Higher Order Markov Chains and Spacey Walks

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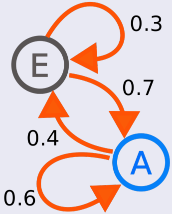
Overview

1. Introduction/review of first-order Markov chains
2. Higher order Markov chains, relation to tensors
3. Stochastic walks on higher order Markov chains
4. Applications of the Spacey walk

Markov Chains

Markov Chains are stochastic models describing a sequence of states with a probability of transitioning between each.

- Defined as matrix: $\mathrm{P} \in \mathbb{R}^{n \times n}$, P_{ij} gives probability of moving to state i from j, for chain with n states.
- Given distribution/state vector $\mathrm{x}^{(n)}$, one step of a random walk is represented by matrix-vector product $\mathrm{x}^{(n+1)} = \mathrm{P}\mathrm{x}^{(n)} \iff x_i^{(n+1)} = \sum_j P_{ij} x_j^{(n)}$.



Transition matrix:

$$\mathrm{P} = \begin{array}{cc} & \begin{array}{cc} A & E \end{array} \\ \begin{array}{c} A \\ E \end{array} & \begin{bmatrix} 0.6 & 0.7 \\ 0.4 & 0.3 \end{bmatrix} \end{array}$$

Figure from `https://commons.wikimedia.org/wiki/File:Markovkate_01.svg`

Definitions

Time Homogeneous

Each transition probability is independent of the time step t.

Irreducible

Every state can be reached from every other state.

Periodic

Periodic markov chain:

$$\exists i \in S \quad s.t. \quad \left(P^d\right)_{ii} \neq 0; \quad d \in \mathbb{Z}, d > 1$$

Periodicity implies a state may only return to itself after some multiple d "hops". If every state has self loops the chain is **aperiodic**.

Canonical Examples

Google PageRank

- Markov chain represents the "idealized" web surfer. States are webpages and transition probability is given by number of outgoing links between pages.
- Ranking is determined by probability of being on certain page.

Board Games

- Each spot on game board is a state.
- Probability of moving between spots is given by dice, spinner, etc.

Weather

- States are possible weather conditions.
- Tomorrow's weather is randomly chosen based on today's conditions.

Steady-State Distribution

Steady state vector $\boldsymbol{\pi} \in \mathbb{R}^n$ does not change when multiplied by Markov chain:
$$\boldsymbol{\pi} = \mathrm{P}\boldsymbol{\pi}$$

- Average distribution as random walk tends to length infinity, $\lim_{k\to\infty} \mathrm{P}^k \mathrm{x}$
- Is equivalent to **Perron vector** of matrix, dominant eigenvector with nonnegative components.
- Compute iteratively with power method: $\mathrm{x}^{(k+1)} = \mathrm{P}\mathrm{x}^{(k)}$.

Unique steady states are guaranteed for **irreducible**, **aperiodic** Markov chains.

Markov Chains with Memory

What if we want our chain to **remember** where it has been? Introduce ***m*-order Markov chain**, where transition probability depends on previous m states.

- Probability is now stored as $\mathrm{P} \in \mathbb{R}^{n \times n^m}$, where columns are a m-tuple of each state permutation.
- Random step becomes slightly more complicated than just a *mat-vec*, will see a better way of doing this.

$$\mathrm{P} = \begin{array}{c c} & \begin{array}{cccc} (s_0, s_0) & (s_1, s_0) & (s_0, s_1) & (s_1, s_1) \end{array} \\ \begin{array}{c} s_0 \\ s_1 \end{array} & \begin{bmatrix} p_{1,1} & p_{1,2} & p_{1,3} & p_{1,4} \\ p_{2,1} & p_{2,2} & p_{2,3} & p_{2,4} \end{bmatrix} \end{array}$$

(Example indexing for 2^{nd} order chain with $n = 2$ states.)

Higher Order Markov Chains

We can **fold the last dimension** of the higher-order Markov matrix to obtain a higher dimensional **tensor**.

