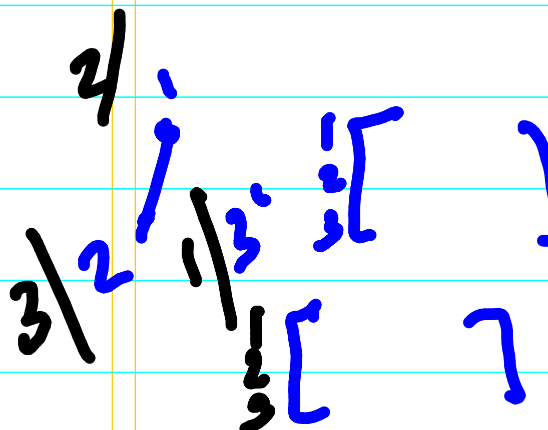
Q1: Is the adjacency matrix a unique representation of a graph (modulo isomorphism)

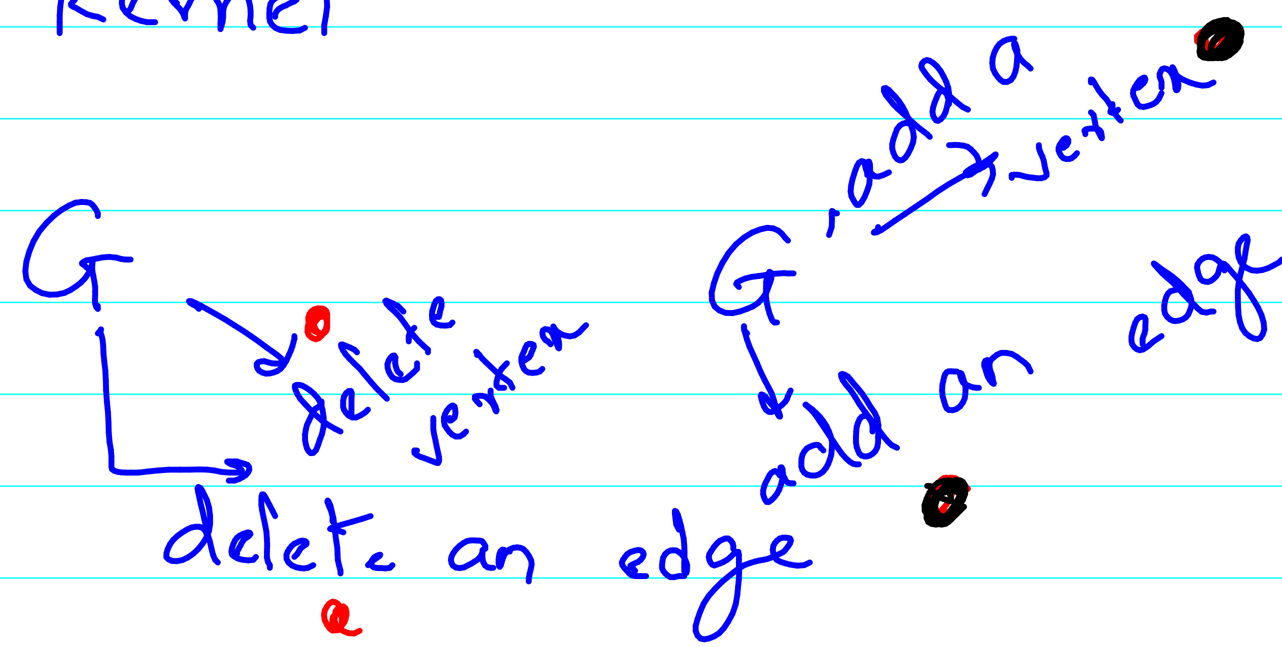


Q2: Is the set of all sub graphs a unique representation?

