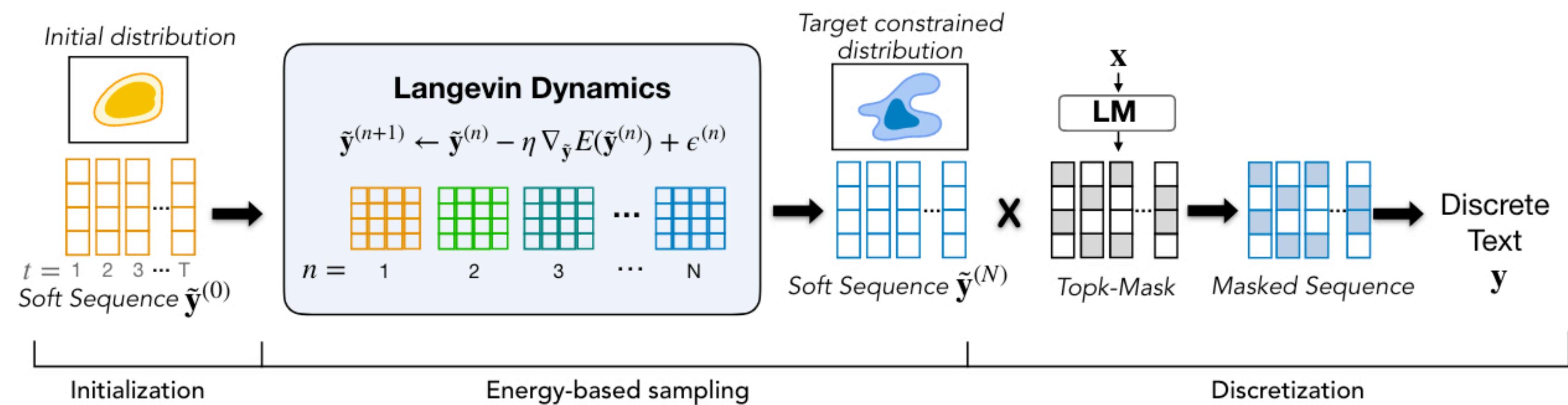
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Initialization. We initialize the soft sequence $\tilde{\mathbf{y}}$ by running greedy decoding with the LM p_{LM} to obtain output logits. In our preliminary experiments, the initialization strategy had limited influence on the generation results.

From soft-tokens to hard tokens

- Top-k mask

$$y_t = \arg \max_{v \in \mathcal{V}_t^k} \tilde{\mathbf{y}}_t(v).$$



- Essentially, the language model gives an idea of what is right
 - Questionable, and ablations reveal that this is critical for their method

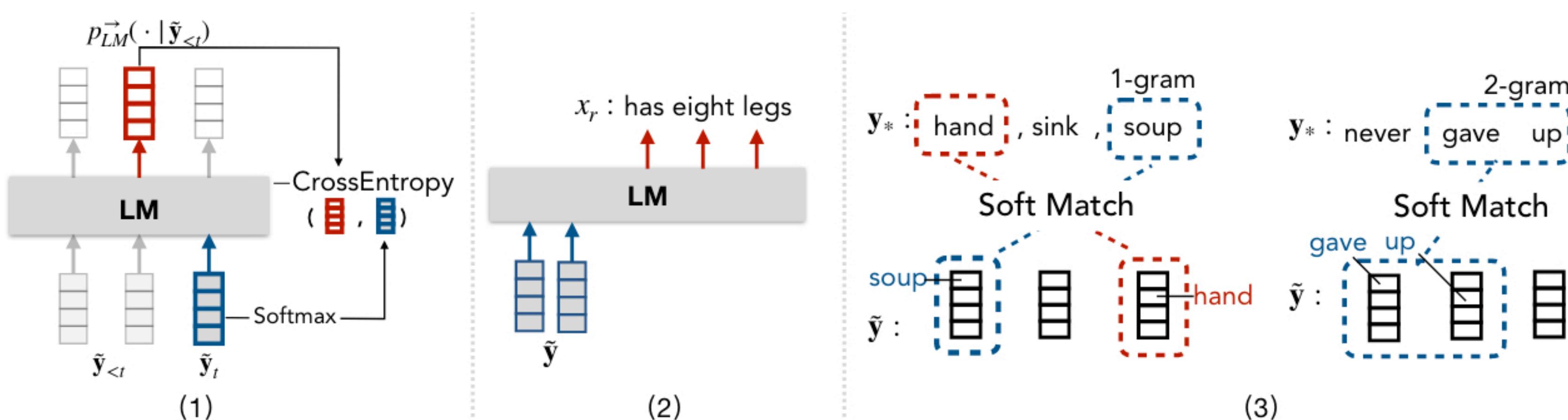
Experiments

Abductive reasoning

- Given a beginning (x_l : ***Tim wanted to learn astronomy***) and end sentence (x_r , ***Tim worked hard in school to become one***), generate a bridge sentence that completes the reasoning chain
 - \tilde{y} : ***Tim took admission in an astronomy program***
- Constraints:
 - The generated text \tilde{y} should have a high-likelihood given the left and right sentences
 - \tilde{y} should predict x_r
 - There should be some common keywords between \tilde{y} , x_l , x_r

Example of constraints

- Soft-fluency constraint: $f_{LM}^{\rightarrow}(\tilde{y}) = \sum_{t=1}^T \sum_{v \in \mathcal{V}} p_{LM}^{\rightarrow}(v | \tilde{y}_{<t}) \log \text{softmax}(\tilde{y}_t(v))$
- To be used in conjunction with other constraints



Experiments

Counterfactual story generation

$$E(\tilde{\mathbf{y}}) = \lambda_a^{lr} f_{\text{LM}}^{\rightarrow}(\tilde{\mathbf{y}}; \mathbf{x}_l) + \lambda_a^{rl} f_{\text{LM}}^{\leftarrow}(\tilde{\mathbf{y}}; \mathbf{x}_r) + \lambda_b f_{\text{pred}}(\tilde{\mathbf{y}}; \mathbf{x}_r) + \lambda_c f_{\text{sim}}(\tilde{\mathbf{y}}; \text{kw}(\mathbf{x}_r) - \text{kw}(\mathbf{x}_l)).$$

Models	Automatic Eval				Human Eval			
	BLEU ₄	ROUGE-L	CIDEr	BERTScore	Grammar	Left-coherence ($\mathbf{x}_l \mathbf{y}$)	Right-coherence ($\mathbf{y} \mathbf{x}_r$)	Overall-coherence ($\mathbf{x}_l \mathbf{y} \mathbf{x}_r$)
LEFT-ONLY	0.88	16.26	3.49	38.48	4.57	3.95	2.68	2.70
DELOREAN	1.60	19.06	7.88	41.74	4.30	4.23	2.83	2.87
COLD (ours)	1.79	19.50	10.68	42.67	4.44	4.00	3.06	2.96

- A number of other shortcuts to get it to work
 - Hyper-parameters appear to be highly tuned (0.3, 0.2, 0.02, 0.48), but no details how
 - The method only generates 10 tokens, and the rest are generated by standard language models

Discussion

- **Summary**
 - There are methods that can generate samples from pre-trained language models that satisfy certain constraints, without re-training
- **Difference between two works?**
 - Formulation and method, but conceptually identical
 - COLD allows drawing multiple samples, but also possible with MuCOCO
 - MuCOCO allows specifying different constraints on weights
- **Non-differentiable objectives**
 - Uses continuous sampling from black box models, but extremely slow

Mix and Match: Learning-free Controllable Text Generation using Energy Language Models

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Modeling dynamics of text using stochastic processes

Published as a conference paper at ICLR 2022

LANGUAGE MODELING VIA STOCHASTIC PROCESSES

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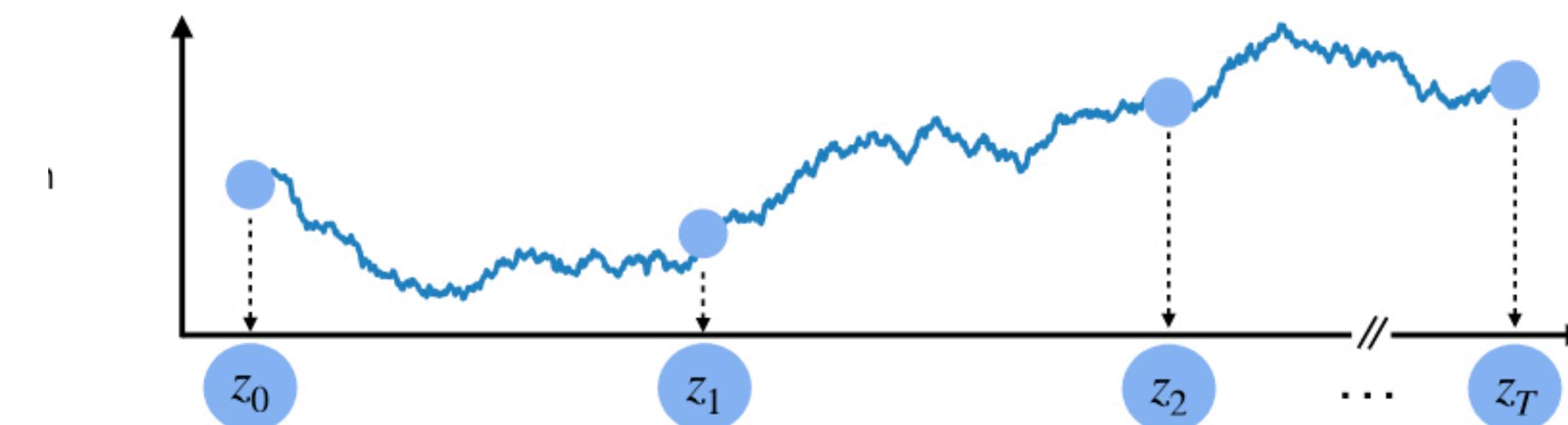
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Introduction

