Deep Generative Models: Markov Models

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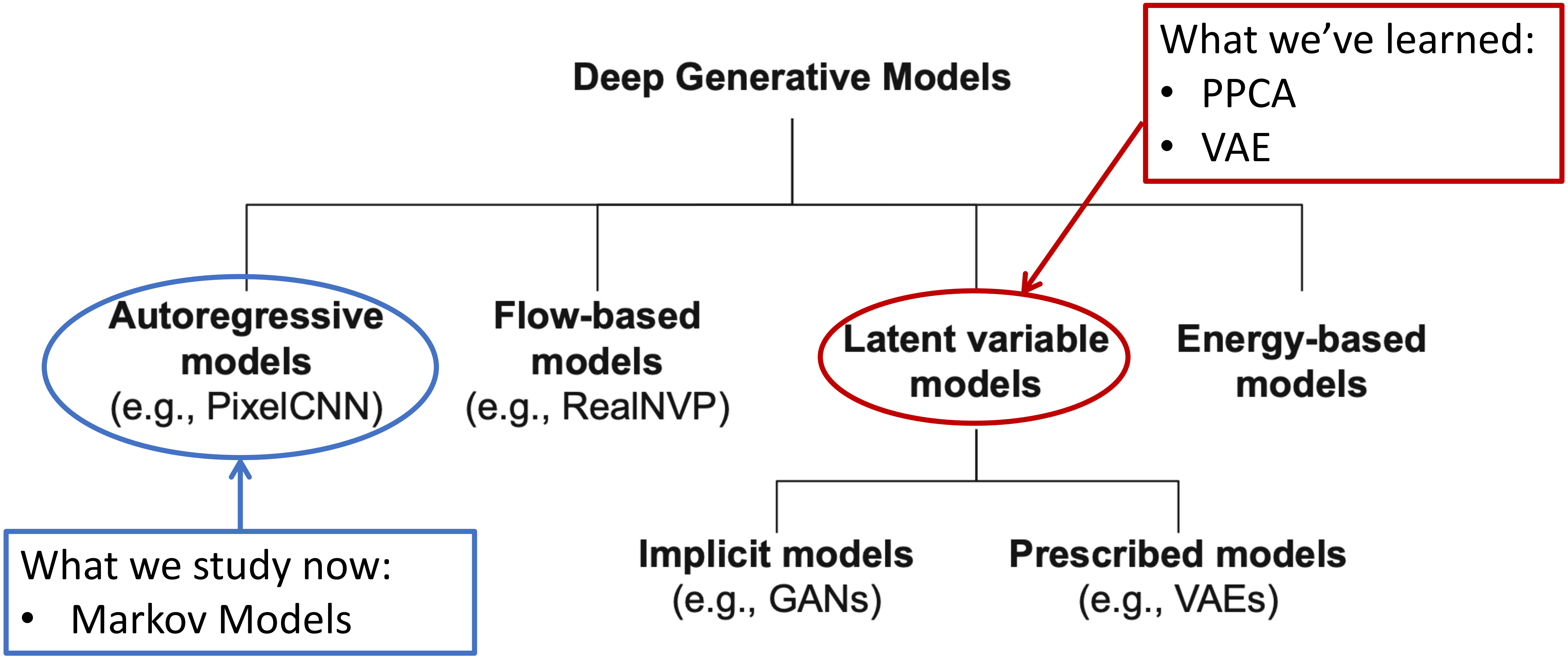
Taxonomy of Generative Models



Lecture Outline

- Stochastic Processes
  - Definition and Examples
- Markov Models and Markov Chains
  - Definition
  - Transition Probability and Transition Matrix
  - Examples
  - Stationarity and Convergence
- Maximum Log-Likelihood for Markov Chains

Stochastic Process

- Definition: A *stochastic process* refers to a sequence of random variables
$$(X_1, X_2, \dots, X_T)$$

- Each X_t takes values from the same sample space Ω (state space)
  - You can assume X_t has K states and $\Omega \coloneqq \{1, \dots, K\}$

- Example (Bernoulli Process):

$$X_t \sim \text{Bernouli}(p), \qquad t = 1, \dots, T$$

  - How many states does X_t has? What is Ω?