Subgraph isomorphism:

G, G': if a sugraph of G is isomorphic to G' then G' is said to be subgraph isomorphic to G

Problems with edit distance kernel



Problem: Each red pt (graph) will need be compared for isomorphism with each black pt (graph)

Topological descriptor:

G → # degree 3 nodes

" " 5 nodes

cliques

simple cycles (only repetition is start node)

of shortest paths of length k

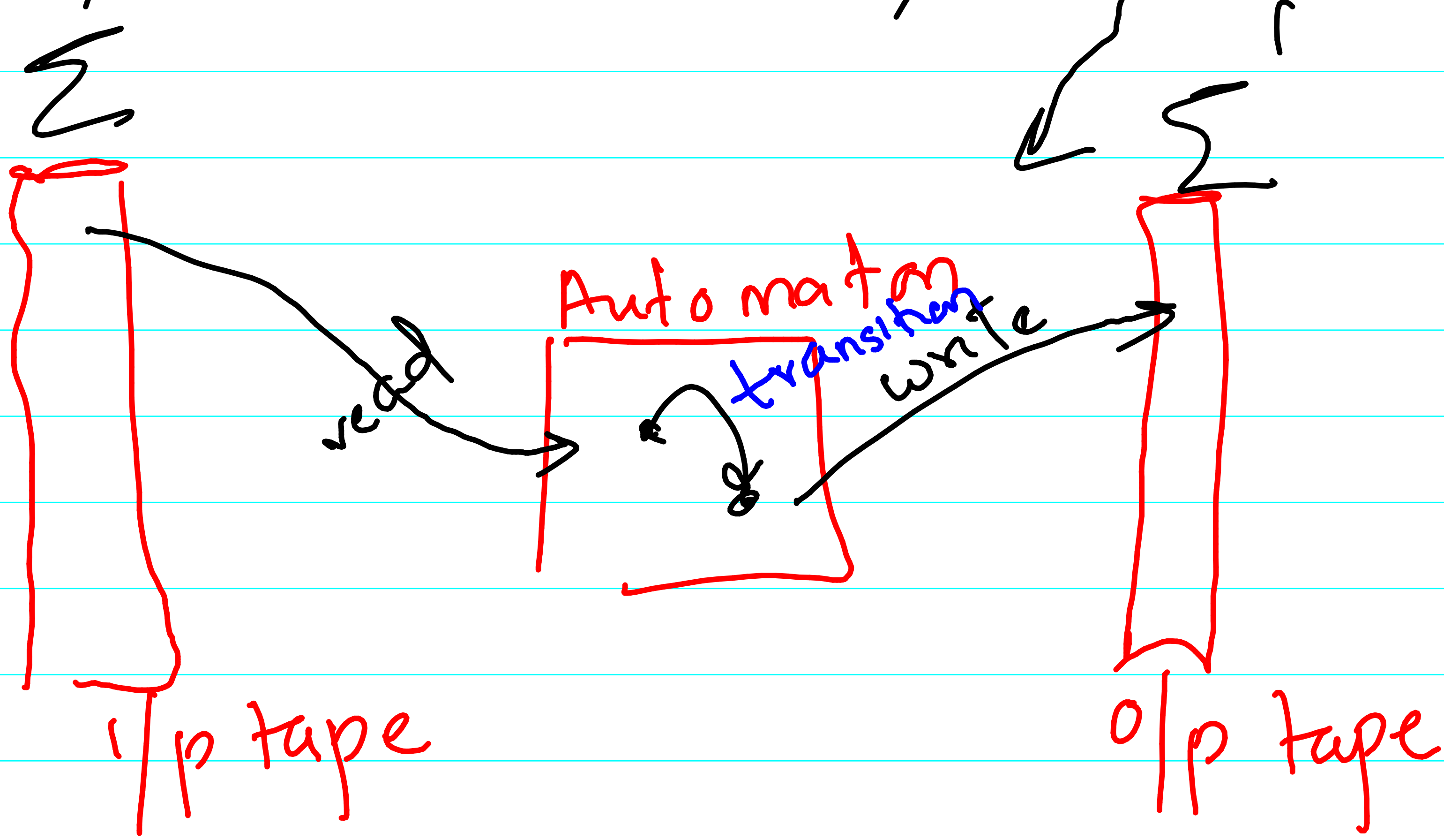
All pairs shortest paths in $O(n^3)$ time

