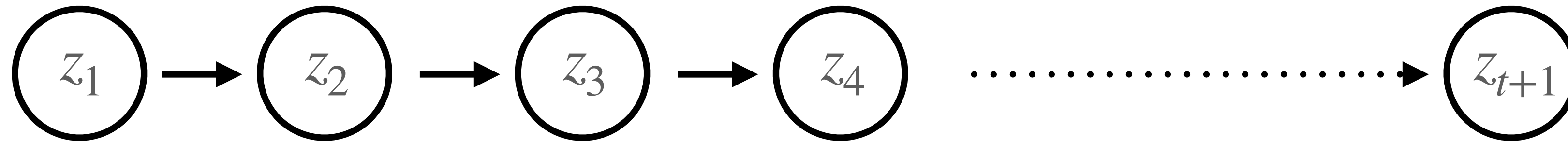


HMMs + LDSs

Some Final Thoughts on FA and PCA

- PCA has simpler understanding in terms of variance and orthogonality
- FA won't be as dependent on scaling
- Important to check that scientific results are robust across methods

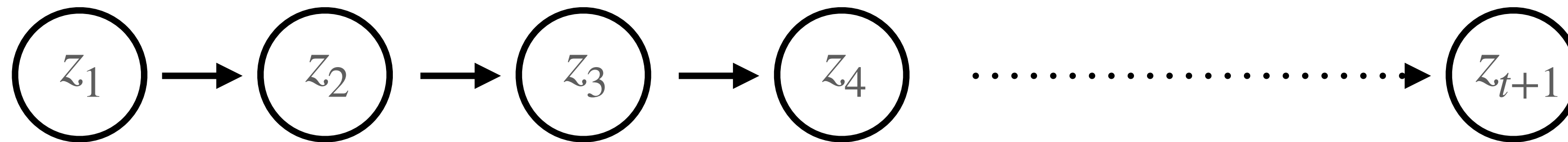
Markov Chains



- The current state only depends on the past state

$$P(z_{t+1} | z_1, z_2, \dots, z_t) = P(z_{t+1} | z_t)$$

Markov Chains



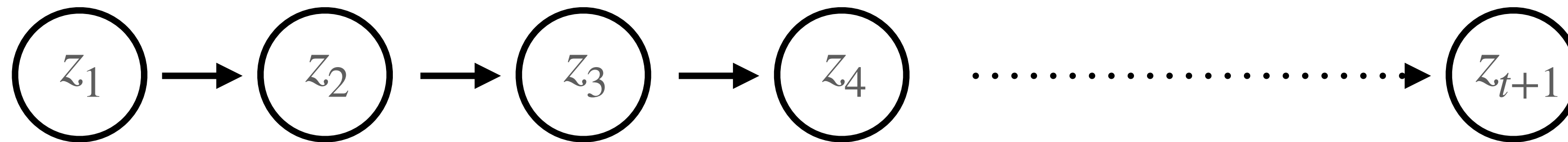
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$$P(z_{t+1} | z_1, z_2, \dots, z_t) = P(z_{t+1} | z_t)$$

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$$P(z_1, z_2, \dots, z_{t+1}) = P(z_1)P(z_2 | z_1) \dots P(z_t | z_{t-1})P(z_{t+1} | z_t)$$

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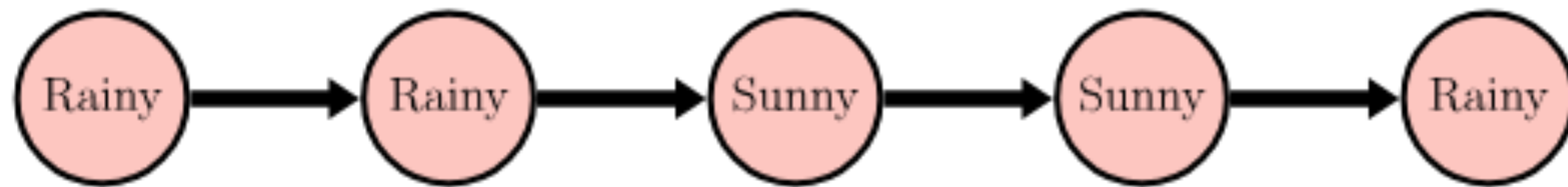
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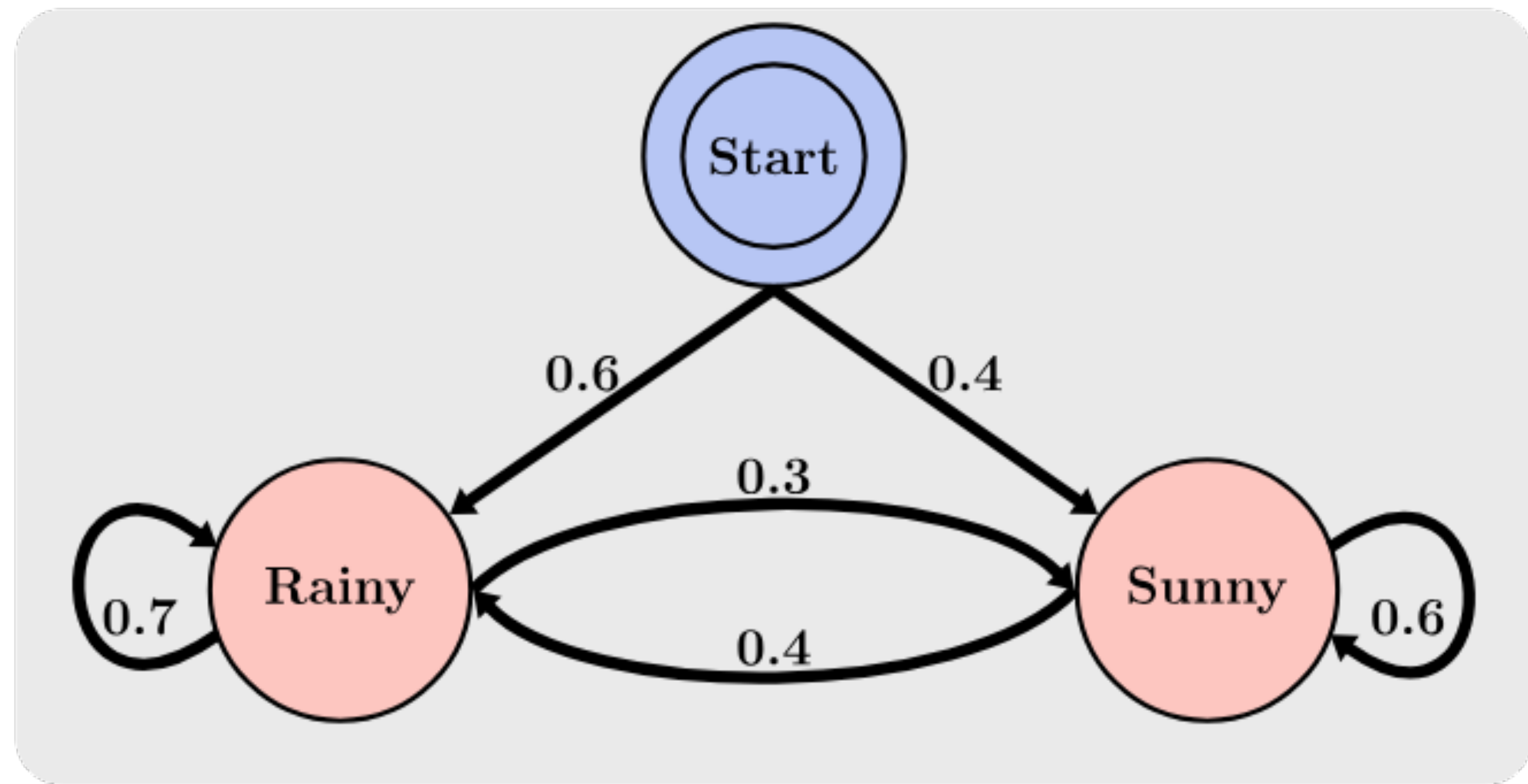
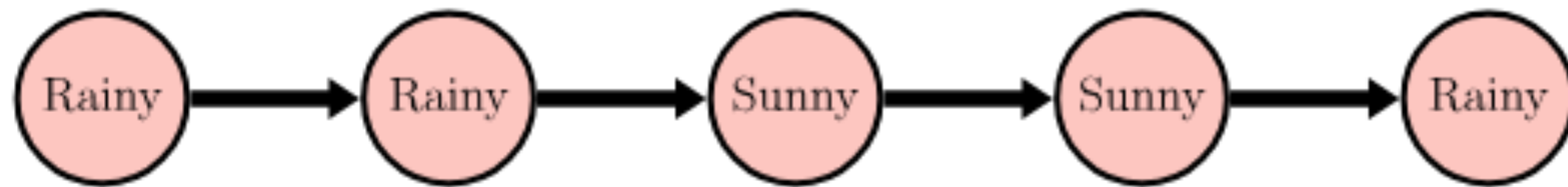
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$$P(z_{1:T}) = P(z_1) \prod_{t=2}^T p(z_t | z_{t-1})$$

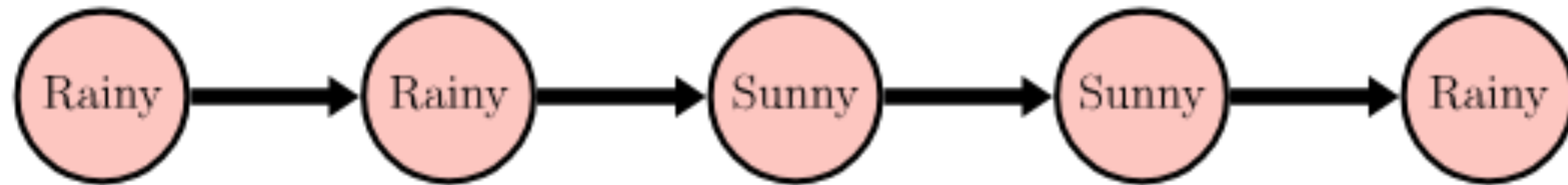
Markov Chains



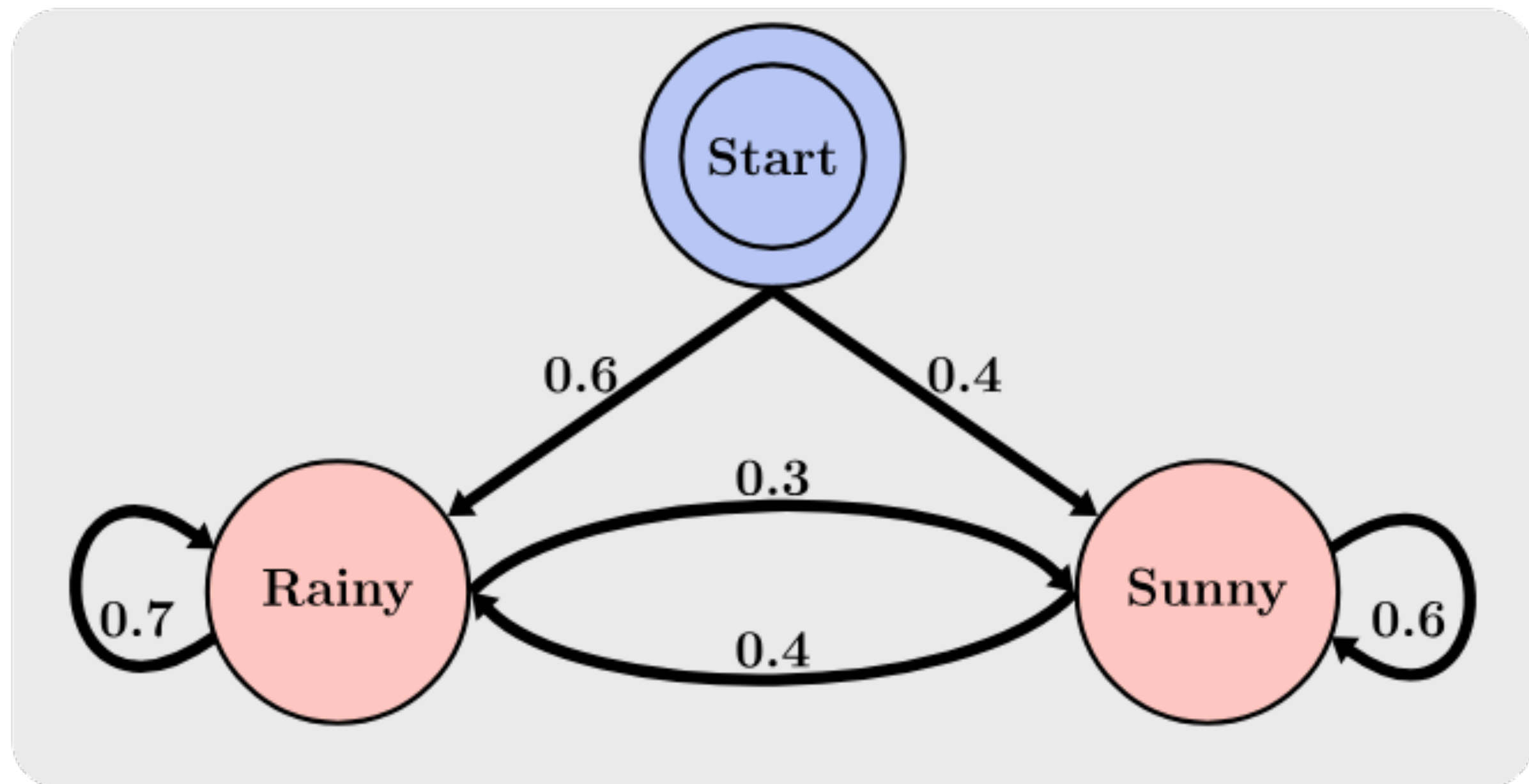
Markov Chains



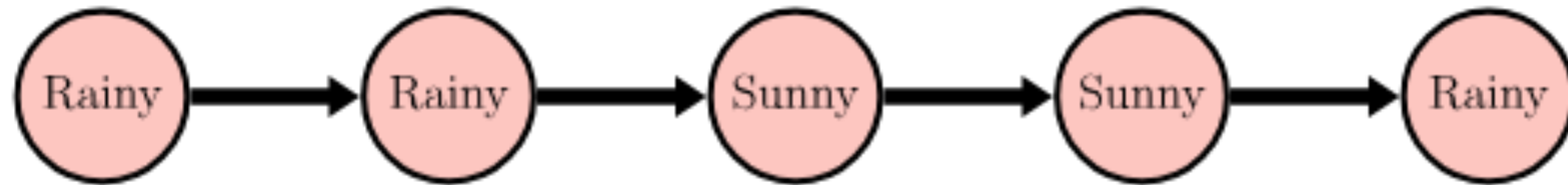
Markov Chains



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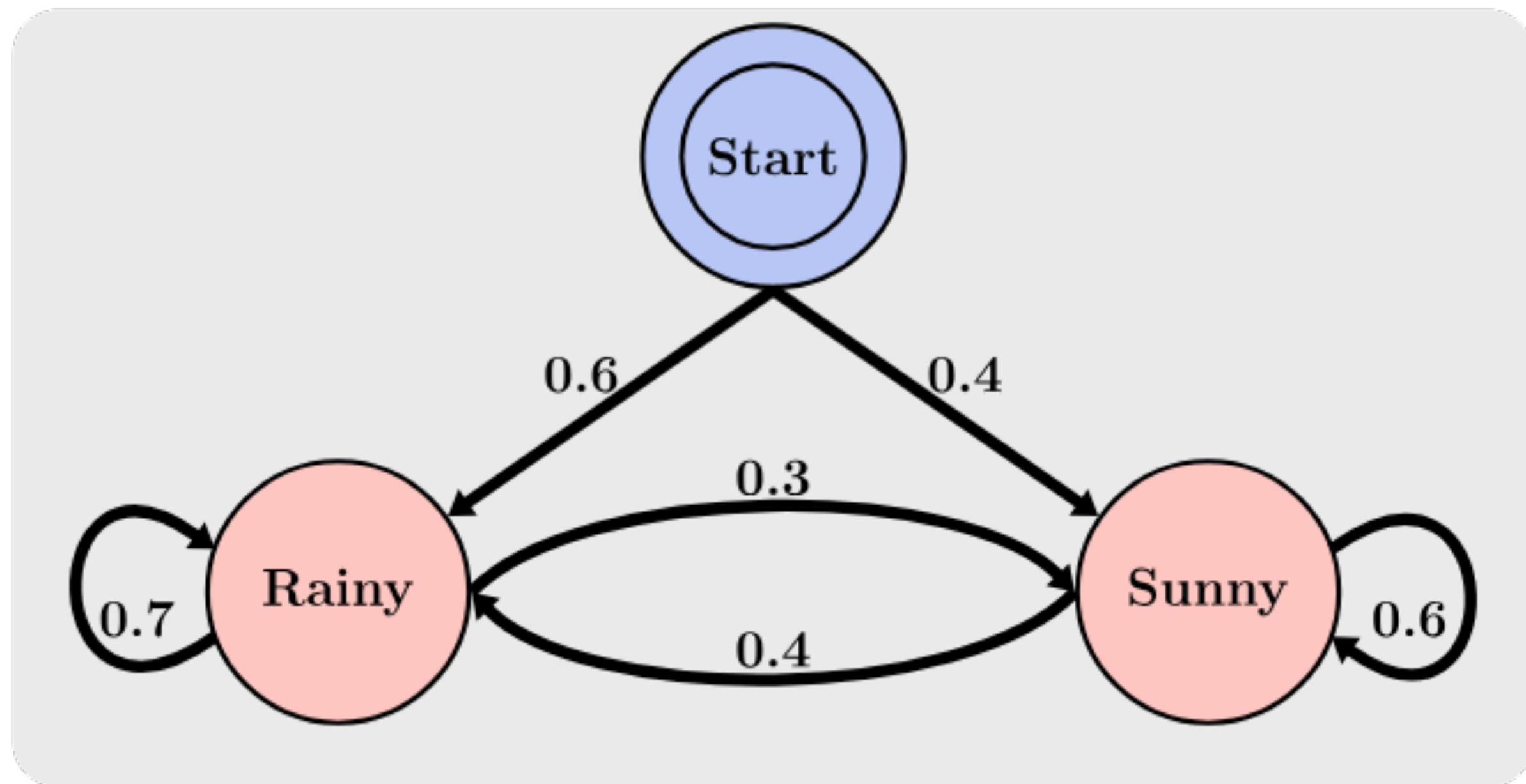
Markov Chains