Markov Property Revisited

- **Issue**: Modeling the joint distribution $\mathbb{P}(X_1, X_2, \ldots, X_T)$ might require exponentially many parameters in the absence of any assumptions on P

- **Conditional Independence Assumption** (Markov property):

$$\overset{\text{future}}{X_{i+1}} \quad \overset{\text{independent}}{\perp} \quad \overset{\text{past}}{X_1, \ldots, X_{i-1}} \quad \overset{\text{given}}{\mid} \quad \overset{\text{present}}{X_i}$$

- **Consequence**: We now only need linearly many parameters:

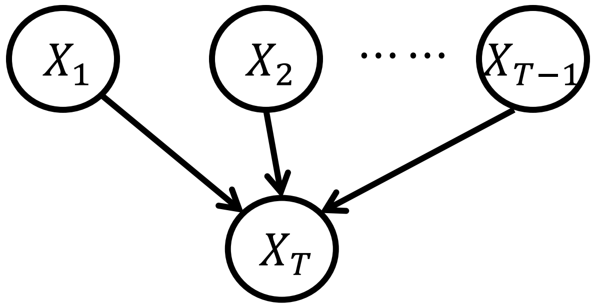
$$\begin{aligned} \mathbb{P}(x_1, \ldots, x_T) &= \mathbb{P}(x_1)\mathbb{P}(x_2 \mid x_1)\mathbb{P}(x_3 \mid \cancel{x_1}, x_2) \cdots \mathbb{P}(x_T \mid \cancel{x_1, \cdots, x_{T-2}}, x_{T-1}) \\ &= \mathbb{P}(x_1)p(x_2 \mid x_1)\mathbb{P}(x_3 \mid x_2) \cdots \mathbb{P}(x_T \mid x_{T-1}) \end{aligned}$$

Markov Chains

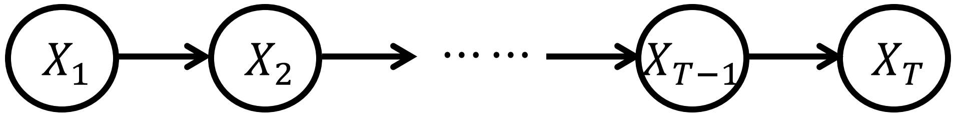
- Definition: A (discrete time) *Markov chain* is a stochastic process $(X_1, X_2, \dots, X_T)$ with the *Markov property*

$$\mathbb{P}(x_1, \dots, x_T) = \mathbb{P}(x_1)\mathbb{P}(x_2 \mid x_1)\mathbb{P}(x_3 \mid x_2) \cdots \mathbb{P}(x_T \mid x_{T-1})$$

  - Without Markov Property:



  - With Markov Property:



Parameters of Markov Chains

- Initial Probability $\pi_1, \dots, \pi_K$: $\pi_i \coloneqq \mathbb{P}(X_1 = i)$.
- Transition Probability a_{ij}:

$$a_{ij} \coloneqq \mathbb{P}(X_{t+1} = j \mid X_t = i) \qquad \forall i, j \in \Omega = \{1, \dots, K\}$$

  - This is the probability that X_t transitions from state i to state j
- Matrix and Vector Notations:

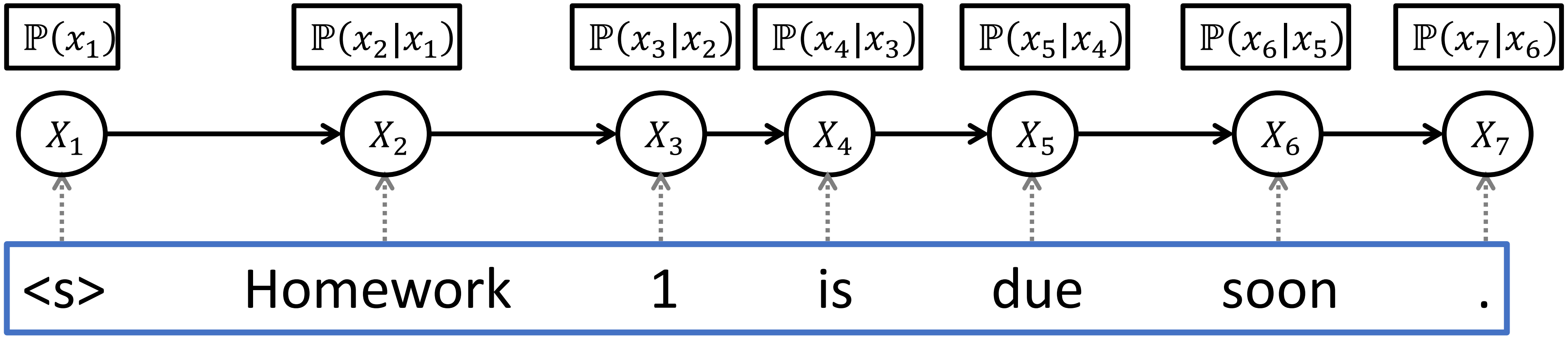
Row Vector

$$A := \begin{bmatrix} a_{11} & \cdots & a_{1K} \\ \vdots & \ddots & \vdots \\ a_{K1} & \cdots & a_{KK} \end{bmatrix} \in \mathbb{R}^{K \times K}, \qquad \pi \coloneqq [\pi_1, \dots, \pi_K] \in \mathbb{R}^{1 \times K}$$

A Markov chain is fully specified by its parameters $\theta := (\pi, A)$

Example: Markov Sentence Model

- State space $\Omega = \{\text{all possible words}\}$
  - The following are viewed as words and included in the state space
    - <s>: the start of the sentence
    - Digits
    - Punctuations
- Each sentence is a Markov chain where the words are random variables:



- Meaning of $\mathbb{P}(x_{t+1}|x_t)$: Given that the current word is x_t, what is the probability that the next word is x_{t+1}?

Example: DNA Sequencing

- State Space $\Omega = \{\mathcal{A}, \mathcal{C}, \mathcal{G}, \mathcal{T}\}$
- Transition Matrix A:

$$
\begin{array}{c|cccc}
 & \mathcal{A} & \mathcal{C} & \mathcal{G} & \mathcal{T} \\
\hline
\mathcal{A} & 0.359 & 0.143 & 0.167 & 0.331 \\
\mathcal{C} & 0.384 & 0.156 & 0.023 & 0.437 \\
\mathcal{G} & 0.306 & 0.199 & 0.150 & 0.345 \\
\mathcal{T} & 0.284 & 0.182 & 0.177 & 0.357
\end{array}
$$

Initial Probability Vector π:

$$
\begin{array}{c|c}
\mathcal{A} & 0.25 \\
\mathcal{C} & 0.25 \\
\mathcal{G} & 0.25 \\
\mathcal{T} & 0.25
\end{array}
$$

- Question 1: Given $\mathcal{C}$, what is the probability of getting DNA sequence $\mathcal{CTGAC}$?
- Answer 1:

$$\mathbb{P}(\mathcal{CTGAC}|X_1 = \mathcal{C}) = \underset{\boxed{0.182}}{\mathbb{P}(\mathcal{C}|\mathcal{T})} \cdot \underset{\boxed{0.345}}{\mathbb{P}(\mathcal{T}|\mathcal{G})} \cdot \underset{\boxed{0.167}}{\mathbb{P}(\mathcal{G}|\mathcal{A})} \cdot \underset{\boxed{0.384}}{\mathbb{P}(\mathcal{A}|\mathcal{C})} \approx 0.00403$$

Example: DNA Sequencing

- State Space $\Omega = \{\mathcal{A}, \mathcal{C}, \mathcal{G}, \mathcal{T}\}$

	$\mathcal{A}$	$\mathcal{C}$	$\mathcal{G}$	$\mathcal{T}$
$\mathcal{A}$	0.359	0.143	0.167	0.331
$\mathcal{C}$	0.384	0.156	0.023	0.437
$\mathcal{G}$	0.306	0.199	0.150	0.345
$\mathcal{T}$	0.284	0.182	0.177	0.357

$\mathcal{A}$	0.25
$\mathcal{C}$	0.25
$\mathcal{G}$	0.25
$\mathcal{T}$	0.25

- Question 2: What's the probability of $X_3 = \mathcal{A}$ given $X_1 = \mathcal{C}$?
- Question 3: What's the probability of $X_3 = \mathcal{A}$?