Properties centred around "special" nodes (eg on web, look at News pages & vicinity

Graph kernels are instances of

Convolution kernels (generalization of parse tree kernels)

Rational kernel



Walk Graph kernels are rational

kernels with following restrictions:

① $\Sigma = \Sigma'$

② $\Sigma = \Sigma' = \{a\}$

walk label

Random walk Kernel:

$$A^2 = \begin{bmatrix} 2 & \cdots & \cdots \\ & & \\ & & \end{bmatrix}$$

corresponds to the fact that I can move out to 2 & back from them

H/W. Q: How to avoid moving back to a node immediately?

One soln: Modify both G_1 & G_2

$G_1 : \langle V_1, E_1 \rangle$ $\qquad$ $G_2 : \langle V_2, E_2 \rangle$

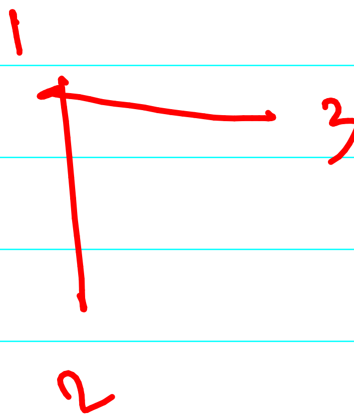
$G_1' : \langle V_1', E_1' \rangle$

$$V_1' = V_1 \cup \{(u,v) \in E_1\}$$

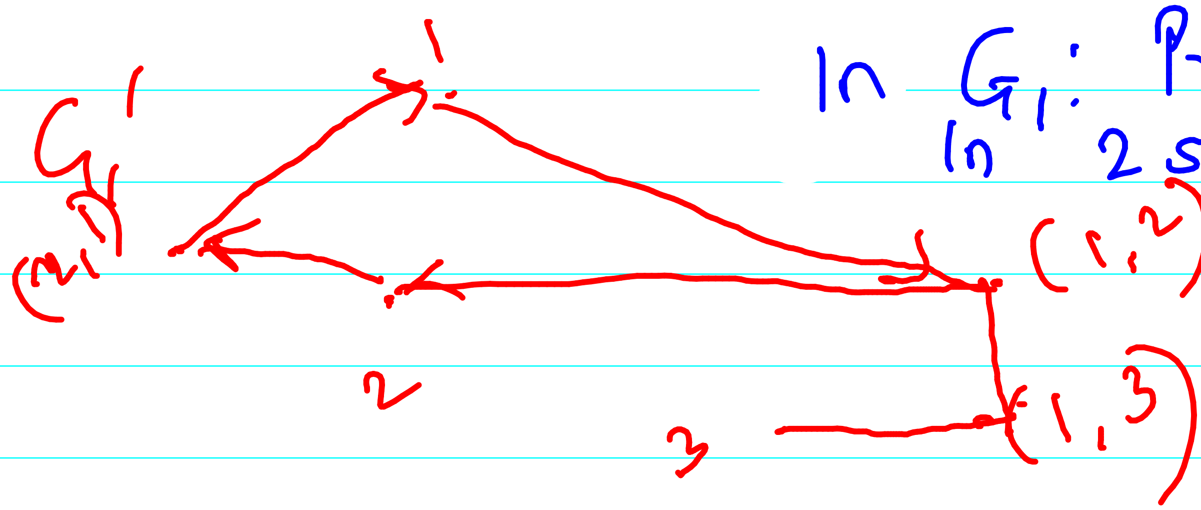
& $E_1' = \{(u, (v,w)) \mid u \in V, (v,w) \in E\}$

$$\bigcup \left\{ ((u,v),(v,w)) \;\middle|\; \begin{array}{l}(u,v) \in E \\ (v,w) \in E\end{array} \right\}$$

G_1 :



