

Expectation Maximization

Junxian He
Oct 17, 2024

Midterm Exam

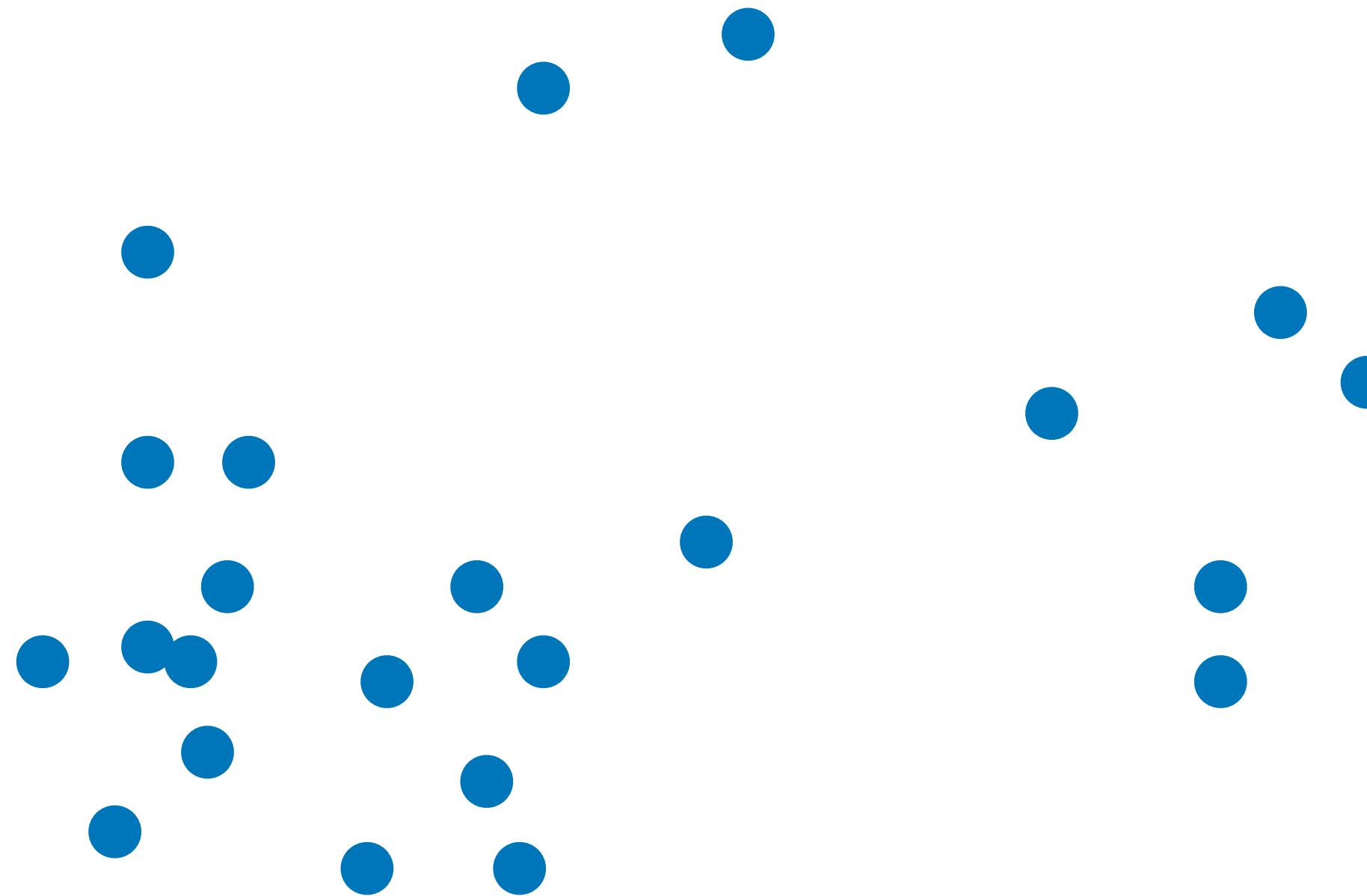
Next Thursday (Oct 24), 120pm-240pm, one A4-size double-sided cheetsheet is allowed (either printing or handwriting is fine)

We have two rooms for the exam for sparse seat plans:

1. For SIS ID ending with an even digit: Room 2303
2. For SIS ID ending with an odd digit: Room 2504

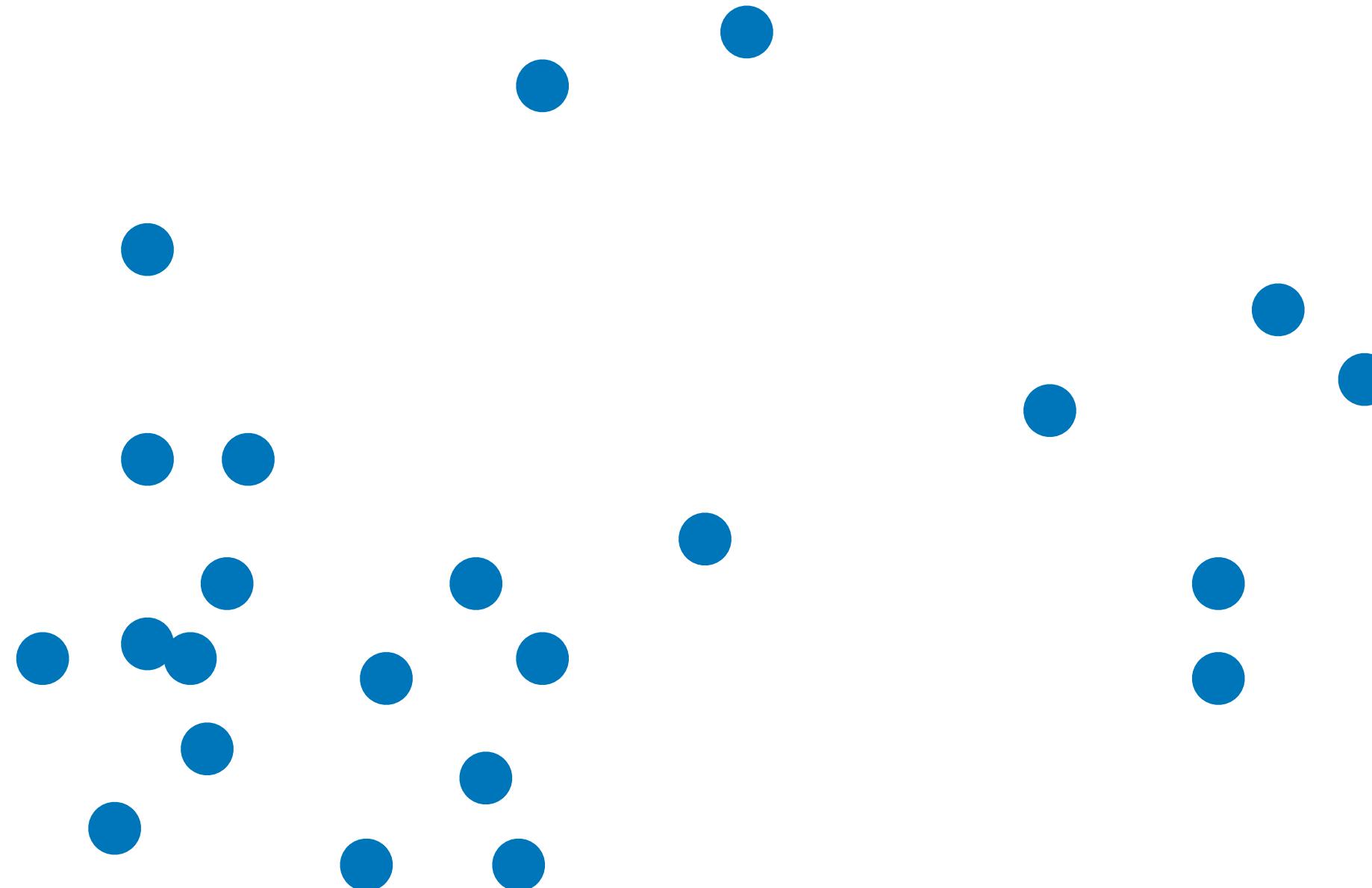
Recap: Generative Models

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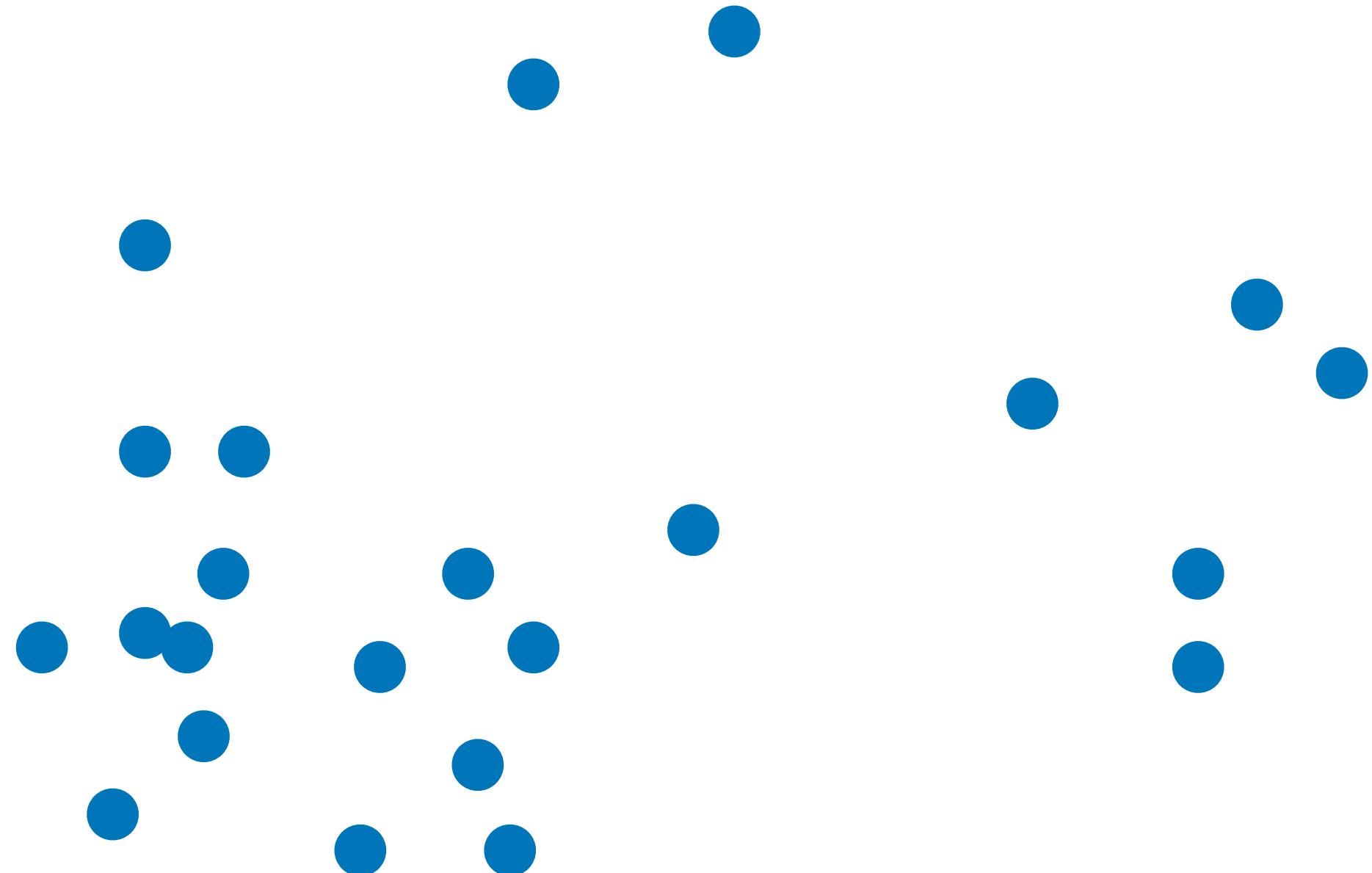
Recap: Generative Models

We want to model $p(x)$



Recap: Generative Models

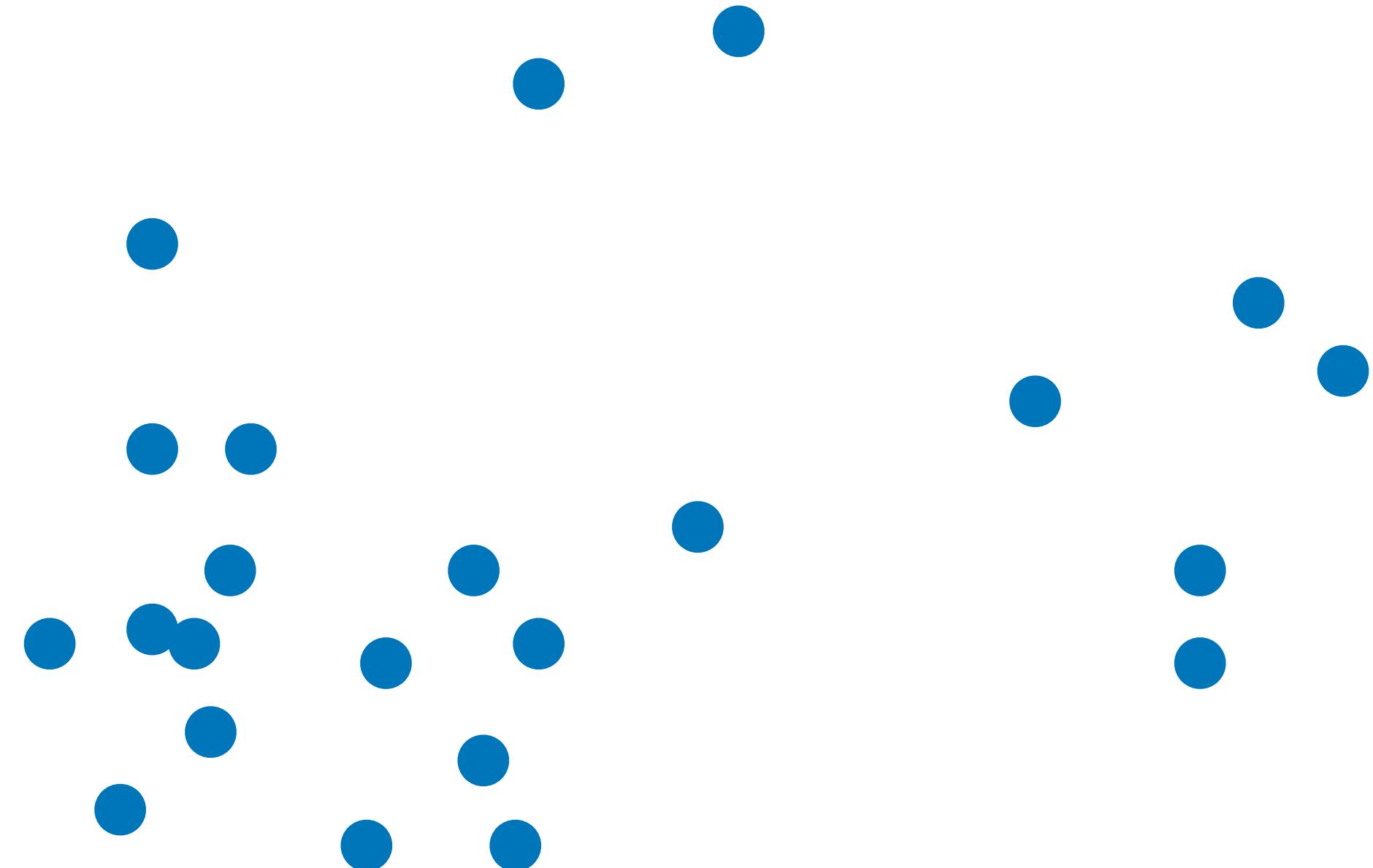
We want to model $p(x)$



In discriminative models, we need to “design” model to make assumption about the function: linear regression, logistic regression, kernel methods