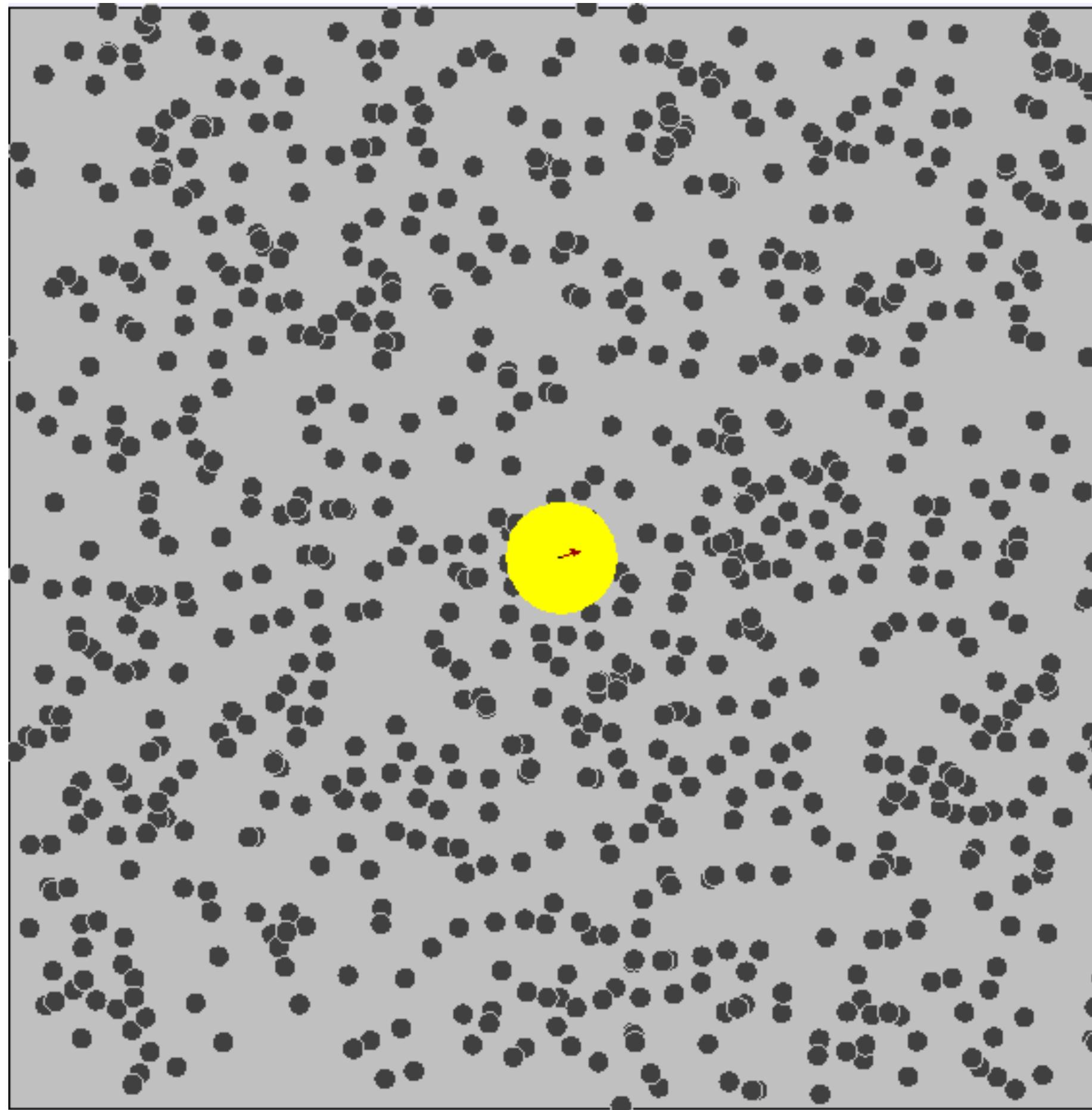
- Long-form generation is important
 - Story generation, document generation
- Current language models struggle
- Possible reason:
 - Auto-regressive models struggle to attend to longer sequences
 - No notion of “evolving” context

Overview

- Generate hidden states for each sentence of a long document
 - The representations should vary ***smoothly***
 - The representations should be ***grounded*** in the start and beginning



Brownian motion

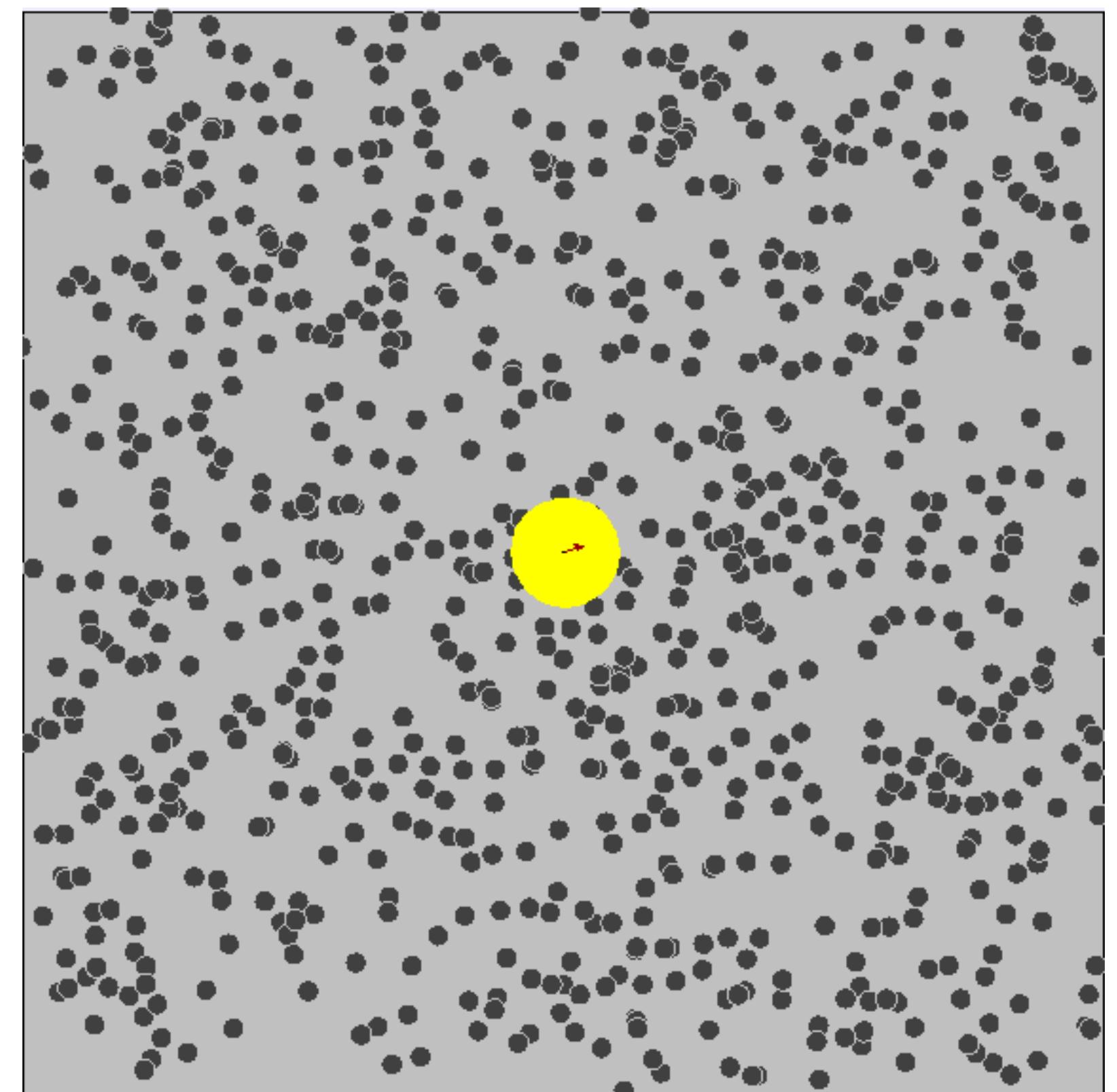
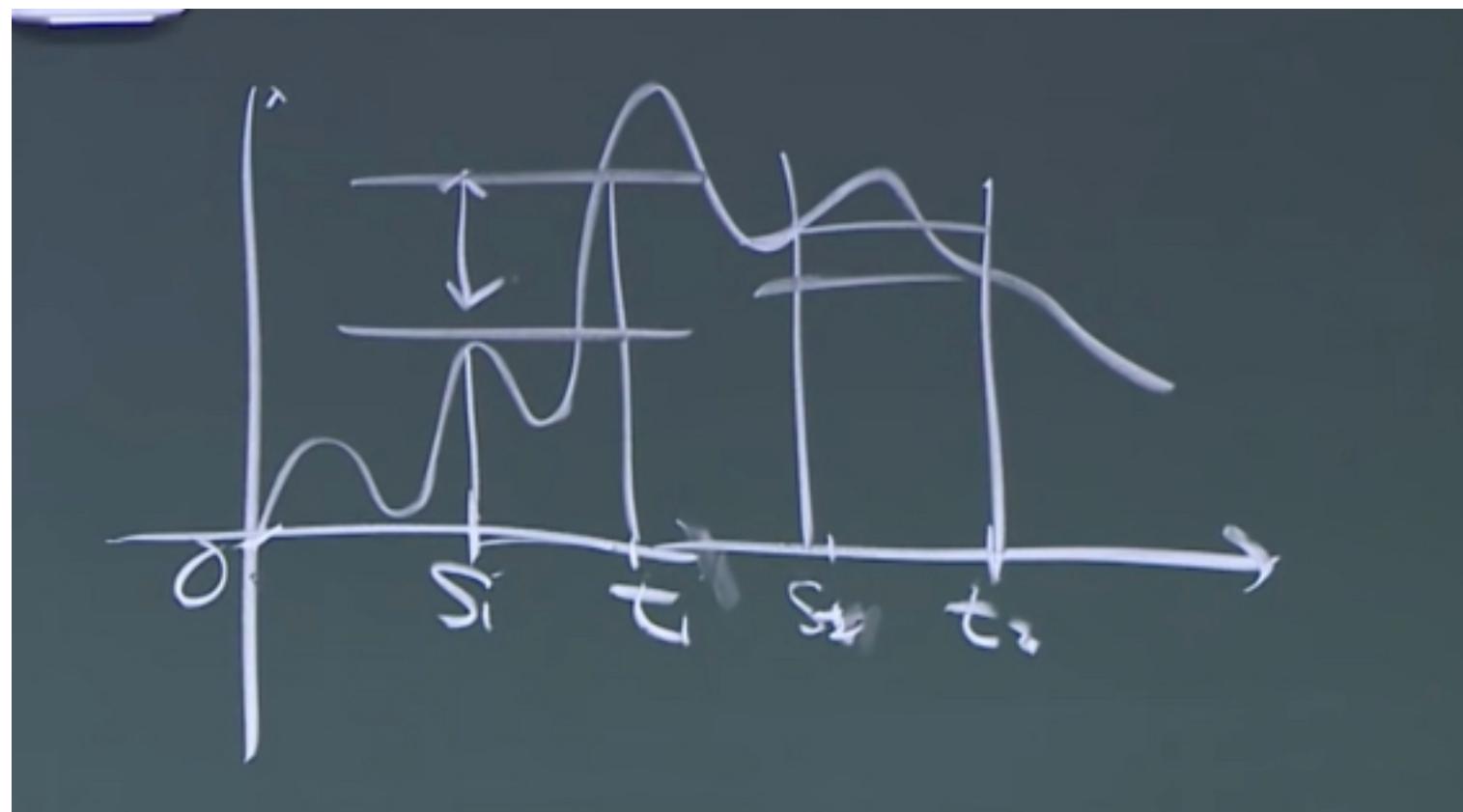