Order m Markov chain with n states is order $m+1$ tensor

$$\mathcal{P} \in \mathbb{R}^{\overbrace{n \times n \times \cdots \times n}^{m+1 \text{ dimensions}}}$$

Transition probability indexed by $P_{i_{(n+1)}, i_{(n)}, i_{(n-1)}, \ldots, i_{(n-m+1)}}$

- State/distribution is stored as order m tensor.
- Example random step for order 2 Markov chain: $X_{ij}^{(n+1)} = \sum_k P_{ijk} X_{jk}^{(n+1)}$

Tensor Notation

- Will write tensors as flattening along first mode, i.e. for $\mathcal{P} \in \mathbb{R}^{2\times 2\times 2}$:

$$\mathcal{P} = \left[\begin{array}{cc|cc} p_{111} & p_{121} & p_{112} & p_{122} \\ P_{211} & p_{221} & p_{212} & p_{222} \end{array}\right]$$

- Each slice is referred to as a **panel**, enumerates transition probabilities given some previous state.
- Note each panel is its own **stochastic matrix**.

Higher Order Steady-State Distribution

Assume 2nd order chains in following slides for notational simplicity – everything generalizes to higher orders though.

Steady state tensor $\mathrm{X} \in \mathbb{R}^{n \times n}$ does not change when multiplied along first mode.

$$X_{ij} = \sum_{k} P_{ijk} X_{jk}$$

- Conceptually simple, but requires $\mathcal{O}\left(n^m\right)$ space to store state tensor.

Replace state tensor with **low rank approximation** $\mathrm{x} \in \mathbb{R}^n$:

$$x_i = \sum_{jk} P_{ijk} x_j x_k$$

Actually just the ***z*-eigenvector** of $\mathcal{P}$!

Stochastic Processes

- For first order, steady state/eigenvector can be represented by a **random walk**.
- Our low rank transformation:

$$X_{ij} = \sum_k P_{ijk} X_{jk} \quad \Rightarrow \quad x_i = \sum_{jk} P_{ijk} x_j x_k$$

is algebraic, is there a **stochastic** process?

Present the concept of a **spacey walk**: upon reaching a new state we *space out* and forget all previous states. State history is then **randomly made up** from previously seen states.

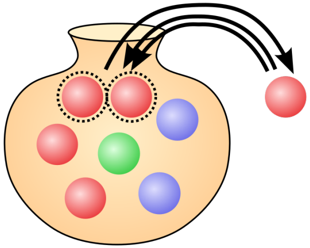
Let $X(0), X(1), \ldots, X(n)$ be the sequence of visited states and N to be the number of states. Define $Y(n)$ as a random previously seen state, each weighted by number of occurrences:

$$P(Y(n) = k \mid \mathcal{F}_n) = \frac{1}{n+N}\left(1 + \sum_{s=1}^{n} \mathbb{1}(X(s) = k)\right)$$

Transition probability is then given by:

$$P(X(n+1) = i \mid X(n) = j, Y(n) = k) = P_{ijk}$$

Pólya Urn



https://commons.wikimedia.org/wiki/File:Urn_problem_qtl5.svg

For simple example of the Spacey walk, consider **Pólya Urn** process. Have urn with red and green balls inside, and repeat the following process:

1. Select a random ball from the urn
2. Put the random ball back in the urn
3. Put another ball of same selected color in the urn

$$\mathcal{P}_{(1)} = \left[\begin{array}{cc|cc} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{array}\right]$$

Vertex-reinforced random walks

This spacey walk is an instance of a **vertex-reinforced random walk**. I.e., a walk that always picks next state based on transition probabilities, but probabilities evolve over time.

Vertex-reinforced walk

$$w_i(n) = \frac{1}{N+n}\left(1 + \sum_{s=1}^{n} \mathbb{1}(X(s) = i)\right)$$

$$P(X(n+1) = i \mid \mathcal{F}_n) = [\mathrm{M}(\mathrm{w}(n))]_{i,X(n)}$$

Where M maps the *occupation vector* w to a stochastic matrix $\mathrm{P} \in \mathbb{R}^{N\times N}$.

For spacey walks, define:

$$M(\mathrm{w}) = \sum_{k=1}^{N} P_{:,:,k} w_k$$

Vertex-reinforced walks and ODEs

Why care about turning the **spacey walk** into a **vertex-reinforced walk**?

Lets us model chain as a **dynamical system**:

$$\frac{dx}{dt} = \pi(M(x)) - x$$

For some π that maps transition matrices to a stationary distribution.

So, to find the tensor eigenvector x, we can solve the ODE for its **fixed points**:

$$\frac{dx}{dt} = 0 \iff x_i = \sum_{ij} P_{ijk} x_j x_k$$

Solution to Steady State

- Now reduced eigenvector problem to matter of **integrating an ODE**.
- Can offer better convergence properties than traditional power method/fixed point iteration.
- Take following periodic Markov chain as example:

$$\mathcal{F}_{(1)} = \left[\begin{array}{cc|cc} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \end{array}\right]$$

When using power iteration:

$$x_i^{n+1} = \sum_{jk} P_{ijk} x_j x_K$$

Oscillates between $\begin{bmatrix} 0 & 1 \end{bmatrix}^T$ and $\begin{bmatrix} 1 & 0 \end{bmatrix}^T$.