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Initial Conditions

$$P(z_1 = R) = 0.6, \quad P(z_1 = S) = 0.4$$



Markov Chains



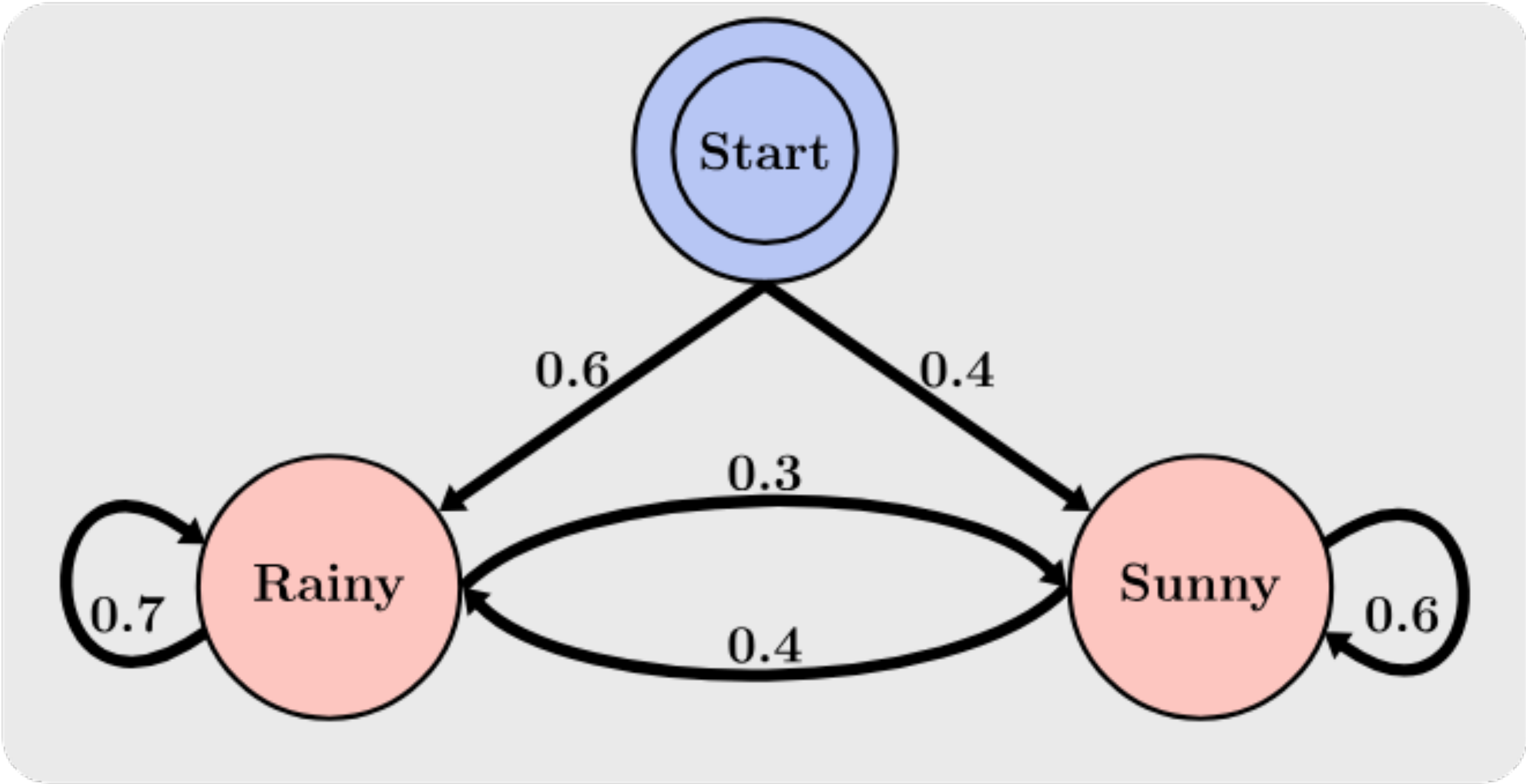
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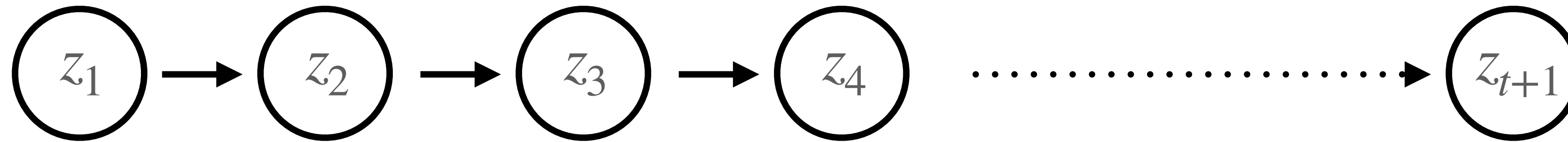
$$P(z_1 = R) = 0.6, \quad P(z_1 = S) = 0.4$$

Transitions Matrix

$P(z_{t+1} = R z_t = R) = 0.7$	$P(z_{t+1} = S z_t = R) = 0.3$
$P(z_{t+1} = R z_t = S) = 0.4$	$P(z_{t+1} = S z_t = S) = 0.6$

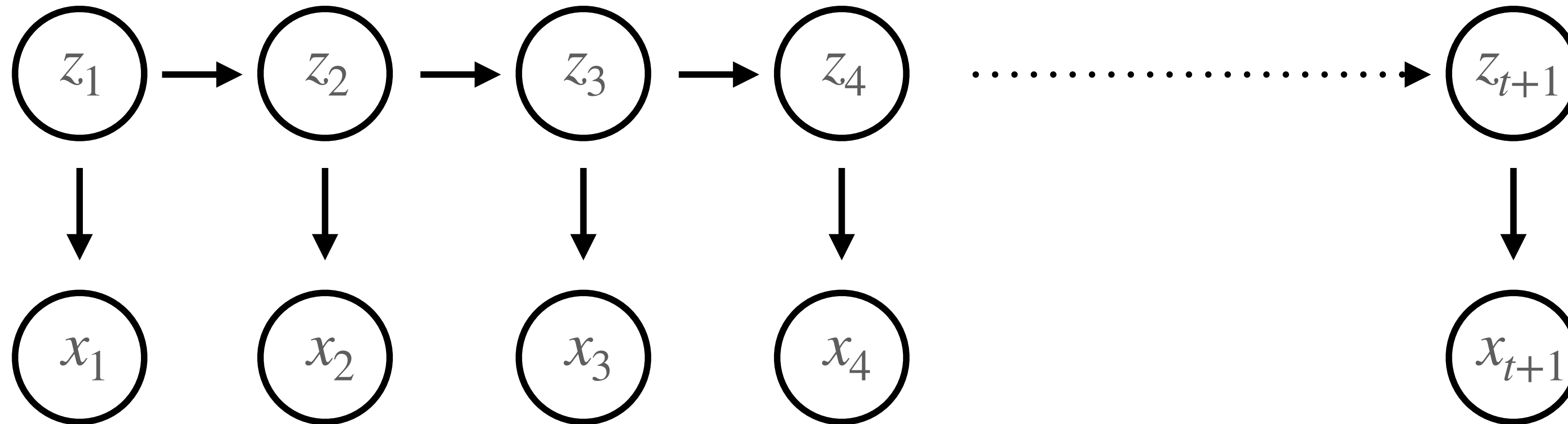


Hidden Markov Models



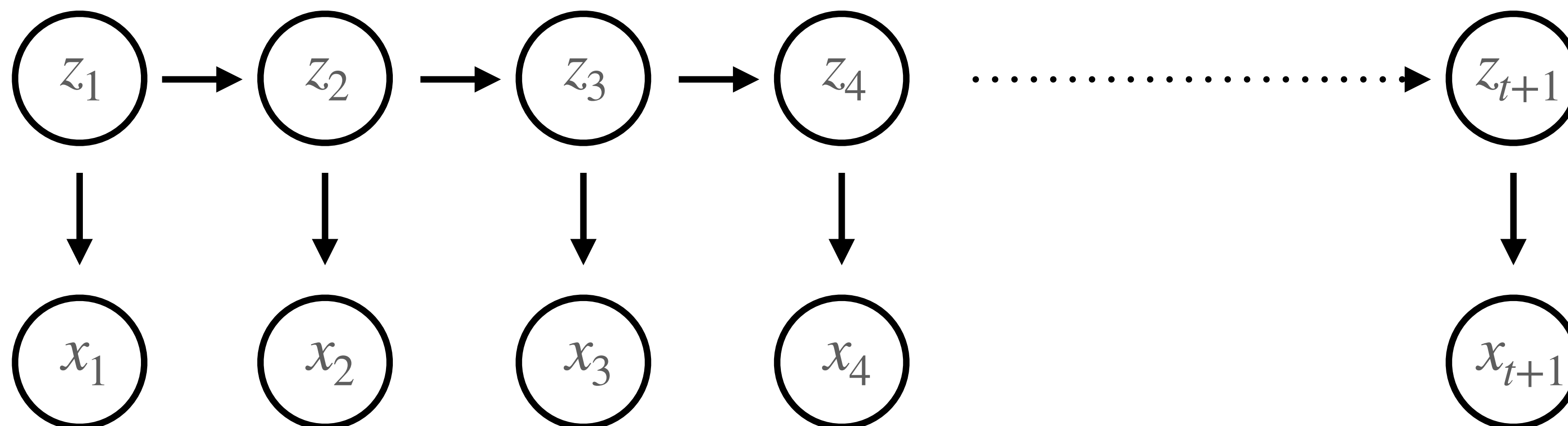
$$P(z_{1:T}) = P(z_1) \prod_{t=2}^T p(z_t | z_{t-1})$$

Hidden Markov Models



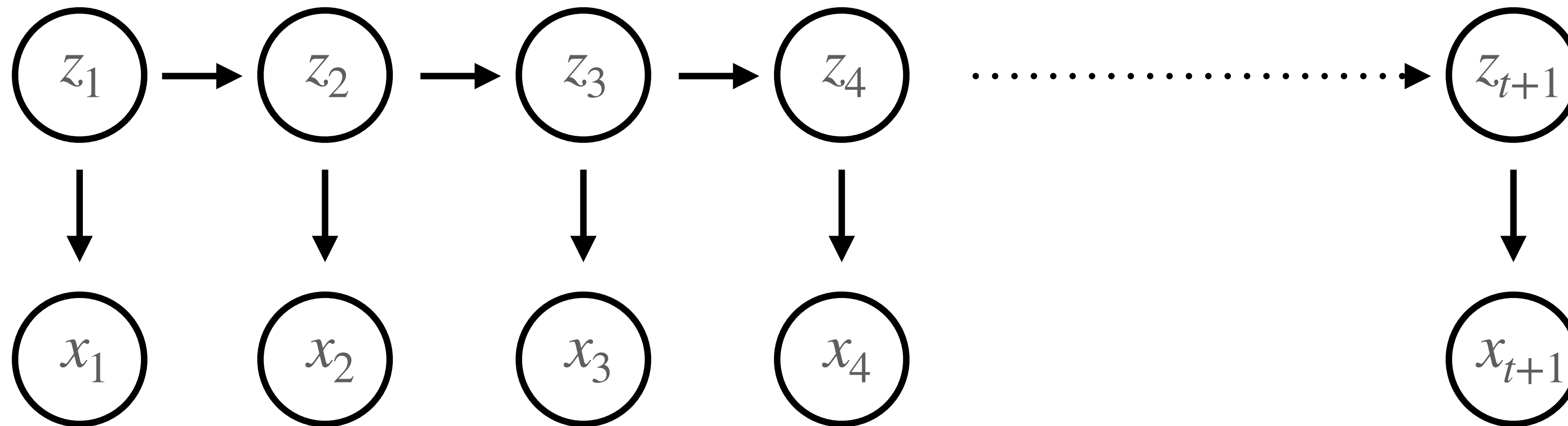
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Hidden Markov Models



$$P(z_{1:T}, x_{1:T}) = P(z_1) \prod_{t=2}^T p(z_t | z_{t-1}) \prod_{t=1}^T p(x_t | z_t)$$

Hidden Markov Models



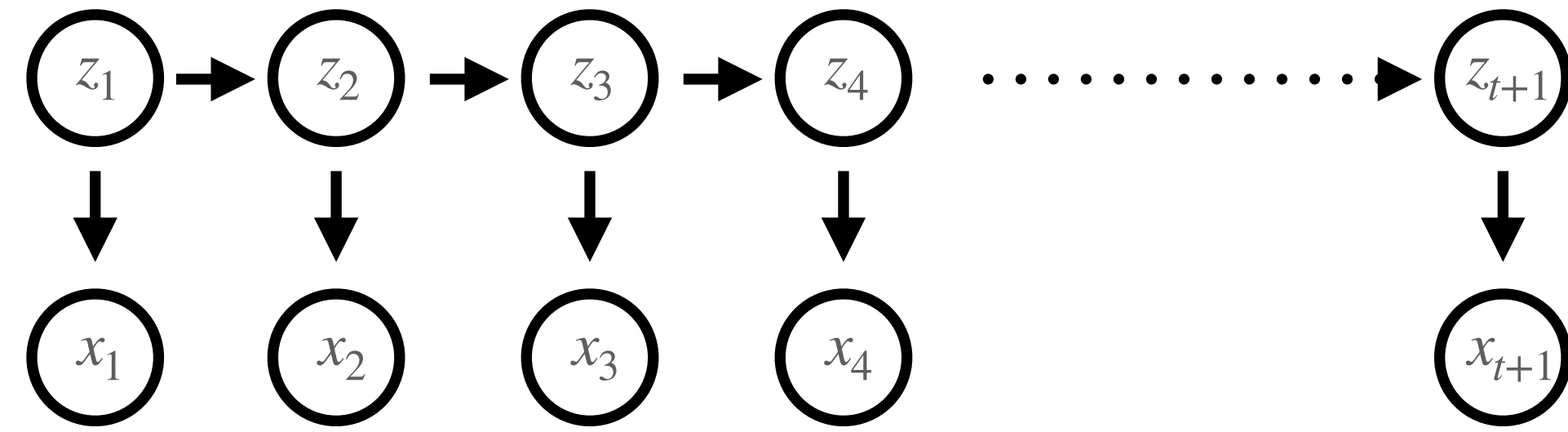
Initial
Probabilities

Transition
Probabilities

Emissions
(Observation)
Probabilities

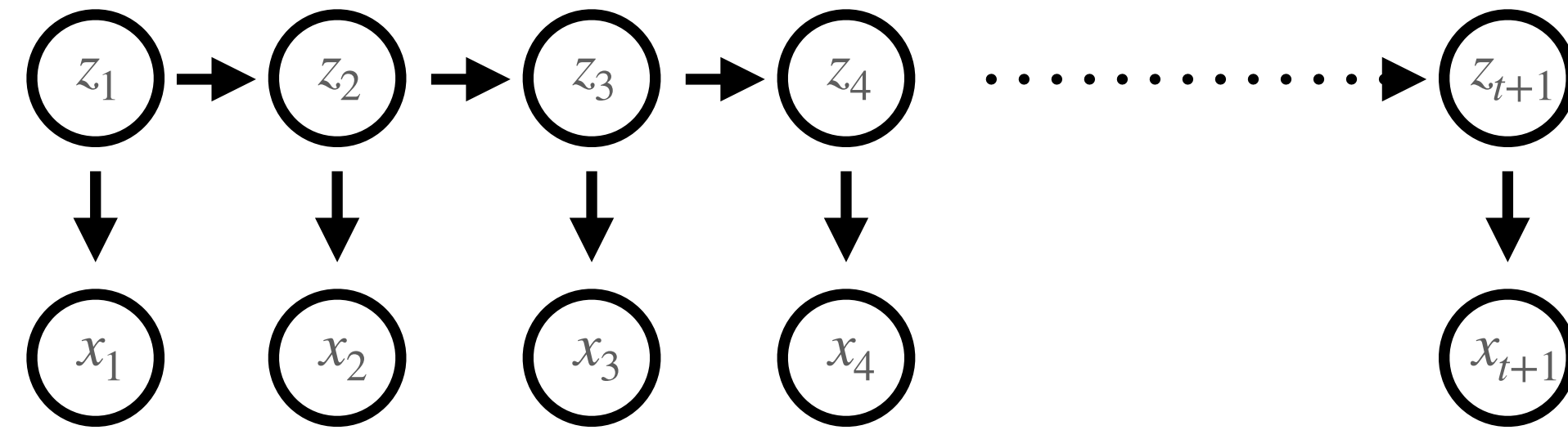
$$P(z_{1:T}, x_{1:T}) = P(z_1) \prod_{t=2}^T p(z_t | z_{t-1}) \prod_{t=1}^T p(x_t | z_t)$$

Hidden Markov Models: Emissions Models



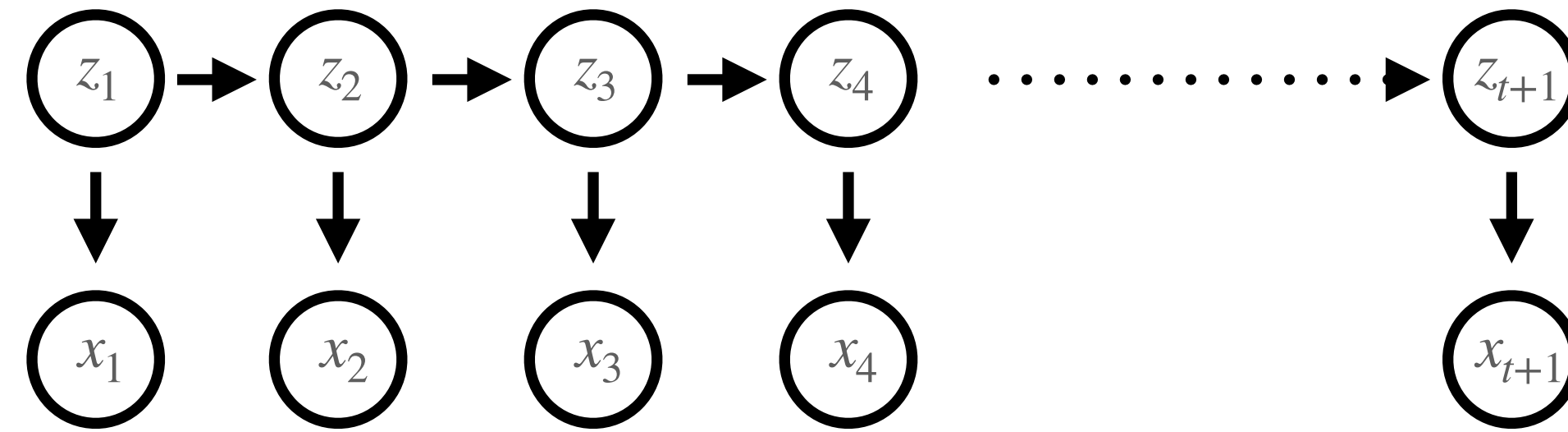
- $P(x|z)$ can take many different forms
 - Gaussian: $P(x_t|z_t) = \mathcal{N}(\mu_{z_t}, \sigma_{z_t})$

Hidden Markov Models: Emissions Models



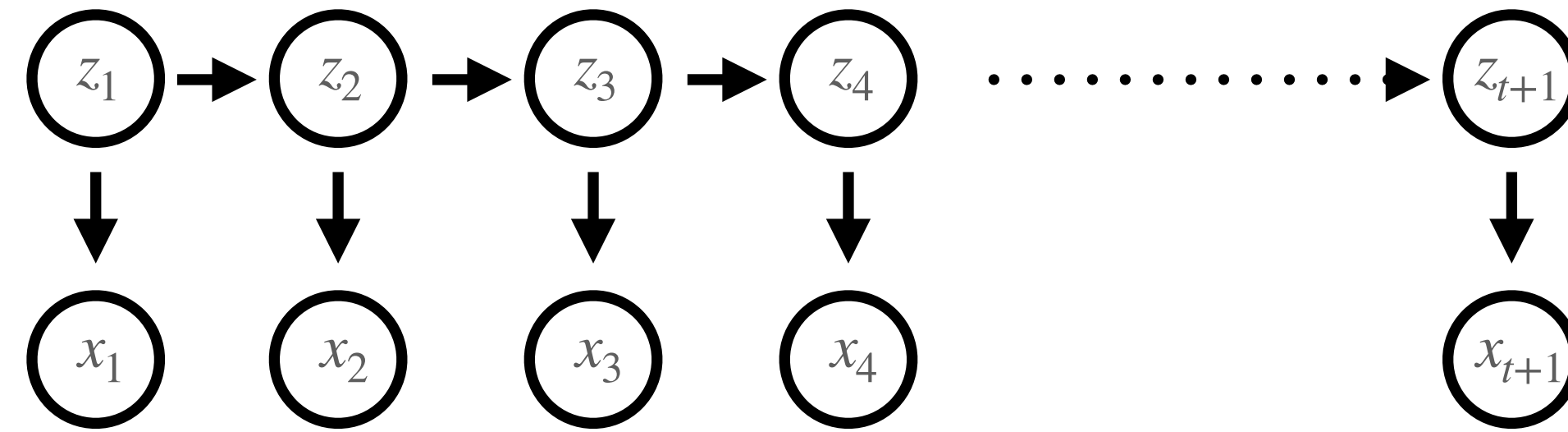
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 - Bernoulli, Poisson, etc.