Brownian motion

Theorem 2.1. *There exists a probability distribution over the set of continuous functions $B : \mathbb{R} \rightarrow \mathbb{R}$ satisfying the following conditions:*

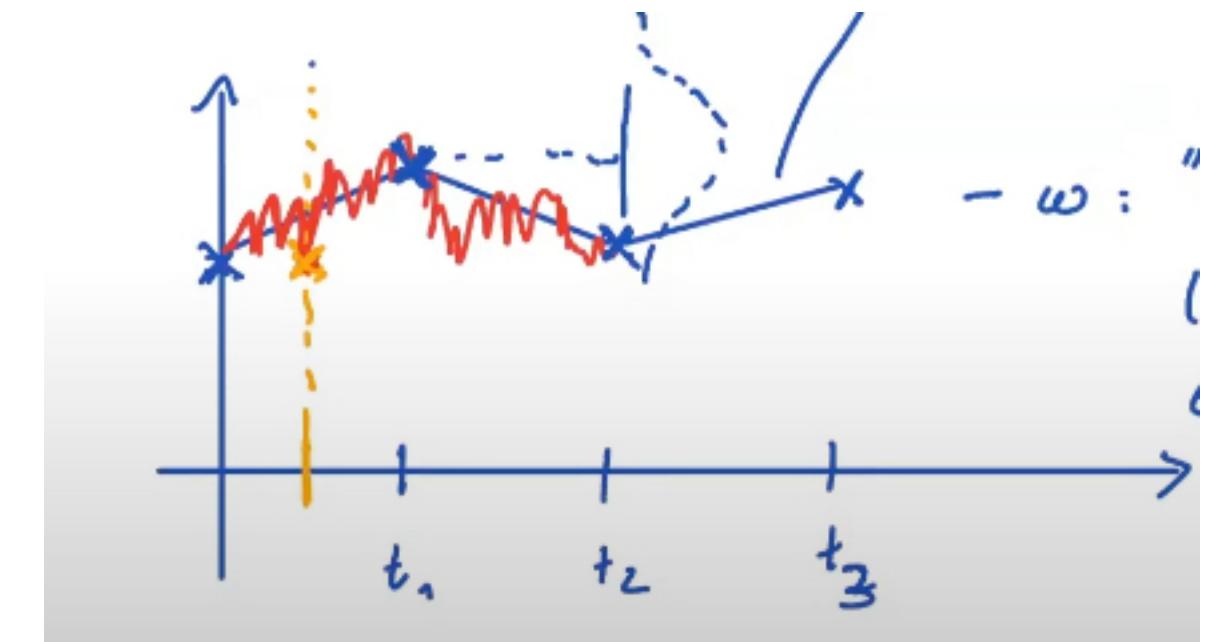
- (i) $B(0) = 0$.
- (ii) (**stationary**) for all $0 \leq s < t$, the distribution of $B(t) - B(s)$ is the normal distribution with mean 0 and variance $t - s$, and
- (iii) (**independent increment**) the random variables $B(t_i) - B(s_i)$ are mutually independent if the intervals $[s_i, t_i]$ are nonoverlapping.

Distribution given by this theorem is brownian motion.



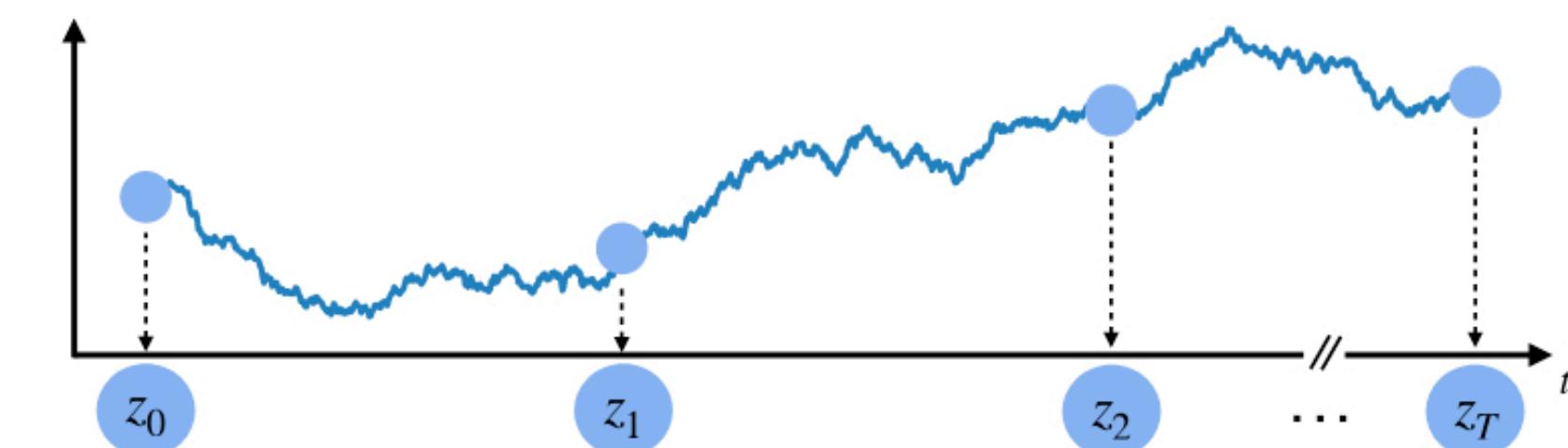
Brownian bridge

- We are given coarse points, and we want to “fill” the path between them with Brownian motion
- key idea: learn latents that create a brownian motion between two given points



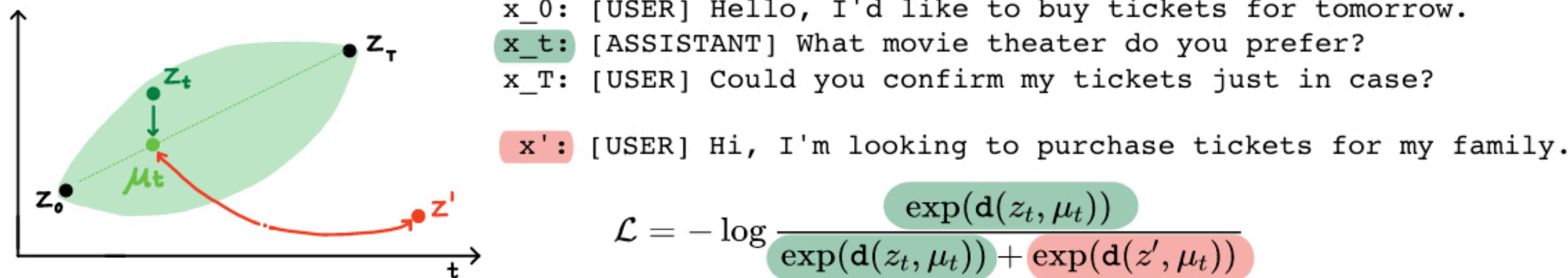
$$p(z_t|z_0, z_T) = \mathcal{N}\left(\left(1 - \frac{t}{T}\right)z_0 + \frac{t}{T}z_T, \frac{t(T-t)}{T}\right).$$

No variance at the beginning or the end
The point is “attached”



Method outline

- Contrastive learning:
 - Three sentences x_0, x_t, x_T from a “document” in a sequence with hidden representations z_0, z_t, z_T
 - A random sentence x' with embedding z'



$$\mathcal{L}_N = \mathbb{E}_X \left[-\log \frac{\exp(\mathbf{d}(x_0, x_t, x_T; f_\theta))}{\sum_{(x_0, x_{t'}, x_T) \in \mathcal{B}} \exp(\mathbf{d}(x_0, x_{t'}, x_T; f_\theta))} \right], \text{ where}$$

$$\mathbf{d}(x_0, x_t, x_T; f_\theta) = -\frac{1}{2\sigma^2} \left\| \underbrace{f_\theta(x_t)}_{z_t} - \underbrace{\left(1 - \frac{t}{T}\right) f_\theta(x_0) - \frac{t}{T} f_\theta(x_T)}_{\text{ }} \right\|_2^2$$

Generating text

- Train a model to generate the sentences conditioned on the latent embeddings
- During inference, generate text conditioned on these latent embeddings

Experiments

- Datasets
 - Wikisection: wikipedia articles on cities split by section, each article has four sections (abstract, history, geography, demographics)
 - Taskmaster-2 (TM-2) (Byrne et al., 2019) contains conversations on finding restaurants between an assistant and a user.
 - TicketTalk (Byrne et al., 2021) contains conversations on booking movie tickets between an assistant and a user. The assistant's and user's turns are similarly marked as in TM-2.
 - ROC Stories (Mostafazadeh et al., 2016) is a short 5-sentence stories dataset.

Results

- Can Time Control model local text dynamics?
- Encode two sentences x_t, x_{t+k} using their method and the baselines
- Order is shuffled, and encodings z_t, z_{t+k} are fed to a classifier