Example: DNA Sequencing

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	$\mathcal{A}$	$\mathcal{C}$	$\mathcal{G}$	$\mathcal{T}$
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$\mathcal{A}$	0.25
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$\mathcal{T}$	0.25

- Question 2: What's the probability of $X_3 = \mathcal{A}$ given $X_1 = \mathcal{C}$?
- Question 3: What's the probability of $X_3 = \mathcal{A}$?
- Answer 2: The state transition is $\mathcal{C} \to x_2 \to \mathcal{A}$ for all possible $x_2 \in \Omega$:

$$\mathbb{P}(X_3 = \mathcal{A} | X_1 = \mathcal{C}) = \sum_{x_2 \in \Omega} \mathbb{P}(X_3 = \mathcal{A} | X_2 = x_2) \cdot \mathbb{P}(X_2 = x_2 \mid X_1 = \mathcal{C})$$

$$= [0.384, 0.156, 0.023, 0.437] \begin{bmatrix} 0.359 \\ 0.384 \\ 0.306 \\ 0.284 \end{bmatrix}$$

  - This is the inner product of the second row and first column of the transition matrix A
  - This is the $(2,1)$-th entry of A^2

Example: DNA Sequencing

- State Space $\Omega = \{\mathcal{A}, \mathcal{C}, \mathcal{G}, \mathcal{T}\}$

	$\mathcal{A}$	$\mathcal{C}$	$\mathcal{G}$	$\mathcal{T}$
$\mathcal{A}$	0.359	0.143	0.167	0.331
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- Answer 2: The state transition is $\mathcal{C} \to x_2 \to \mathcal{A}$ for all possible $x_2 \in \Omega$:

$$\mathbb{P}(X_3 = \mathcal{A} | X_1 = \mathcal{C}) = \sum_{x_2 \in \Omega} \mathbb{P}(X_3 = \mathcal{A} | X_2 = x_2) \cdot \mathbb{P}(X_2 = x_2 \mid X_1 = \mathcal{C})$$

- Answer 3: The state transition is $x_1 \to x_2 \to \mathcal{A}$ for all possible $x_1, x_2 \in \Omega$:

$$\mathbb{P}(X_3 = \mathcal{A}) = \sum_{x_1 \in \Omega} \mathbb{P}(X_3 = \mathcal{A} | X_1 = x_1) \cdot \mathbb{P}(X_1 = x_1)$$

Question 2

Initial Probability

Generalizing the DNA Sequencing Example

- State Space $\Omega = \{1, \dots, K\}$
- $(A^s)_{ij}$: the (i,j)-th entry of A^s
- $(A^s)_{:j}$: the j-th column of A^s
- $(\cdot)_j$: the j-th entry of a vector

Transition Matrix A and initial probability distribution π :

$$A := \begin{bmatrix} a_{11} & \cdots & a_{1K} \\ \vdots & \ddots & \vdots \\ a_{K1} & \cdots & a_{KK} \end{bmatrix} \in \mathbb{R}^{K \times K}, \qquad \pi := [\pi_1, \dots, \pi_K] \in \mathbb{R}^{1 \times K}$$

- Claim 1: $\mathbb{P}(X_{t+s} = j \mid X_t = i) = (A^s)_{ij} \qquad (\forall s, t, i, j)$
- Claim 2: $\mathbb{P}(X_{s+1} = j) = (\pi A^s)_j \qquad (\forall s, j)$
- Proof of Claim 2:

$$\mathbb{P}(X_{s+1} = j) = \sum_{i \in \Omega} \mathbb{P}(X_{s+1} = j \mid X_1 = i) \cdot \mathbb{P}(X_1 = i) \underset{\text{Claim 1}}{=} \sum_{i \in \Omega} (A^s)_{ij} \cdot \pi_i = \pi (A^s)_{:j} = (\pi A^s)_j$$

- Proof of Claim 1: By induction (next page)

Proof of Claim 1

- State Space $\Omega = \{1, \dots, K\}$
- $(A^s)_{ij}$: the (i,j)-th entry of A^s
- $(A^s)_{:j}$: the j-th column of A^s
- $(\cdot)_j$: the j-th entry of a vector

Transition Matrix A and initial probability distribution π :

$$A := \begin{bmatrix} a_{11} & \cdots & a_{1K} \\ \vdots & \ddots & \vdots \\ a_{K1} & \cdots & a_{KK} \end{bmatrix} \in \mathbb{R}^{K \times K}, \qquad \pi := [\pi_1, \dots, \pi_K] \in \mathbb{R}^{1 \times K}$$