Recap: Generative Models

We want to model $p(x)$



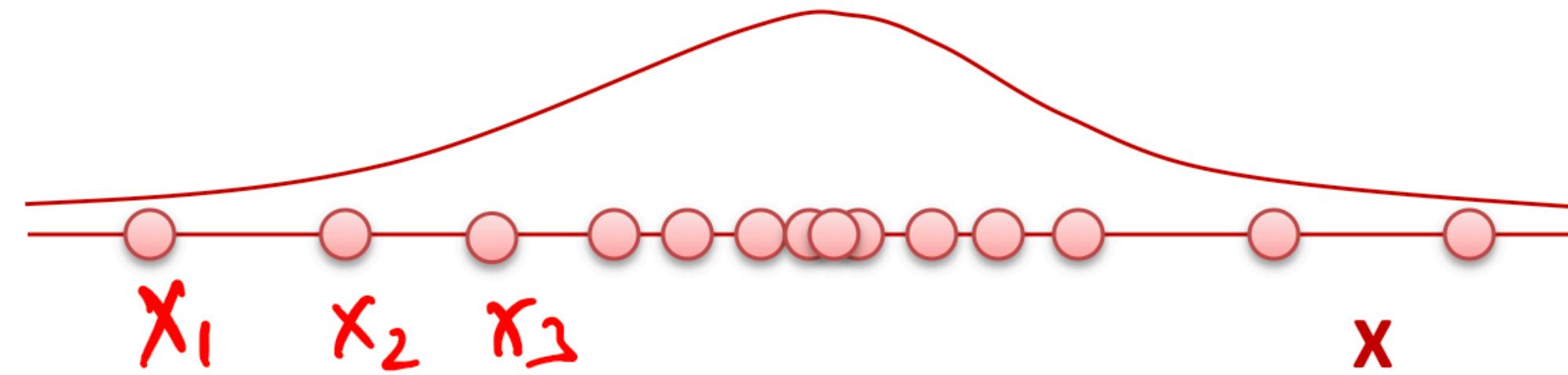
In discriminative models, we need to “design” model to make assumption about the function: linear regression, logistic regression, kernel methods

In generative models, we “design” the model and make assumptions about the data, through defining a distribution family

Recap: Generative Models

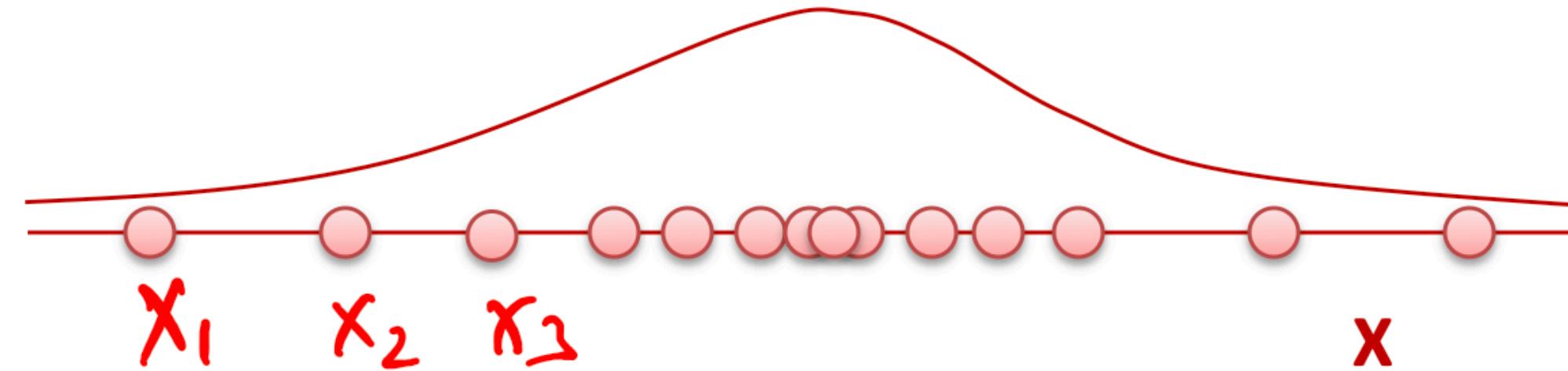
Recap: Generative Models

Data, $D =$



Recap: Generative Models

Data, $D =$

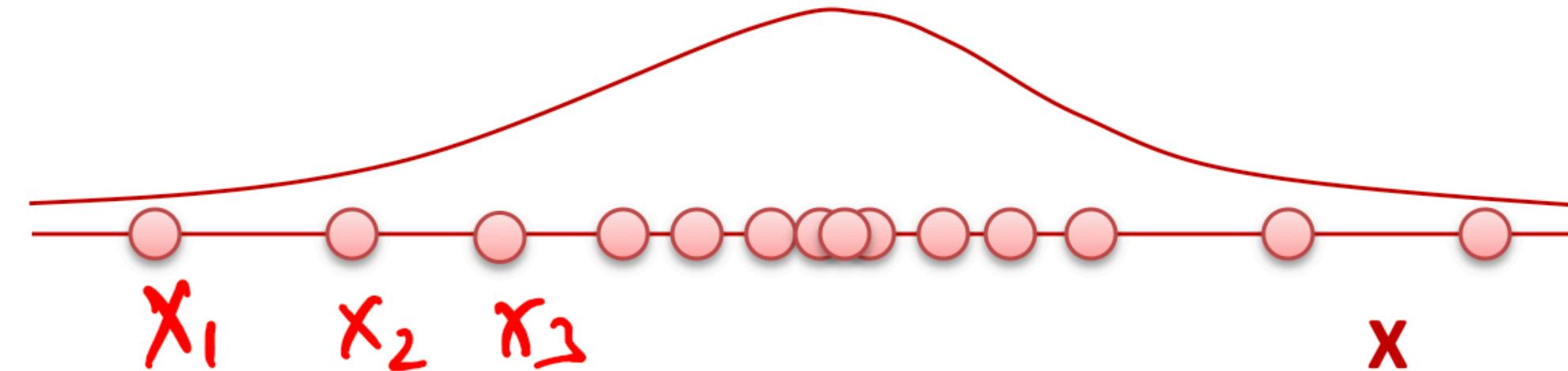


As a simplest case, we directly assume $x \sim N(\mu, \Sigma)$



Recap: Generative Models

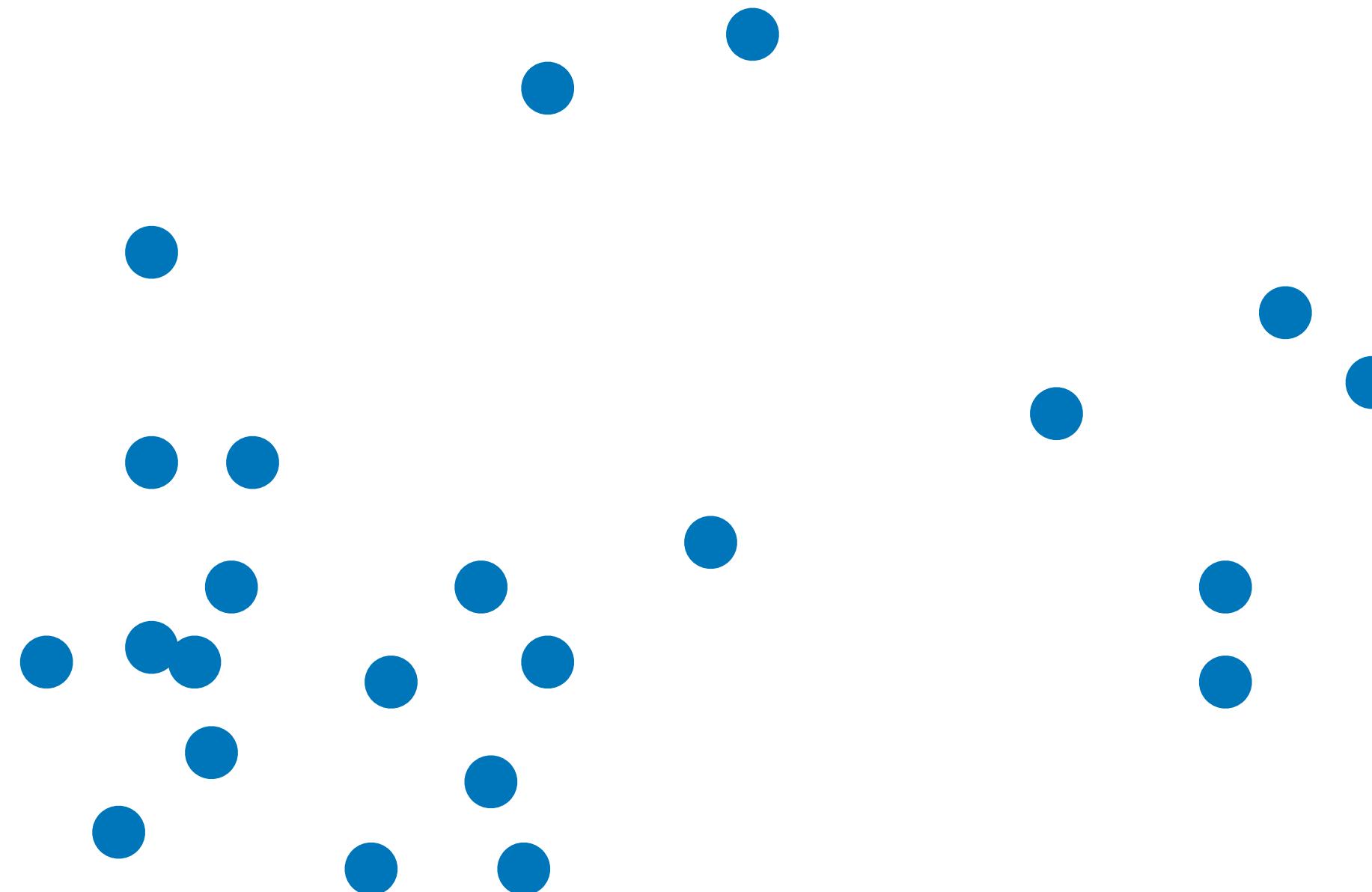
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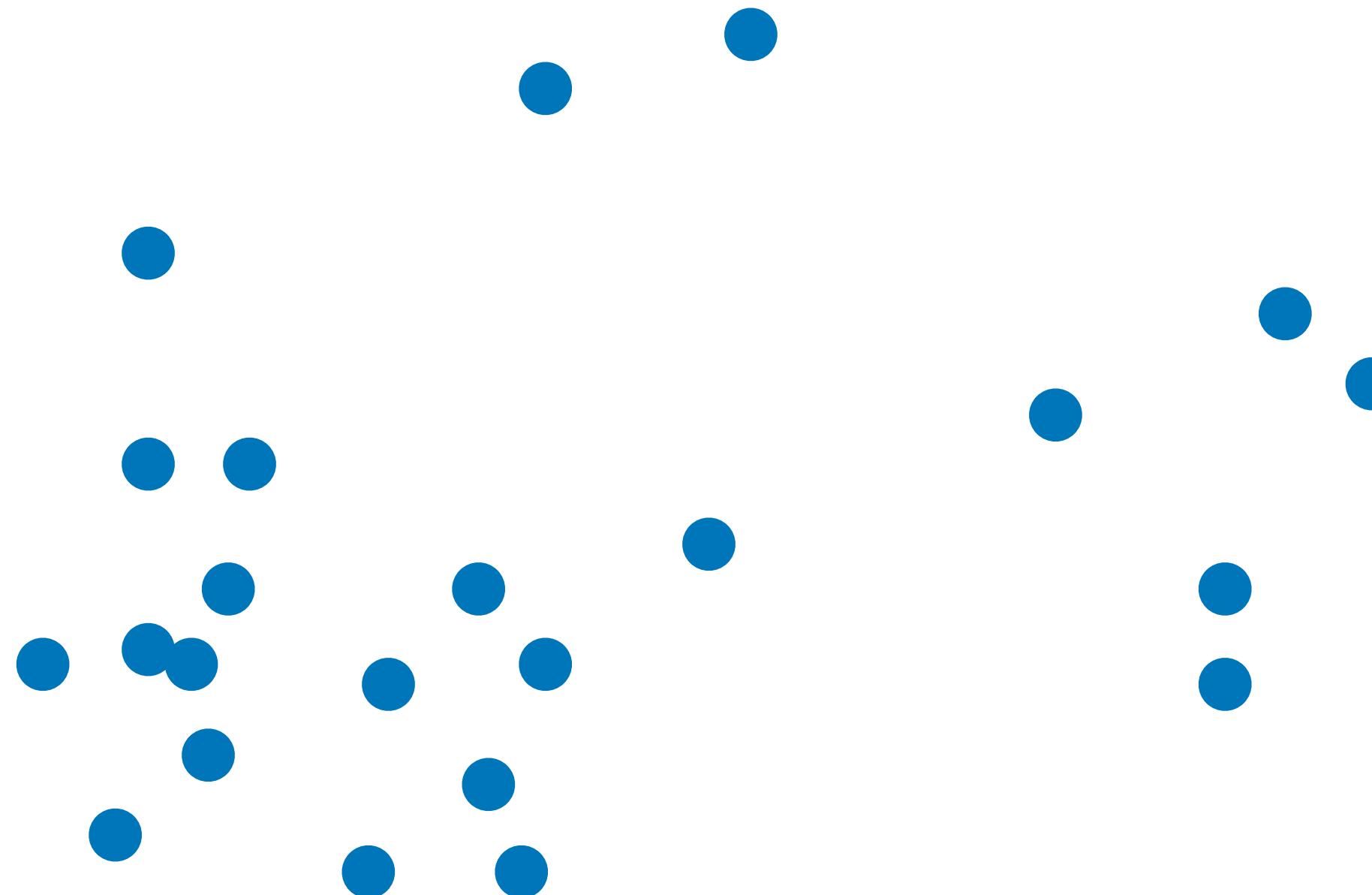
By varying the parameters (μ, Σ) , the model represents different distributions that belong to the Gaussian family

Recap: Generative Models



How to construct more complex distribution family?