Hidden Markov Models: Emissions Models



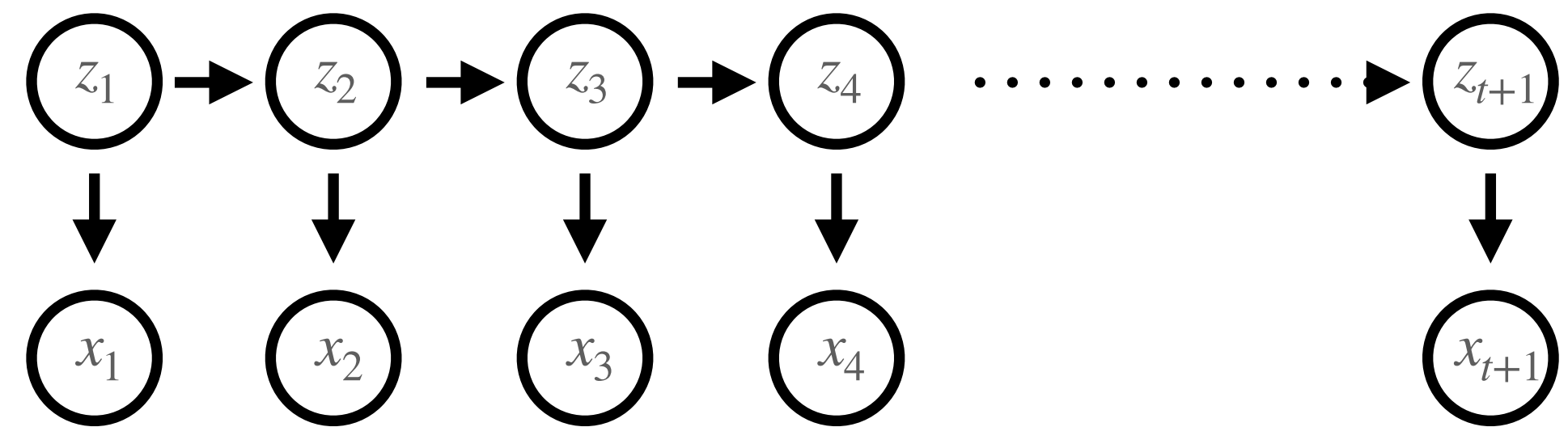
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 - Autoregressive HMM (ARHMM):
 - Different dynamics in each discrete state: $P(x_t|z_t) = \mathcal{N}(y_{t-1} - A_{z_t}y_t, \sigma_{z_t})$

Hidden Markov Models: Emissions Models

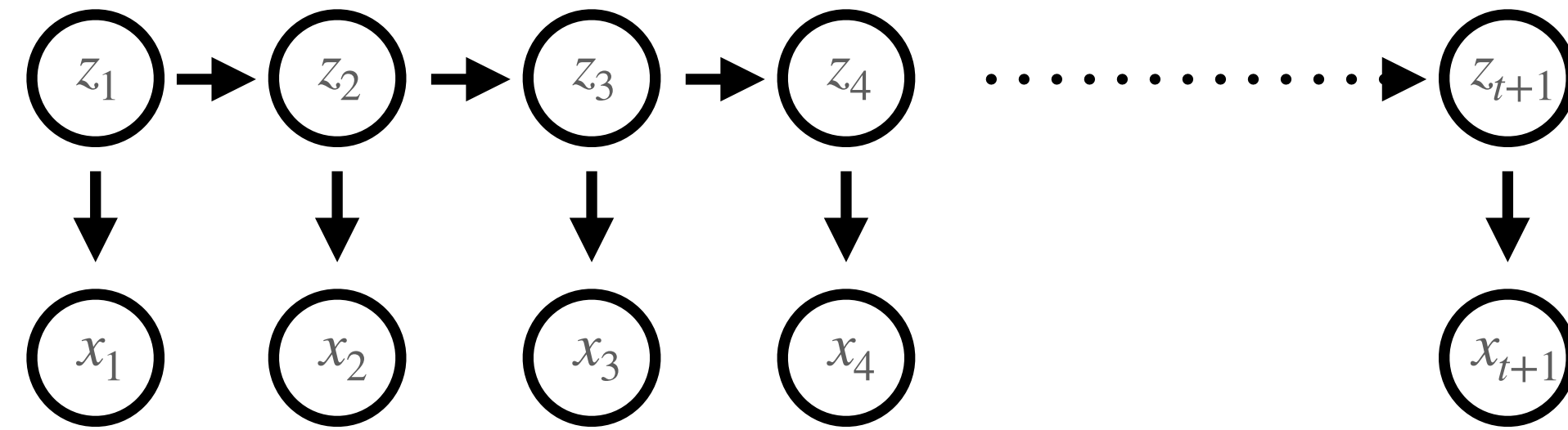


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 - Autoregressive HMM (ARHMM):
 - Different dynamics in each discrete state: $P(x_t|z_t) = \mathcal{N}(y_{t-1} - A_{z_t}y_t, \sigma_{z_t})$
 - GLM-HMM:
 - different GLM weights in each discrete state

Simulating from an HMM

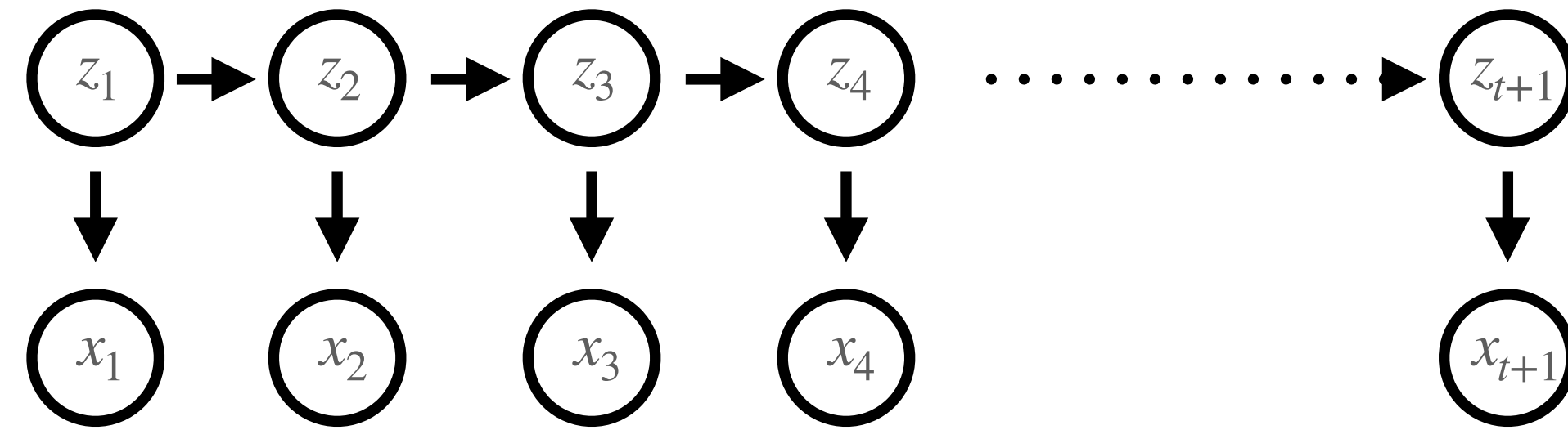


Simulating from an HMM



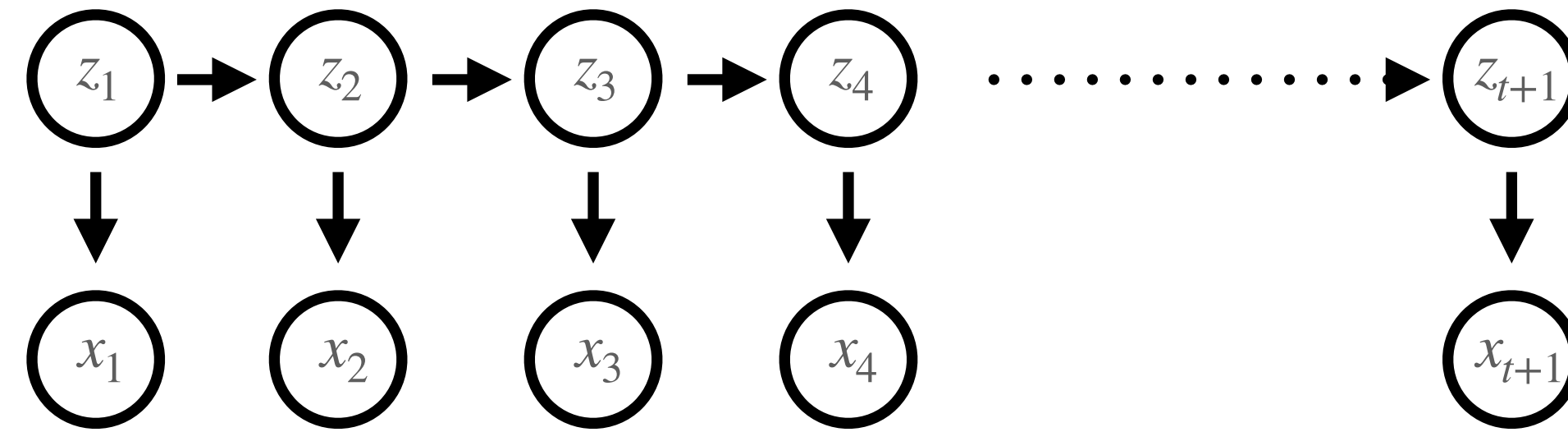
- Sample from $P(z_1)$

Simulating from an HMM



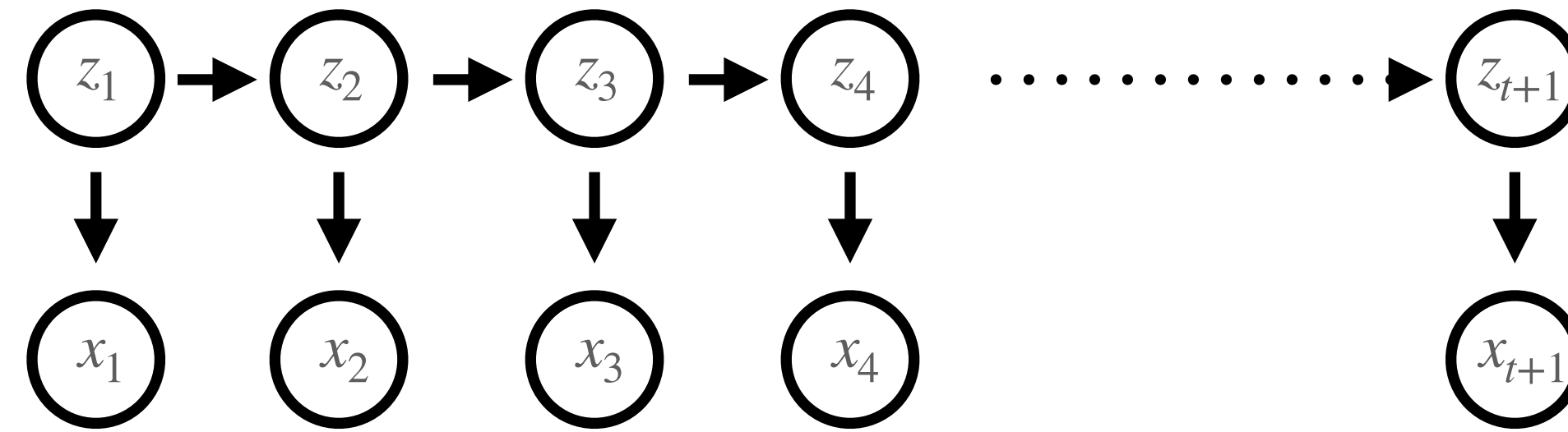
- Sample from $P(z_1)$
- Sample from $P(x_1 | z_1)$

Simulating from an HMM



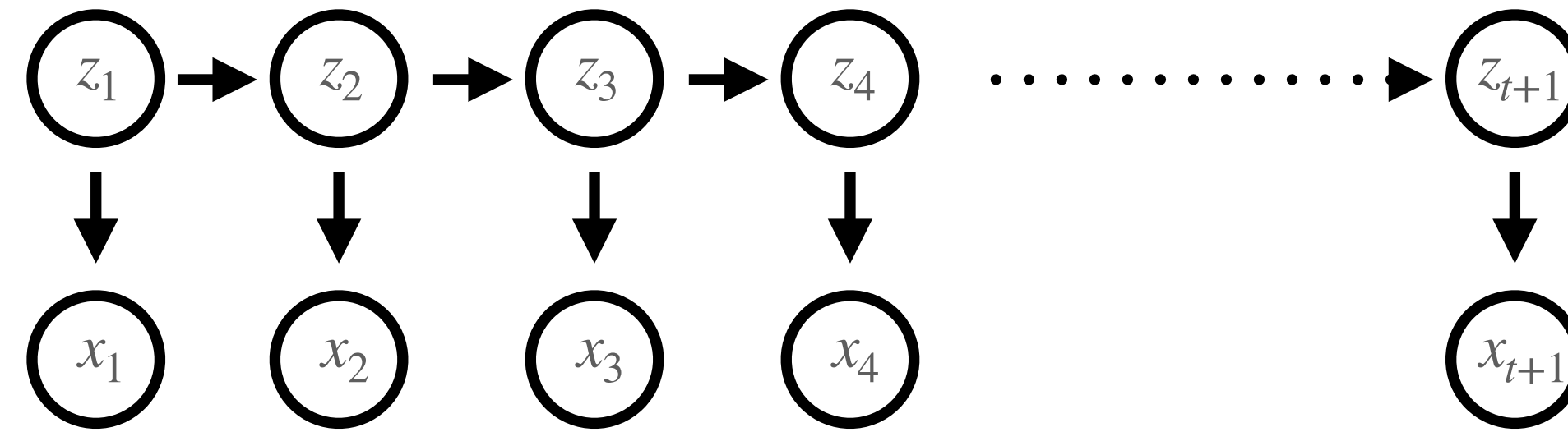
- Sample from $P(z_1)$
- Sample from $P(x_1 | z_1)$
- For all future time steps:
 - Sample $P(z_{t+1} | z_t)$
 - Sample $P(x_{t+1} | z_{t+1})$

HMM: Goals



- Given some data:
 - Fit the model!
 - Infer discrete latent states
 - Infer model parameters (transition probabilities, emissions model)
 - Determine the likelihood of the data given the model parameters

HMM: Goals

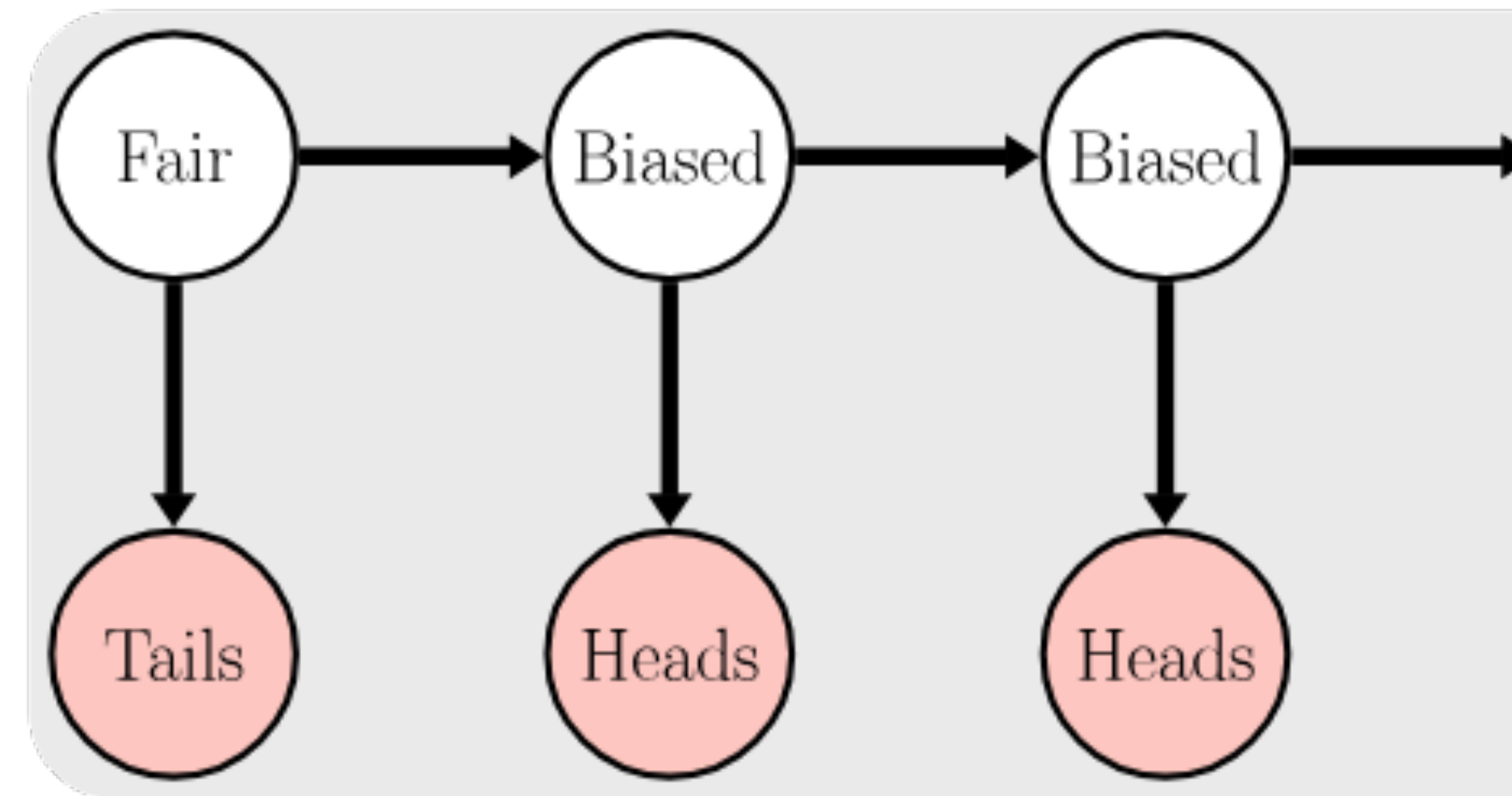


- Given some data:
 - Fit the model!
 - Infer discrete states
 - Infer model parameters (transition probabilities, emissions model)
 - **Determine the likelihood of the data given the model parameters**