- Claim 1: $\mathbb{P}(X_{t+s} = j \mid X_t = i) = A_{ij}^s$
- Proof of Claim 1 (Induction):
  - $\forall s, t$, it is easy to prove shift invariance: $\mathbb{P}(X_{t+s} = j \mid X_t = i) = \mathbb{P}(X_{1+s} = j \mid X_1 = i)$
  - Next we prove $\mathbb{P}(X_{1+s} = j \mid X_1 = i) = A_{ij}^s$ by induction on s:
    - The base case $s = 1$ follows from the definition of A
    - Suppose we have $\mathbb{P}(X_s = j \mid X_1 = i) = A_{ij}^{s-1}$ then:

$$\mathbb{P}(X_{1+s} = j \mid X_1 = i) = \sum_{k \in \Omega} \mathbb{P}(X_{s+1} = j \mid X_s = k) \cdot \mathbb{P}(X_s = k \mid X_1 = i) = \sum_{k \in \Omega} a_{kj} \cdot (A^{s-1})_{ik} = (A^s)_{ij}$$

Limiting Behavior of Markov Chains

- We have just proved

$$\mathbb{P}(X_{t+s} = j \mid X_t = i) = (A^s)_{ij} \qquad (\forall s, t, i, j)$$

$$\mathbb{P}(X_{s+1} = j) = (\pi A^s)_j \qquad (\forall s, j)$$

- Our next goal is to understand the limits $\lim_{s \to \infty} A^s$, $\lim_{s \to \infty} \pi A^s$.
- The two limits are related to the eigenvalues of A:
  - Assume A is diagonalizable and write $A = U\Lambda \mathrm{U}^{-1}$ with eigenvalues $\Lambda = \mathrm{diag}(\lambda_1, \dots, \lambda_K)$
    - The diagonalizability assumption is not necessary but to simplify the exposition…
  - Then we have

$$\lim_{s \to \infty} A^s = U \left(\lim_{s \to \infty} \Lambda^s \right) U^{-1}, \qquad \lim_{s \to \infty} \pi A^s = \pi U \left(\lim_{s \to \infty} \Lambda^s \right) U^{-1}$$

- Hence, a necessary condition for the limits to exist is that $|\lambda_k| \le 1$ for all k.

Eigenvalues of Transition Matrix

$$A := \begin{bmatrix} a_{11} & \cdots & a_{1K} \\ \vdots & \ddots & \vdots \\ a_{K1} & \cdots & a_{KK} \end{bmatrix} \in \mathbb{R}^{K \times K}$$

- Proposition. Let $\lambda_1, \ldots, \lambda_K$ be eigenvalues of A. Then
$$\max_{k=1,\ldots,K} |\lambda_k| = 1.$$
- Proof. We first show $|\lambda_k| \leq 1$. Let (λ, u) be an eigen-pair with $Au = \lambda u$, $||u||_2 = 1$ and $u = [u_1, \ldots, u_K]^\top$. Let i be the index such that $|u_i|$ is maximized, i.e.,
$$i = \operatorname{argmax}_j |u_j|.$$

Then $Au = \lambda u$ implies $\sum_j a_{ij} u_j = \lambda u_i$, which furthermore gives
$$|\lambda| \leq \left| \frac{\sum_j a_{ij} u_j}{u_i} \right| \leq \sum_j |a_{ij}| \cdot \left| \frac{u_j}{u_i} \right| \leq \sum_j |a_{ij}| = \sum_j a_{ij} = 1.$$

Finally, A always has an eigenvalue 1: $A \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}$

$|\lambda_k| \leq 1$ is not sufficient for convergence

- Intuition:
  - Assume A is diagonalizable and write $A = U\Lambda\mathrm{U}^{-1}$ with eigenvalues $\Lambda = \mathrm{diag}(\lambda_1, \dots, \lambda_K)$
    - The diagonalizability assumption is not necessary but to simplify the exposition…

  - Then $\lim_{s\to\infty} A^s = U\left(\lim_{s\to\infty} \Lambda^s\right)U^{-1} = U\left(\mathrm{diag}\left(\lim_{s\to\infty} \lambda_1^s, \dots, \lim_{s\to\infty} \lambda_K^s\right)\right)U^{-1}$

  - And $\lim_{s\to\infty} \lambda_k^s$ …
    - is equal to 0 if $|\lambda_k| < 1$
    - is equal to 1 if $\lambda_k = 1$
    - does not exist if $\lambda_k = -1$

  - λ_k can even be a complex eigenvalue with $|\lambda_k| = 1$

Lesson

- Existence. In order for $\lim_{s\to\infty} A^s$, $\lim_{s\to\infty} \pi A^s$ to exist, we need to make assumptions such that:
  - A has no eigenvalues of magnitude 1 other than 1 itself.