Recap: Generative Models

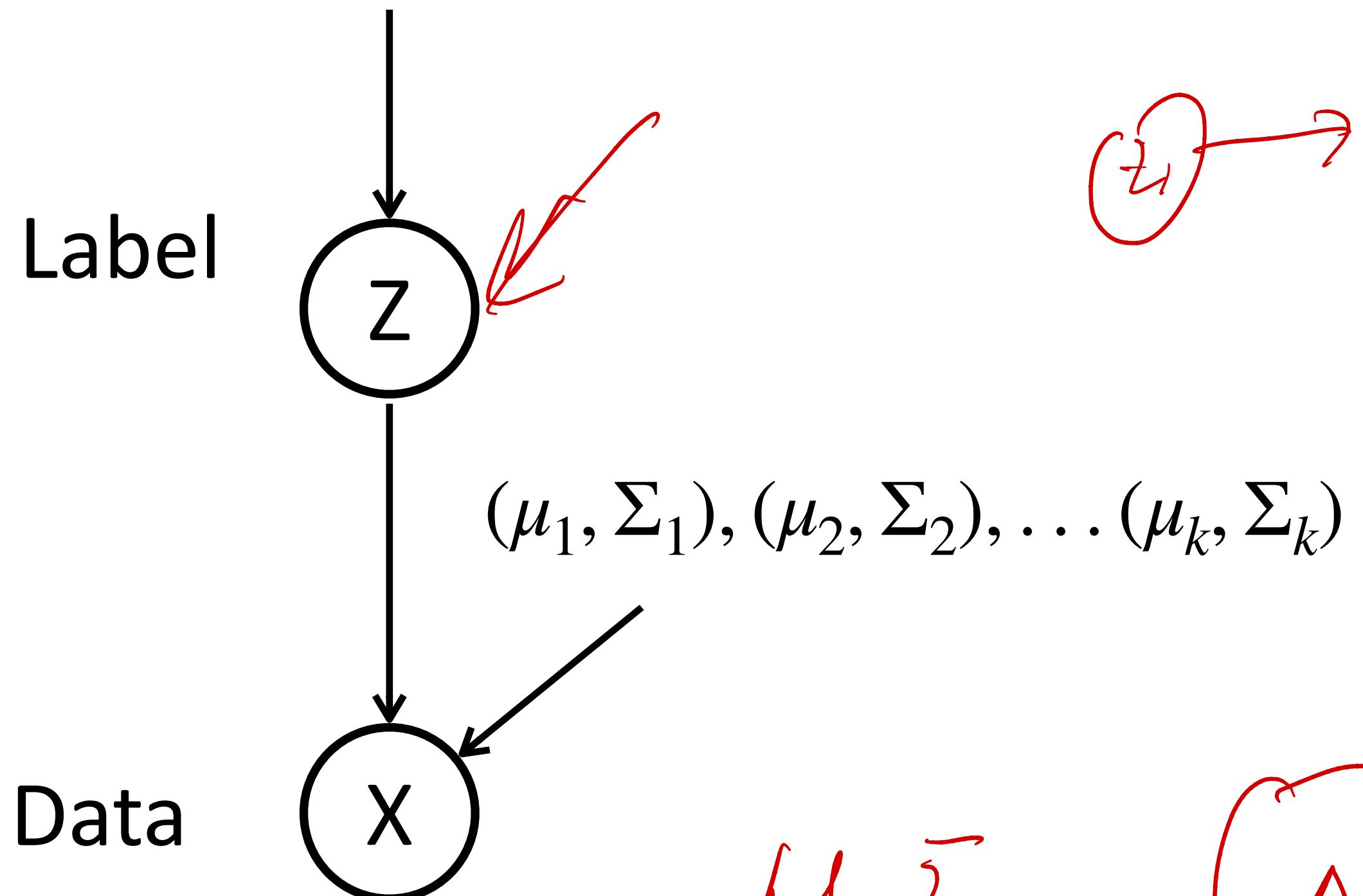


How to construct more complex
distribution family?

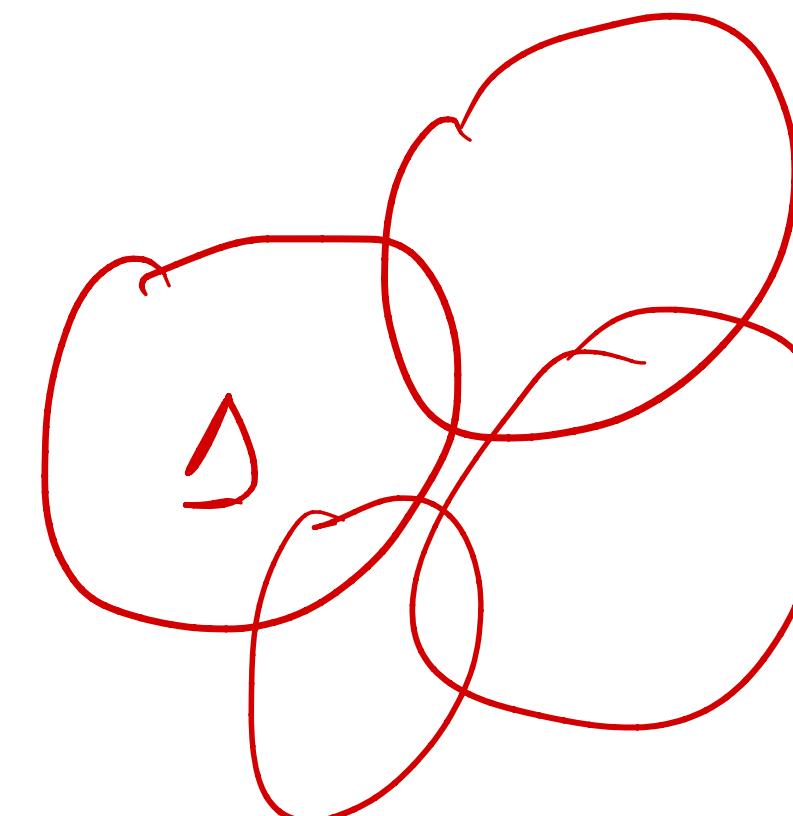
Introducing more latent variables

Recap: Gaussian Mixture Model

$p(z)$: multinomial , k
classes(e.g. uniform)



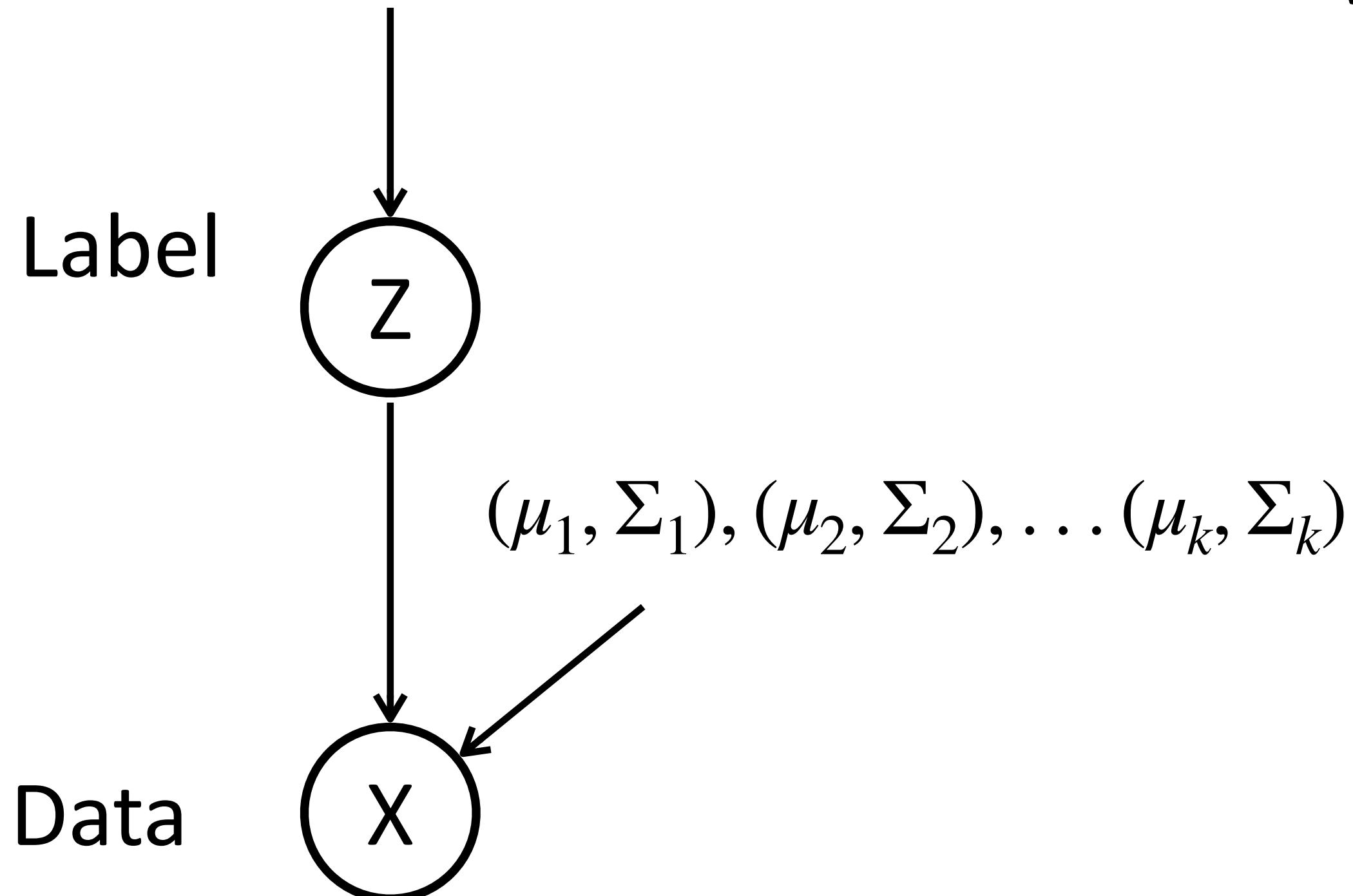
$$\mu, \Sigma$$



Recap: Gaussian Mixture Model

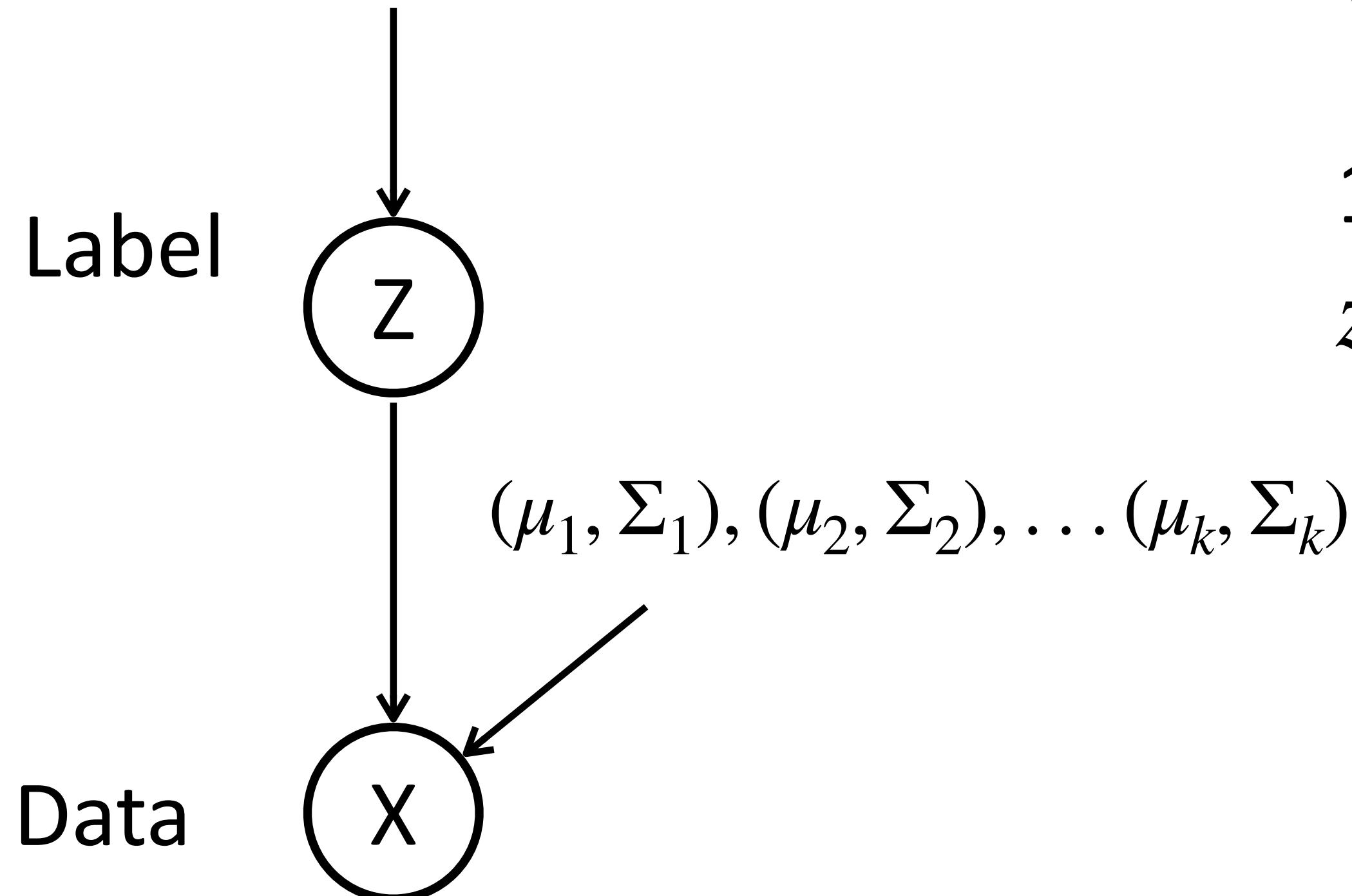
$p(z)$: multinomial , k
classes(e.g. uniform)

We assume the generative process as:



Recap: Gaussian Mixture Model

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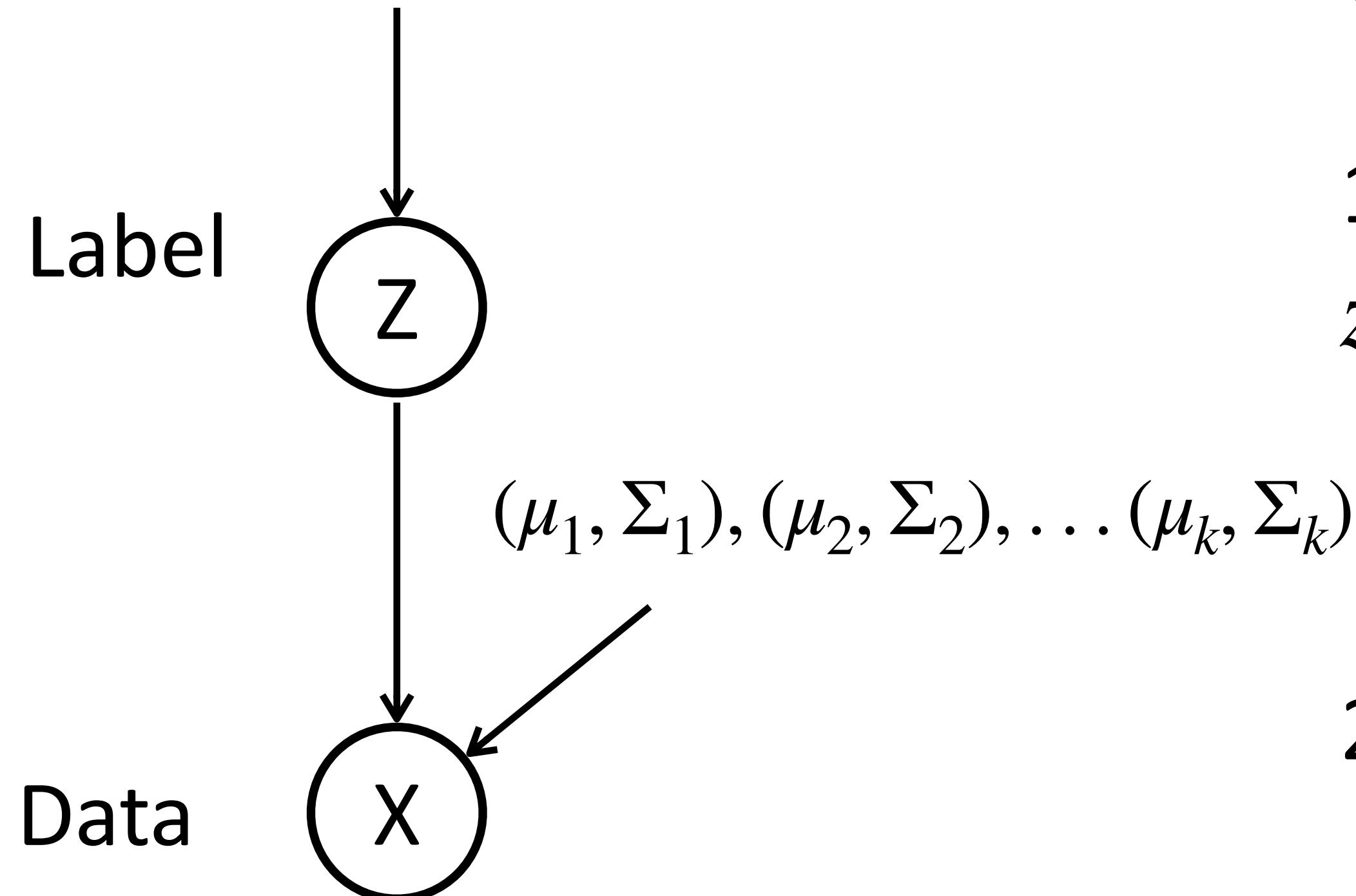