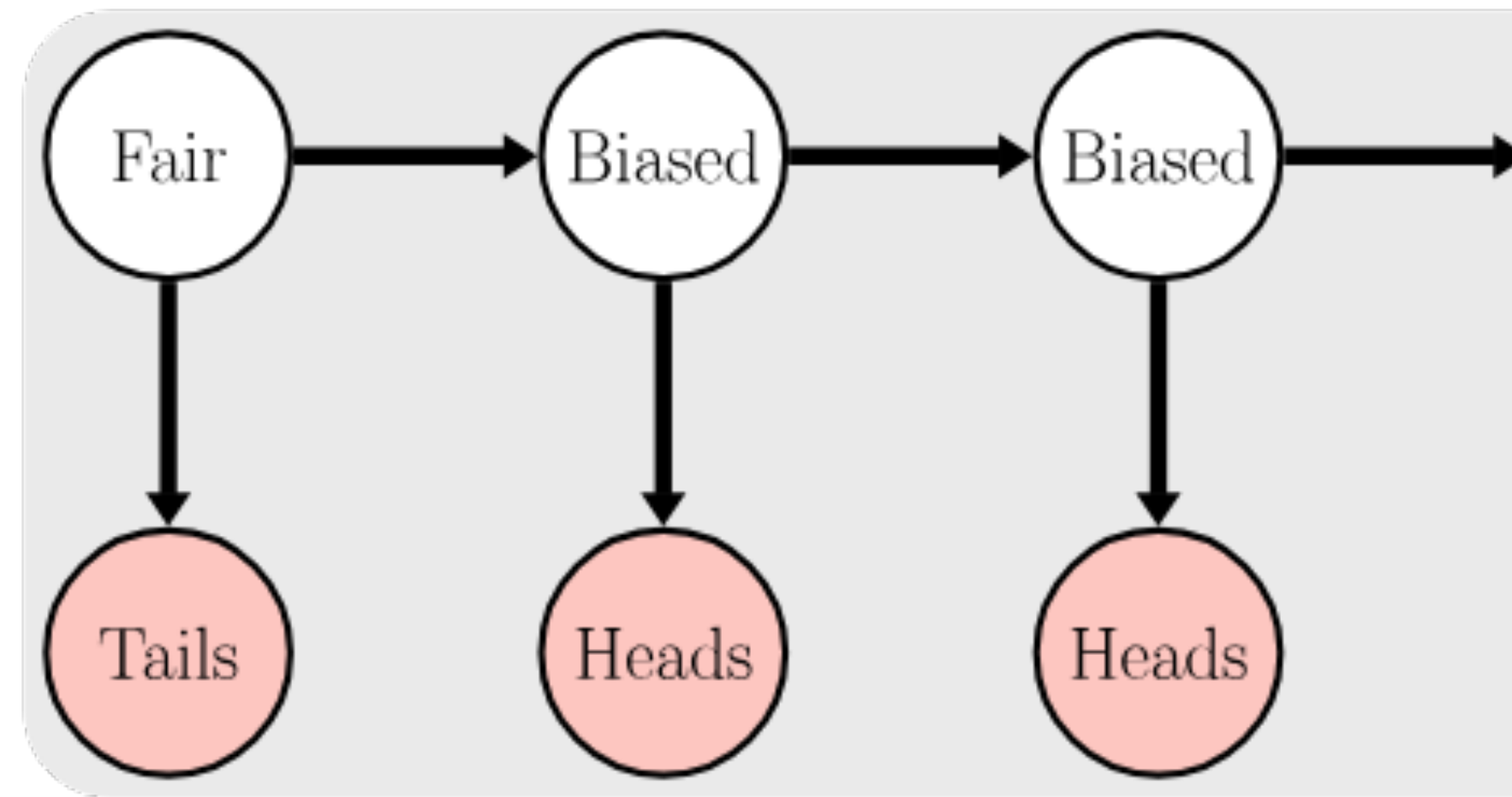
HMMs: Evidence Likelihood

- Estimate the likelihood, $L(X|\theta)$, of the observed data, $X = \{x_1, x_2 \dots x_T\}$ given the HMM parameters θ

HMMs: Evidence Likelihood



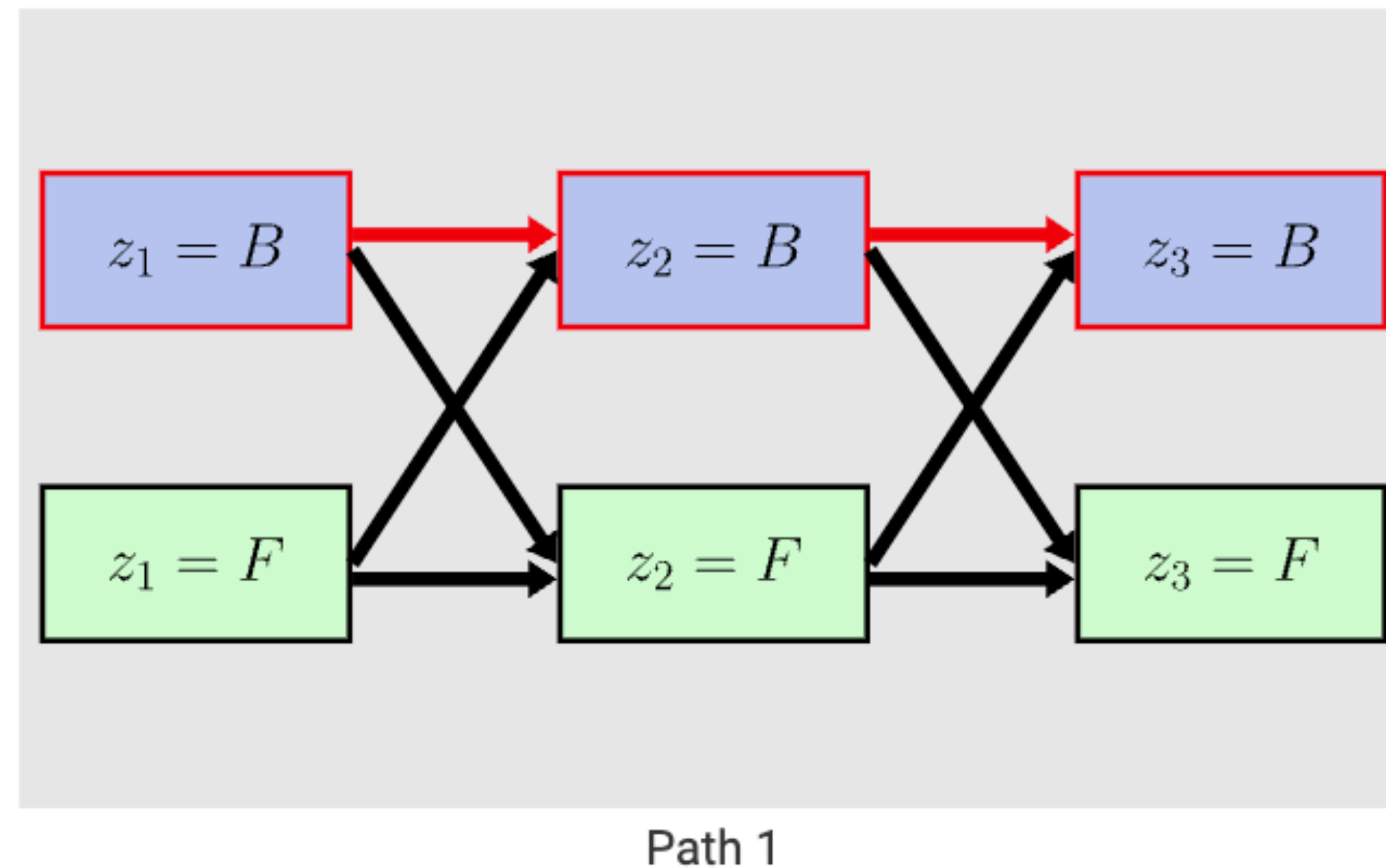
HMMs: Evidence Likelihood



- Example: How can we compute $L(HHH | \theta)$?

HMMs: Evidence Likelihood

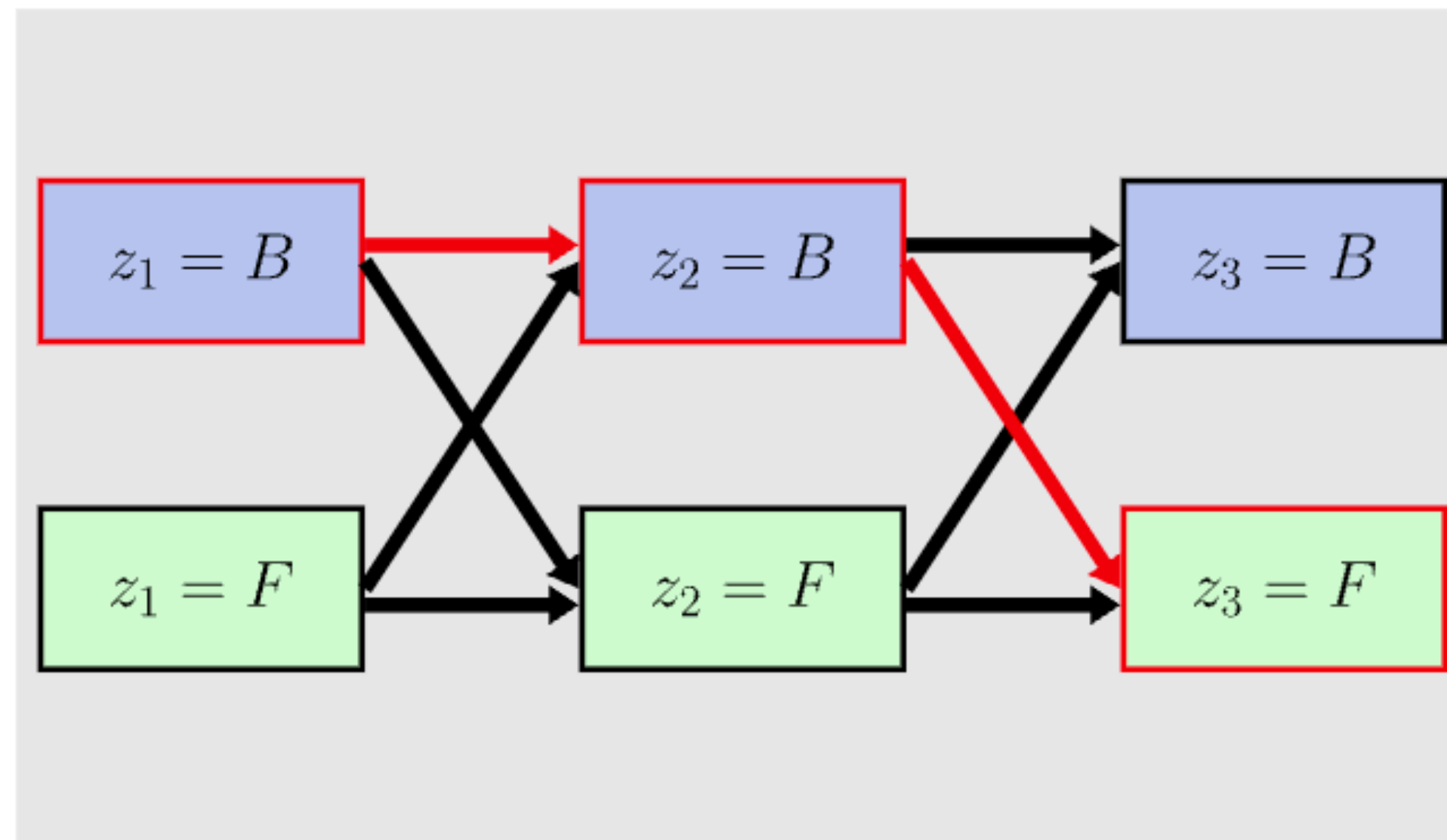
- Example: How can we compute $L(HHH|\theta)$?



$$P(HHH|BBB) = P(B)P(H|B)P(B|B)P(H|B)P(B|B)P(H|B)$$

HMMs: Evidence Likelihood

- Example: How can we compute $L(HHH|\theta)$?

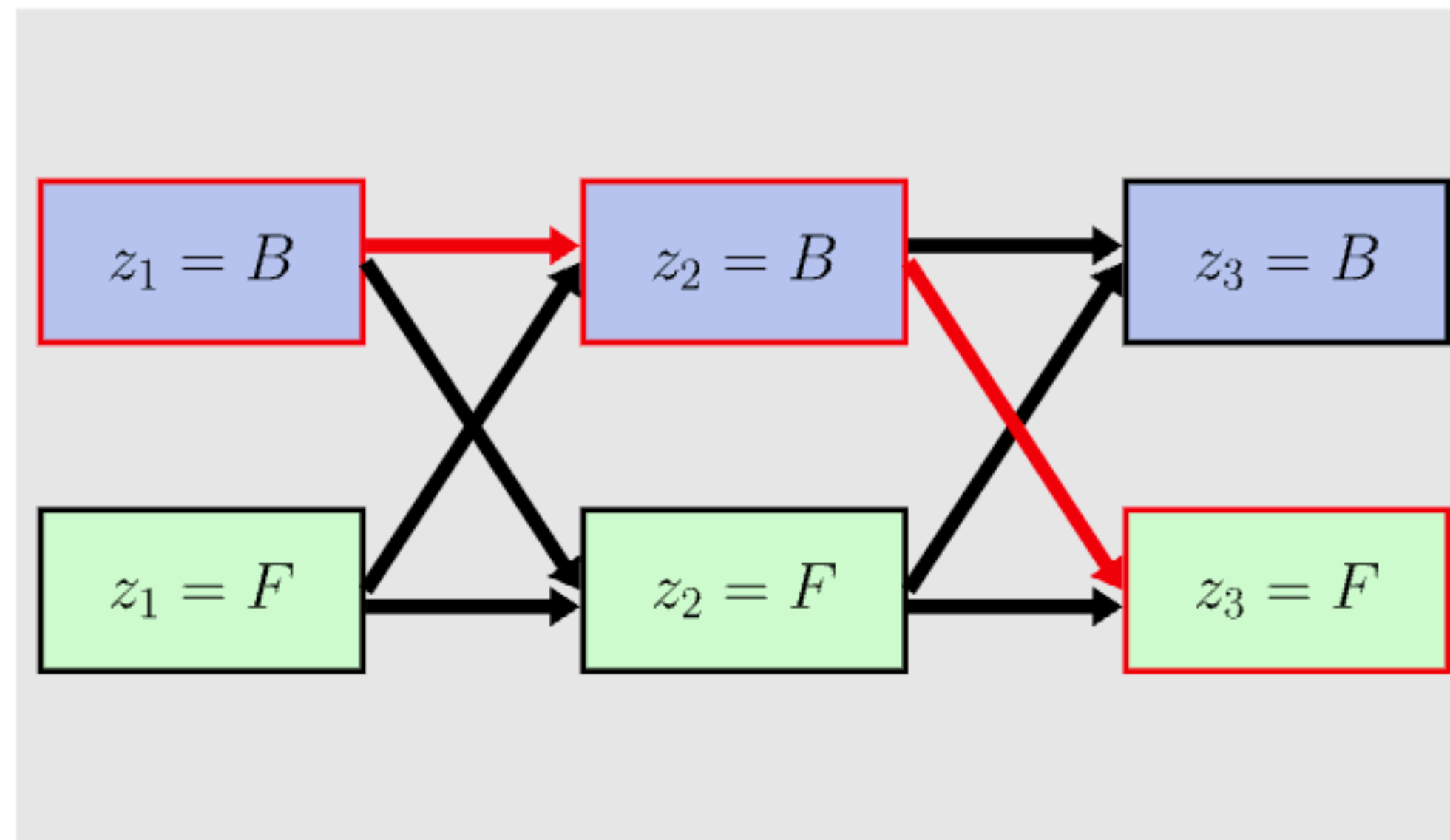


Path 2

$$P(HHH|BBF) = P(B)P(H|B)P(B|B)P(H|B)P(F|B)P(H|F)$$

HMMs: Evidence Likelihood

- Example: How can we compute $L(HHH|\theta)$?



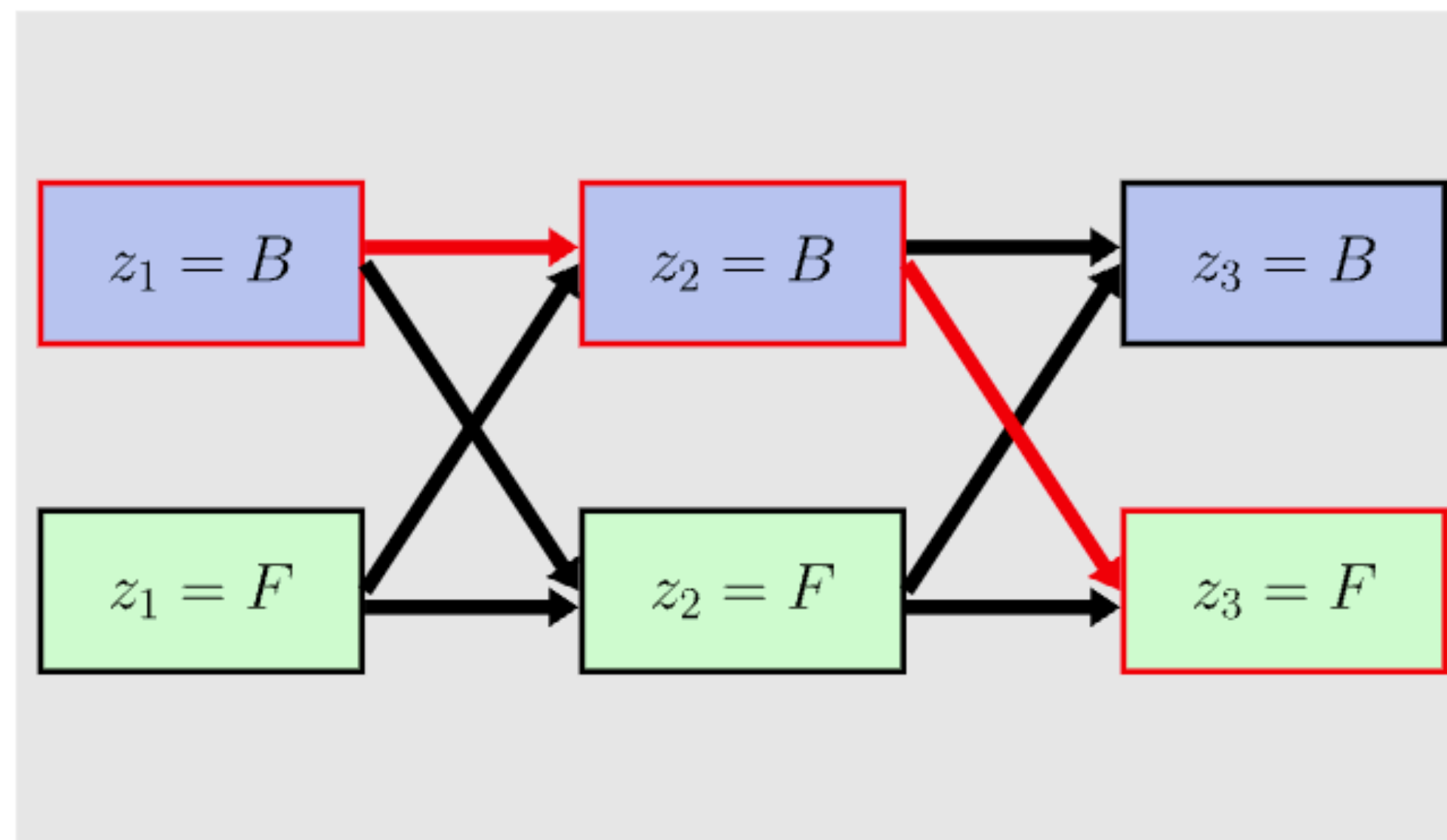
Path 2

$$P(HHH|BBF) = P(B)P(H|B)P(B|B)P(H|B)P(F|B)P(H|F)$$

- Here, for $K = 2$ and $T = 3$, there are $2^3 = 8$ possible paths
- $L(HHH|\theta)$ is the sum of probabilities across the 8 paths

HMMs: Evidence Likelihood

- Example: How can we compute $L(HHH|\theta)$?