- Uniqueness. In order for $\lim_{s\to\infty} \pi A^s$ to be the same for different initial distribution π, we need to make assumptions such that:
  - 1 is the eigenvalue of A of geometric/algebraic multiplicity 1

- The assumptions should be “interpretable” in terms of Markov chains or states
  - e.g., assuming A to be diagonalizable is not interpretable

Irreducibility and Strongly Connected Graph

- Definition. A directed graph is called *strongly connected* if there is a path in each direction between each pair of vertices of the graph.

- Definition. A transition matrix A is called *irreducible* if every state can be reached from any other state, i.e., for any i, j, there is some t such that
$$\mathbb{P}(X_t = j \mid X_1 = i) > 0.$$

- Remark. Each state can be denoted by a vertex and, if $a_{ij} > 0$ then we add a directed edge from vertex i to vertex j. This way, we obtain a directed graph. We can see that A is irreducible if and only if the graph is strongly connected

Limiting Behavior of Markov Chains

- Theorem. Assume A is irreducible, then there is some $v = [v_1, \dots, v_K]$ such that
  - For any initial distribution π we have:
  $$\lim_{s\to\infty} \frac{I + A + \cdots + A^{s-1}}{s} = ev, \qquad \lim_{s\to\infty} \pi\left(\frac{I + A + \cdots + A^{s-1}}{s}\right) = v$$
  $$\boxed{e \coloneqq \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}}$$
  - If furthermore there is some $a_{ii} > 0$, then for any initial distribution π we have
  $$\lim_{s\to\infty} A^s = ev, \qquad \lim_{s\to\infty} \pi A^s = v$$
- Remark. In the latter case, v is called the stationary distribution as it is the unique vector that satisfies:
$$vA = v, \qquad v_i > 0\ (\forall i), \qquad \sum_i v_i = 1$$
- Remark on Proof. This result is related to Perron–Frobenius Theory (Google search it). For its proof, see Chapter 7 (Perron–Frobenius Theory) of "*Matrix Analysis and Applied Linear Algebra*", *Second Edition (Carl D. Meyer, 2023)*.

Example

- Let $A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ and $v = [0.5, 0.5]$ and $I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$. Note that $a_{11} = a_{22} = 0$
  - A has two eigenvalues, 1 and -1.
  - We have $A^{2t} = I$ and $A^{2t+1} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ for any t, so $\lim_{s\to\infty} A^s$ does not exist.
  - We have $vA = [0.5, 0.5] \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = [0.5, 0.5] = v$, so $\lim_{s\to\infty} vA^s = [0.5, 0.5]$. However, for any initial distribution π different from v, $\lim_{s\to\infty} \pi A^s$ does not exist.
  - On the other hand, we have $\left(\frac{I+A}{2}\right)^2 = \begin{bmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{bmatrix} = \frac{I+A}{2}$, which implies

$$\lim_{s\to\infty} \left(\frac{I+A}{2}\right)^s = \frac{I+A}{2} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} [0.5, 0.5] = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \pi$$

Estimate Transition Parameters θ from Data

- We have derived some results based on the transition matrix …

- In practice, we are given data samples rather than the transition matrix

- We will assume the data are sampled from a Markov chain, and then compute the transition matrix from data via **maximum likelihood estimation (MLE)**

MLE of Markov Chains

$$X_1 \to X_2 \to \cdots\cdots \to X_{T-1} \to X_T$$

- Assume we have N i.i.d. samples $\{\boldsymbol{x}^{(n)}\}_{n=1}^{N}$ from distribution $p_\theta(\boldsymbol{x})$
  - $\boldsymbol{x} \coloneqq (x_1, \ldots, x_T)$ each x_t has K status
  - $\theta = (A, \pi)$: unknown transition matrix and initial probability distribution
- MLE:

$$(\hat{A}_{ML}, \hat{\pi}_{ML}) = \mathrm{argmax}_{A,\pi} \prod_{n=1}^{N} p_{A,\pi}(\boldsymbol{x}^{(n)})$$