We assume the generative process as:

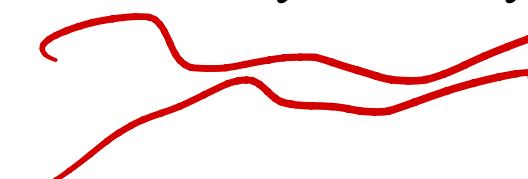
1. For each data point, sample its label z_i from $p(z)$

Recap: Gaussian Mixture Model

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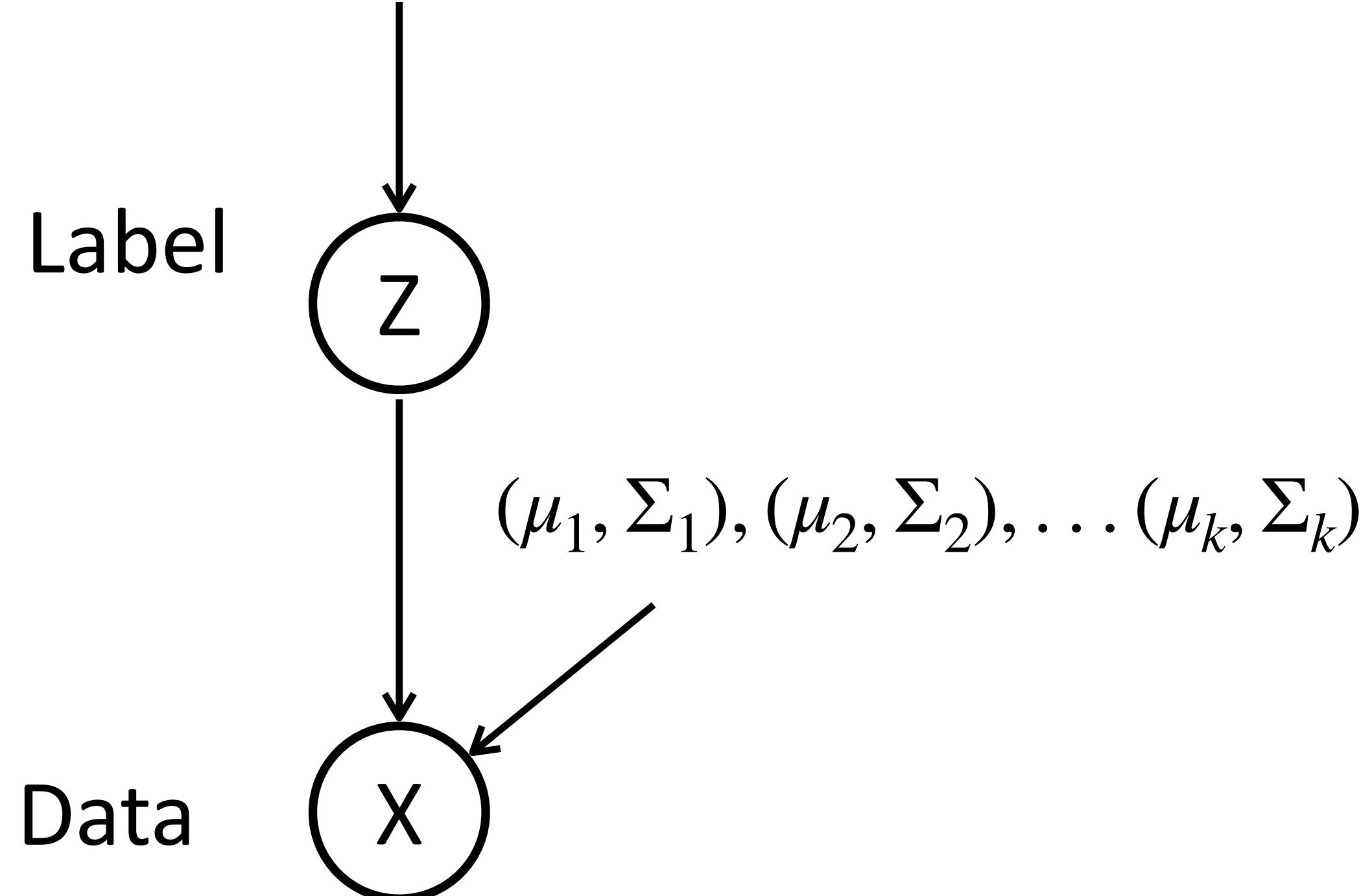


We assume the generative process as:

1. For each data point, sample its label z_i from $p(z)$
 2. Sample $x_i \sim N(\mu_{z_i}, \Sigma_{z_i})$
- 

Recap: MLE for GMM

$p(z)$: multinomial , k classes(e.g. uniform)



$\phi \rightarrow p(z)$
Unsupervised:

$$\operatorname{argmax}_{\phi, \mu, \Sigma} \log p(x)$$

How to compute this?

$\operatorname{argmax}_{\phi, \mu, \Sigma} \log P(x, z)$

easy

Recap: MLE for GMM

$$\begin{aligned}\ell(\phi, \mu, \Sigma) &= \sum_{i=1}^n \log p(x^{(i)}; \phi, \mu, \Sigma) \\ &= \sum_{i=1}^n \log \sum_{z^{(i)}=1}^k p(x^{(i)}|z^{(i)}; \mu, \Sigma) p(z^{(i)}; \phi).\end{aligned}$$

marginalization

Recap: MLE for GMM

$$\begin{aligned}\ell(\phi, \mu, \Sigma) &= \sum_{i=1}^n \log p(x^{(i)}; \phi, \mu, \Sigma) \\ &= \sum_{i=1}^n \log \sum_{z^{(i)}=1}^k p(x^{(i)}|z^{(i)}; \mu, \Sigma) p(z^{(i)}; \phi).\end{aligned}$$

$\not\exists$ continuous $\log \int_t^\infty$ ---

1. Intractable (no closed-form for the solution)

Recap: MLE for GMM

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$\sum_z f \cdot P(z) = E_{z \sim p(z)}$

$\log [E_{z \sim p(z)} P(f(z))]$

1. Intractable (no closed-form for the solution)
2. Large variance in gradient descent

Recap: MLE for GMM

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$\log P(x)$

GANs VAEs diffusion

1. Intractable (no closed-form for the solution)
2. Large variance in gradient descent

Expectation Maximization is to address the MLE optimization problem

Things are easy when we know z..

In case we know z

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$$\{v_y \mathcal{P}(x, z)$$

$$\ell(\phi, \mu, \Sigma) = \sum_{i=1}^n \log p(x^{(i)} | z^{(i)}; \mu, \Sigma) + \log p(z^{(i)}; \phi).$$



Things are easy when we know z..

In case we know z

$$\ell(\phi, \mu, \Sigma) = \sum_{i=1}^n \log p(x^{(i)} | z^{(i)}; \mu, \Sigma) + \log p(z^{(i)}; \phi).$$

$$\phi_j = \frac{1}{n} \sum_{i=1}^n 1\{z^{(i)} = j\},$$

$$\mu_j = \frac{\sum_{i=1}^n 1\{z^{(i)} = j\} x^{(i)}}{\sum_{i=1}^n 1\{z^{(i)} = j\}},$$

$$\Sigma_j = \frac{\sum_{i=1}^n 1\{z^{(i)} = j\} (x^{(i)} - \mu_j)(x^{(i)} - \mu_j)^T}{\sum_{i=1}^n 1\{z^{(i)} = j\}}.$$

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~~Expectation maximization is to infer the latent variables first (z here), and maximize the likelihood given the inferred z iteratively~~

Expectation Maximization for GMM

Repeat until convergence:

{

}

Expectation Maximization for GMM

Repeat until convergence:

{

(E-step) For each i, j , set

inference

$$w_j^{(i)} := p(z^{(i)} = j | x^{(i)}; \phi, \mu, \Sigma)$$



}

Expectation Maximization for GMM

Repeat until convergence:

{

(E-step) For each i, j , set

$$w_j^{(i)} := p(z^{(i)} = j | x^{(i)}; \phi, \mu, \Sigma)$$

Compute the posterior distribution,
given current parameters

}

Expectation Maximization for GMM

Repeat until convergence:

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No parameter change in E-step

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(M-step) Update the parameters:

}

$$\begin{aligned}\phi_j &:= \frac{1}{n} \sum_{i=1}^n w_j^{(i)}, \\ \mu_j &:= \frac{\sum_{i=1}^n w_j^{(i)} x^{(i)}}{\sum_{i=1}^n w_j^{(i)}}, \\ \Sigma_j &:= \frac{\sum_{i=1}^n w_j^{(i)} (x^{(i)} - \mu_j)(x^{(i)} - \mu_j)^T}{\sum_{i=1}^n w_j^{(i)}}\end{aligned}$$

Expectation Maximization

- Why does it work?
- What is its relation to MLE estimation?
is EM still MLE?
- How is convergence guaranteed?
- When we perform EM, what is the real objective that we are optimizing?

General EM Algorithm

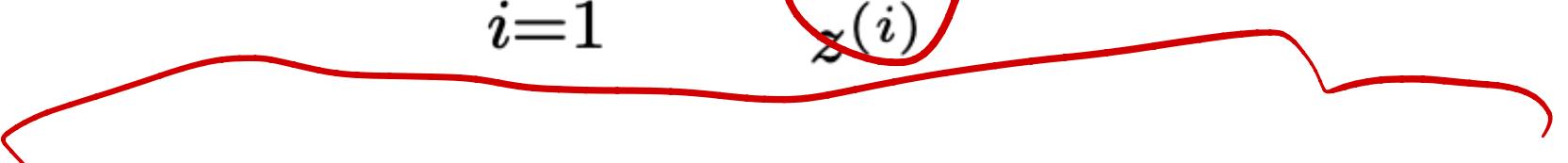
General EM Algorithm

$$p(x; \theta) = \sum_z p(x, z; \theta)$$

z

General EM Algorithm

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$$\begin{aligned} \cancel{\max} \ell(\theta) &= \sum_{i=1}^n \log p(x^{(i)}; \theta) \\ &= \sum_{i=1}^n \log \left(\sum_{z^{(i)}} p(x^{(i)}, z^{(i)}; \theta) \right). \end{aligned}$$


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Let Q to be a distribution over z



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Let Q to be a distribution over z

$$\begin{aligned}\log p(x; \theta) &= \log \sum_z p(x, z; \theta) \\ &= \log \sum_z Q(z) \frac{p(x, z; \theta)}{Q(z)} \\ &\geq \sum_z Q(z) \log \frac{p(x, z; \theta)}{Q(z)}\end{aligned}$$

Jensen's inequality

General EM Algorithm

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This lower bound holds for any $Q(z)$

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ELBO

This lower bound holds for any Q(z)

$$\log p(x; \theta) = \log \sum_z p(x, z; \theta)$$

$$= \log \sum_z Q(z) \frac{p(x, z; \theta)}{Q(z)}$$

$$\geq \sum_z Q(z) \log \frac{p(x, z; \theta)}{Q(z)}$$

tight

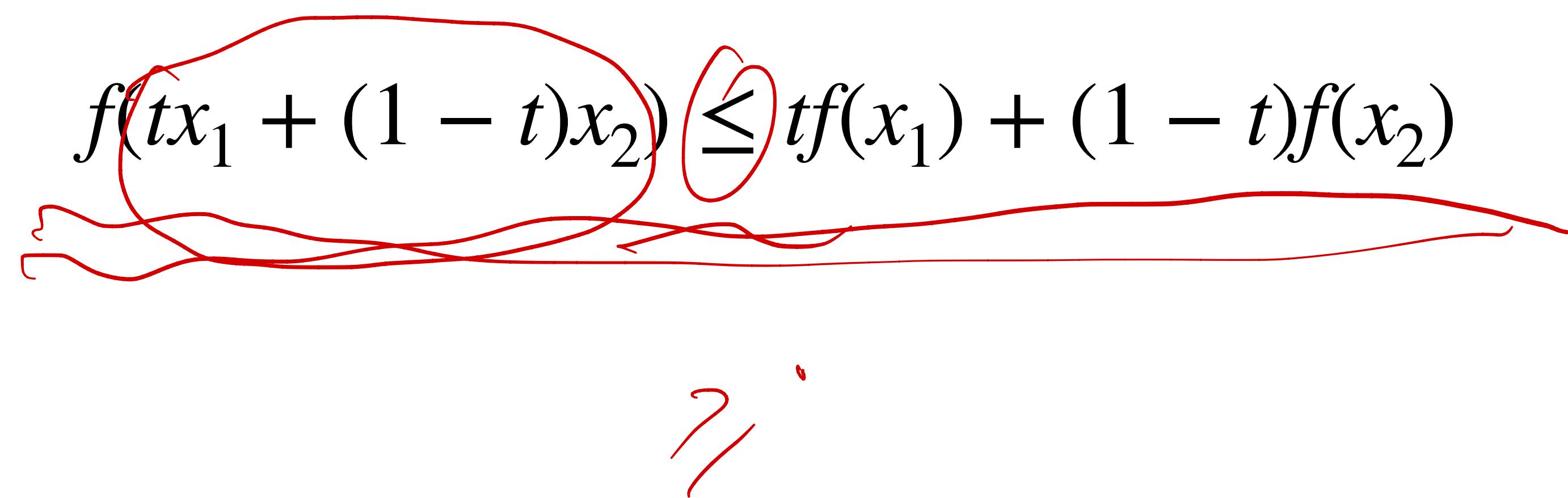
Jensen inequality

$\log(\cdot)$

concave

Jensen Inequality

For a convex function f , and $t \in [0,1]$



Jensen Inequality

For a convex function f , and $t \in [0,1]$

$$f(tx_1 + (1 - t)x_2) \leq tf(x_1) + (1 - t)f(x_2)$$

In probability:

$$f(\mathbb{E}[X]) \leq \mathbb{E}[f(X)]$$
$$f(P_1x_1 + P_2x_2 + \dots + P_kx_k) \leq \sum P_i f(x_i)$$
$$\sum P_i = 1$$

Jensen Inequality

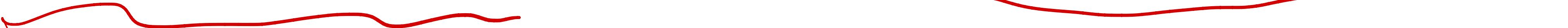
For a convex function f , and $t \in [0,1]$

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In probability:

$$f(\mathbb{E}[X]) \overset{?}{\leq} [f(X)]$$

If f is strictly convex, then equality holds only when X is a constant



Evidence Lower Bound (ELBO)