Forward-stepping ODE

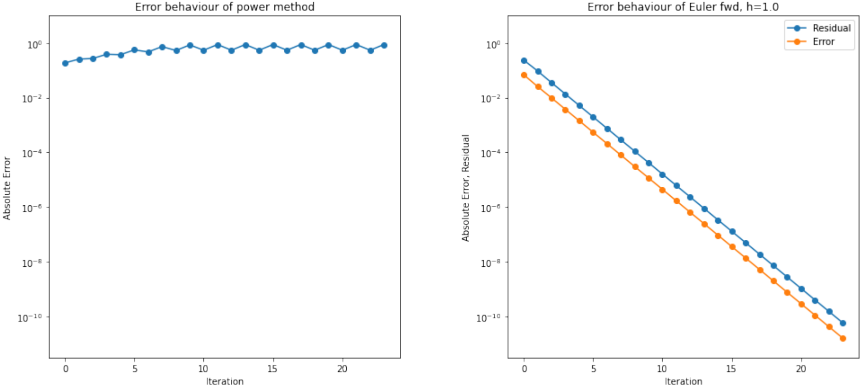
$$\frac{dx}{dt} = \pi\left(\mathrm{M}\left(\mathrm{x}\right)\right) - \mathrm{x}$$

with Euler converges to analytical solution $\left[\left(\sqrt{5}-1\right)/2 \quad \left(3-\sqrt{5}\right)/2\right]^T$.

Solution to Steady State (contd)

$$\mathcal{F}_{(1)} = \left[\begin{array}{cc|cc} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \end{array}\right]$$

Both methods, with starting guess of $x = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \end{bmatrix}^T$:

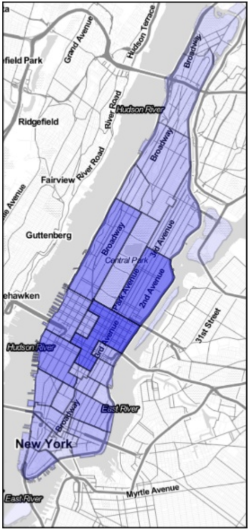


Population genetics study dynamics of allele distribution, or type of each organism. Suppose we have n types, the possibility of passing each type to child is given by:

$$P\left(\text{child is type } i \mid \text{parents are types } j, k\right) = P_{ijk}$$

- Parent ordering doesn't matter, have natural symmetry $P_{ijk} = P_{ikj}$.
- Spacey walk models how population dynamics evolve over time.
- Stationary type distribution satisfies $\mathrm{x}_i = \sum_{jk} P_{ijk} x_j x_k$.

Taxi Trajectory Modeling



(Benson, Gleich, Lim)

- Model taxicab as **spacey walk** $\mathcal{P}_{ijk}$, with N states being possible locations.
- Passenger at location k gets picked up at j and goes to i with probability P_{ijk}.
- Assume passengers are likely to be picked up nearby where they are dropped off, i.e. at airport.
- Difficult to solve, higher order gives better performance (RMSE) than first order:

First Order	Second Order	Spacey Walk
0.846	0.835	0.835

Ranking and Clustering

Can extend "classical" PageRank to **multilinear PageRank**, z-eigenvector problem:

$$x = \alpha \mathcal{P}_{(1)} (x \otimes x) + (1 - \alpha) v$$

where $v \in \mathbb{R}^n$ is the **teleport vector**, and $1 - \alpha$ is the probability of teleporting to a random state. Unique steady state when $\alpha < \frac{1}{m-1}$, forward euler converges as $h \to 0$.

Can also use this for clustering – partitioning graph into sets of similar nodes.

Conclusion

- Introduce high order Markov chain as having **memory of previous states**.
- High order Markov chains can be represented as **tensor** of transition probabilities.
- Tensor form naturally emits eigenvector steady-state.
- Z-eigenvector is the limiting distribution of the **spacey random walk**.
- Random walk can be turned into equivalent ODE construction.
- We can solve an ODE to find the tensor eigenvector!
- The Spacey walk is a generalization of the **Pólya process**, has interesting applications.

References

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