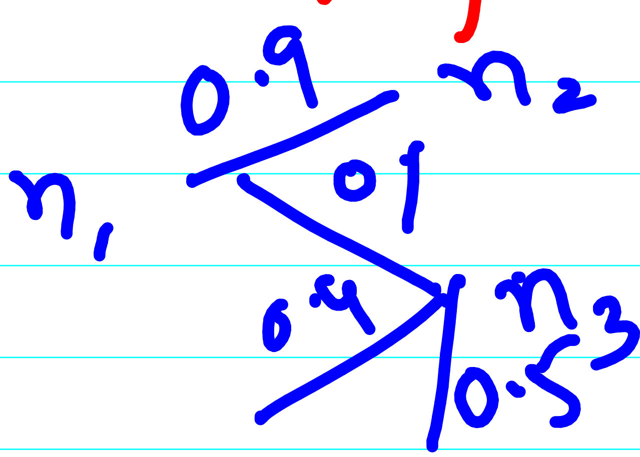
In G_1: $\Pr(1 \to 1$ in 2 steps$) > 0$

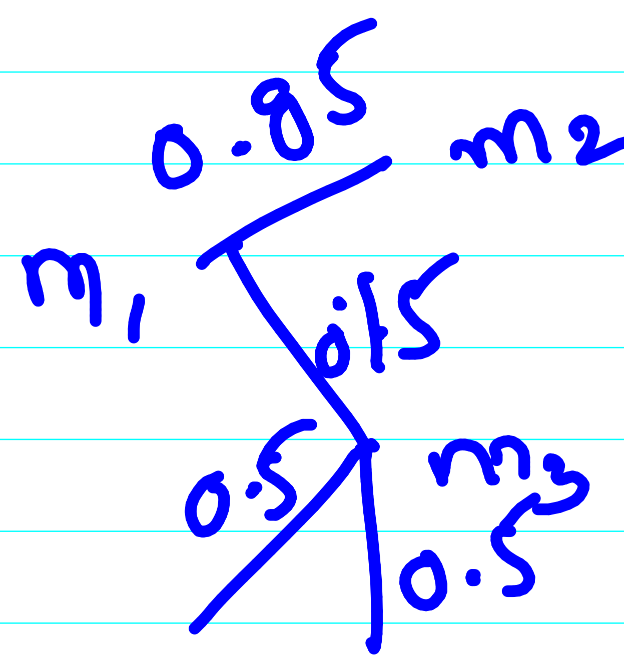


In G_1': $\Pr(1 \to 1$ in 2 steps$) = 0$

$\Pr(1 \to 1$ in 4 steps$) > 0$

Random walk kernel goal:
Nodes similar (as per random walks) in one graph should be similar to node pairs (with similar "similarity" neighbourhood) in other graph





2 choices: for $\mu(k)$

$$k(i,j) = \left[\sum_{k=0}^{\infty} \mu(k) A^k\right]_{i,j}$$

Similarity between 2 nodes in same graph

$\mu(k)$

λ^k

$\frac{\lambda^k}{k!}$.

$$K(G_1, G_2) = \frac{1}{|G_1||G_2|} \sum_{i} \sum_{j} \left(\sum_{k=0}^{\infty} \mu(k) A_{\times}^k\right)$$

Similarity between 2 graphs

$$= \frac{1}{|G_1||G_2|} \sum_{k=0}^{\infty} \mu(k) e^T A_{\times}^k e$$

e is a column vector of 1's

i.e

$$\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

Let us prove that

$K(G_1, G_2)$ is p.s.d.

① Understand $A_\otimes$

② Prove that

$$K(G_1, G_2) = \frac{1}{|G_1||G_2|} \sum_{k=0}^{\infty} \lambda^k p_\otimes^T A_\otimes^k q_\otimes$$

is p.s.d kernel

Hint: ① $(A \otimes B)(C \otimes D) = AC \otimes BD$

② For our problem

$A_\otimes = A_1 \otimes A_2$

(where A_1 & A_2 are adj

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matrices of G_1 & G_2 resp.)

Similarly: $q_{\otimes} = q_1 \otimes q_2$

$$p_{\otimes} = p_1 \otimes p_2$$