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$$\begin{aligned}\log p(x; \theta) &= \log \sum_z p(x, z; \theta) \\ &= \log \sum_z Q(z) \frac{p(x, z; \theta)}{Q(z)} \\ &\geq \sum_z Q(z) \log \frac{p(x, z; \theta)}{Q(z)}\end{aligned}$$

ELBO

$\log P(x)$

Evidence Lower Bound (ELBO)

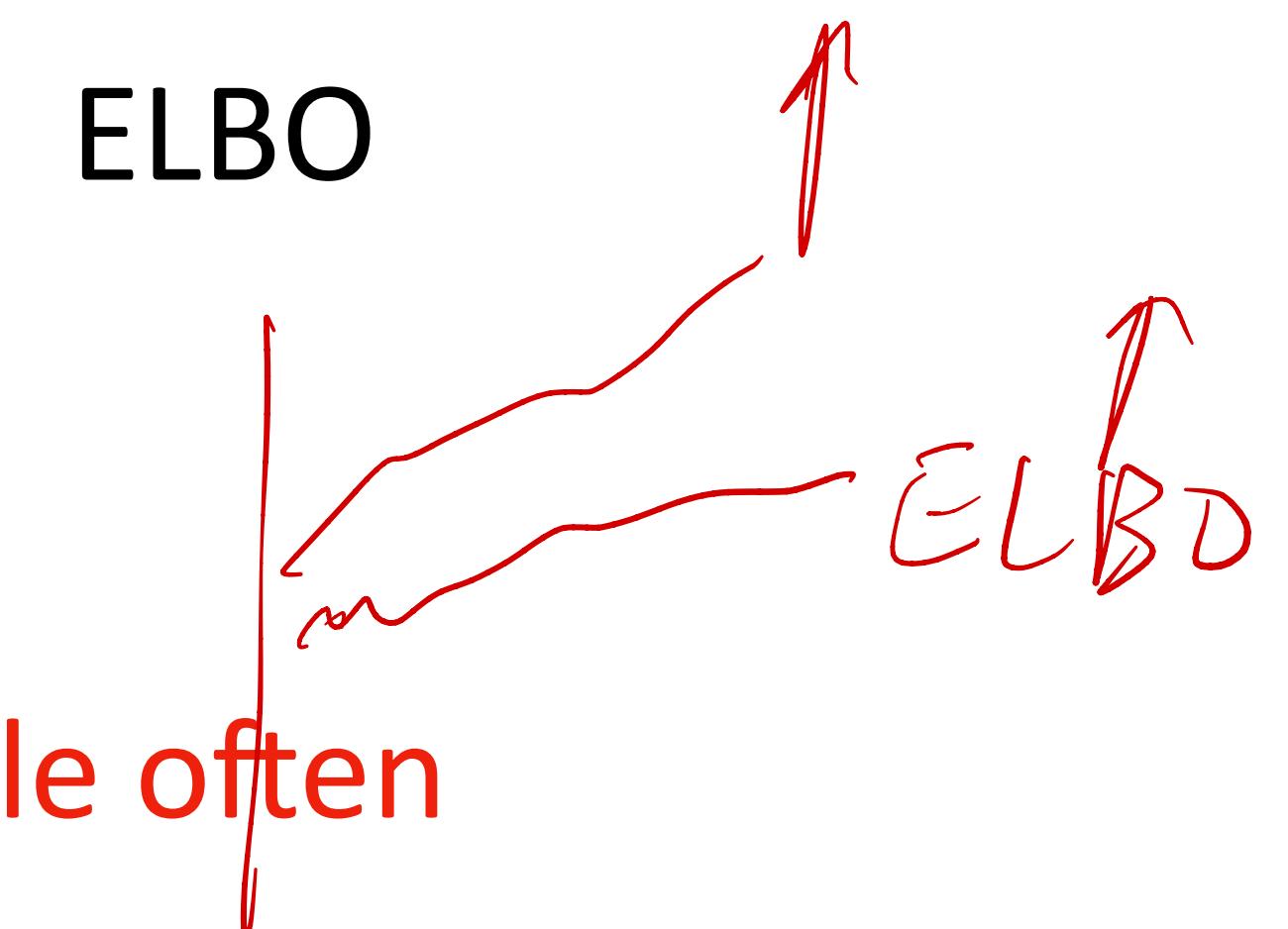
$$\begin{aligned}\log p(x; \theta) &= \log \sum_z p(x, z; \theta) \\ &= \log \sum_z Q(z) \frac{p(x, z; \theta)}{Q(z)} \quad \text{ELBO} \\ &\geq \sum_z Q(z) \log \frac{p(x, z; \theta)}{Q(z)}\end{aligned}$$

Evidence Lower Bound (ELBO)

$$\begin{aligned}\log p(x; \theta) &= \log \sum_z p(x, z; \theta) \\ &= \log \sum_z Q(z) \frac{p(x, z; \theta)}{Q(z)} \\ &\geq \sum_z Q(z) \log \frac{p(x, z; \theta)}{Q(z)}\end{aligned}$$

Because the log likelihood is intractable, people often optimize its lower bound instead

$$\underbrace{\max}_{\text{max ELBO}} \log p(x)$$



Evidence Lower Bound (ELBO)



$$\begin{aligned}\log p(x; \theta) &= \log \sum_z p(x, z; \theta) \\ &= \log \sum_z Q(z) \frac{p(x, z; \theta)}{Q(z)} \\ &\geq \sum_z Q(z) \log \frac{p(x, z; \theta)}{Q(z)}\end{aligned}$$

ELBO

Because the log likelihood is intractable, people often optimize its lower bound instead

Why optimizing lower bound works? How to choose $Q(z)$, why we computed posterior in the E step, what is the benefit?

EM

Evidence Lower Bound (ELBO)

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Evidence Lower Bound (ELBO)

$$\begin{aligned}\log p(x; \theta) &= \log \sum_z p(x, z; \theta) \\ &= \log \sum_z Q(z) \frac{p(x, z; \theta)}{Q(z)} \\ &\geq \sum_z Q(z) \log \frac{p(x, z; \theta)}{Q(z)} \\ &\stackrel{?}{\equiv}\end{aligned}$$

When is the lower bound tight?

Jensen inequality $\stackrel{?}{\equiv}$ is constant

Evidence Lower Bound (ELBO)

$$\begin{aligned}\log p(x; \theta) &= \log \sum_z p(x, z; \theta) \\ &= \log \sum_z Q(z) \frac{p(x, z; \theta)}{Q(z)} \\ &\geq \underbrace{\sum_z Q(z) \log}_{\sim} \frac{p(x, z; \theta)}{Q(z)}\end{aligned}$$

When is the lower bound tight?

no matter what τ is

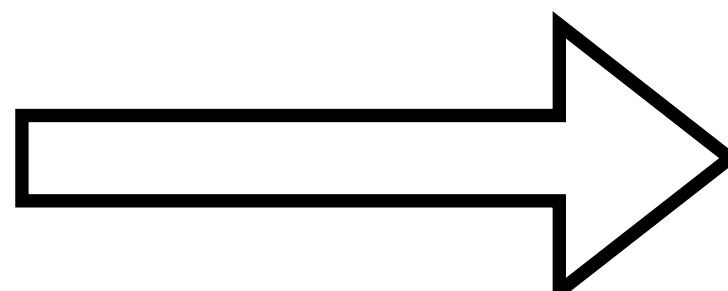
$$\frac{p(x, z; \theta)}{Q(z)} = c$$
$$Q(z) = \frac{P(x, z; \theta)}{c}$$
$$Q(z) = \frac{P(x, z)}{\sum_{\tau} P(x, z)}$$
$$= \frac{P(x, z)}{P(x)}$$

Evidence Lower Bound (ELBO)

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When is the lower bound tight?

$$\frac{p(x, z; \theta)}{Q(z)} = c$$



$$\begin{aligned}Q(z) &= \frac{p(x, z; \theta)}{\sum_z p(x, z; \theta)} \\ &= \frac{p(x, z; \theta)}{p(x; \theta)} \\ &= p(z|x; \theta)\end{aligned}$$

Evidence Lower Bound (ELBO)

Evidence Lower Bound (ELBO)

Verify $\sum_z Q(z) \log \frac{p(x, z; \theta)}{Q(z)}$ when $Q(z) = p(z|x)$?

$$\begin{aligned} \text{ELBO} &= \sum_x P_{Cz|x} \log \left(\frac{P_{Cx, z; \theta}}{P_{Cz|x}} \right) \\ &= \left(\sum_z P_{Cz|x} \right) \log P_{Cx} \\ &= \log P_{Cx} \left(\sum_z P_{Cz|x} \right) \\ &= \log P_{Cx} \end{aligned}$$

Evidence Lower Bound (ELBO)

Verify $\sum_z Q(z) \log \frac{p(x, z; \theta)}{Q(z)}$ when $Q(z) = p(z|x)$?

$$\text{ELBO}(x; Q, \theta) = \sum_z Q(z) \log \frac{p(x, z; \theta)}{Q(z)}$$

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$$\forall Q, \theta, x, \quad \log p(x; \theta) \geq \text{ELBO}(x; Q, \theta)$$



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$$\forall Q, \theta, x, \quad \log p(x; \theta) \geq \text{ELBO}(x; Q, \theta)$$

For a dataset of many data samples

$$\begin{aligned} \ell(\theta) &\geq \sum_i \text{ELBO}(x^{(i)}; Q_i, \theta) \\ &= \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta)}{Q_i(z^{(i)})} \end{aligned}$$

Evidence Lower Bound (ELBO)

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Evidence Lower Bound (ELBO)

$$\text{ELBO}(x; Q, \theta) = \sum_z Q(z) \log \frac{p(x, z; \theta)}{Q(z)}$$

What is $\operatorname{argmax}_{Q(z)} \text{ELBO}(x; Q, \theta)$?

$Q(z) = ?$

$$\log P(x) \geq \text{ELBO}(x; Q, \theta)$$

$$\underbrace{Q(z) = P(z|x)}$$

$\log P(x)$ is constant varying $Q(z)$

The General EM Algorithm

Repeat until convergence {

(E-step) For each i , set

$$Q_i(z^{(i)}) := p(z^{(i)}|x^{(i)}; \theta).$$

(M-step) Set

$$\theta := \arg \max_{\theta} \sum_{i=1}^n \text{ELBO}(x^{(i)}; Q_i, \theta)$$

$$= \arg \max_{\theta} \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta)}{Q_i(z^{(i)})}.$$

}

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Based on current θ , model parameters does not change in E-step



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Q_{cur} is fixed

$Q(z)$ is not relevant to θ , and $Q(z)$ does not change in the M-step

}

The General EM Algorithm

Repeat until convergence {

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ELBO(θ) $(Q(z))$

Based on current θ , model parameters does not change in E-step

(M-step) Set

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$$= \arg \max_{\theta} \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta)}{Q_i(z^{(i)})}.$$

$Q(z)$ is not relevant to θ , and $Q(z)$ does not change in the M-step

}

E-step is maximizing ELBO over $Q(z)$, M-step is maximizing ELBO over θ

The General EM Algorithm

Repeat until convergence {

(E-step) For each i , set

$$Q_i(z^{(i)}) := p(z^{(i)}|x^{(i)}; \theta).$$

Based on current θ , model parameters does not change in E-step

(M-step) Set

$$\theta := \arg \max_{\theta} \sum_{i=1}^n \text{ELBO}(x^{(i)}; Q_i, \theta)$$

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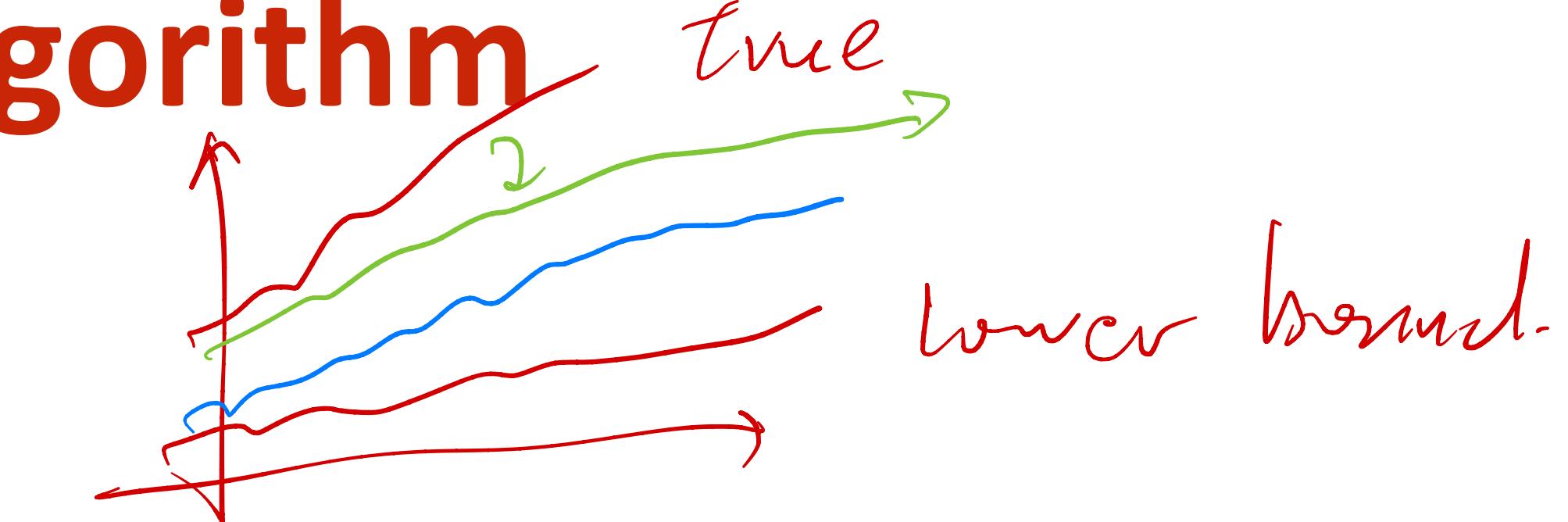
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Why is maximizing lower-bound sufficient?