	Method	Wikisection		TM-2		TicketTalk	
		$k = 5$	$k = 10$	$k = 5$	$k = 10$	$k = 5$	$k = 10$
Classical methods	GPT2	50.3 ± 5.8	50.2 ± 6.3	55.7 ± 5.3	63.6 ± 7.3	54.7 ± 6.1	65.0 ± 8.1
	BERT	50.9 ± 4.9	47.8 ± 9.0	68.8 ± 3.5	80.7 ± 3.8	68.4 ± 5.1	80.4 ± 6.3
	ALBERT	49.9 ± 12.1	49.6 ± 18.0	81.6 ± 4.0	86.1 ± 7.3	78.4 ± 6.7	89.4 ± 3.1
	S-BERT	50.8 ± 6.0	48.0 ± 9.1	73.4 ± 3.5	83.3 ± 4.3	72.1 ± 5.3	84.2 ± 5.2
	Sim-CSE	49.1 ± 6.4	48.1 ± 8.5	75.4 ± 3.8	86.2 ± 3.9	75.1 ± 5.9	85.2 ± 3.1
Implicit dynamics	VAE (8)	49.5 ± 5.5	50.5 ± 5.1	50.5 ± 4.4	51.5 ± 6.0	49.9 ± 1.0	51.2 ± 1.0
	VAE (16)	50.1 ± 5.8	51.3 ± 4.7	48.8 ± 4.8	50.8 ± 4.9	50.1 ± 1.0	49.5 ± 1.0
	VAE (32)	50.5 ± 5.1	50.0 ± 6.0	48.0 ± 5.1	47.3 ± 5.9	50.0 ± 1.0	49.3 ± 1.0
Brownian motion	ID (8)	49.8 ± 5.9	50.1 ± 5.0	60.3 ± 5.2	65.2 ± 6.8	59.2 ± 1.9	66.5 ± 1.1
	ID (16)	53.3 ± 5.4	55.8 ± 6.2	60.5 ± 5.0	67.7 ± 6.8	60.3 ± 1.0	68.4 ± 6.4
	ID (32)	50.0 ± 5.0	50.1 ± 5.0	60.4 ± 5.3	67.6 ± 7.1	61.0 ± 1.0	67.9 ± 6.5
Their method	BM (8)	49.8 ± 5.4	50.0 ± 5.4	49.8 ± 5.4	49.9 ± 5.2	49.7 ± 5.0	50.6 ± 5.8
	BM (16)	50.3 ± 5.5	50.5 ± 5.2	49.9 ± 4.3	51.1 ± 6.0	50.3 ± 4.6	50.8 ± 5.5
	BM (32)	49.3 ± 5.6	48.8 ± 5.8	49.5 ± 4.7	49.6 ± 5.2	49.5 ± 5.6	49.1 ± 6.1
$d(x_t, x_{t'}; f_\theta) = -\frac{1}{2\sigma^2} \left\ \underbrace{f_\theta(x_{t'})}_{z_{t'}} - \underbrace{f_\theta(x_t)}_{z_t} \right\ _2^2$	TC (8)	49.23 ± 5.72	48.3 ± 6.8	77.6 ± 7.8	87.7 ± 6.9	71.6 ± 2.9	82.9 ± 4.1
	TC (16)	57.25 ± 5.30	65.8 ± 5.4	78.2 ± 8.1	88.0 ± 7.1	71.3 ± 3.3	82.9 ± 4.1
	TC (32)	50.1 ± 4.8	49.8 ± 5.8	77.9 ± 7.9	87.9 ± 7.4	72.0 ± 3.9	84.4 ± 3.9

Results

Infilling

- Five-sentence stories: x_0, x_1, x_2, x_3, x_4
- Generate $x_2 \mid x_0, x_1, x_3, x_4$
- Encode $z_0 \leftarrow x_0 \parallel x_1, z_T \leftarrow x_3 \parallel x_4$

Method	BLEU (\uparrow)
LM	1.54 ± 0.02
ILM	3.03 ± 0.11
VAE (8)	0.75 ± 0.17
VAE (16)	0.62 ± 0.07
VAE (32)	0.03 ± 0.0
ID (8)	2.9 ± 0.3
ID (16)	0.9 ± 0.0
ID (32)	1.0 ± 0.1
TC (8)	3.80 ± 0.06
TC (16)	4.30 ± 0.02
TC (32)	5.4 ± 0.11

Table 2: BLEU on ground truth infill and generated sentence.

Potential next steps

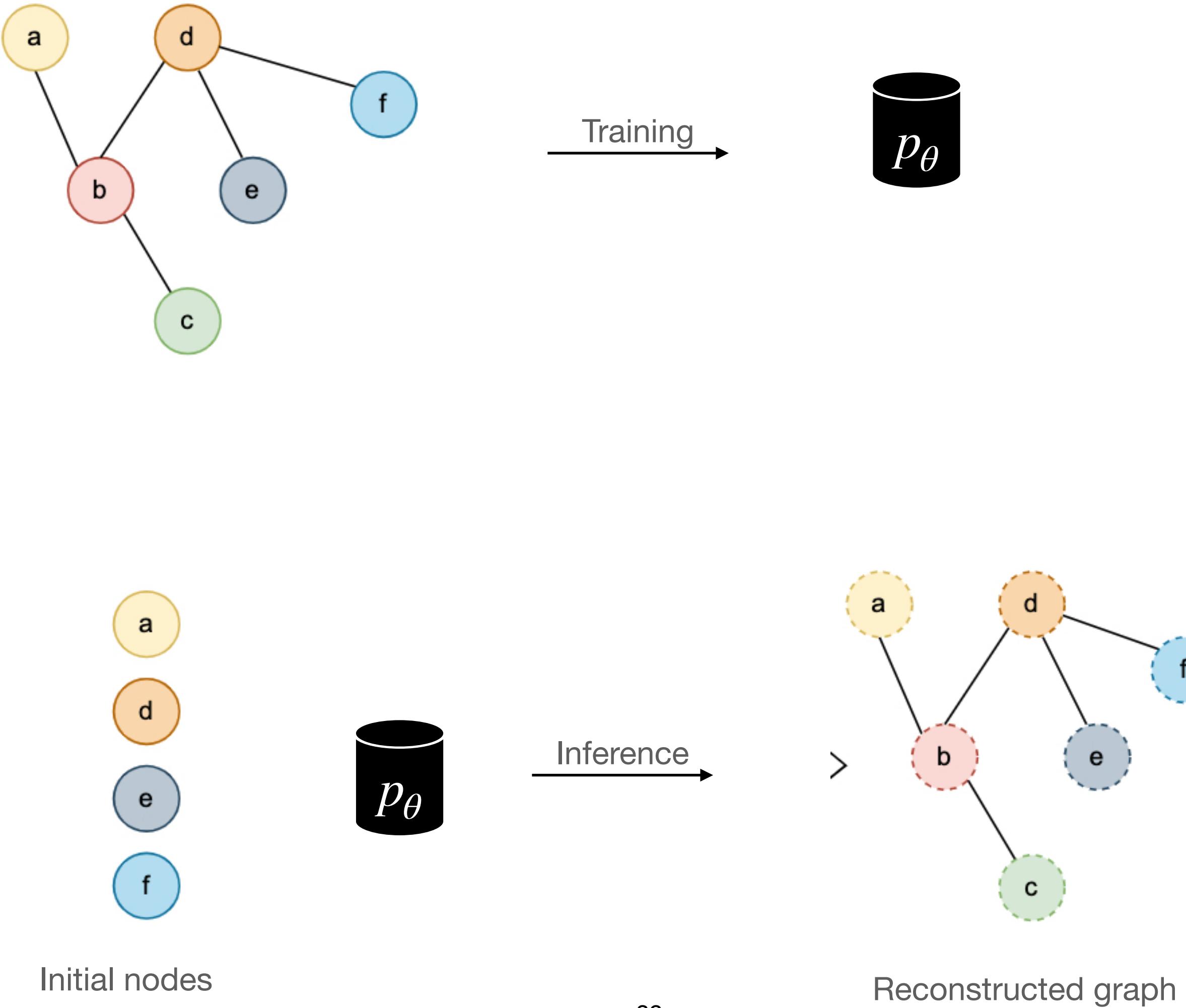
- Aligning brownian processes across sequences
- Pinning down to more than three points?

FLOWGEN: Fast and slow graph generation

Aman Madaan, Yiming Yang
(WIP)

Graph generation

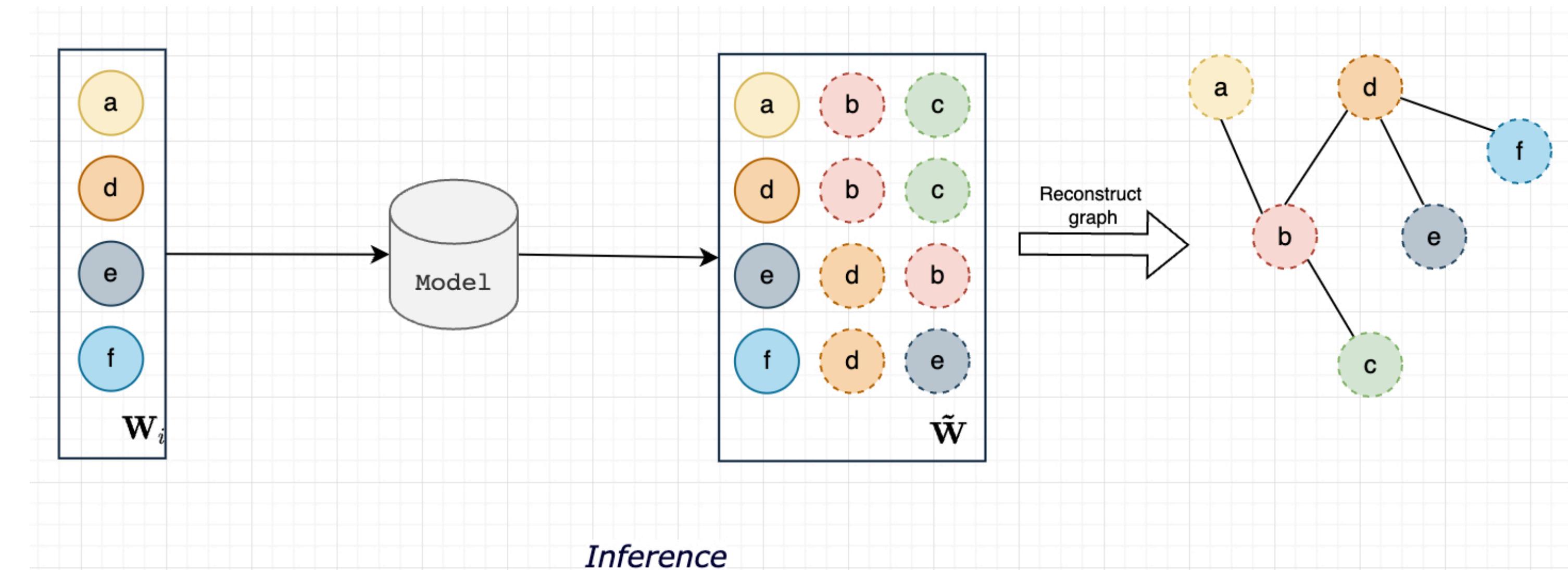
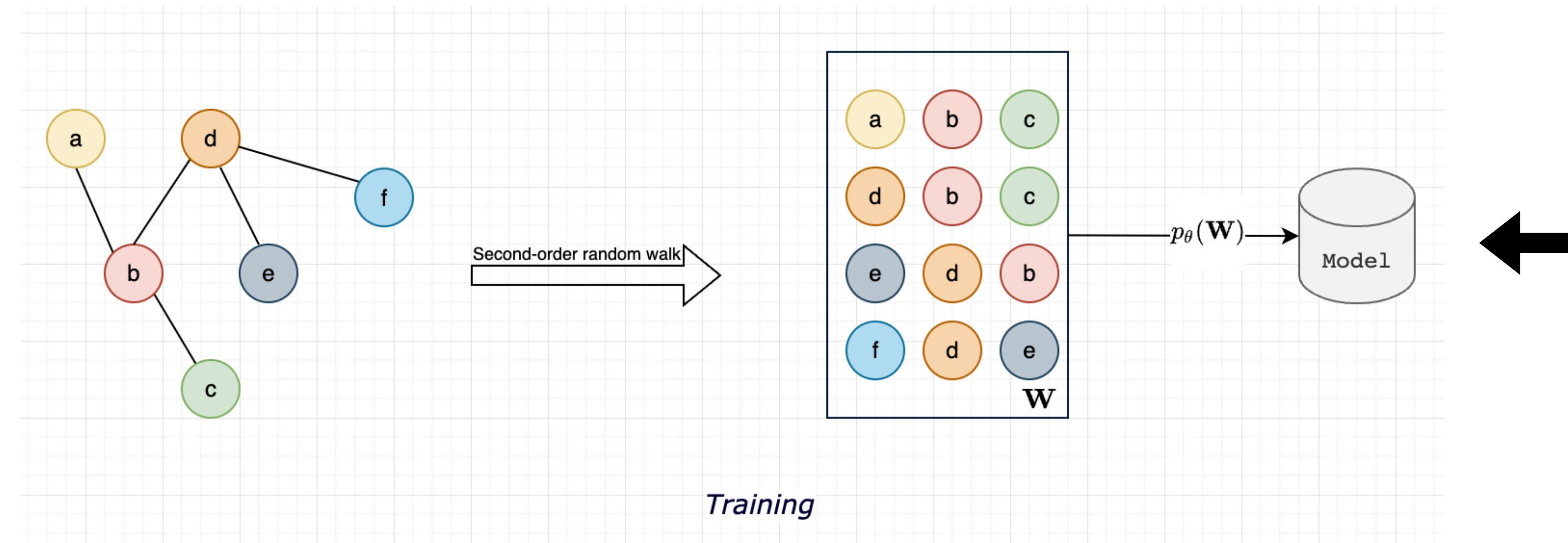
- Overview: learn a model for a (typically large) graph