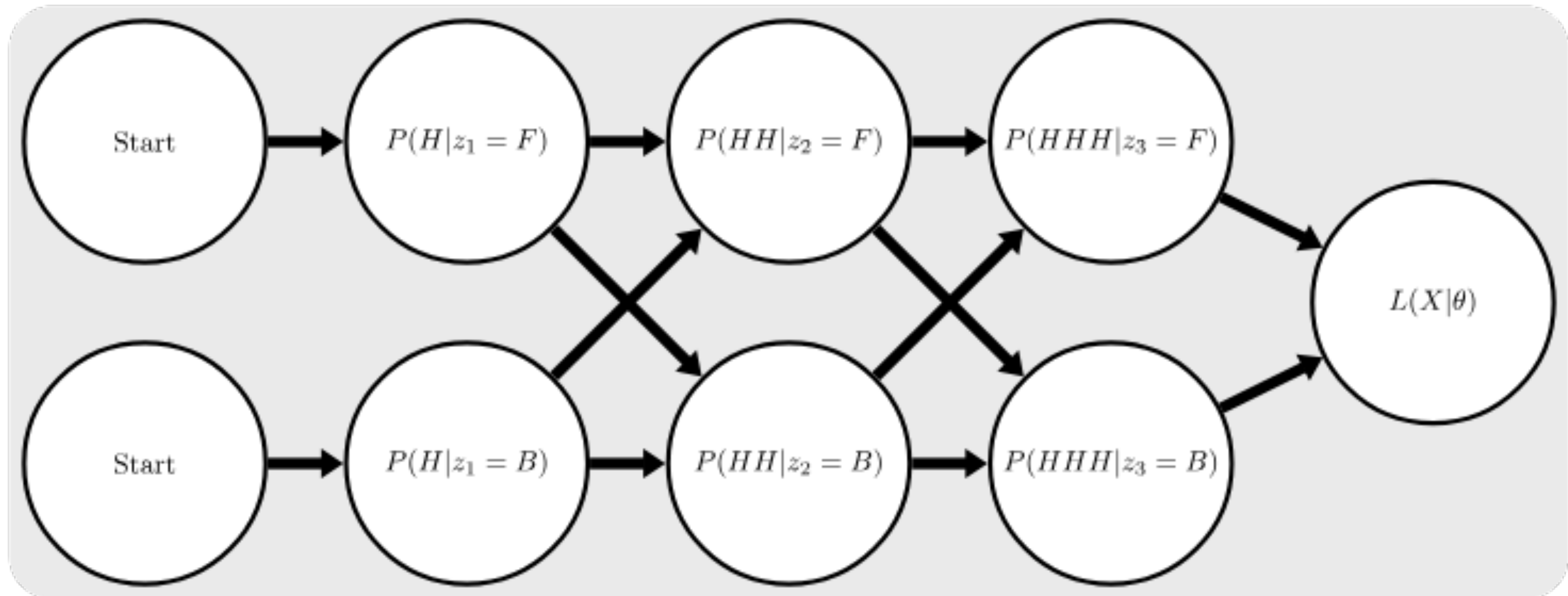
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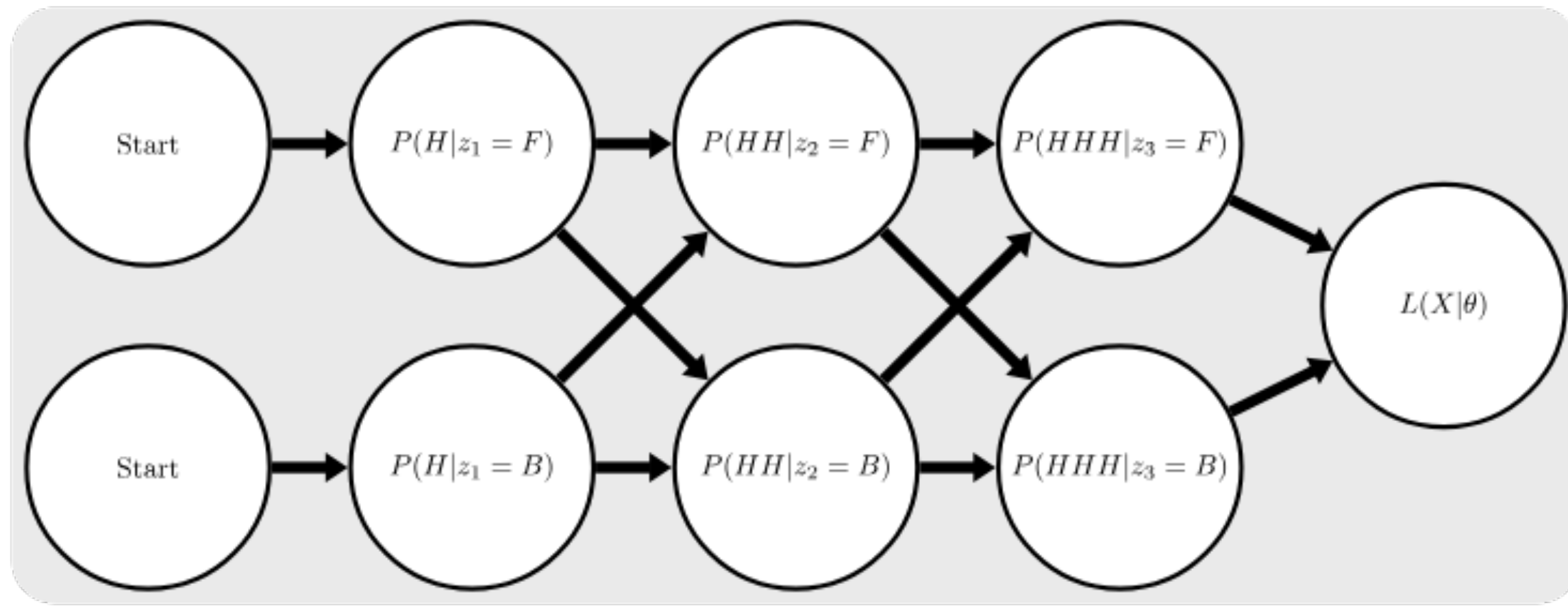
- Here, for $K=2$ and $T=3$, there are $2^3 = 8$ possible paths
- $L(HHH|\theta)$ is the sum of probabilities across the 8 paths
- In general, there are K^T paths

HMMs: Efficient Calculation via Forward Algorithm

HMMs: Efficient Calculation via Forward Algorithm



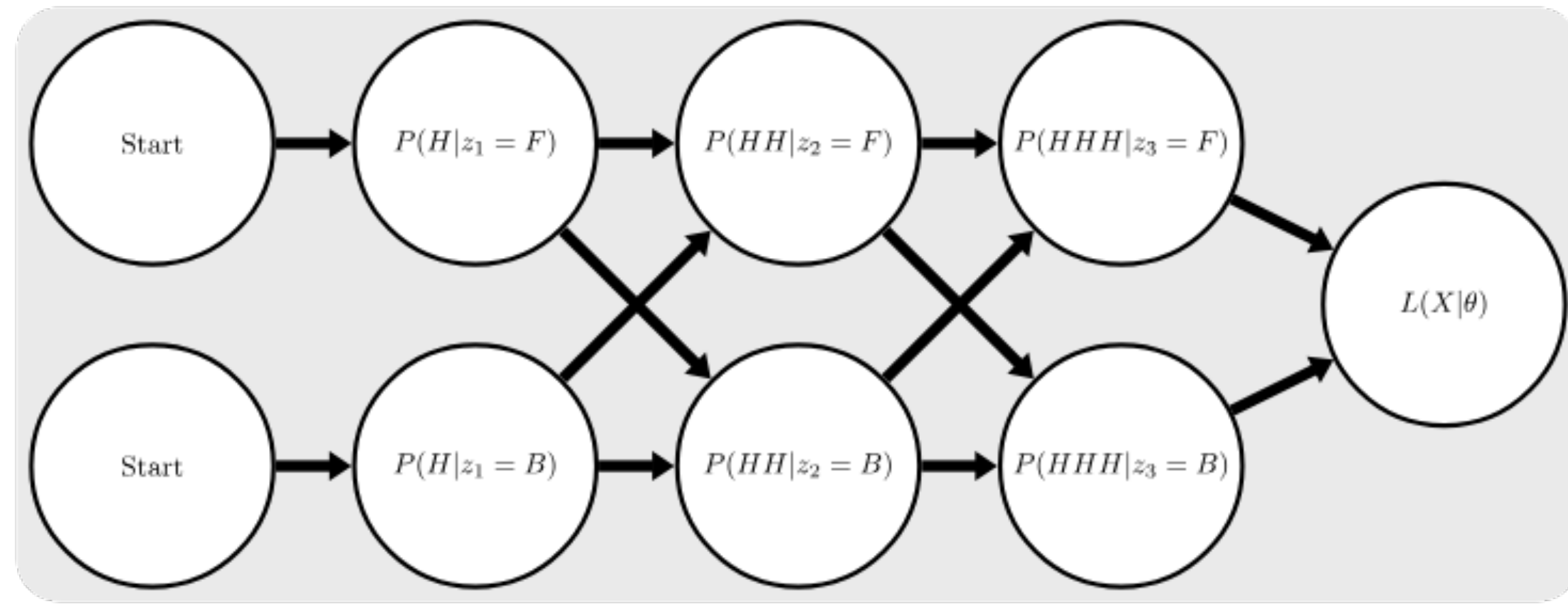
HMMs: Forward Algorithm



$$\alpha_t(i) = P(X_{1:t} | z_t = i)$$

- The probability of data up to time t given a particular latent at time t

HMMs: Forward Algorithm



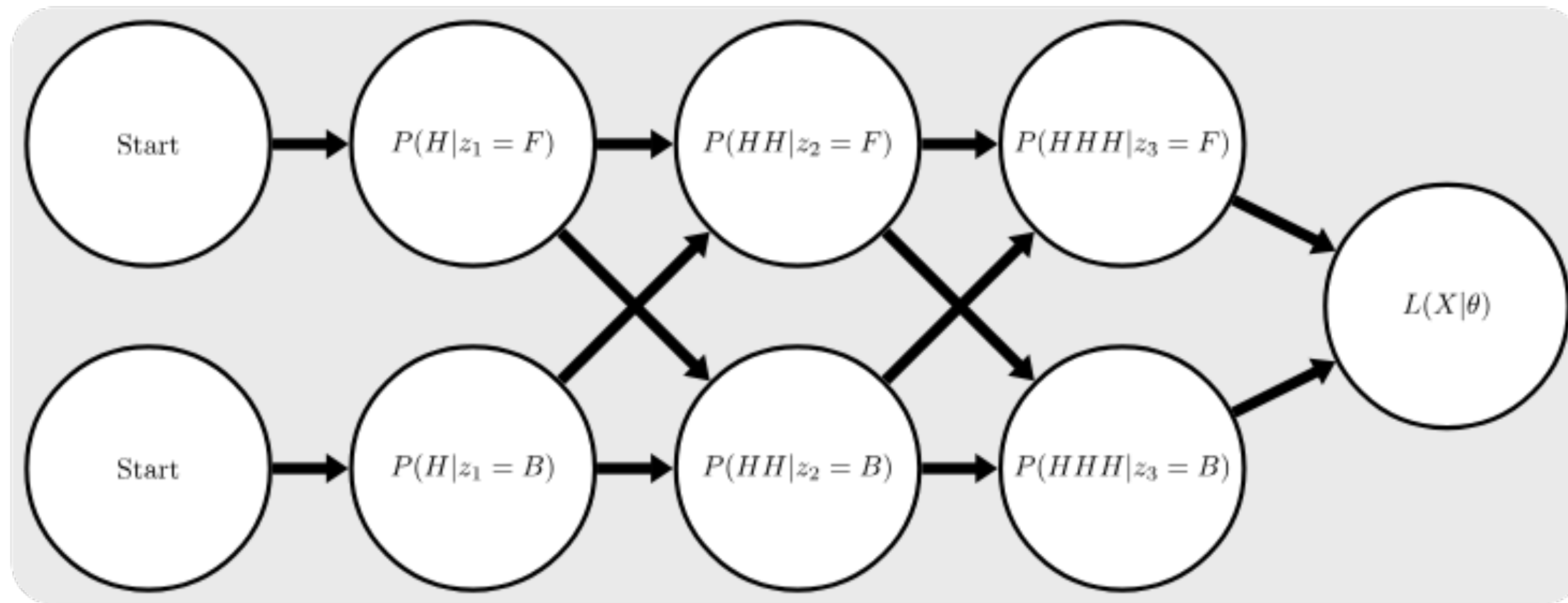
Initial Step:

$$\begin{aligned}\alpha_1(i) &= P(x_1 = i) \cdot P(x_1 | z_1 = i) \\ &= \pi_i \cdot \phi_j(x_1)\end{aligned}$$

$$\alpha_t(i) = P(X_{1:t} | z_t = i)$$

- The probability of data up to time t given a particular latent at time t

HMMs: Forward Algorithm



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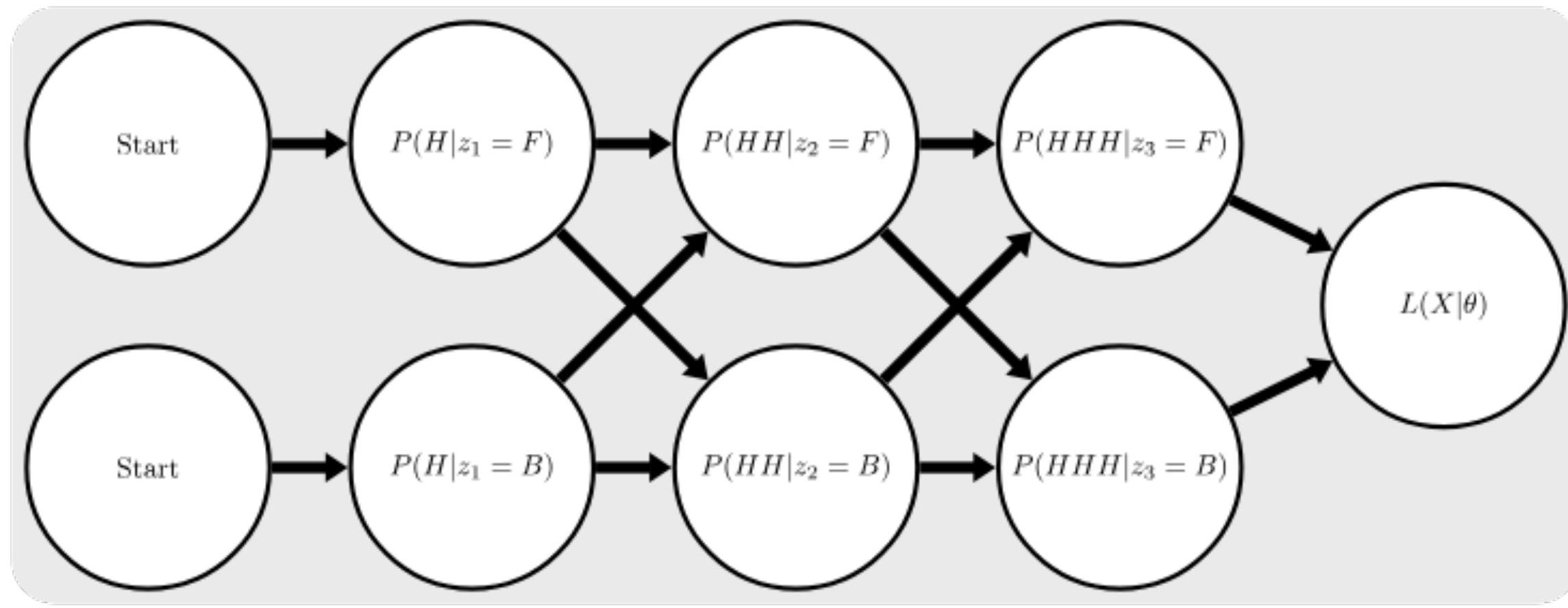
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Future Steps:

$$\begin{aligned}\alpha_{t+1}(j) &= \left\{ \sum_{i=1}^K \alpha_t(i) \cdot P(z_{t+1} = j | P(z_t = i)) \right\} \cdot P(x_{t+1} | z_{t+1} = j) \\ &= \left\{ \sum_{i=1}^K \alpha_t(i) \cdot A_{ij} \right\} \cdot \phi_j(x_{t+1})\end{aligned}$$

HMMs: Forward Algorithm



$$\alpha_t(i) = P(X_{1:t} | z_t = i)$$

- The probability of data up to time t given a particular latent at time t

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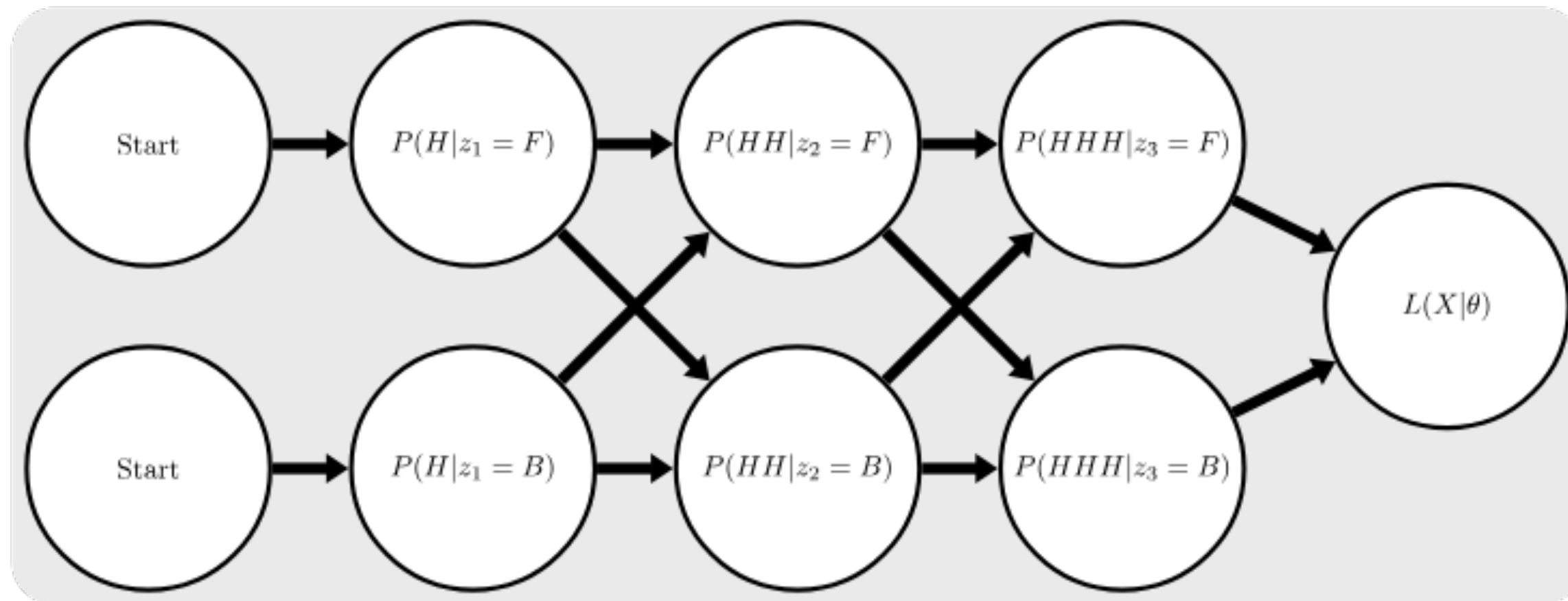
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$$\alpha_{t+1} = \phi_{t+1} \circ (A^T \alpha_t)$$

HMMs: Forward Algorithm



$$\alpha_t(i) = P(X_{1:t} | z_t = i)$$

- The probability of data up to time t given a particular latent at time t

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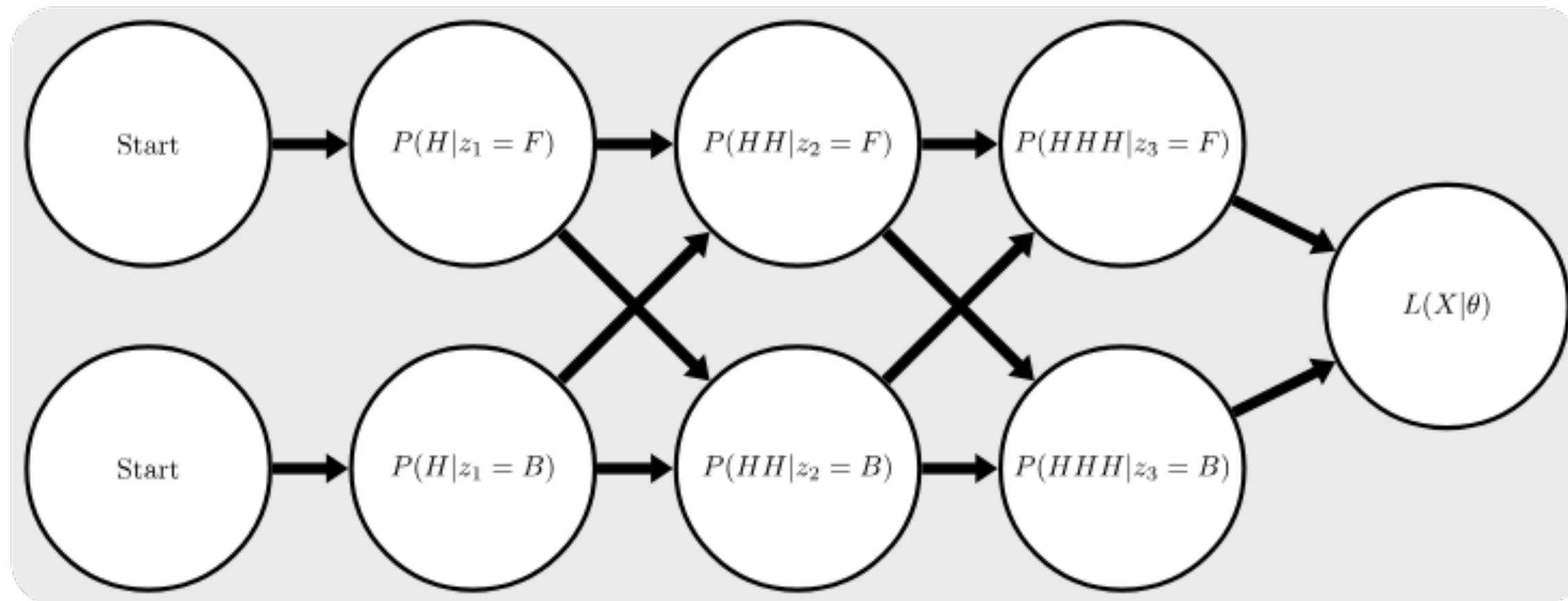
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$$\alpha_{t+1} = \phi_{t+1} \circ (A^T \alpha_t)$$

- At each step, normalize so the α 's sum to 1!