Markov Property

$$(\hat{A}_{ML}, \hat{\pi}_{ML}) = \mathrm{argmax}_{A,\pi} \prod_{n=1}^{N} p_\pi\left(x_1^{(n)}\right) \prod_{t=2}^{T} p_A\left(x_t^{(n)} \mid x_{t-1}^{(n)}\right)$$

Similar to estimating $\hat{A}_{ML}$, so left as an exercise

Variables are separable

$$\hat{\pi}_{ML} = \mathrm{argmax}_\pi \prod_{n=1}^{N} p_\pi\left(x_1^{(n)}\right)$$

Our focus next

$$\hat{A}_{ML} = \mathrm{argmax}_A \prod_{n=1}^{N} \prod_{t=2}^{T} p_A\left(x_t^{(n)} \mid x_{t-1}^{(n)}\right)$$

Simplifying The MLE

$$\boxed{\hat{A}_{ML} = \operatorname{argmax}_A \prod_{n=1}^{N} \prod_{t=2}^{T} p_A\left(x_t^{(n)} \mid x_{t-1}^{(n)} \right)}$$

- $\mathbb{I}(\cdot)$: indicator function
- N_{ij}: the number of samples with transitions from state i to state j, i.e.,

$$N_{ij} \coloneqq \sum_{n=1}^{N} \sum_{t=2}^{T} \mathbb{I}\left(x_t^{(n)} = j, x_{t-1}^{(n)} = i\right)$$

Then we have:

1. $p_A\left(x_t^{(n)} \mid x_{t-1}^{(n)} \right) = \prod_{i=1}^{K} \prod_{j=1}^{K} (a_{ij})^{\mathbb{I}\left(x_t^{(n)}=j,\, x_{t-1}^{(n)}=i\right)}$
2. $\prod_{n=1}^{N} \prod_{t=2}^{T} p_A\left(x_t^{(n)} \mid x_{t-1}^{(n)} \right) = \prod_{n=1}^{N} \prod_{t=2}^{T} \prod_{i=1}^{K} \prod_{j=1}^{K} (a_{ij})^{\mathbb{I}\left(x_t^{(n)}=j,\, x_{t-1}^{(n)}=i\right)}$

$$= \prod_{i=1}^{K} \prod_{j=1}^{K} \left(a_{ij}\right)^{N_{ij}}$$

This gives:

$$\boxed{\hat{A}_{ML} = \operatorname{argmax}_A \prod_{i=1}^{K} \prod_{j=1}^{K} \left(a_{ij}\right)^{N_{ij}}}$$

Simplifying The MLE

$$\hat{A}_{ML} = \text{argmax}_A \prod_{i=1}^{K} \prod_{j=1}^{K} \left(a_{ij}\right)^{N_{ij}}$$

- N_{ij}: the number of samples with transitions from state i to state j

Taking logarithm and adding constraints $\sum_j a_{ij} = 1$:

$$\hat{A}_{ML} = \text{argmax}_A \sum_{i=1}^{K} \sum_{j=1}^{K} N_{ij} \log a_{ij} \quad \text{subject to} \quad \sum_{j=1}^{K} a_{ij} = 1 \ (\forall i)$$

$\downarrow$ Variables are separable

Solve the following for every $i = 1, \dots, K$:

$$\widehat{a_{ij}}_{ML} = \text{argmax}_{a_{ij}} \sum_{j=1}^{K} N_{ij} \log a_{ij} \quad \text{subject to} \quad \sum_{j=1}^{K} a_{ij} = 1$$

Remark: We have seen how to solve it using Lagrangian multipliers (recall *EM for Gaussian Mixture Models*)

$$\widehat{a_{ij}}_{ML} = \frac{N_{ij}}{\sum_{j=1}^{K} N_{ij}}$$

Remark: The optimal transition matrix can be found by simply counting and classifying the number of the transitions of the sample states!

Conclusion

- Markov chains have several applications

- For irreducible transition matrix with at least one positive entry, the Markov chain will eventually a stationary distribution

- The transition matrix can be learned from data via maximum likelihood estimation