Foundations of Data Science & Machine Learning

Summary — Week 08
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Abstract

This week's lectures discusses random walks on directed graphs and its properties. Further we discuss stationary distributions of random walks with its real life applications.

1 Random Walks on Graphs

Definition: A **Random Walks** consists of a 'walk' on graph where the destination is chosen according to the current state and outgoing path probabilities. The sum of probabilities of outgoing paths from a state is equal to 1.

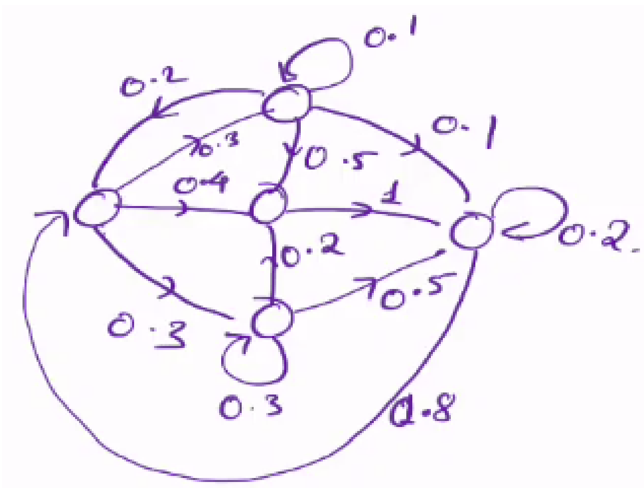


Fig 1.0 A sample Graph

→ A good example for random walk can be (web pages, hyperlinks).

Fig 1.1 Weight of edge representing the probability P_{ij}

→ Edge weights = Transition probability

$$P_{ij} = P[Next\,State = j/Current\,State = i]$$

$$Hence\,\forall i \in V(G), \sum_{j \in V(G)} P_{ij} = 1$$

→ Transition Probability Matrix (TPM):

$$P = \begin{bmatrix} P_{11} & ... & P_{1n} \\ P_{21} & ... & P_{2n} \\ : & & \\ P_{n1} & ... & P_{nn} \end{bmatrix}_{n \times n}$$

$$\begin{bmatrix} P_{11} & ... & P_{1n} \\ P_{21} & ... & P_{2n} \\ : & & \\ P_{n1} & ... & P_{nn} \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ : \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ : \\ 1 \end{bmatrix}$$

→ P1 ≡ Every row of P sums to 1.
→ P is not symmetric as it's not necessary that $P_{ij} = P_{ji}$
→ Hence 1I = $[1, 1, ..., 1]^T$ is a (right) eigen vector of P with eigen value 1.
In fact, if P is real non-negative matrix then,
P is a stochastic matrix <=> P 1I = 1I

Corollary: If P_1 and P_2 are n × n stochastic matrices, then so is P_1P_2

$$P_1P_21| = P_1(P_21|) = P_11| = 1|$$

Corollary: If P is a stochastic matrix, then $\forall k \in \mathbb{N}, P^k$ is a stochastic matrix. (proof using previous corollary)

$$P^k[i, j] = P[\text{State after k steps = j / current step = i}]$$

Proposition: All eigen values of P have magnitude ≤ 1. i.e. Px = $\lambda x \Rightarrow |\lambda| \leq 1$
Proof: Let x = $(x_1, x_2, ...x_n)$ be a eigen vector corresponding to λ s.t. some $|x_j| \leq 1 \forall j$

$$Px = \lambda x$$

$$< (i^{th}\,row\,of\,P), x >= \lambda x_i$$

$$\sum_{j=1}^{n} P_{ij}x_j = \lambda 1$$

$$|\lambda| \leq \sum_{j=1}^{n} P_{ij}|x_j| \leq \sum_{j=1}^{n} P_{ij}1 = 1$$

→ What is multiplicity of $\lambda = 1$?
If $\lambda = 1$, then $x_j = 1 \forall j$ s.t $P_{ij} \neq 0$
If every vertex is reachable from i, then $x_j = 1 \forall j \Rightarrow x = 1I$.

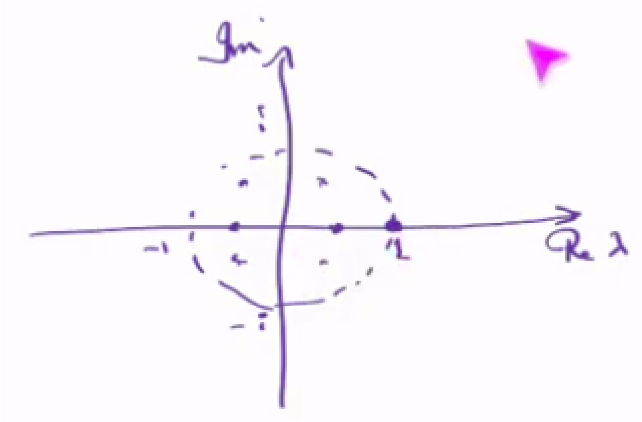


Fig 1.2 Eigen value

Proposition: If the embedding graph G is strongly connected then the eigen value 1 has the multiplicity 1.