$\left[\log p(x) \right]$



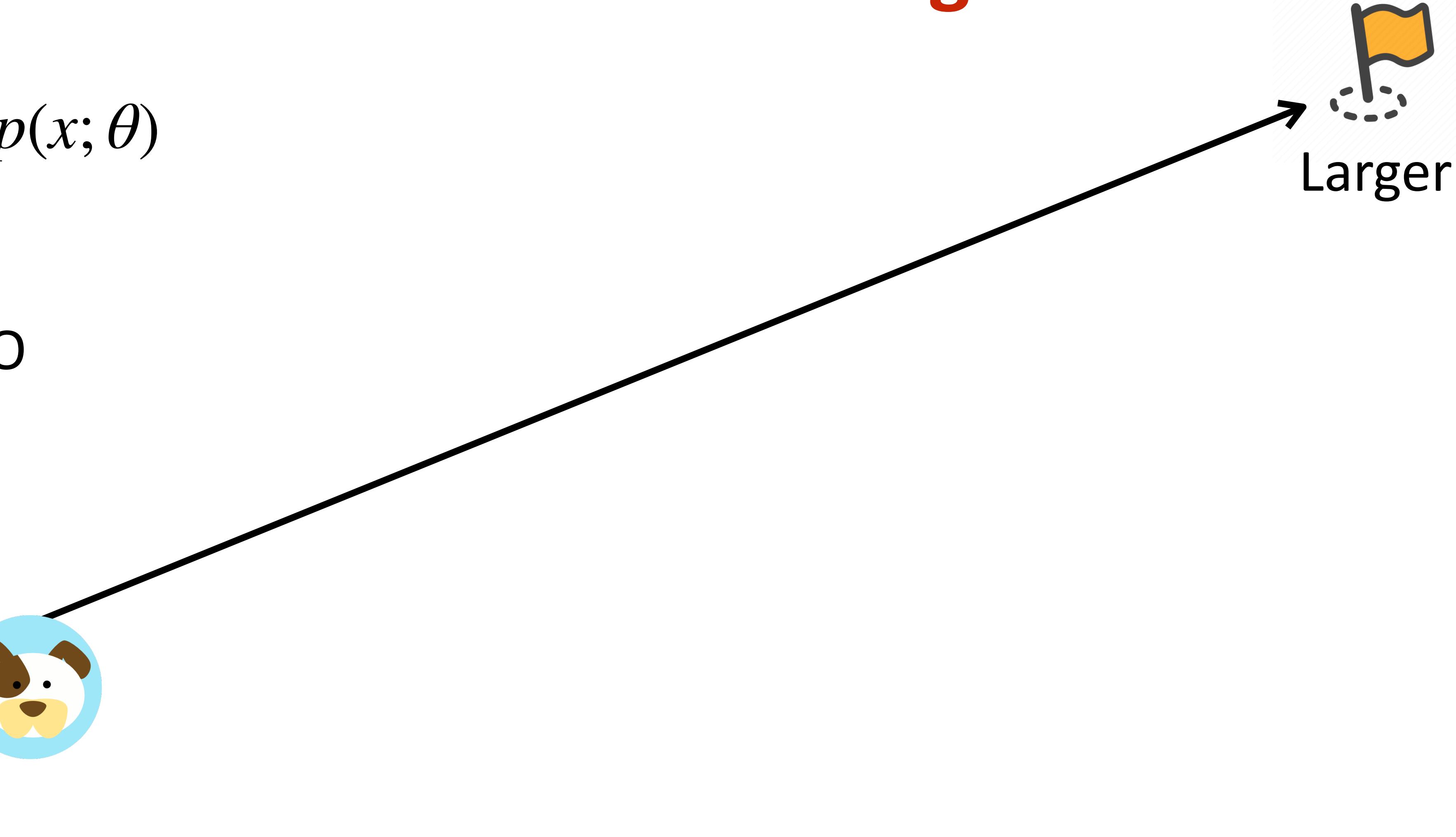
EM is Hill Climbing



$\log p(x; \theta)$



ELBO



EM is Hill Climbing

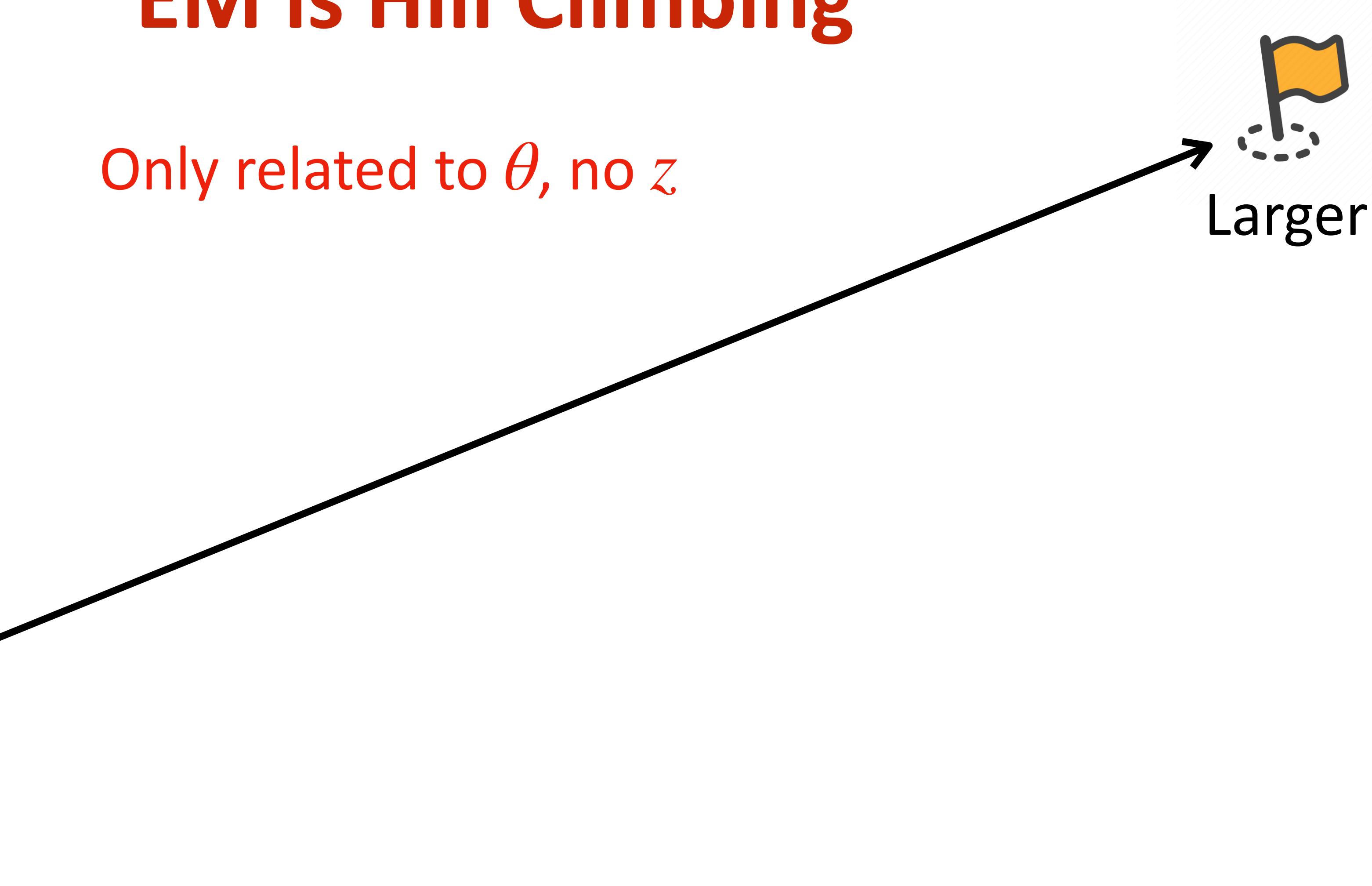


$\log p(x; \theta)$

Only related to θ , no z



ELBO



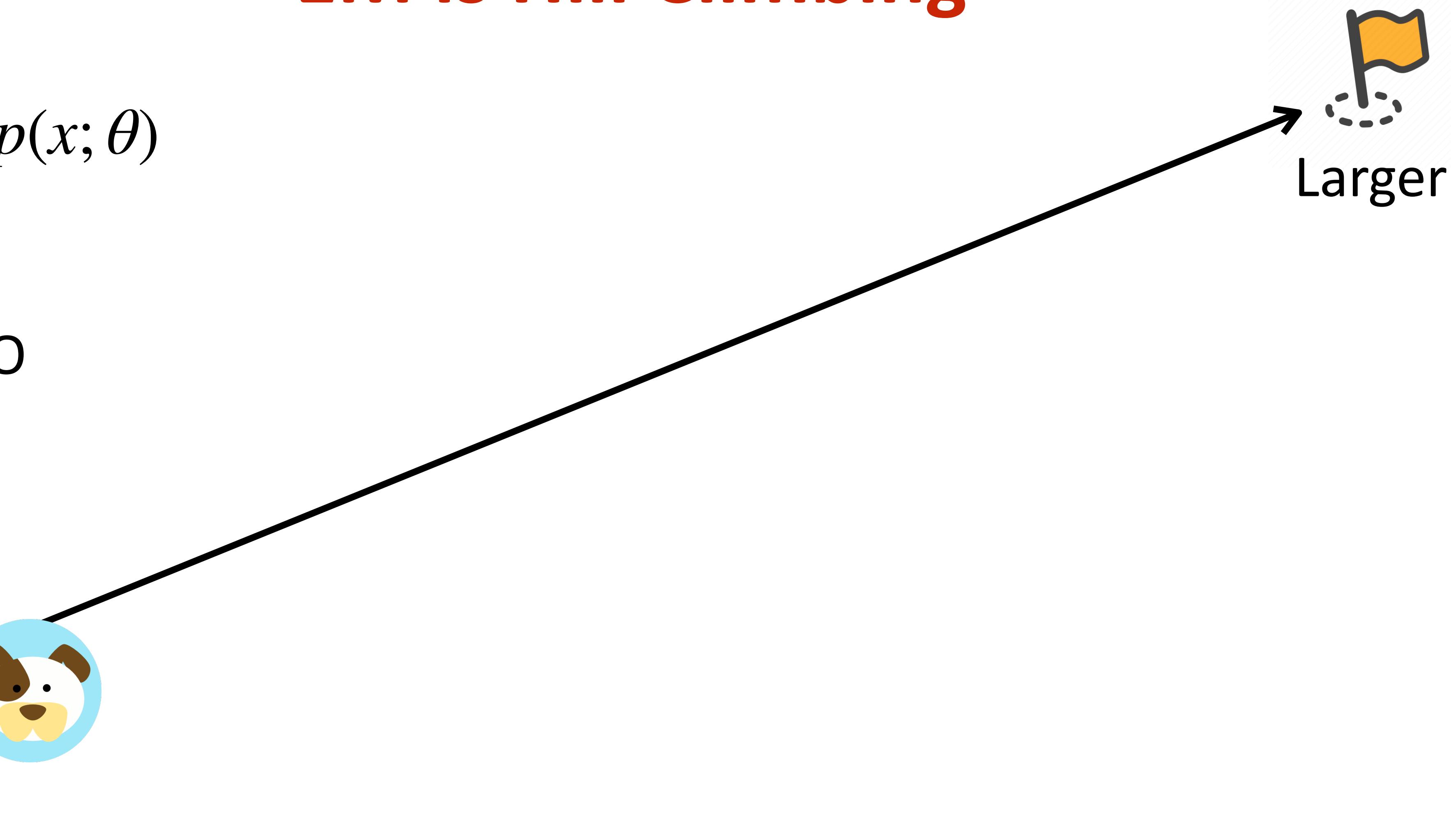
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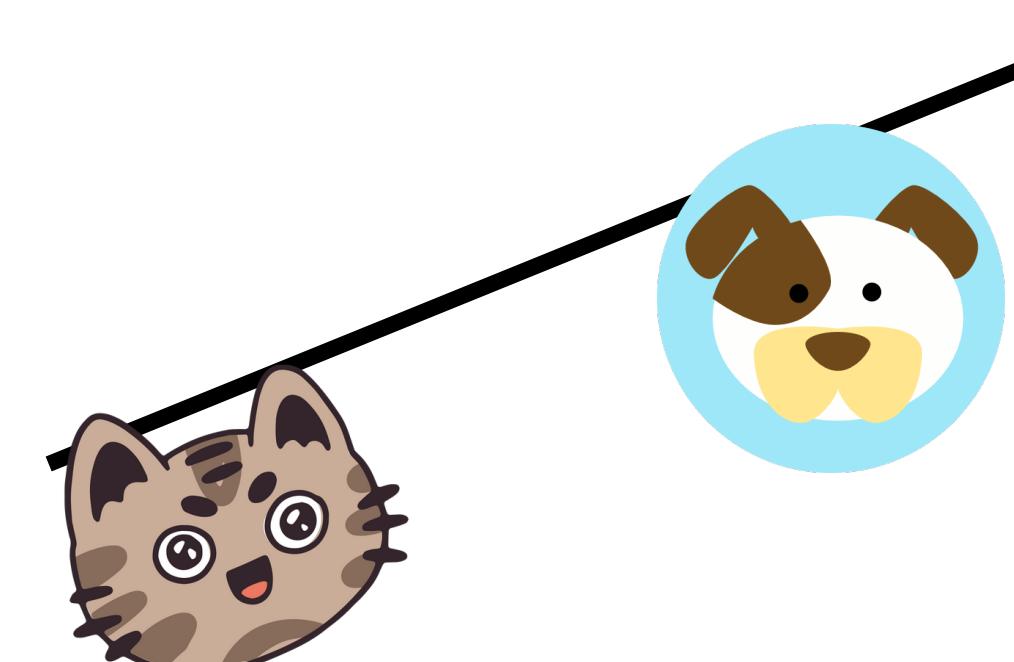
EM is Hill Climbing



$\log p(x; \theta)$



ELBO



E-step: $Q(z) = p(z | x; \theta)$, making ELBO tight



Larger

EM is Hill Climbing



$\log p(x; \theta)$



ELBO



E-step: $Q(z) = p(z | x; \theta)$, making ELBO tight

“dog” doesn’t change, because θ does not change



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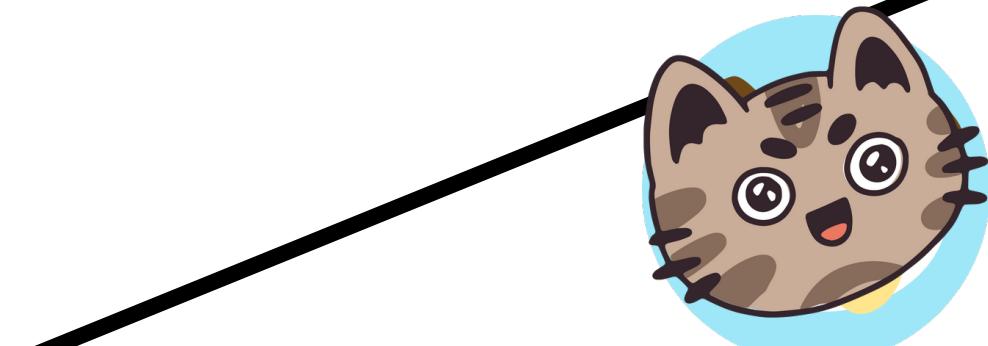
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$\log p(x; \theta)$