Evaluating graph generation models

- **Structural:** how closely does \mathbf{G}' look like \mathbf{G} ?
 - Max degree
 - Triangle count
 - Clustering coefficient
 - Can be gamed by a model that memorizes all the edges
- **Downstream task:**
 - Tests generalization
 - During training, entire \mathbf{G} is not used and some edges are held out
 - What % of those edges are generated in \mathbf{G}' ?

Autoregressive graph generation (our method)



N layer transformer
architecture with
self-attention

Alternative interpretation:
matrix completion

Autoregressive graph generation

Results

- Outperforms existing baselines + Not sensitive to hyper-parameters tuning

Method	CORAML	CITESEER	POLBLOGS
Adamic/Adar	92.16	88.69	85.43
DC-SBM	96.03	94.77	95.46
node2vec	92.19	95.29	85.10
VGAE	95.79	95.11	93.73
NetGAN	95.19	96.30	95.51
FLOWGEN (ours)	96.93	97.03	95.00

Table 3: Area under the curve (AUC) for link prediction. FLOWGEN outperforms or matches strong baselines.

	N_{LCC}	E_{LCC}
CORAML	2,810	7,981
CITESEER	2,110	3,757
POLBLOGS	1,222	16,714

Graph	Max. degree	Assortativity	Triangle Count	Power law exp.	Inter-comm unity density	Intra-comm. unity denisty	Cluster-ing coeff.	Charac. path len.
CORA-ML	240	-0.075	2,814	1.860	4.3e-4	1.7e-3	2.73e-3	5.61
Netgan	233	-0.066	1,588	1.793	6.0e-4	1.4e-3	2.44e-3	5.20
FLOWGEN (ours)	224	-0.080	2,123	1.857	5.4e-4	1.3e-3	2.50e-3	5.40

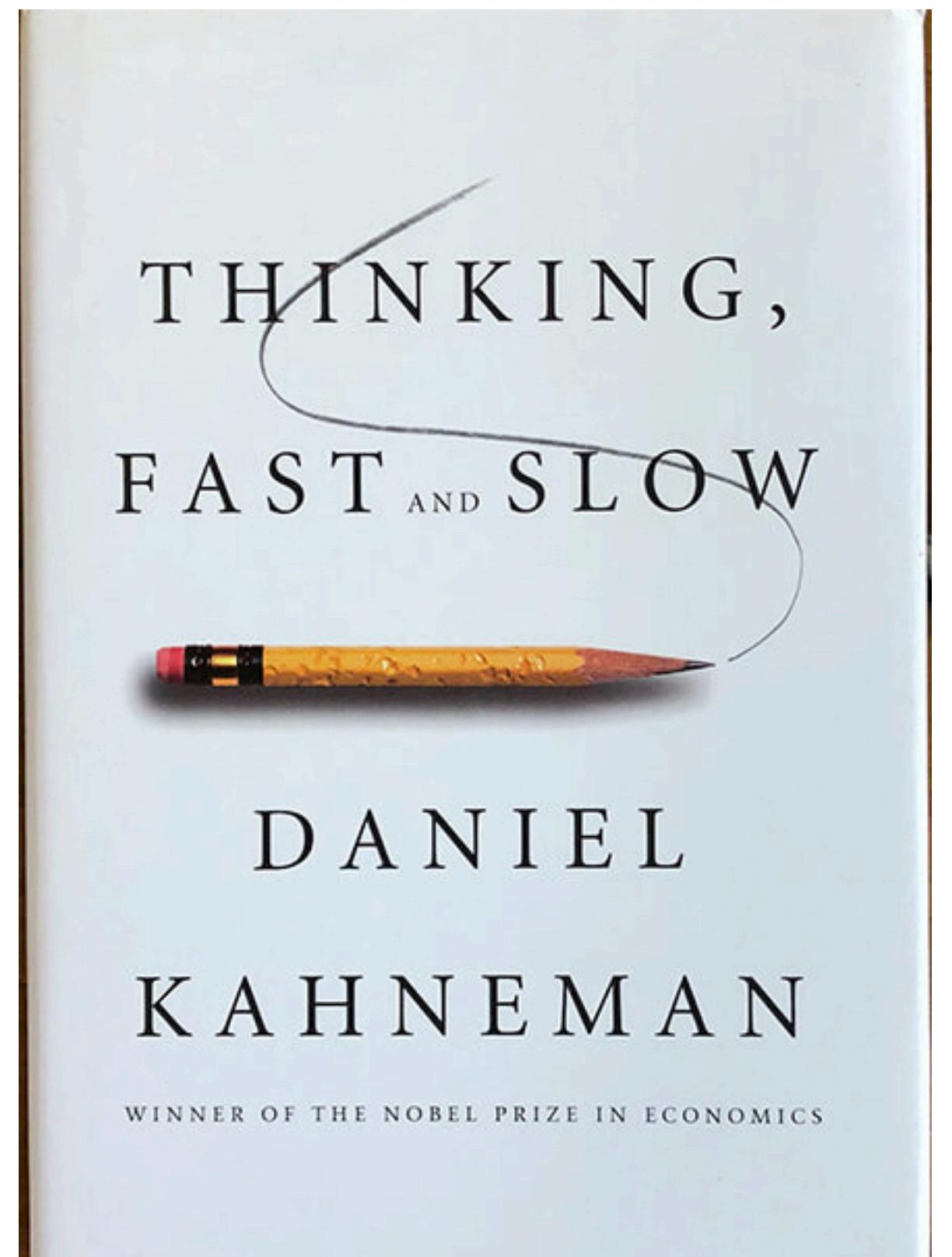
Table 2: Comparison of FLOWGEN with Netgan for structural metrics for CORAML. The ground truth values are listed in the top-row, and the value closer to the ground truth is highlighted in bold. FLOWGEN closely matches the ground truth graph on a larger number of metrics.

2 * 2 = ?

$$19 * 3 = ?$$

Dual-process theory of mind

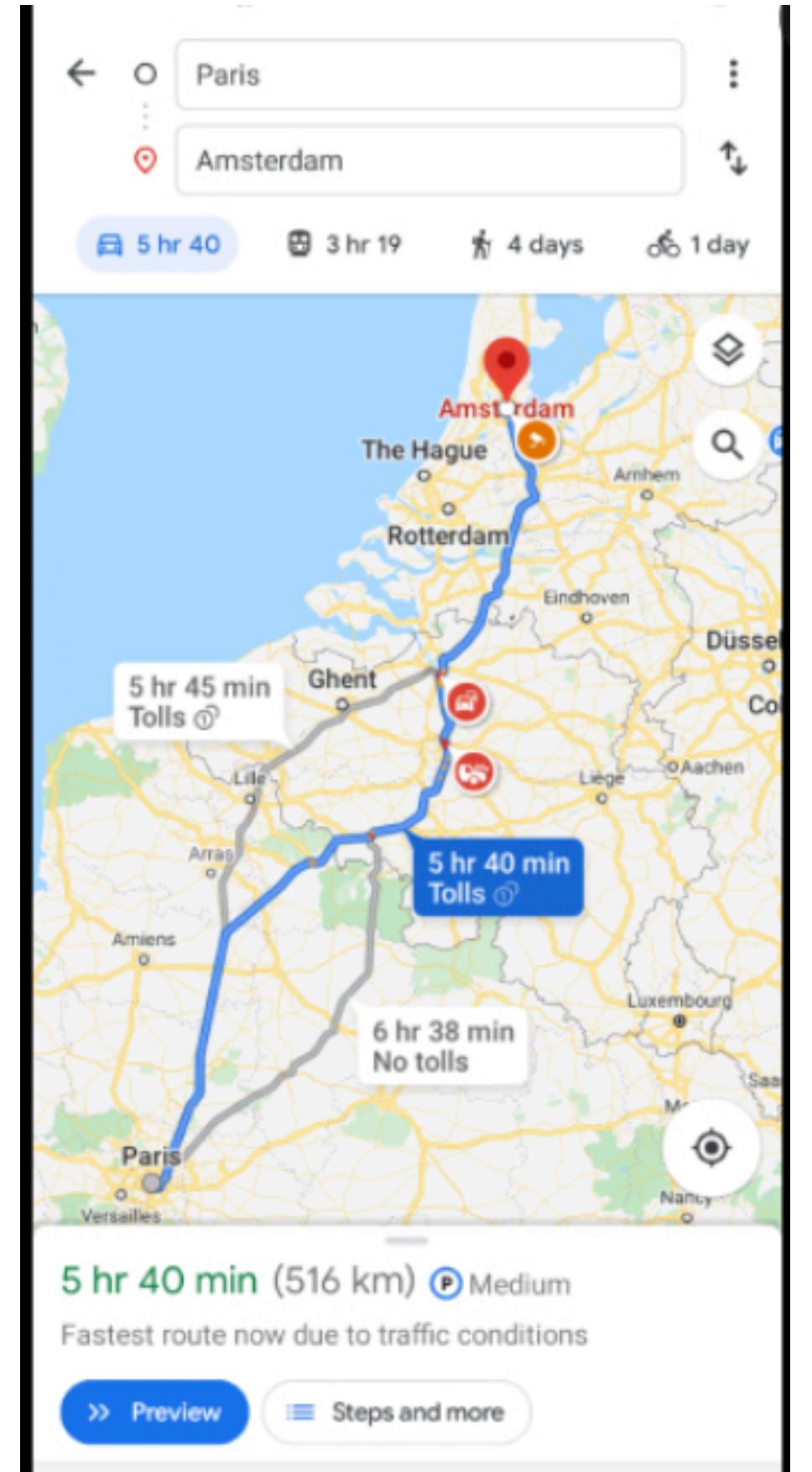
- Humans use different metaphorical parts of the brain to solve problems of various difficulties:
 - System 1: **fast**, instinctive, pattern-matcher, good for easy problems
 - System 2: **slow**, analytical, deep-thinker, good for hard problems
- Current machine learning models:
 - Always use the same hammer for problems of all levels of difficulty
- Practical implications:
 - More efficient systems
 - Critical in the age of large language models