$\equiv$ 1I is the unique eigen vector (upto scaling) for $\lambda = 1$.

$\rightarrow$ Converse? (Exercise)

(Hint: Sink component)

$\rightarrow$ When do we get $\lambda = -1$?

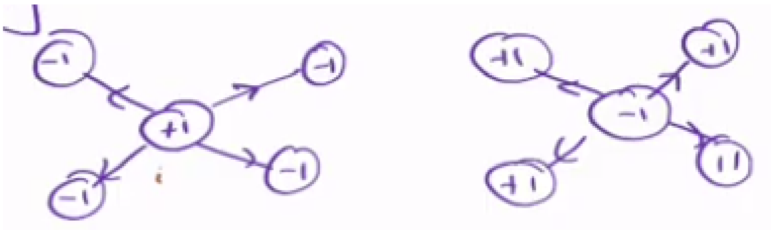


Fig 1.3 Graph in $\lambda = -1$ case

This could happen when G is bipartite graph

Strongly connected $\Rightarrow$ -1 also has multiplicity 1.

$\rightarrow$ Is P full rank?

Not necessarily.

A possible case when P is full rank:

$$\begin{bmatrix} 1/3 & 1/3... & 1/3 \\ 1/3 & 1/3... & 1/3 \\ \vdots & & \\ 1/3 & 1/3... & 1/3 \end{bmatrix}$$

Interestingly the n $\times$ (n+1) matrix P - I : 1I has rank n. (exercise)

$\rightarrow$ In an undirected graph case, $P_{ij} = P_{ji}$ and the P is symmetric matrix.

$\rightarrow$ P^T? ... It capture "evolution of random walk"

P^T is more important than P. Let p = $(p_1, p_2, ..., p_n)$ be the node probabilities at current step. Then, $p' = P^T p$ gives the node probability at the next step.

$$p'_i = \sum_{j=1}^{n} P_{ji} p_j = [P^T p]_i$$

$$p(t+1) = P^T p(t)$$

$\rightarrow$ $x = (x_1, x_2, ..., x_n)$ is called probability vector if $x_i \geq 0 \, \forall i$ and $\sum_{i=1}^{n} x_i = 1$
$\rightarrow$ Properties of P^T:

- Eigen values (and multiplicities) pf P and P^T are the same. (Proof using determinents: $\det(P^T - \lambda I) = \det((P - \lambda I)^T) = \det((P - \lambda I)))$.

- x is a prob. vector $\Rightarrow$ P^T x is a prob. vector

  Proof: Let $y = P^T x$, $y_i \geq 0$ obviously

$$\sum_{i=1}^{n} y_i = 1|^T y = 1|^T P^T x = (P\,1|)^T x = (1|)^T x = 1|$$

- P^T also has a unique eigen vector (upto scaling) for $\lambda = 1$. (considering strongly connected graph for 'unique'). But is it a prob. vector? YES!

2 Stationary Distributions of Random Walks

Definition: $\pi \in \mathbb{R}^n$ is called a **Stationary Distribution** of a random walk with transition matrix P if:
(i) π is a prob. vector &
(ii) $P^T \pi = \pi$

Theorm 1: (Fundamental theorm of finite Markov Chain)
$\rightarrow$ A random walk on every finite graph has a stationary distribution.
Observation: Finiteness is necessary.
Standard Proof: Key idea: **"Fixed Point Theorems"**
Let $f : X \rightarrow X$, then a point $x \in X$ s.t. f(x) = x is called a **fixed point** of f.
Example: Any continuous function from a closed interval [a,b] to itself has a fixed point.
Let f : [a,b] $\rightarrow$ [a,b], continuous

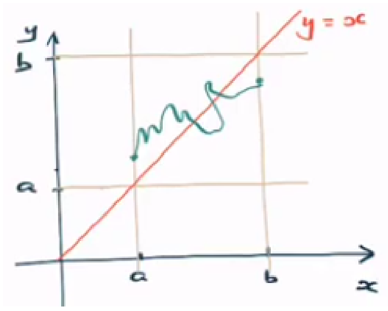


Fig 2.0 function f

Since f is continuous function, f will intersect with function y = x at at least one point. Hence there will be at least one fixed point independent of what f is.
Fact 1: If X is closed a compact convex set and f is continuous, then f has a fixed point. (Brouwer's FP theorm)
Fact 2: Closed and bounded sets in $\mathbb{R}^n$ are compact.
$\rightarrow$ What's our X?
X = set of all prob. vectors in $\mathbb{R}^n$. $(n = |V(G)|)$
$= \{(p_1, .., p_n) : p_i \geq 0, \sum p_i = 1\}$

→ Verify that X is:

(i) convex ($p, q \in X$, $then\, \lambda p + (1-\lambda)q \in X$)

(ii) bounded ($||x||_\infty : max x_i$, $then \{||x||_\infty : x \in X\} \leq B = 1$)

(iii) closed

→ Then f : X → X

x $\mapsto P^T x$

→ Verify f is continuous.