HMMs: Forward Algorithm



$$\alpha_t(i) = P(X_{1:t} | z_t = i)$$

- The probability of data up to time t given a particular latent at time t

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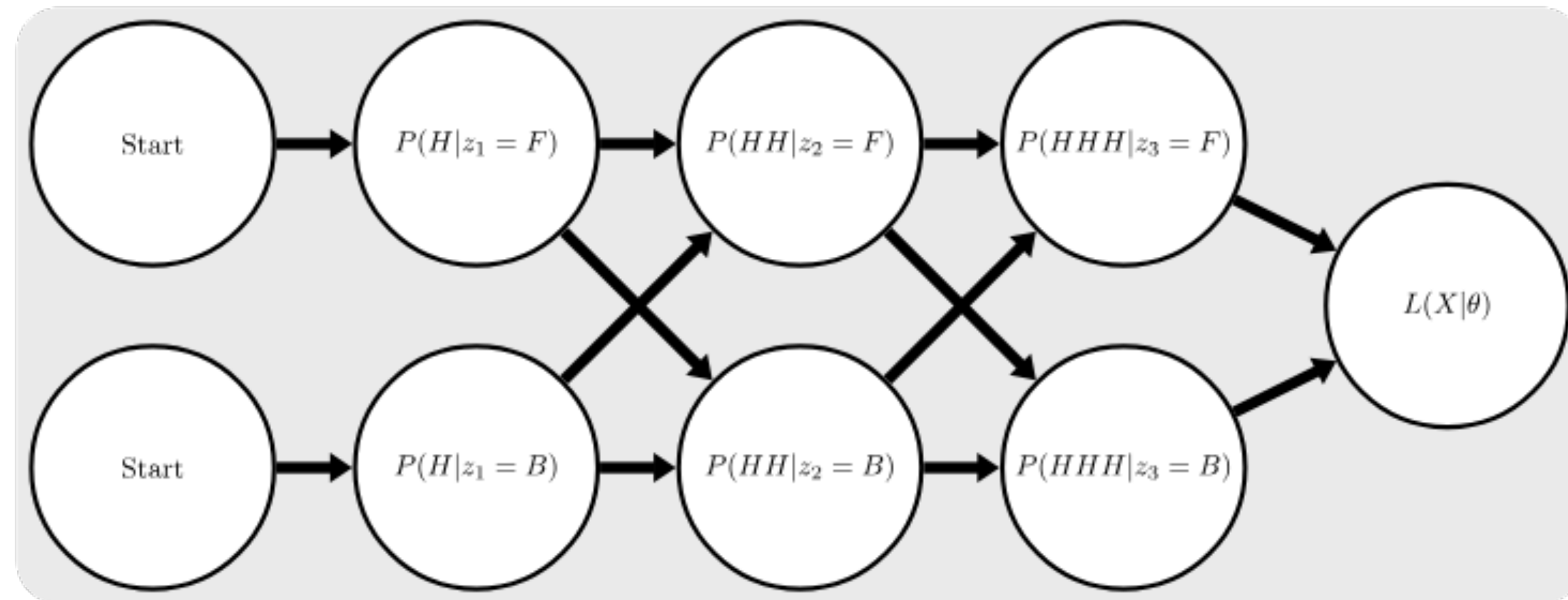
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- At each step, normalize so the α 's sum to 1!
- We can view $\alpha_t(i)$ as the probability of being in latent state i given the data up to time t

HMMs: Forward Algorithm



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- At each step, normalize so the α 's sum to 1!
- We can view $\alpha_t(i)$ as the probability of being in latent state i given the data up to time t
- Time complexity of $O(TK^2)$

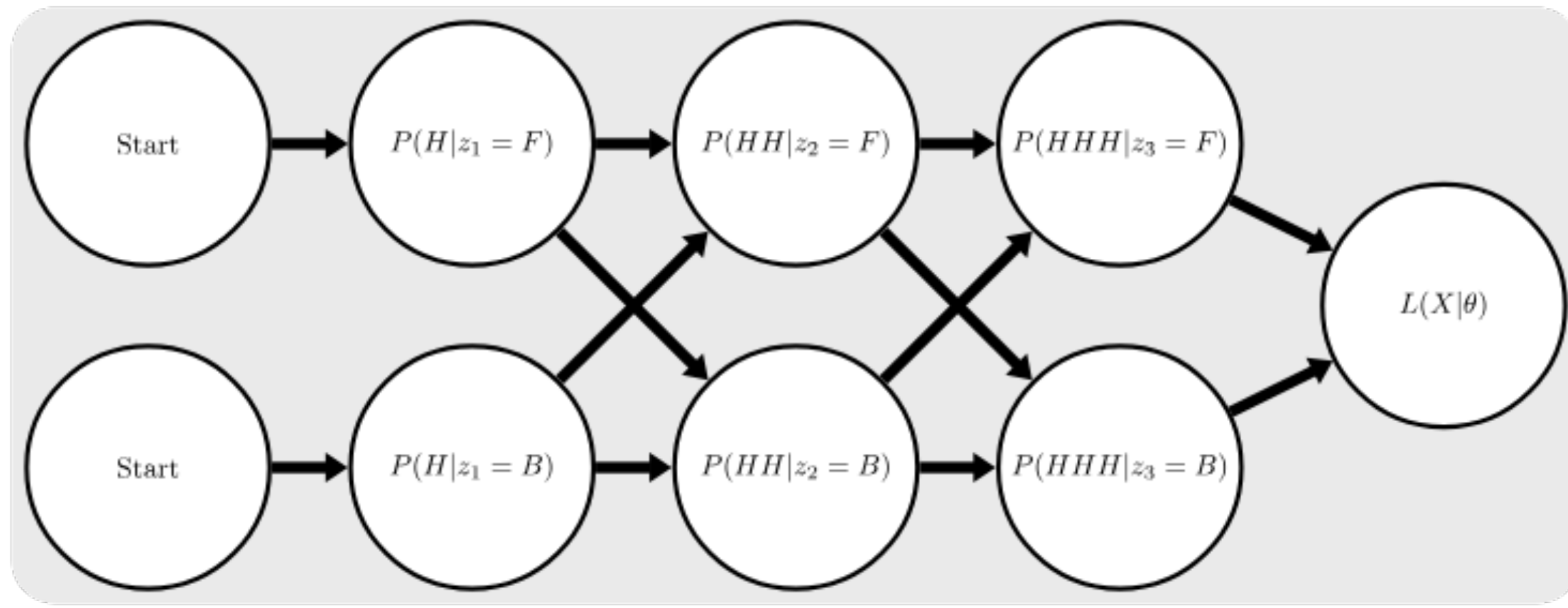
HMMs: EM Algorithm

- E-step: Learn expected states and transitions
- M-step: Optimize parameters

HMMs: E step

- Want to learn $P(z_t | X_{1:T})$
- Can get that from $P(X_{1:T} | z_t)$ and Bayes' Rule
- Forward algorithm gave us $P(X_{1:t} | z_t)$
- But what about $P(X_{t+1:T} | z_t)$?
 - Backward algorithm!

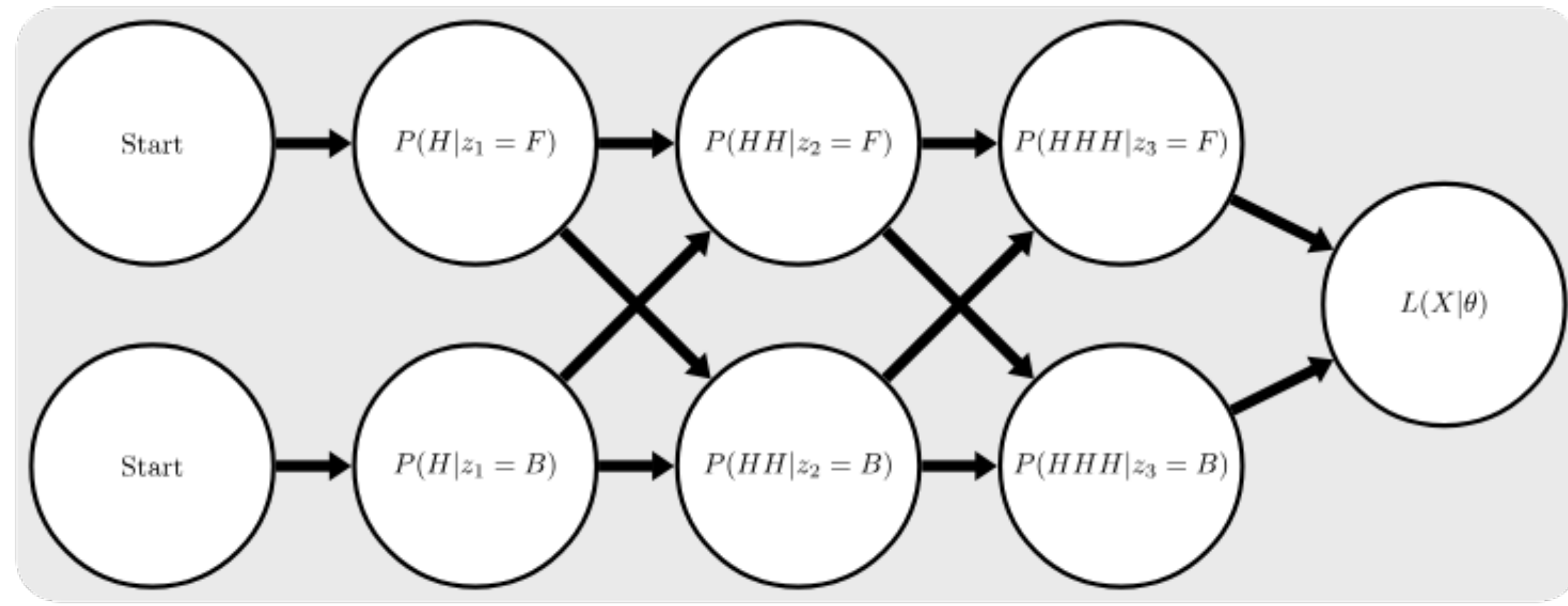
HMMs: Backward Algorithm



$$\beta_t(i) = P(X_{t+1:T} | z_t = i)$$

- The probability of data after time t given a particular latent at time t

HMMs: Backward Algorithm



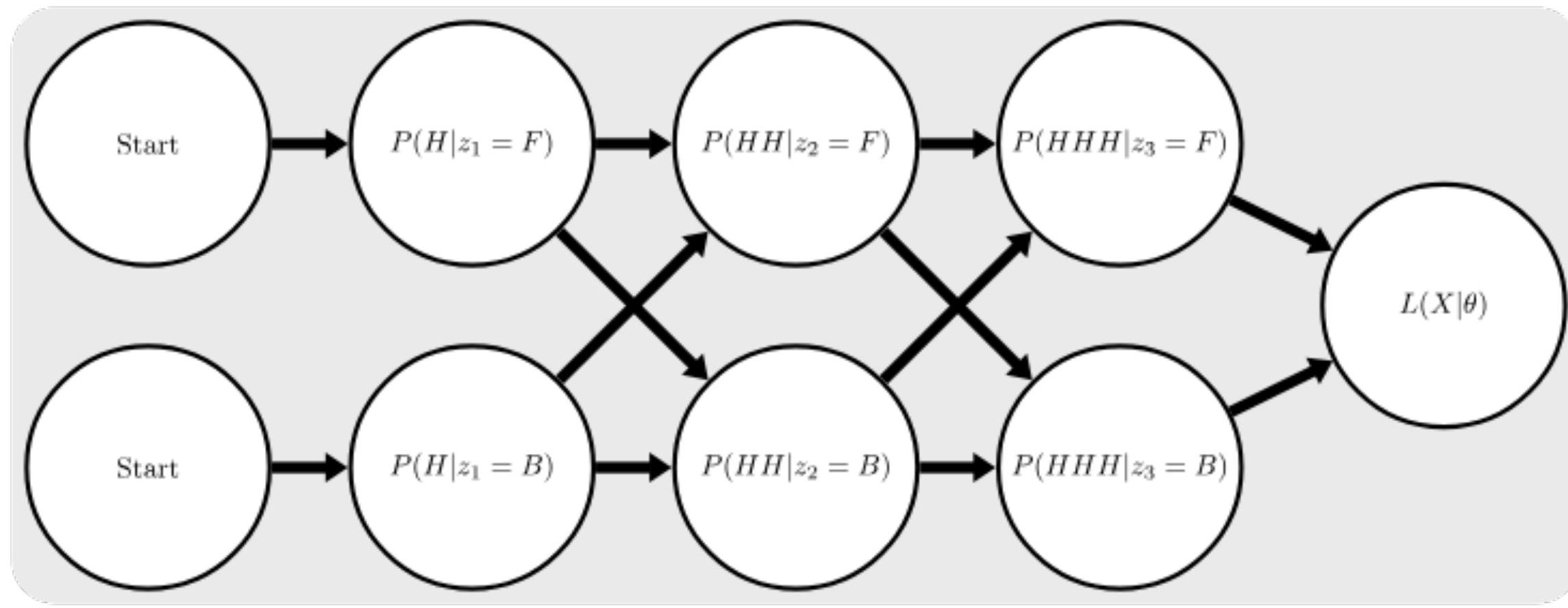
Initial Step:

$$\beta_T(i) = 1$$

$$\beta_t(i) = P(X_{t+1:T} | z_t = i)$$

- The probability of data after time t given a particular latent at time t

HMMs: Backward Algorithm



$$\beta_t(i) = P(X_{t+1:T} | z_t = i)$$

- The probability of data after time t given a particular latent at time t

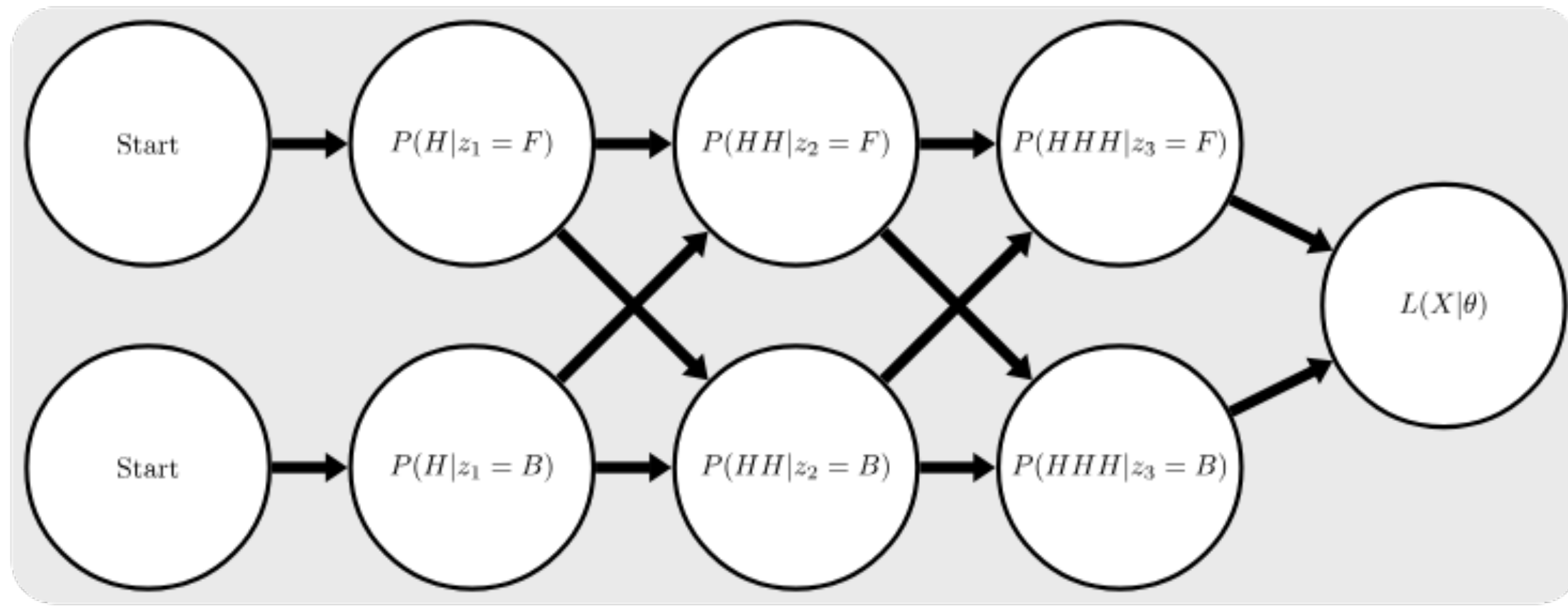
Initial Step:

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Future Steps:

$$\begin{aligned} \beta_t(j) &= \sum_{i=1}^K \beta_{t+1}(i) \cdot P(x_{t+1} | z_{t+1} = i) \cdot P(z_{t+1} = i | P(z_t = j)) \\ &= \sum_{i=1}^K \beta_{t+1}(i) \cdot \phi_i(x_{t+1}) \cdot A_{ji} \end{aligned}$$