FLOWGEN

Generating graphs fast and slow

- Our method relies on using random walks for reconstructing the graph
- A random walk begins from a fixed, given node v_1
 - Generating the 2nd point requires reasoning about 2-hops $p(v_2 \mid v_1)$
 - Generating the 3rd point requires $p(v_3 \mid v_2, v_1)$
 - Intuitively, the process gets more difficult with sequence
- Need assistance only when generating walks in the later part



FLOWGEN

Overview

- Train two models: **fast** (transformer with 1 layer) and **slow** (transformer with 6 layers)
- Start random walk generation with a **fast** model, **switch** to a slow model ***when the walk is starting to feel lost***
- **Switch**
 - Easy because of auto-regressive setup: the walk generated so far is a prefix to the slower model
- ***When the walk is starting to feel lost***
 - In general, known to be a challenging issue
 - Relates to uncertainty estimation, model calibration

How Can We Know *When* Language Models Know?
On the Calibration of Language Models for Question Answering

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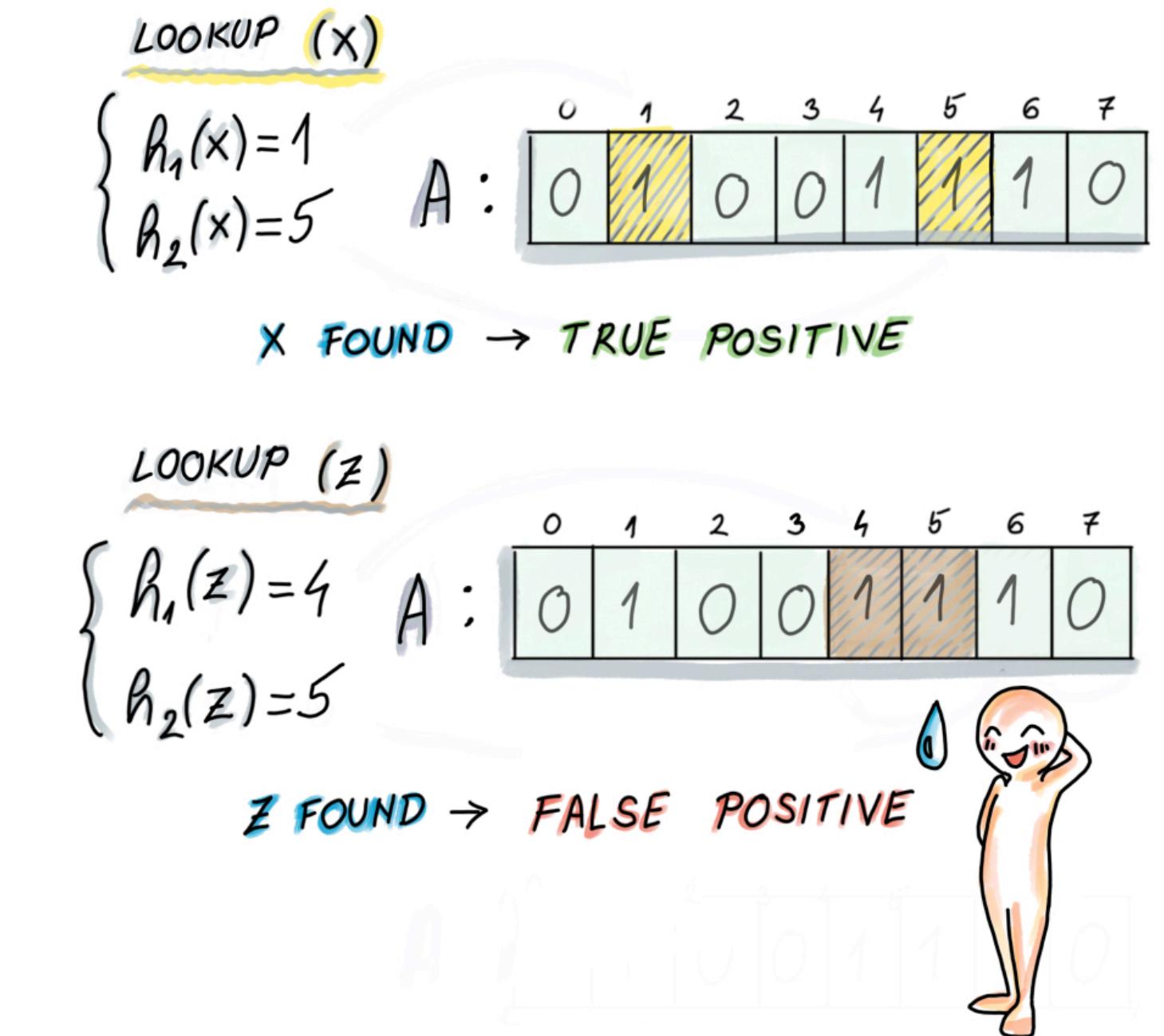
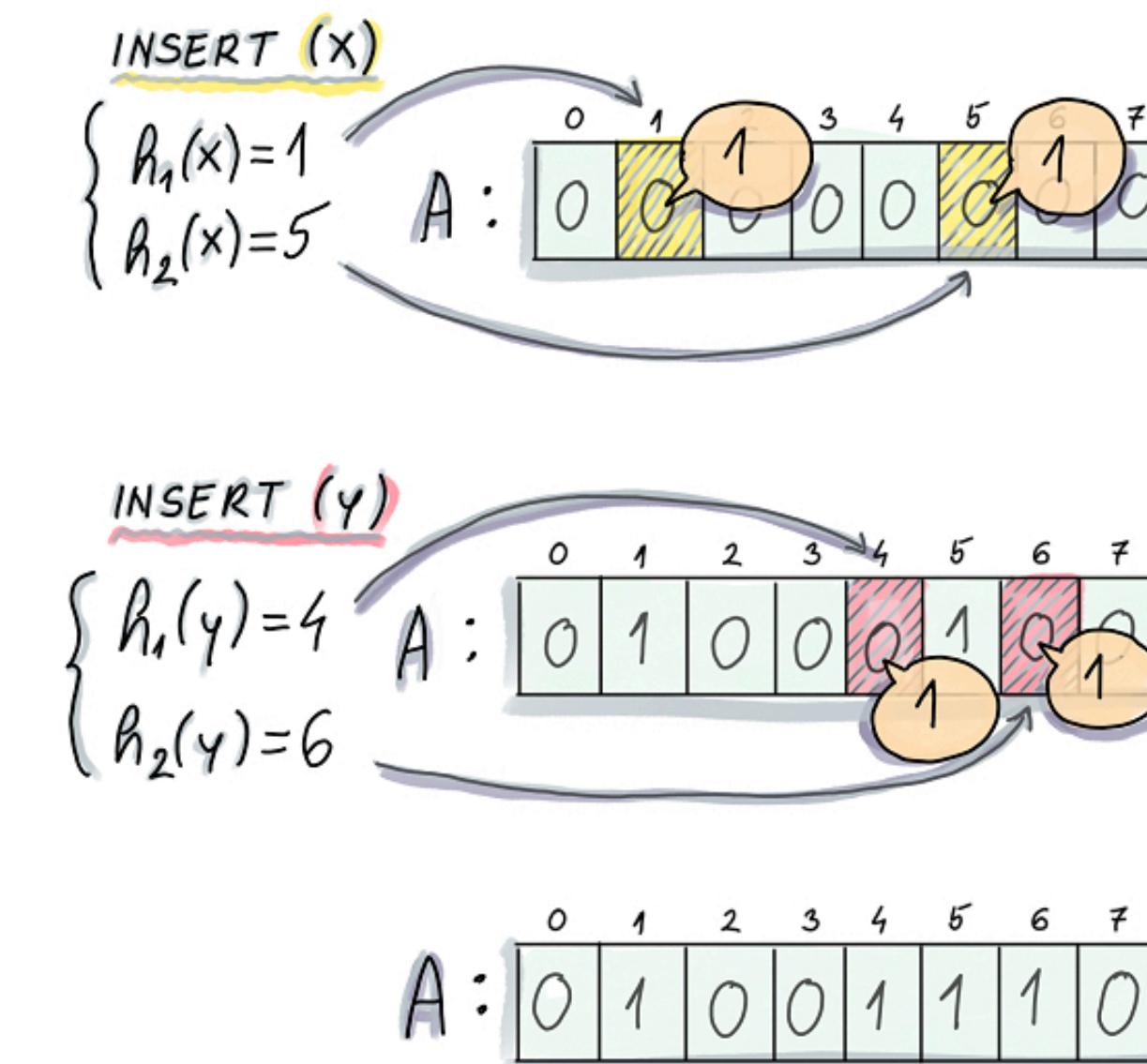
FLOWGEN

How do we know when the model is getting lost?