ELBO



M-step: $\max_{\theta} ELBO$

ELBO becomes larger, and it is not tight anymore because posterior changes



EM is Hill Climbing



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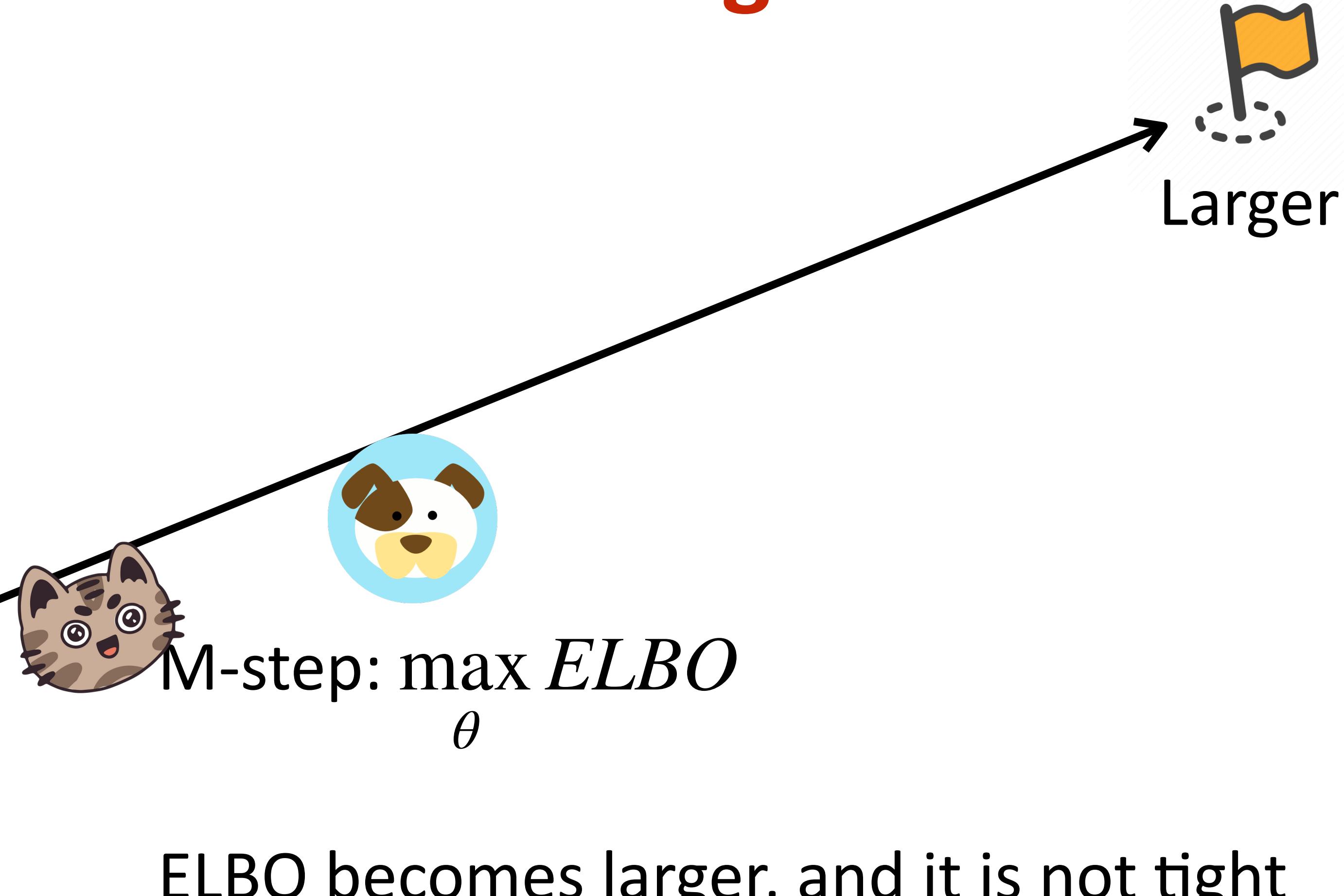
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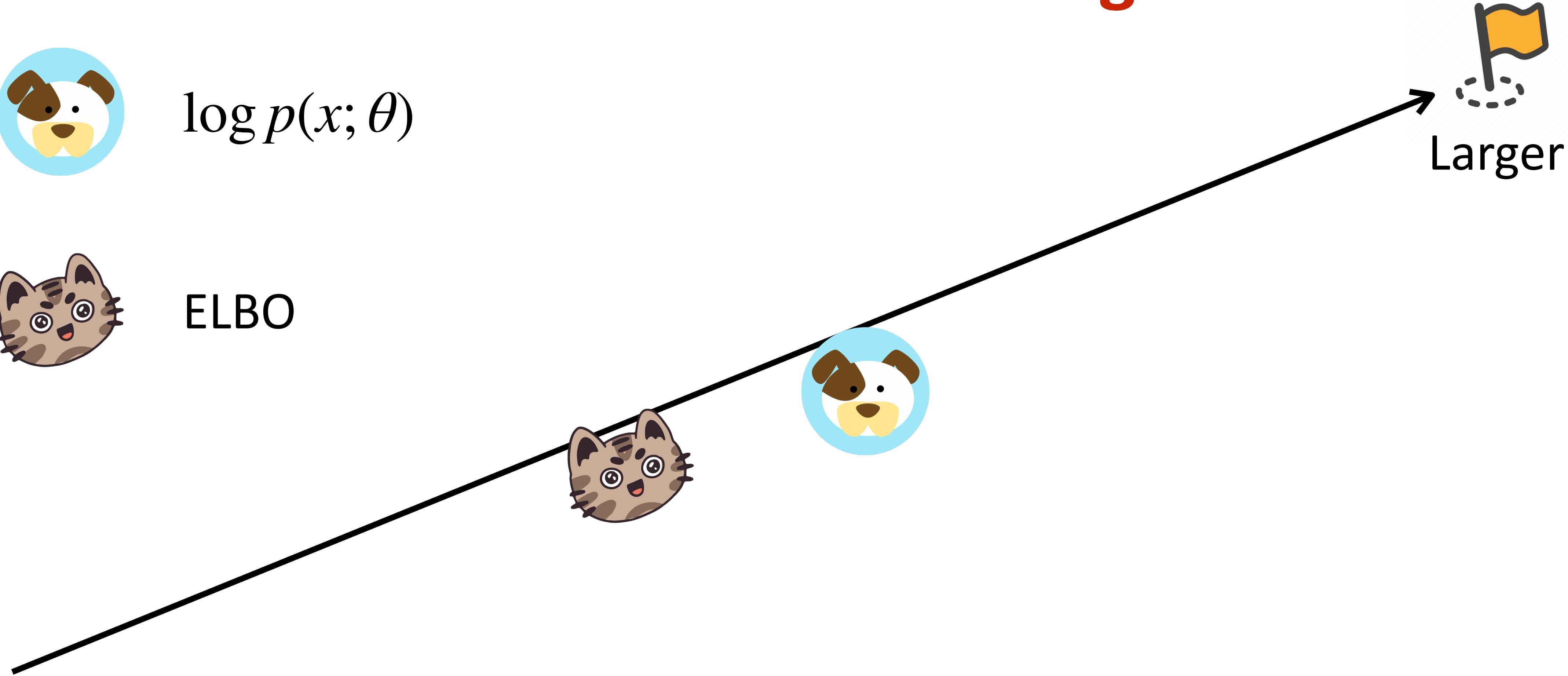
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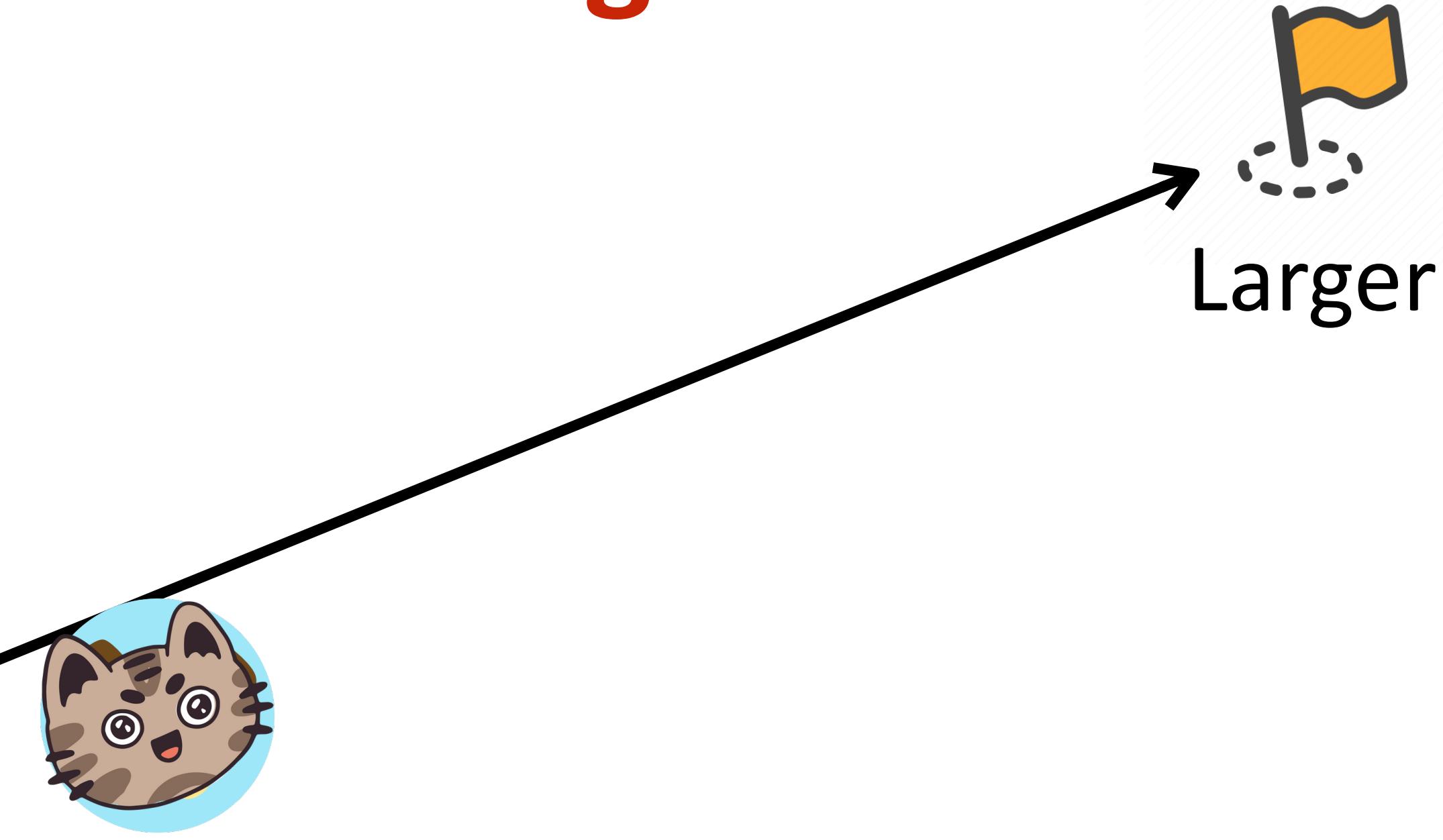
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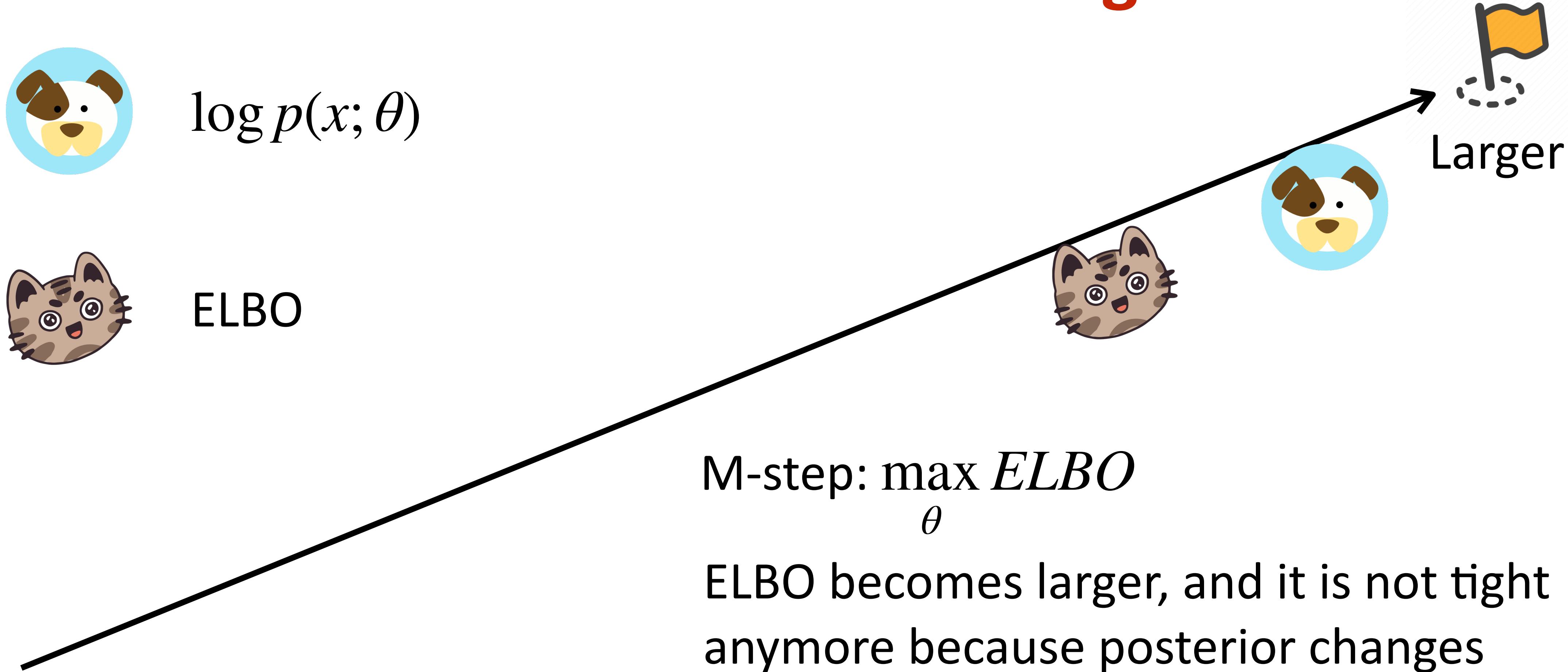
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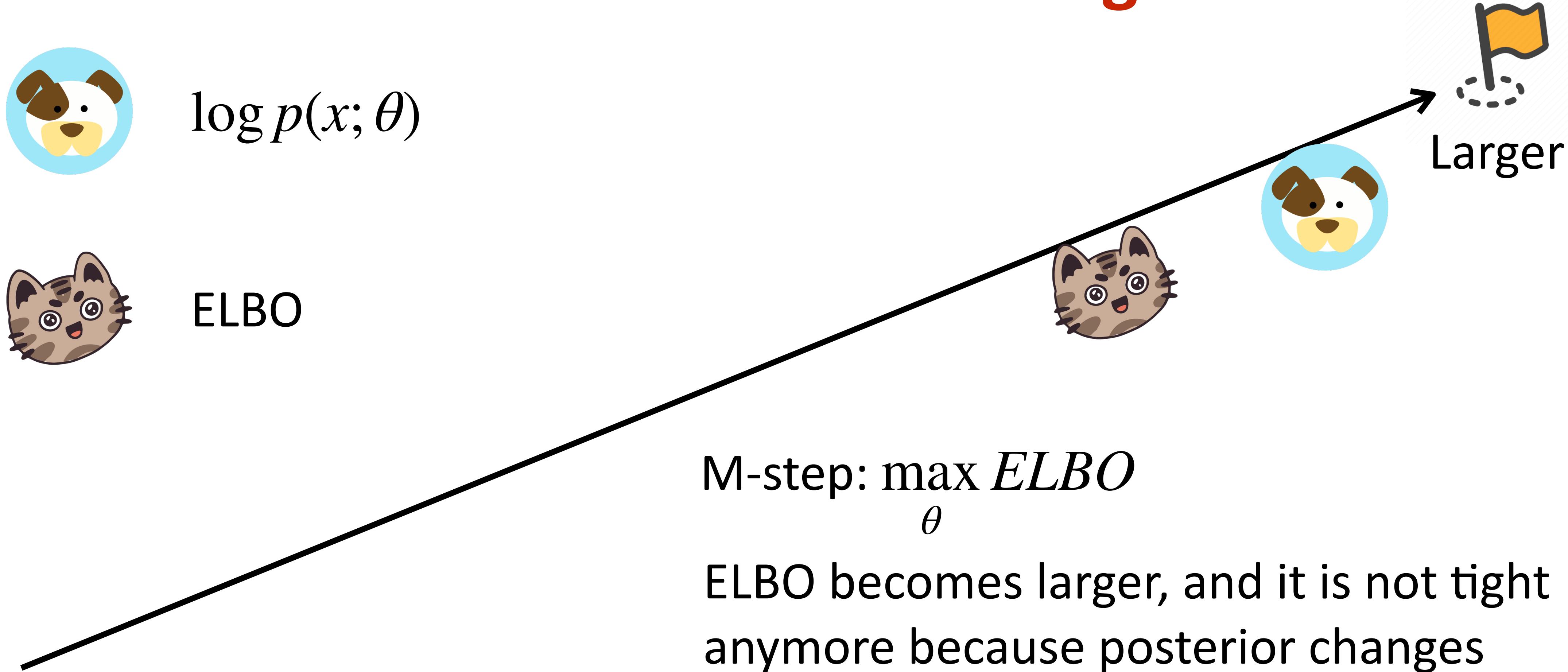
EM is Hill Climbing



$\log p(x; \theta)$



ELBO



$\log p(x; \theta)$ is monotonically increasing!