HMMs: Backward Algorithm



$$\beta_t(i) = P(X_{t+1:T} | z_t = i)$$

- The probability of data after time t given a particular latent at time t

Initial Step:

$$\beta_T(i) = 1$$

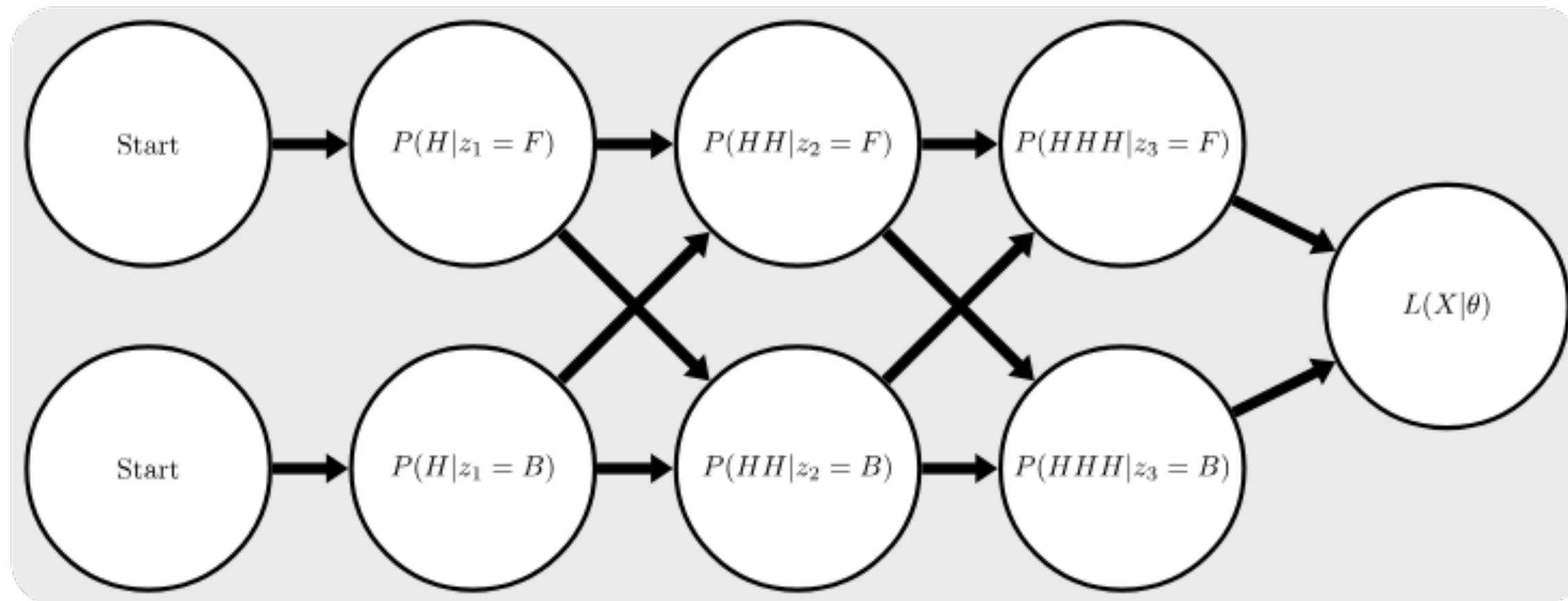
Future Steps:

$$\beta_t(j) = \sum_{i=1}^K \beta_{t+1}(i) \cdot P(x_{t+1} | z_{t+1} = i) \cdot P(z_{t+1} = i | P(z_t = j))$$

$$= \sum_{i=1}^K \beta_{t+1}(i) \cdot \phi_i(x_{t+1}) \cdot A_{ji}$$

$$\beta_t = A(\phi_{t+1} \circ \beta_{t+1})$$

HMMs: Backward Algorithm



$$\beta_t(i) = P(X_{t+1:T} | z_t = i)$$

- The probability of data after time t given a particular latent at time t

Initial Step:

$$\beta_T(i) = 1$$

Future Steps:

$$\beta_t(j) = \sum_{i=1}^K \beta_{t+1}(i) \cdot P(x_{t+1} | z_{t+1} = i) \cdot P(z_{t+1} = i | P(z_t = j))$$

$$= \sum_{i=1}^K \beta_{t+1}(i) \cdot \phi_i(x_{t+1}) \cdot A_{ji}$$

$$\beta_t = A(\phi_{t+1} \circ \beta_{t+1})$$

- At each step, normalize so the β 's sum to 1!
- We can view $\beta_t(i)$ as the probability of being in latent state i given the data after time t

HMMs: E step

$$P(z_t = i | X_{1:T}) \propto P(X_{1:T} | z_t = i) \quad \text{If the prior is uniform}$$

$$= P(X_{1:t} | z_t = i) P(X_{t+1:T} | z_t = i)$$

$$= \alpha_t(i) \beta_t(i)$$

- Expected number of times of being in state i at time t

HMMs: E step

- Expected number of times of being in state i at time t
 - Let $\gamma_t(i) = P(z_t = i | X_{1:T})$

HMMs: E step

- Expected number of times of being in state i at time t
 - Let $\gamma_t(i) = P(z_t = i | X_{1:T})$
- Expected number of transitions from state i to j at time t .
 - $\epsilon_t(i, j) = P(z_t = i, z_{t+1} = j | X_{1:T})$

HMMs: M step

Updating π

$\hat{\pi}_k$ denotes the expected fraction of sequences with $z_1 = k$.

$$\hat{\pi}_k = \frac{\text{Expected number of sequences that start with } z_k}{\text{Total number of sequences}}$$

$$\hat{\pi}_k = \frac{\sum_{n=1}^N \gamma_{n,1}(k)}{N}$$

Assume there are N sequences
and $\gamma_{n,t}$ is for sequence n at time t

HMMs: M step

Updating A

\hat{A}_{jk} denotes the expected probability of transitions from state i to state j .

$$\begin{aligned}\hat{A}_{jk} &= \frac{\text{Expected number of transitions from state } i \text{ to state } j}{\text{Expected number of transitions from state } i} \\ &= \frac{\sum_{n=1}^N \sum_{t=1}^{T_i-1} \epsilon_{n,t}(j, k)}{\sum_{k=1}^K \sum_{n=1}^N \sum_{t=1}^{T_n-1} \epsilon_{n,t}(j, k)}\end{aligned}$$

HMMs: M step

- With Bernoulli observations:

Updating ϕ

$\hat{\phi}_{jl}$ denotes the expected probability of observing l from state j .

$$\begin{aligned}\hat{\phi}_{jl} &= \frac{\text{Expected number of times in state } j \text{ and observing } l}{\text{Expected number of times in state } j} \\ &= \frac{\sum_{n=1}^N \sum_{t \text{ where } x_{nt}=l}^{T_i} \gamma_{n,t}(j)}{\sum_{n=1}^N \sum_{t=1}^{T_i} \gamma_{n,t}(j)}\end{aligned}$$

HMMs: M step

- With Gaussian observations:

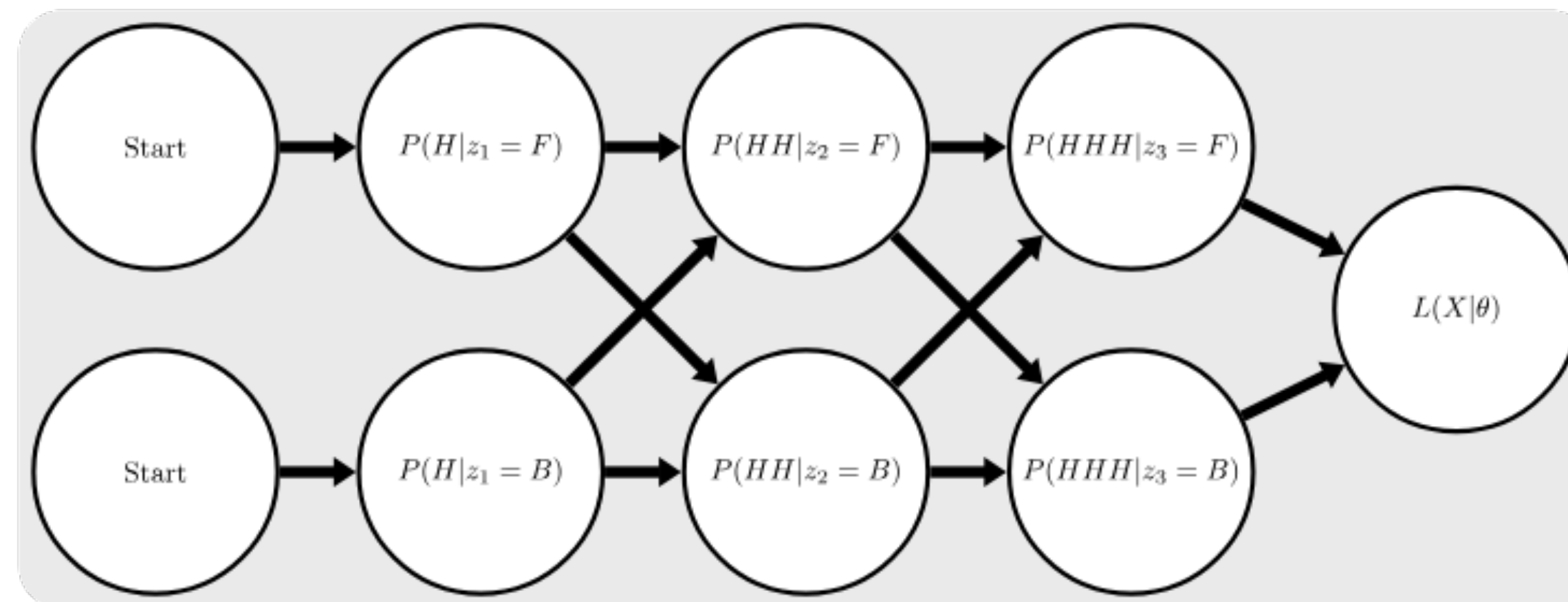
$$\mu_j = \frac{\text{Expected sum of observations in state } j}{\text{Expected number of times in state } j}$$

$$\mu_j = \frac{\sum_{n=1}^N \sum_{t=1}^T \gamma_{n,t}(j) x_{n,t}}{\sum_{n=1}^N \sum_{t=1}^T \gamma_{n,t}(j)}$$

- Not shown: there is also a covariance parameter

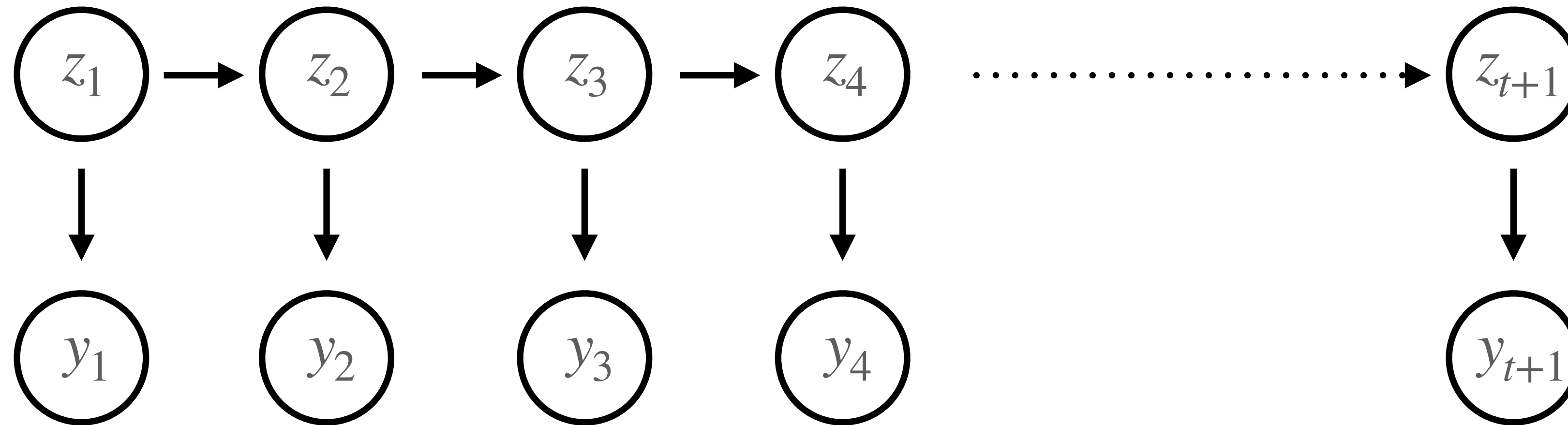
HMMs: Viterbi Algorithm

- Another common goal is to find the single most likely sequence of discrete states: $\operatorname{argmax}_{z_{1:T}} P(z_{1:T} | X_{1:T})$
- Note that $P(z_t | X_{1:T})$ does not necessarily give this!
- Viterbi Algorithm is another iterative dynamic programming algorithm to find this sequence



Linear Dynamical Systems

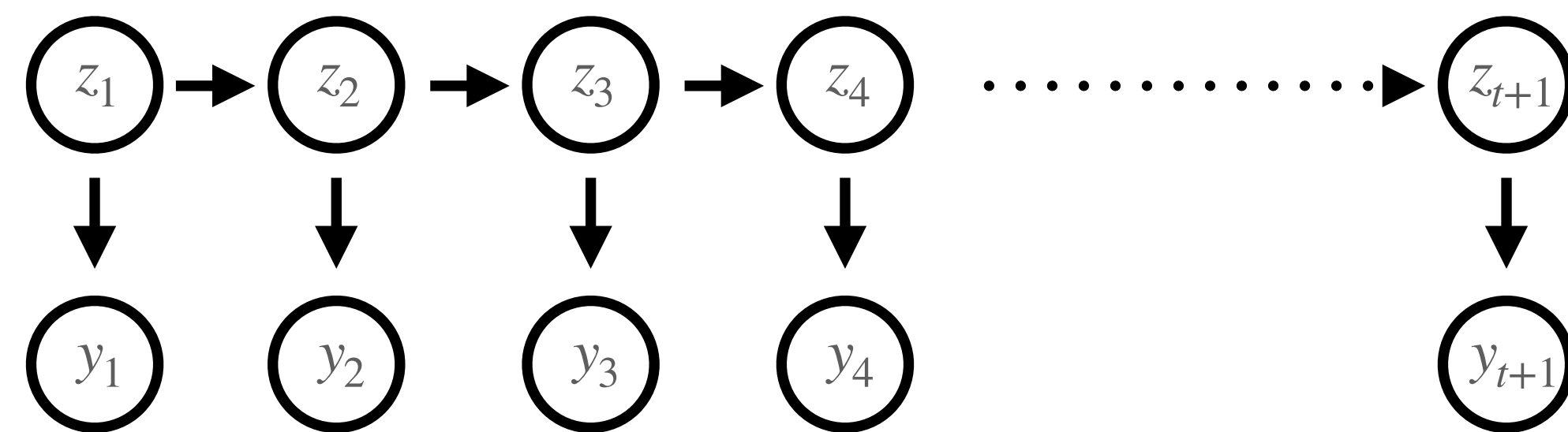
Linear Dynamical Systems



$$P(z_{1:T}, y_{1:T}) = P(z_1) \prod_{t=2}^T p(z_t | z_{t-1}) \prod_{t=1}^T p(y_t | z_t)$$

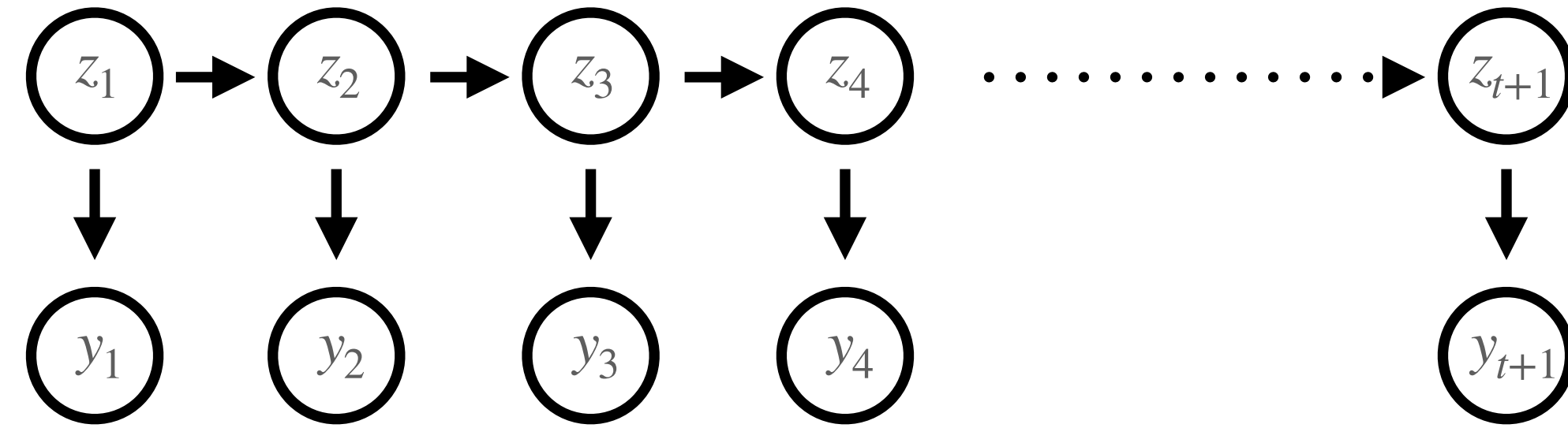
- Same graphical model as an HMM, but now z is continuous!
- Note the change in notation from $x \rightarrow y$

Linear Dynamical Systems



$$P(z_{1:T}, y_{1:T}) = P(z_1) \prod_{t=2}^T p(z_t | z_{t-1}) \prod_{t=1}^T p(y_t | z_t)$$

Linear Dynamical Systems



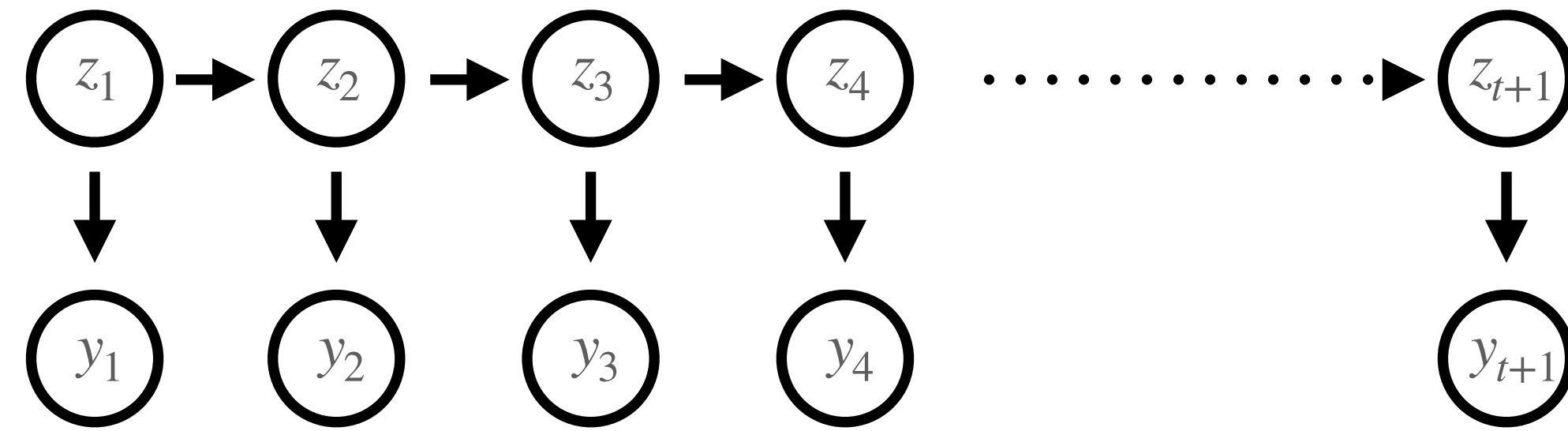
$$P(z_{1:T}, y_{1:T}) = P(z_1) \prod_{t=2}^T p(z_t | z_{t-1}) \prod_{t=1}^T p(y_t | z_t)$$

$$\mathcal{N}(z | \mathbf{0}, \mathbf{I})$$

$$\mathcal{N}(z_t | \mathbf{F}_t z_{t-1}, \mathbf{Q}_t)$$

$$\mathcal{N}(y_t | \mathbf{H}_t z_t, \mathbf{R}_t)$$

Linear Dynamical Systems



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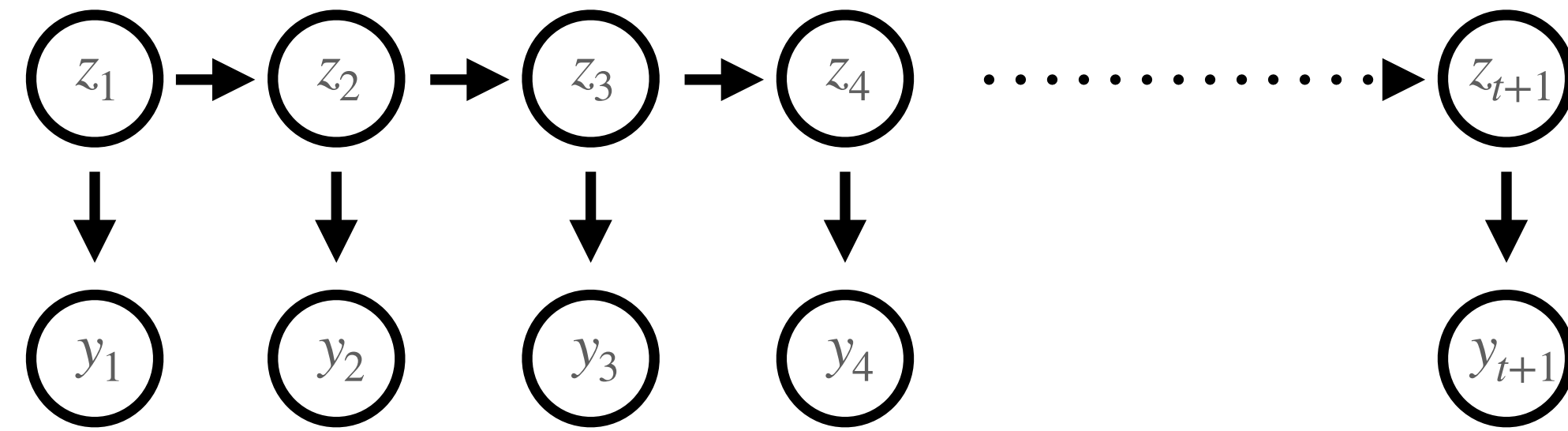
Or more fully:

$$\mathcal{N}(z_t | \mathbf{F}_t z_{t-1} + \mathbf{B}_t \mathbf{u}_t + \mathbf{b}_t, \mathbf{Q}_t)$$