- Define $N = [v_i, v_{i+1}, v_{i+2}, v_{i+3}]$ to be a neighborhood of four consecutive nodes in the true graph, \mathcal{R} to be all the random walks of length 4
- We want an estimate of $P(N \in \mathcal{R})$
 - For smaller graphs, \mathcal{R} can be enumerated and fed to a balanced-binary tree for efficient search (aka hashmap)
 - Not an option for our case
 - Graphs are large, exponential possible \mathcal{R}
 - Can use distributed lookup caches, but if switch detection takes all the time, we will miss out on any gains by fast + slow interplay
- Want a quick estimate of $P(N \in \mathcal{R})$
 - Noisy estimate is okay
 - **Bloom-filters** are meant for exactly this use case
- **Interpretation:** random walks are brownian motion in the limit, we want to determine if a set of consecutive points was sampled from the process defining brownian motion

Bloom filters

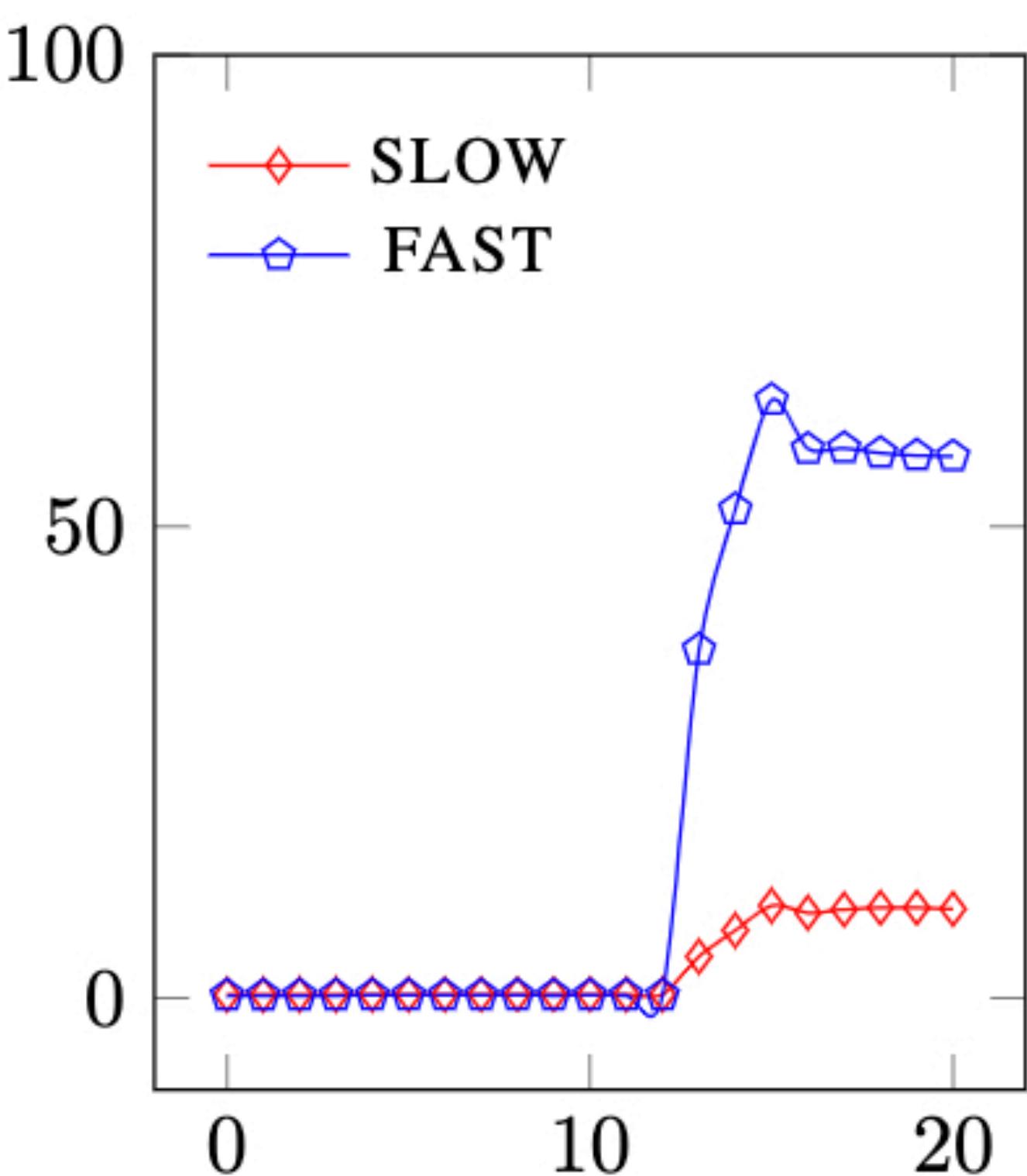
- Probabilistic data structures for efficiently answering set-membership queries
- Parameters:
 - m bits
 - k hash functions
 - n elements to be inserted
- Tunable False positive rate: $\epsilon \approx (1 - e^{\frac{-kn}{m}})^k$

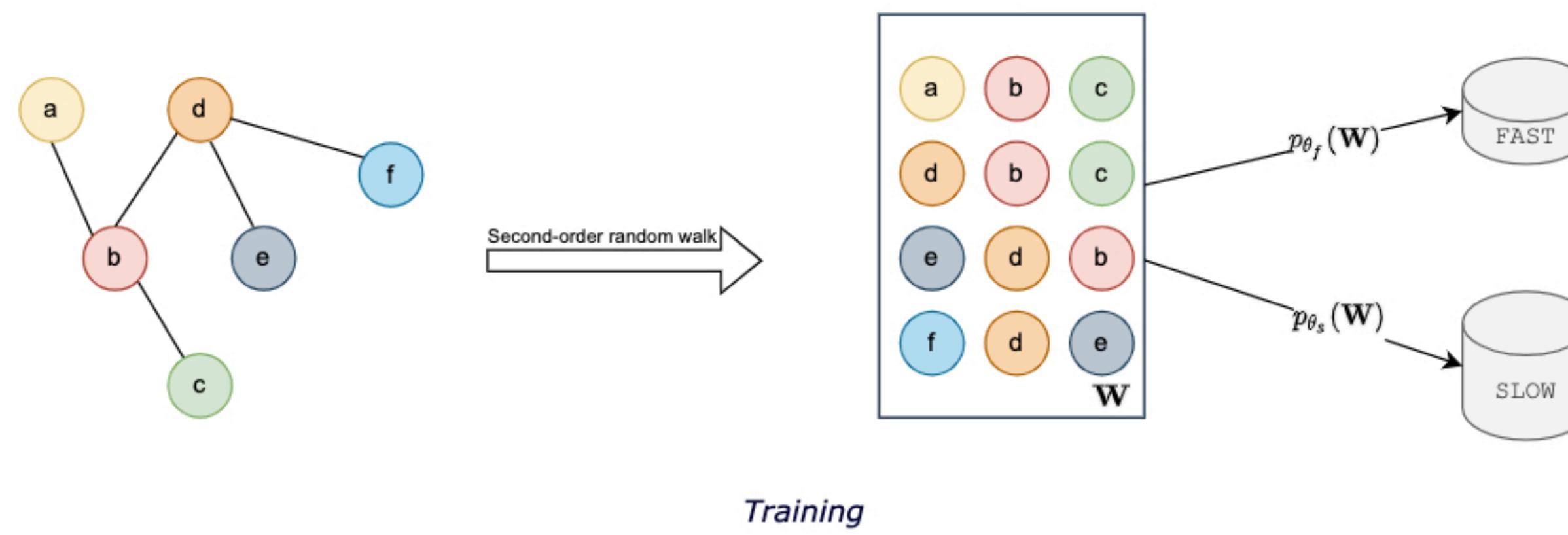


FLOWGEN

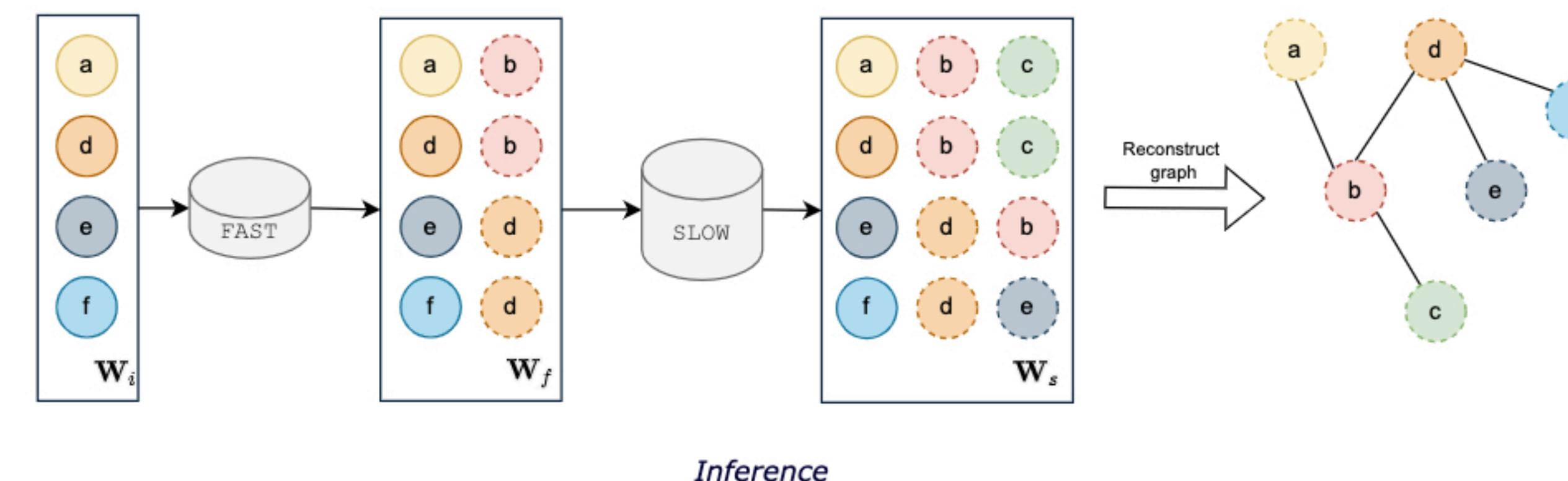
Detecting exploration

- Store a large fraction of neighborhoods in the training data in a bloom filter \mathcal{B}
- Approximately 1 bit per walk
 - 130x less space to store the entire graph for doing search queries
- Random walk can be in “exploring” or “exploiting” phase:
 - When a neighborhood is not found in \mathcal{B} , random walk is “exploring”, otherwise random walk is exploiting
 - Let $EL(N)$ be 1 if the neighborhood is likely to be exploratory
 - $\frac{dEL(N)}{dt}$ rate of change of exploration with time
 - Switch at $t = \text{argmax}_t \frac{dEL(N)}{dt}$
- Generate 10k walks from fast and slow model, detect when they switch by finding the rate of new neighborhoods





Training



Inference

Results

Same accuracy at 50% less time

	FAST	SLOW	FLOWGEN
CORAML (500k)	76.8 (288)	92.2 (806)	90.8 (484)
CORAML (100M)	91.5 (50k)	96.7 (180k)	96.9 (110k)
CITESEER (500k)	90.9 (313)	94.6 (862)	93.3 (687)
CITESEER (100M)	96.1 (62k)	96.8 (172k)	96.5 (137k)
POLBLOGS (500k)	61.9 (309)	85.4 (854)	86.5 (686)
POLBLOGS (100M)	66.2 (48k)	93.8 (156k)	93.8 (108k)