So f has a fixed point in X. That is your stationary distribution.

Direct Proof:

Let x be any prob. vector

Consider the sequence of prob. vector - $x, xP, xP^2, xP^3, ...$ (Evolution of the random walk x(0), x(1), ... where $x(t) = xP^t$)

Let **"long-term average"** be a(t) = (1/t)(x(0) + x(1) + ... x(t-1))
$= (1/t)(x + xP + ... + xP^{t-1})$

Claim 1: $\forall t$, a(t) is a prob. vector

therefore, a(1), a(2), ... $\in X$

X is bounded ⇒ a(1), a(2), ... contains a convergent subsequence $a(t_1), a(t_2), ...$(proof: pigeonhole principle)

X is closed ⇒ $lim_{n \to \infty} a(t_n) = a \in X$. (i.e. a is a prob. vector)

$$\forall t,\, a(t)P - a(t) = (1/t)(xP + xP^2 + ... + xP^t) - (1/t)(x + xP + ... + xP^{t-1})$$

$$= (1/t)(xP^t - x)$$

$$||a(t)P - a(t)||_\infty \leq (1/t) \quad - (*)$$

$$||a(t_n)P - a(t_n)||_\infty \leq (1/t_n) \to 0\, as\, n \to \infty$$

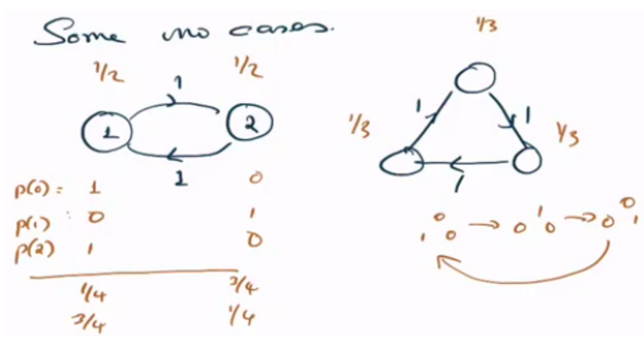
$$\Rightarrow ||aP - a||_\infty = 0$$

$$aP = a$$

Hence a is a stationary distribution.

Question. If p(0) is an arbitrary starting distribution. Does $p(n) = p(0)P^n \to \pi\ as\ n \to \infty$ **?**

Ans. Not always but Yes in most cases.



(Fig 2.1)

Yes iff gcd of lengths of all directed cycles in G is 1.

2.1 Summary

1. Every random walk on a finite graph has a stationary distribution π. $(\pi P = \pi)$
2. If the graph is strongly connected then the stationary distribution is unique and $a(t) \to \pi \; as \; t \to \infty$
3. If the graph G is strongly connected and gcd(cycle length) = 1, for any prob. vector p(0), $p(t) \to \pi \; as \; t \to \infty$

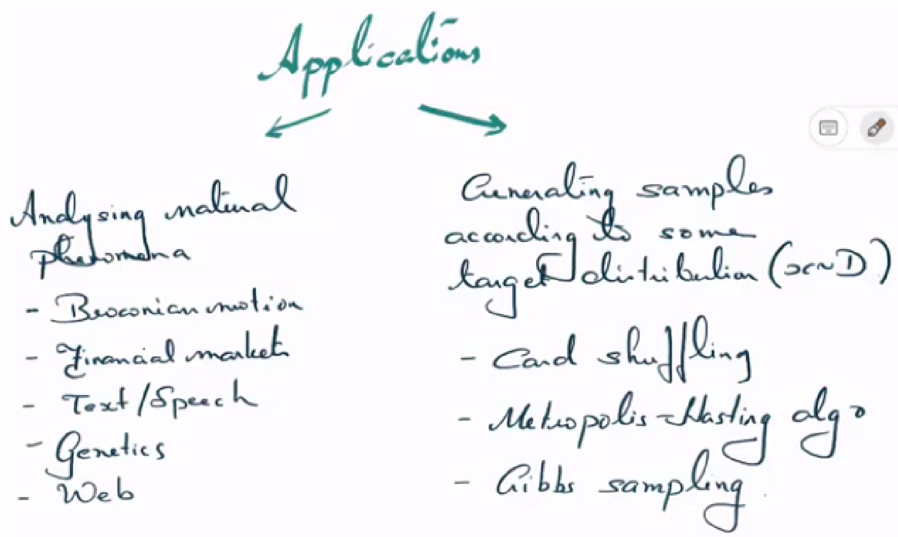


Fig 2.2 applications of point(3.)