Or more fully:

$$\mathcal{N}(y_t | \mathbf{H}_t z_t + \mathbf{D}_t \mathbf{u}_t + \mathbf{d}_t, \mathbf{R}_t)$$

Linear Dynamical Systems



$$P(z_{1:T}, y_{1:T}) = P(z_1) \prod_{t=2}^T p(z_t | z_{t-1}) \prod_{t=1}^T p(y_t | z_t)$$

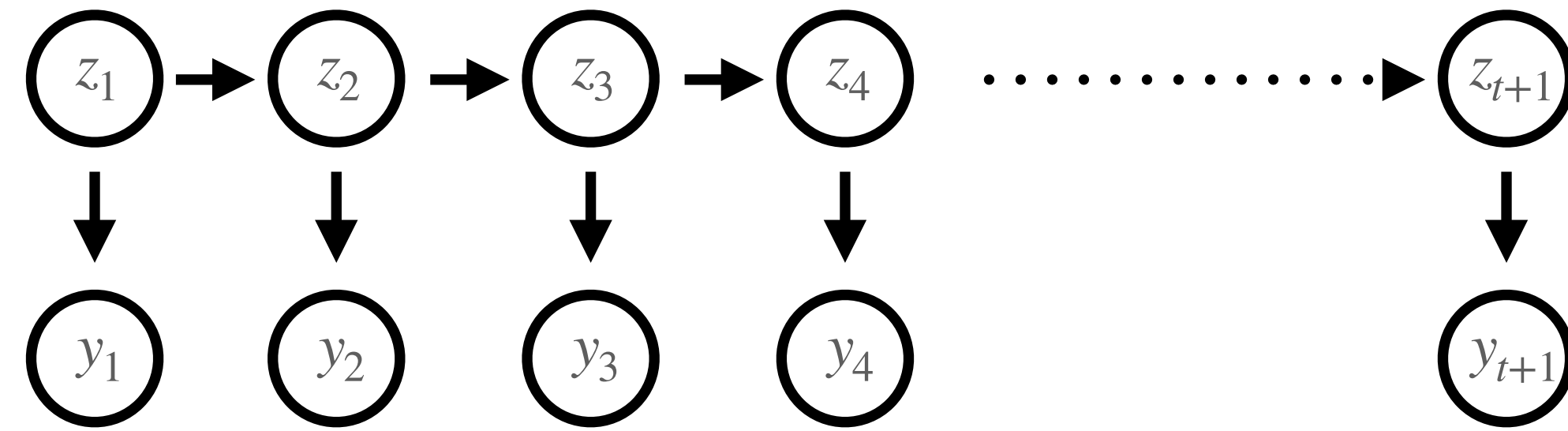
$$\mathcal{N}(z | \mathbf{0}, \mathbf{I})$$

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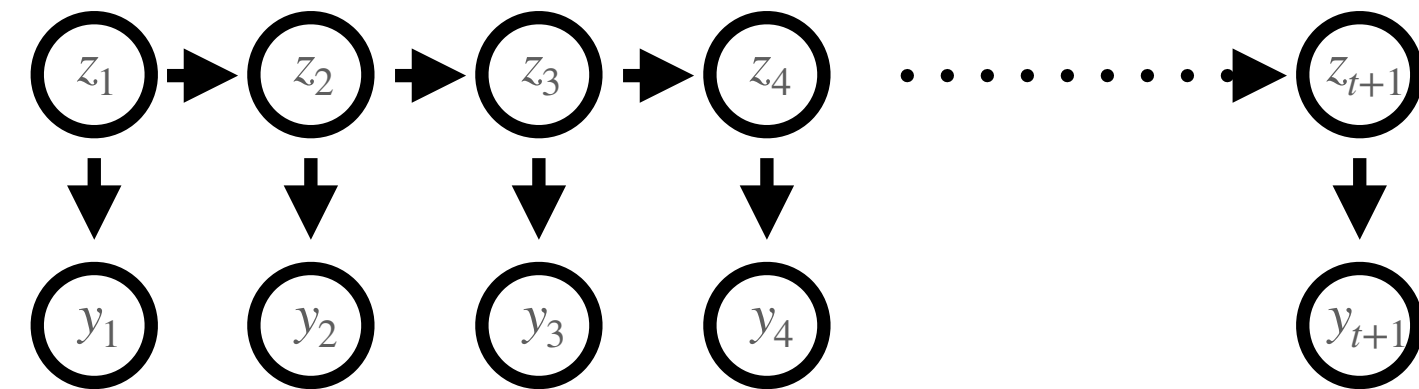
*Just like the Factor Analysis Model,
but now with a dynamics term!*

Simulating from an ~~HMM~~ LDS

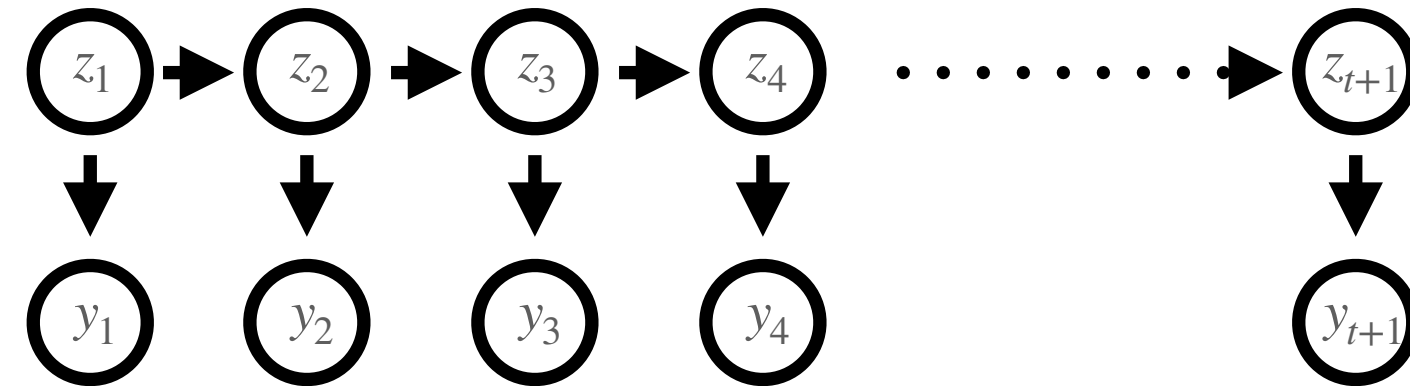


- Sample from $P(z_1)$
- Sample from $P(y_1 | z_1)$
- For all future time steps:
 - Sample $P(z_{t+1} | z_t)$
 - Sample $P(y_{t+1} | z_{t+1})$

LDS: Inferring the Latent States with a Kalman Filter

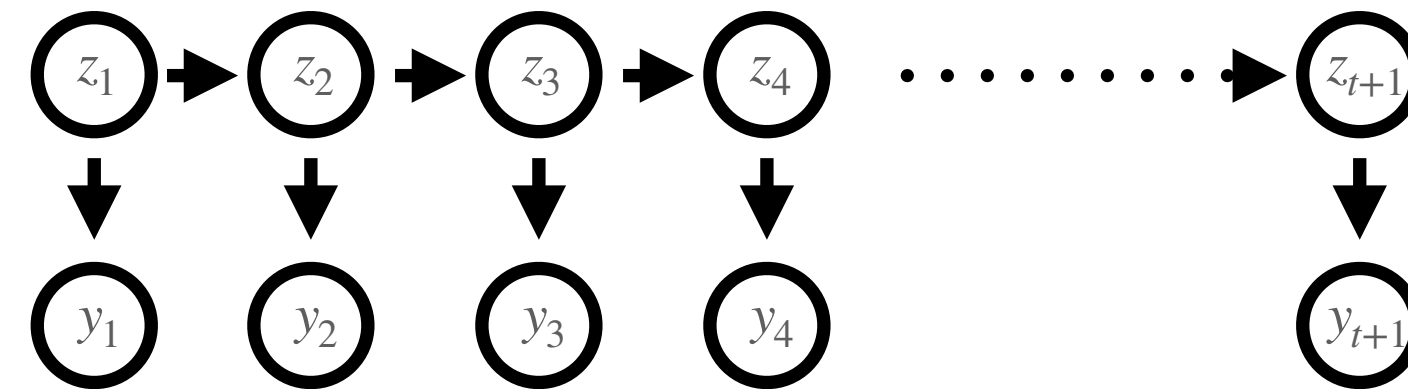


LDS: Inferring the Latent States with a Kalman Filter



- Predict Step:
 - Predict forward in time with dynamics model
- Update Step:
 - Use observations to modify dynamics-only prediction from above

LDS: Inferring the Latent States with a Kalman Filter

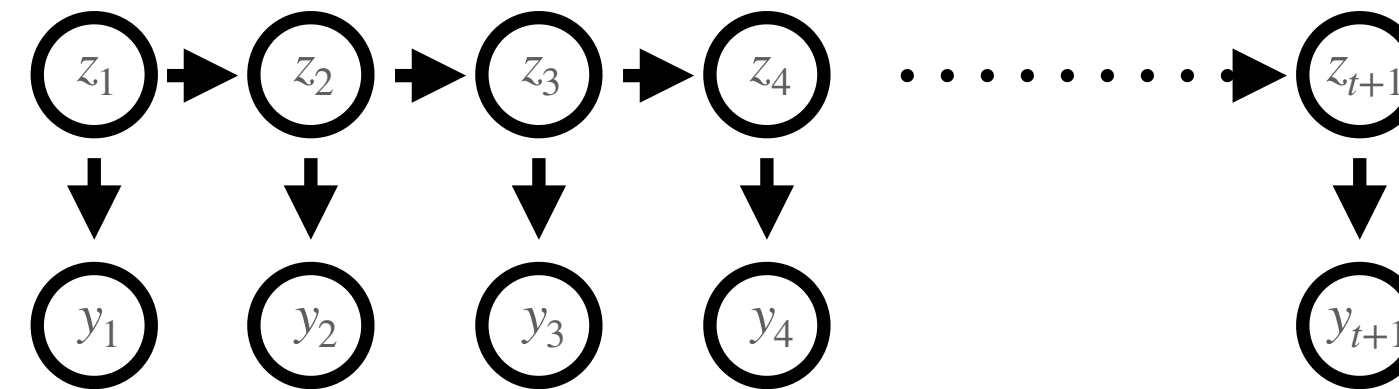


$$\mathcal{N}(z_t | \mathbf{F}_t z_{t-1}, \mathbf{Q}_t)$$

$$\mathcal{N}(y_t | \mathbf{H}_t z_t, \mathbf{R}_t)$$

- Predict Step:
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LDS: Inferring the Latent States with a Kalman Filter



$$\mathcal{N}(z_t | \mathbf{F}_t z_{t-1}, \mathbf{Q}_t)$$

$$\mathcal{N}(y_t | \mathbf{H}_t z_t, \mathbf{R}_t)$$

- Predict Step:

- Predict forward in time with dynamics model

$$p(z_t | \mathbf{y}_{1:t-1}, \mathbf{u}_{1:t}) = \mathcal{N}(z_t | \boldsymbol{\mu}_{t|t-1}, \boldsymbol{\Sigma}_{t|t-1})$$

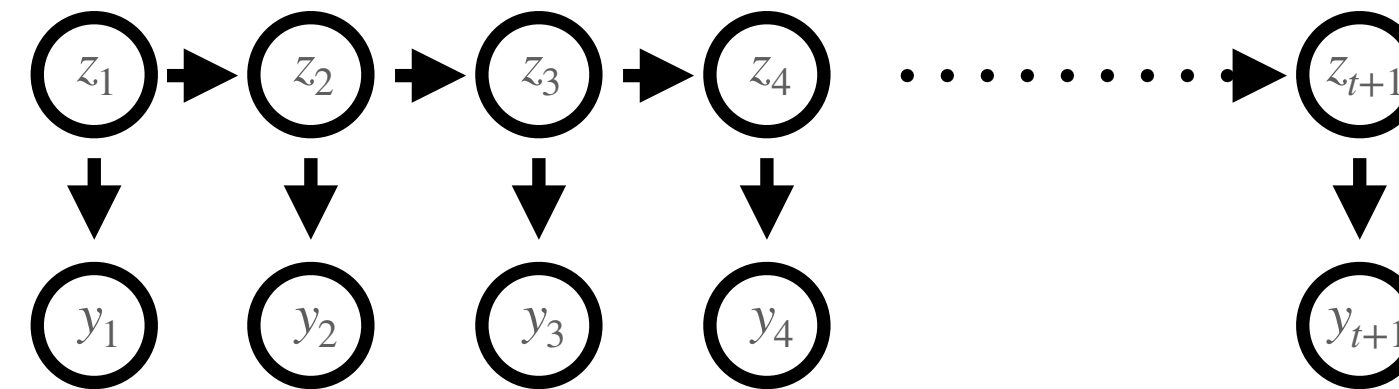
$$\boldsymbol{\mu}_{t|t-1} = \mathbf{F}_t \boldsymbol{\mu}_{t-1|t-1} + \mathbf{B}_t \mathbf{u}_t + \mathbf{b}_t$$

$$\boldsymbol{\Sigma}_{t|t-1} = \mathbf{F}_t \boldsymbol{\Sigma}_{t-1|t-1} \mathbf{F}_t^\top + \mathbf{Q}_t$$

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LDS: Inferring the Latent States with a Kalman Filter



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$$p(z_t | \mathbf{y}_{1:t}, \mathbf{u}_{1:t}) = \mathcal{N}(z_t | \boldsymbol{\mu}_{t|t}, \boldsymbol{\Sigma}_{t|t})$$

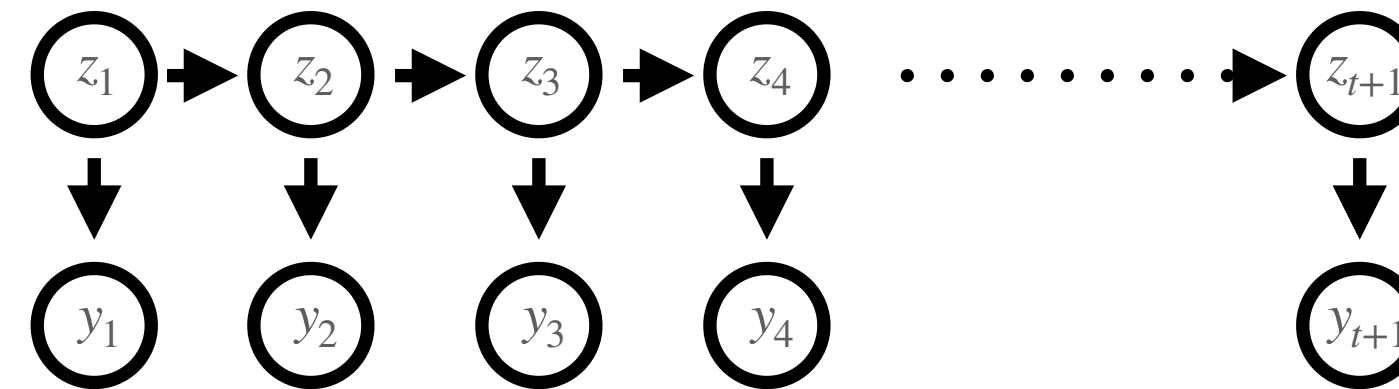
$$\hat{\mathbf{y}}_t = \mathbf{H}_t \boldsymbol{\mu}_{t|t-1} + \mathbf{D}_t \mathbf{u}_t + \mathbf{d}_t$$

$$\mathbf{S}_t = \mathbf{H}_t \boldsymbol{\Sigma}_{t|t-1} \mathbf{H}_t^\top + \mathbf{R}_t$$

$$\mathbf{K}_t = \boldsymbol{\Sigma}_{t|t-1} \mathbf{H}_t^\top \mathbf{S}_t^{-1}$$

$$\boldsymbol{\mu}_{t|t} = \boldsymbol{\mu}_{t|t-1} + \mathbf{K}_t (\mathbf{y}_t - \hat{\mathbf{y}}_t)$$

LDS: Inferring the Latent States with a Kalman Filter



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$$\mathbf{S}_t = \mathbf{H}_t \boldsymbol{\Sigma}_{t|t-1} \mathbf{H}_t^\top + \mathbf{R}_t$$

$$\mathbf{K}_t = \boldsymbol{\Sigma}_{t|t-1} \mathbf{H}_t^\top \mathbf{S}_t^{-1}$$

Dynamics Noise

Observations Noise

$$\boldsymbol{\mu}_{t|t} = \boldsymbol{\mu}_{t|t-1} + \mathbf{K}_t (\mathbf{y}_t - \hat{\mathbf{y}}_t)$$

LDS: Inferring the Latent States with a Kalman Smoother

- The Kalman Filter finds $p(z_t | y_{1:t}, u_{1:t})$
 - Comparable to the “forward” algorithm for HMMs

LDS: Inferring the Latent States with a Kalman Smoother

- The Kalman Filter finds $p(z_t | y_{1:t}, u_{1:t})$
 - Comparable to the “forward” algorithm for HMMs
- The Kalman Smoother finds $p(z_t | y_{1:T}, u_{1:T})$
 - Also includes a calculation going backwards in time, and is comparable to the “forward-backward” algorithm for HMMs

LDS: Model Fitting

- Most standard is EM
 - E-step is Kalman Smoother
 - M-step optimizes parameters
 - Can learn interesting things about the dynamics too!
- Subspace Identification (SSID) is also used

Resources

- Probabilistic Machine Learning Book 2, Chapter 29
 - <https://probml.github.io/pml-book/book2.html>
- Interactive HMM Website
 - <https://nipunbatra.github.io/hmm/>