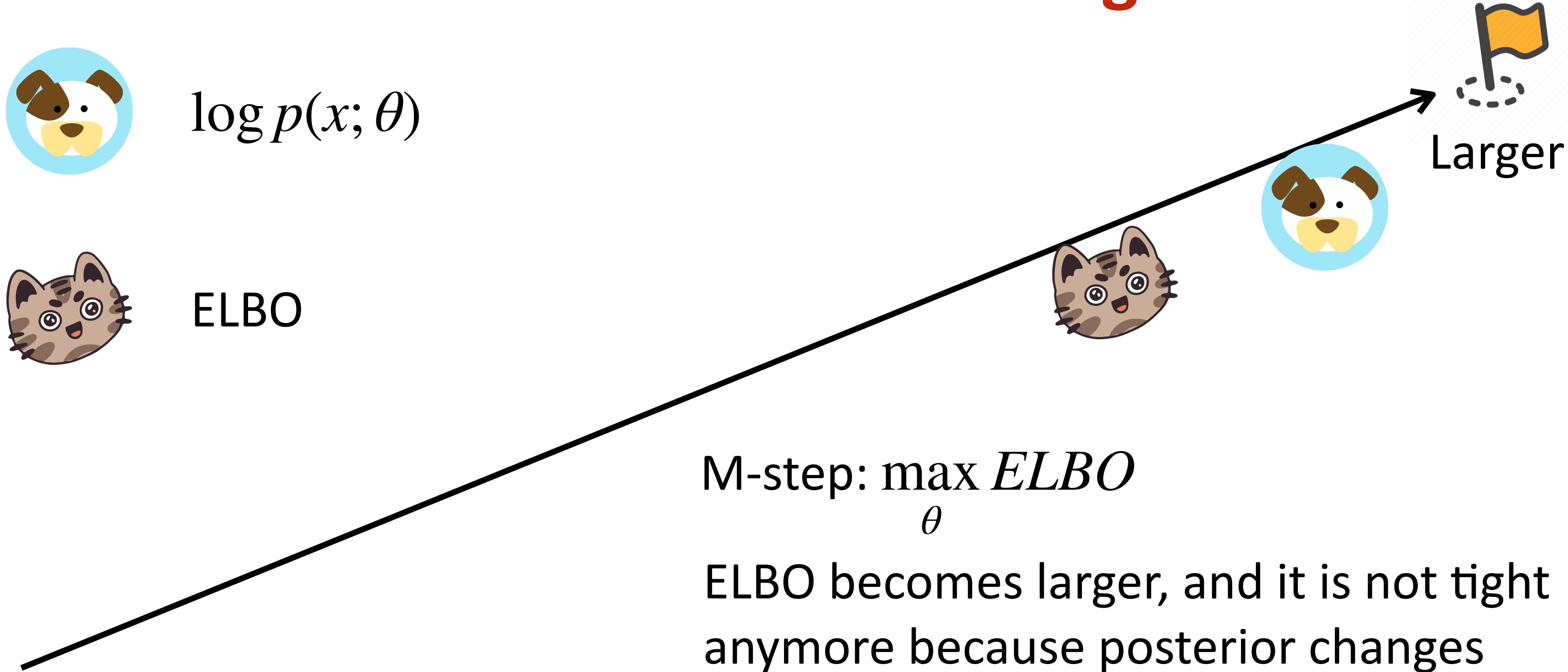
EM is Hill Climbing



$\log p(x; \theta)$



ELBO



$\log p(x; \theta)$ is monotonically increasing!

We are doing MLE implicitly!

EM is Hill Climbing



$\log p(x; \theta)$



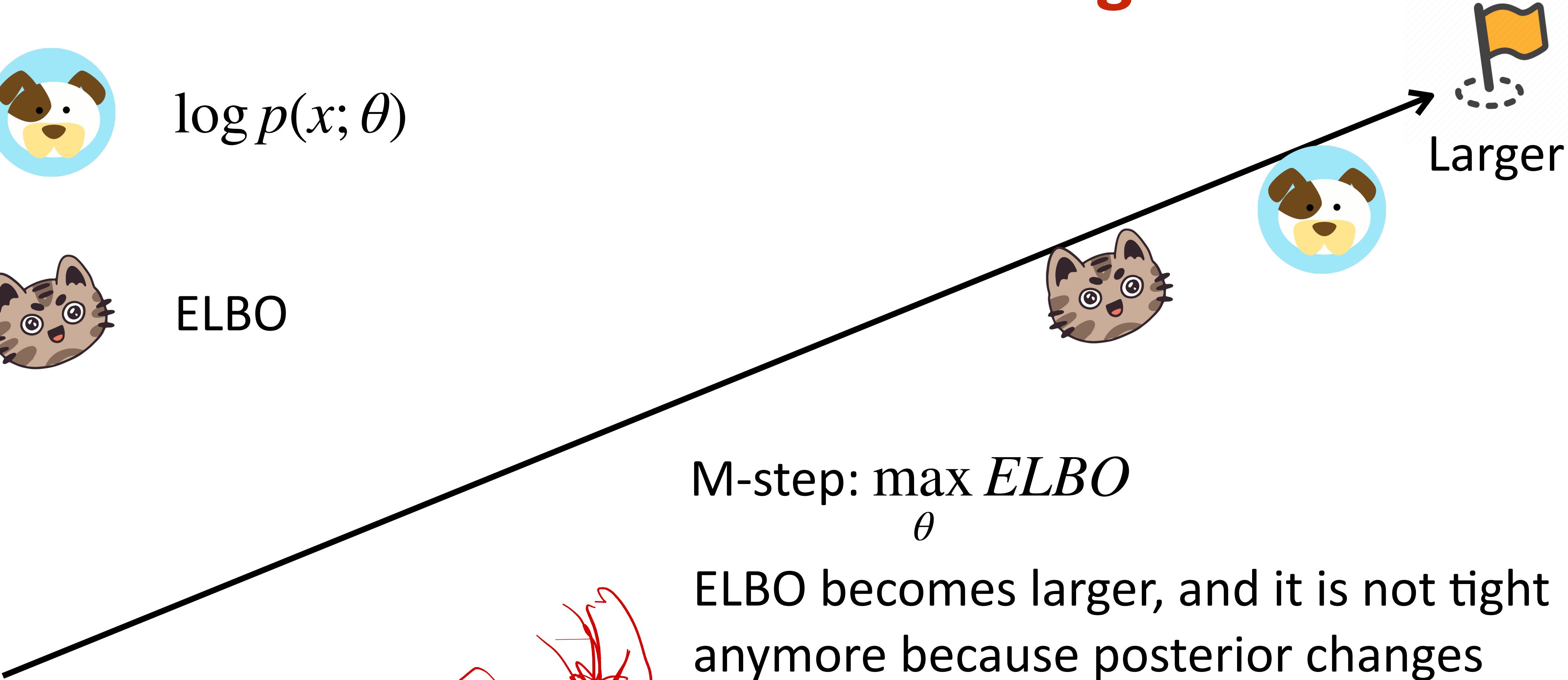
ELBO



$\log p(x; \theta)$ is monotonically increasing!

We are doing MLE implicitly!

Convergence is guaranteed



ELBO loss function

ELBO

VAE

E-step

maximize ELBO
 $Q(z)$

$$Q(z) = P(z|x)$$

until converge

M-step

maximize ELBO
 θ

ELBO loss function

Revisit the E-Step

Repeat until convergence {

(E-step) For each i , set

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(M-step) Set

$$\begin{aligned}\theta &:= \arg \max_{\theta} \sum_{i=1}^n \text{ELBO}(x^{(i)}; Q_i, \theta) \\ &= \arg \max_{\theta} \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta)}{Q_i(z^{(i)})}.\end{aligned}$$

}

Revisit the E-Step

Repeat until convergence {

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Computable posterior is important. If $Q(z)$ is not the posterior, then there is no guarantee that $\log p(x)$ is improved at every iteration

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Still remember conjugate prior? Which is for easy-to-compute posterior

$$\begin{aligned} \mathbb{Z} &\downarrow \\ \mathcal{P}_{CZ} & \quad \text{family} \\ (\mathcal{P}_{CZ|x}) & \equiv P(x) \end{aligned}$$

$$(Q_{CZ} = \mathcal{P}_{CZ}|x)$$

$$\mathbb{E}_{z \sim Q_{CZ}} \log \frac{P(x, z)}{Q_{CZ}}$$

Q_{CZ} easy to sample from

Revisit the M-Step

Revisit the M-Step

$$\operatorname{argmax}_{\theta} \sum_z Q(z) \log \frac{p(x, z; \theta)}{Q(z)} = \operatorname{argmax}_{\theta} \sum_z Q(z) \log p(x, z; \theta)$$

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We can use Monte-Carlo sampling to approximate the expectation

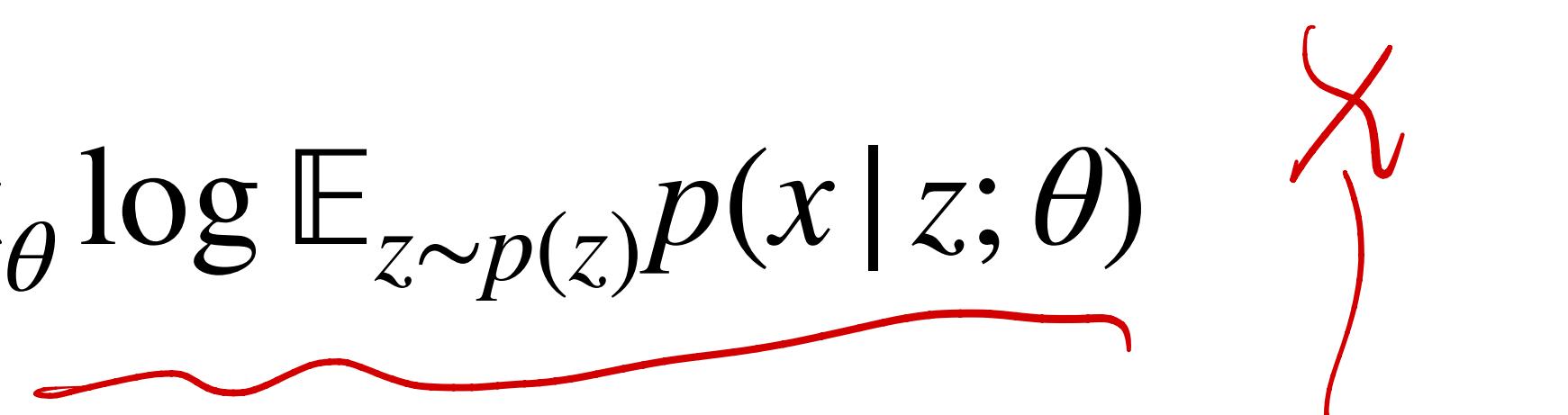
Comparing Direct Maximization and EM

Direct maximization:

$$\operatorname{argmax}_{\theta} \log \sum_z p(x | z; \theta) p(z) = \operatorname{argmax}_{\theta} \log \mathbb{E}_{z \sim p(z)} p(x | z; \theta)$$

Comparing Direct Maximization and EM

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M-Step in EM:

$$\operatorname{argmax}_{\theta} \sum_z Q(z) \log p(x, z; \theta) = \operatorname{argmax}_{\theta} \mathbb{E}_{z \sim Q(z)} \log p(x, z; \theta)$$


Comparing Direct Maximization and EM

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Why don't we use MC sampling to approximate expectation in direct maximization?

Comparing Direct Maximization and EM

Direct maximization:

$$\operatorname{argmax}_{\theta} \log \sum_z p(x|z; \theta) p(z) = \operatorname{argmax}_{\theta} \log \mathbb{E}_{z \sim p(z)} p(x|z; \theta)$$

x is given $p(x|z)$
 $z \sim p(z)$
 $Q(z) = P(z|x)$

M-Step in EM:

$$\operatorname{argmax}_{\theta} \sum_z Q(z) \log p(x, z; \theta) = \operatorname{argmax}_{\theta} \mathbb{E}_{z \sim Q(z)} \log p(x, z; \theta)$$

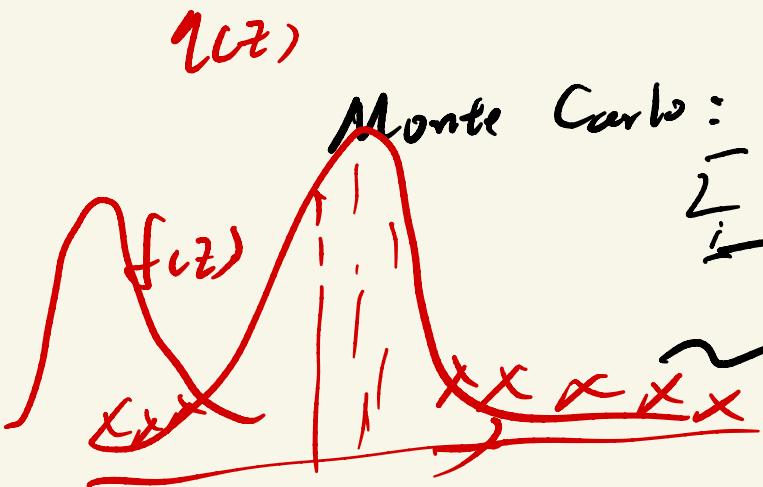
Why don't we use MC sampling to approximate expectation in direct maximization?

It may need a large number of samples to have a good approximation

$$E_{z \sim q(z)} f(z) = \sum_i q(z_i) f(z_i)$$

↑

$f(z_i)$ is large



Monte Carlo:

$$\frac{\sum_i f(z^{(i)})}{N}$$

$$z^{(i)} \sim q(z)$$

$z^{(i)}$ where $f(z_i)$ and $q(z_i)$ uniform 100 sample $q(z_i)$ are large

$f(z_i)$

Other Interpretations of ELBO

$$\text{ELBO}(x; Q, \theta) = \mathbb{E}_{z \sim Q} [\log p(x, z; \theta)] - \mathbb{E}_{z \sim Q} [\log Q(z)]$$

$$= \mathbb{E}_{z \sim Q} [\log p(x|z; \theta)] - D_{KL}(Q||p_z)$$

Regularize $Q(z)$ towards the prior $p(z)$

AE
reconstru
constant

$p(z|x)$

$$\text{ELBO}(x; Q, \theta) = \log p(x) - D_{KL}(Q||p_{z|x})$$

$D_{KL}(Q||p_{z|x}) \geq 0$

Maximizing ELBO over $Q(z)$ is essentially solving the posterior distribution $p(z|x)$

$$Q = P_{CZ|x}$$

Further Questions

Further Questions

E step $\vartheta = \underline{P(z|x)}$

- What if we do not have closed-form model posterior? $\underline{P(z|x)}$

Further Questions

- What if we do not have closed-form model posterior? —> Variational EM



inference

$$P(z|x)$$

Further Questions

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The process of approximating the model posterior is called variational inference

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- What if we do not have closed-form model posterior? → Variational EM

The process of approximating the model posterior is called variational inference

We will learn variational autoencoder later

Thank You!
Q & A