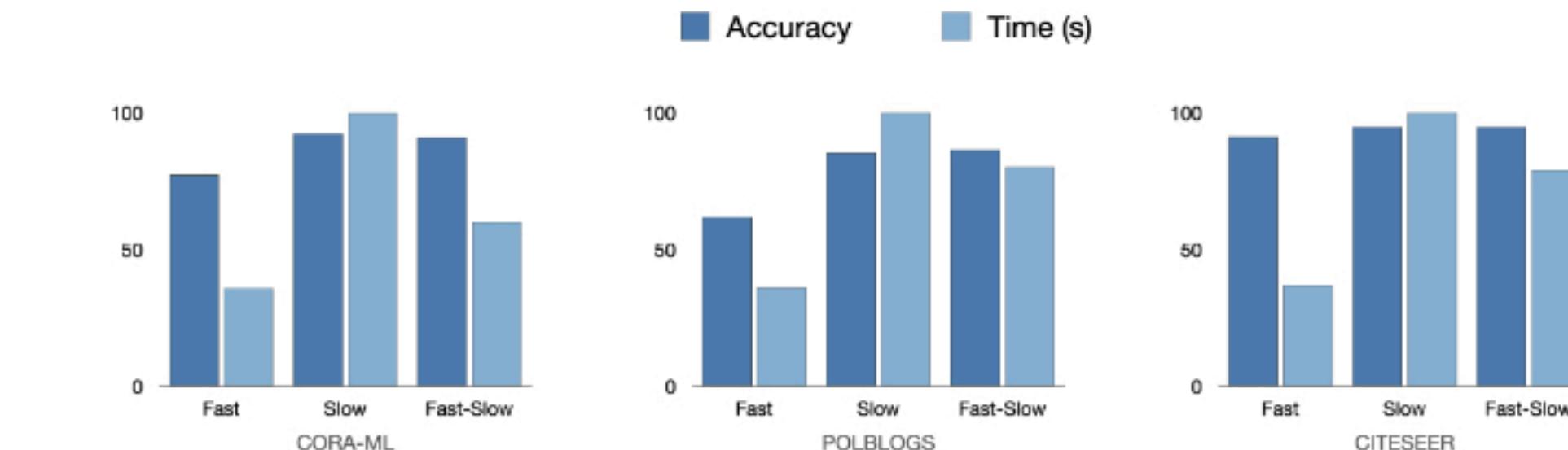
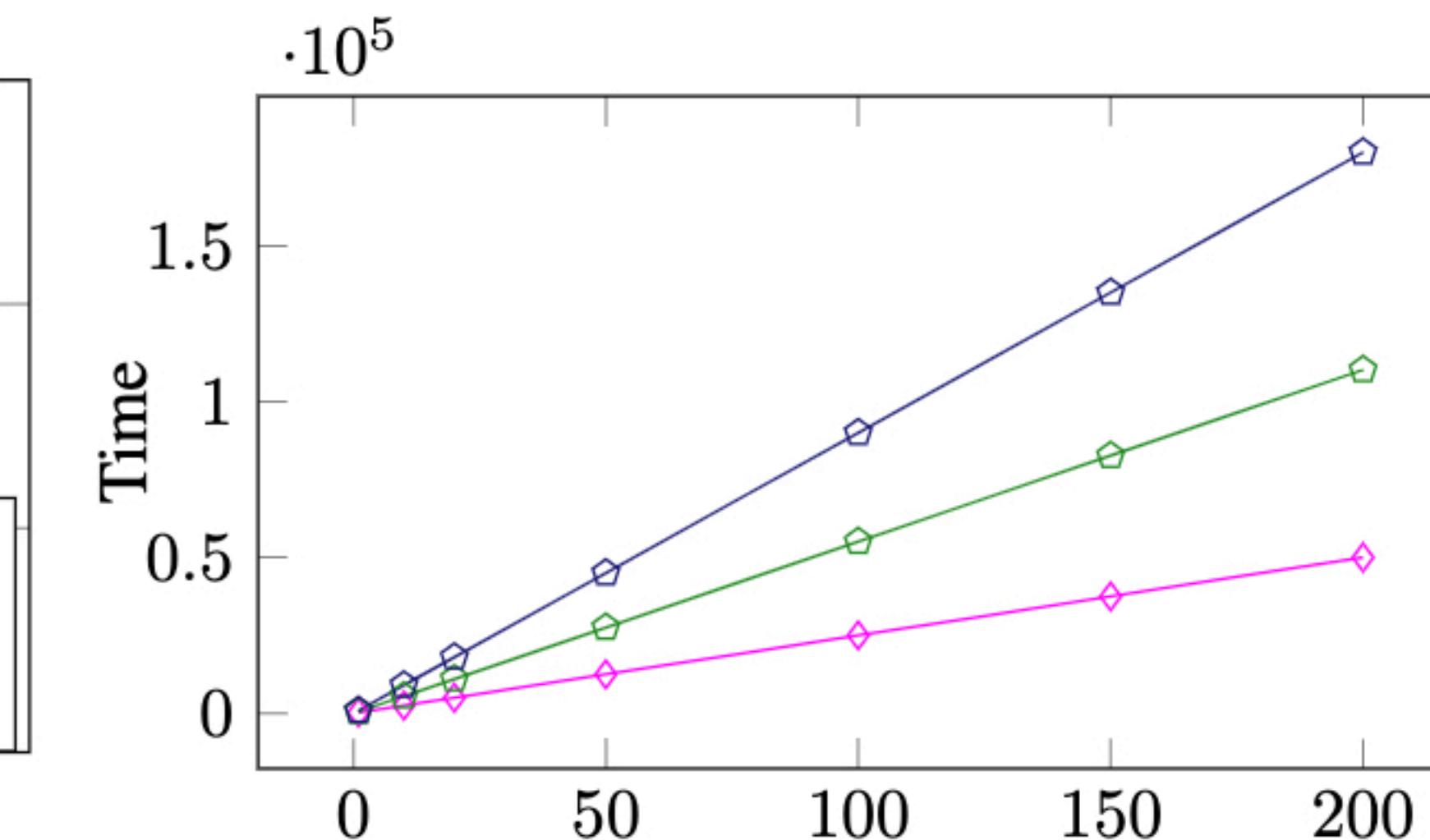
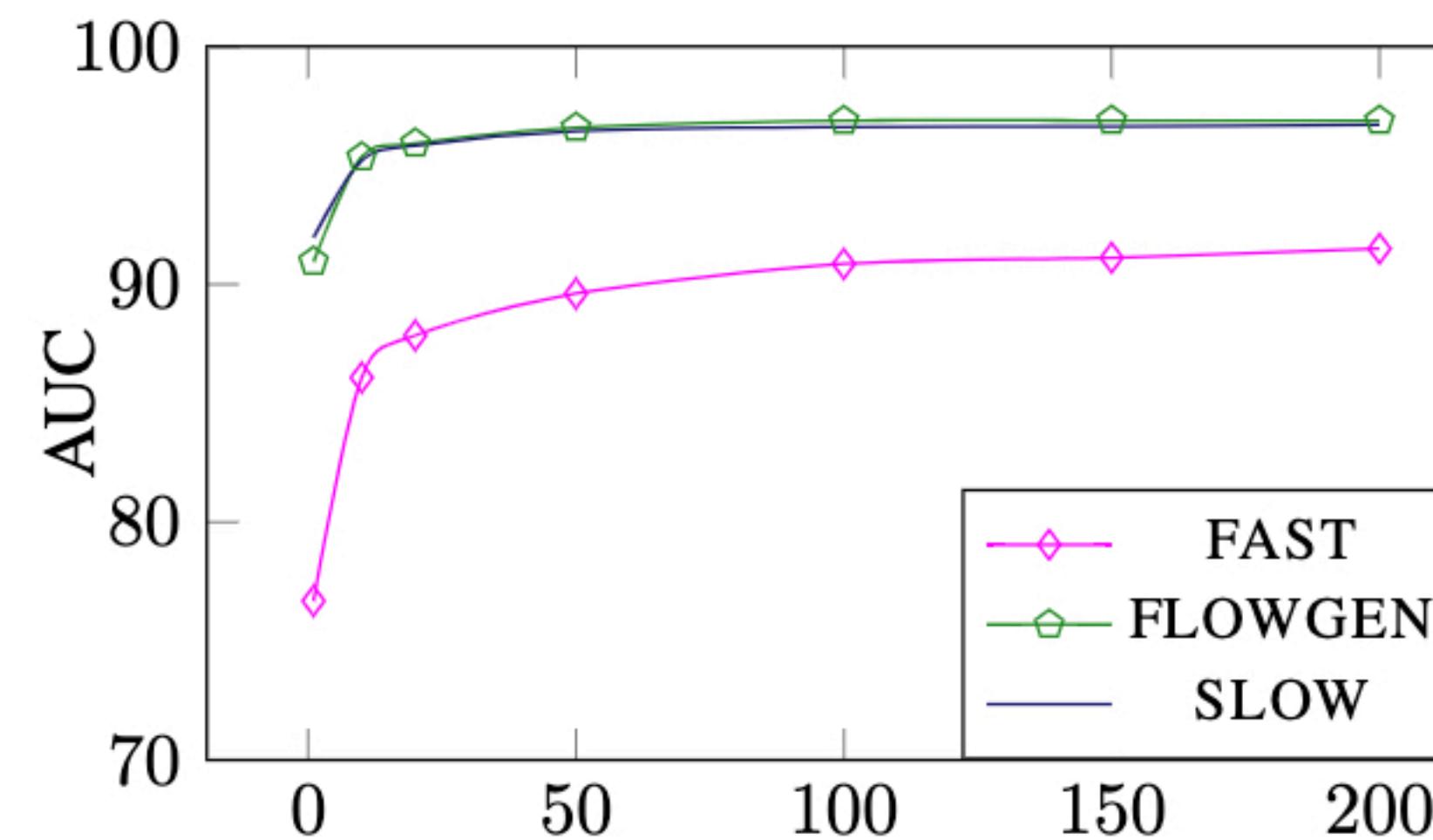


Figure 4: Average precision vs. time taken for the three settings. The FAST and SLOW model speed-accuracy trade-off is apparent: FAST model is fast but less accurate (average precision $\sim 75\%$, compared to the SLOW model which is slower but has average precision of 92%). FLOW combines the strengths of the two modes: it achieves an accuracy of 90% while being $\sim 50\%$ faster than the SLOW model. Note that the time is normalized relative to SLOW (SLOW takes 100% of the time).



Take home message

- Beyond vanilla seq2seq
 - Gradient-based optimization
 - Sampling from energy models
 - Gradient-free sampling
 - Generation as brownian process
 - Fast-slow generation with bloom filters
- Next steps:
 - Gradient based methods that actually work
 - Fitting a brownian motion model to the random walk for determining the switch point more efficiently