Course: CSC591/791, Graph Data Mining: Theory, Algorithms, and Applications
Final Exam: Comprehensive, home-take exam.
STUDENT's ID: avshirod

This exam is intended to be an **individual** effort. You are allowed to use and reference the materials posted on Moodle, cited in the exam, your homework assignments, your notes, the class slides, and the lecture assignments. You are **NOT** allowed to use the other sources, such as your classmates and the internet at large.

1. Good luck!
2. You get BONUS 5 points if your solution is in LaTeX (both source and PDF)
3. Otherwise, a PDF (even a scanned hand-written solution) must be uploaded into Moodle
4. The Total Exam Score by the TA: ______ out of **(100 points)**

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Agreed: *avshirod* Date: *December 1st, 2016*

1. ________ out of **(15 points)**: Given an infectious disease following the SIS virus propagation model with transmission probability $\beta = 0.3$ and healing probability $\delta = 0.5$, in a contact network with 10 nodes and the following edges: $\{(0, 1), (0, 3), (1, 4), (2, 3), (2, 6), (5, 6), (5, 7), (6, 7), (7, 9), (8, 9)\}$, answer:

   (a) ________ out of **(1 point)**: What is the spectral radius of the network?

   (b) ________ out of **(1 point)**: What is the effective strength of the virus?

   (c) ________ out of **(1 point)**: According to the theorem studied in class [1], can the infection result in an epidemic?

   (d) ________ out of **(9 points)**: Using the NetShield algorithm [2], which 3 nodes should be immunized to minimize the spread of the infection?

   (e) ________ out of **(3 points)**: After immunizing the 3 nodes selected in (4), can the infection result in an epidemic?

References:

1 B. A. Prakash, D. Chakrabarti, M. Faloutsos, N. Valler, C. Faloutsos. Got the Flu (or Mumps)? Check the Eigenvalue! arXiv:1004.0060 [physics.soc-ph], 2010.

2 H. Tong, B. A. Prakash, C. Tsourakakis, T. Eliassi-Rad, C. Faloutsos, D. H. Chau. On the Vulnerability of Large Graphs. In ICDM, 2010.

Ans:
VPM - SIS

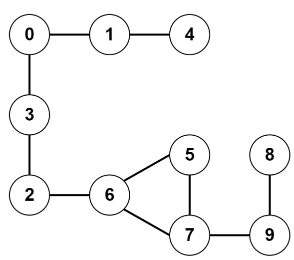


Figure 1: Visualizing the SIS network graph

$\beta = 0.3$ # Nodes $n = 10$
$\delta = 0.5$ # Edges $e = 10$

(a) Spectral Radius = 2.373 (Max eigenvalue of AdjMat - λ_1)

(b) Effective Strength
$S = \lambda_1 * C_{VPM} = \lambda_1 * \frac{\beta}{\delta} = 2.373 * \frac{0.3}{0.5} = 1.4238$

(c) Epidemic?
As effective strength $S = 1.4238 > 1$,
$\therefore$ Epidemic.

(d) 3 nodes that should be immunized to minimize the spread of the infection, as per *NetShield* algorithm $= \{6, 7, 5\}$

(e) Vaccinate above nodes. Epidemic now?
λ_1 of modified graph $= 1.732$
$S = \lambda_1 * C_{VPM} = 1.732 * 0.6 = 1.0392 > 1$
$\therefore$ Still Epidemic.

NOTE:
Although the NetShield algorithm implemented below is giving nodes $[6, 7, 5]$ as the output, it is not the optimum output (because it does not stop the epidemic.
If we vaccinate nodes $[6, 7, 0]$ instead, then we get eigenvalue as 1 and $S = 0.6 < 1$. And we'll be able to stop the epidemic.

Listing 1: Code for NetShield Algorithm

```
import networkx as nx
import numpy as np
from scipy.sparse import linalg

g = nx.Graph()
g = nx.read_edgelist('q1edges.txt', nodetype=int)

def get_largest_eigens(graph):
    adj = nx.to_scipy_sparse_matrix(graph, dtype=
        float)
    eigenvalue, eigenvector = linalg.eigs(adj.T, k=1,
         which='LR')
    return eigenvalue, eigenvector
# largest = u1.flatten().real

g.A = nx.adjacency_matrix(g)
g.eig = nx.linalg.adjacency_spectrum(g)
lambda_1, mu_1 = get_largest_eigens(g)

def shield_value_score(graph, node):
    eigenval, eigenvec = get_largest_eigens(graph)
    eigenvector = eigenvec.flatten()
    score = 2 * eigenval.real * (eigenvector[node].
        real ** 2)
    return score
```

```python
def netshield(graph, k):
    lambda_1, mu_1 = get_largest_eigens(graph)
    svs = [shield_value_score(graph, node) for node
        in graph.nodes()]
    s = []
    while (len(s) < k):

        def get_netshield_score(node):
            adj = nx.adjacency_matrix(graph)
            score = svs[node] - 2 * (adj[:,s] * mu_1[
                s].real) * mu_1[node].real
            return score

        scores = np.array([get_netshield_score(node)
            for node in graph.nodes()])
        scores[s] = -99999
        scores = scores.tolist()
        s.append(scores.index(max(scores)))
    return s

k = 3
to_vaccinize = netshield(g, 3)
print("Nodes to Vaccinize = %r" % to_vaccinize)

g_vacc = g.copy()
g_vacc.remove_nodes_from(to_vaccinize)
g_vacc.eig = nx.linalg.adjacency_spectrum(g_vacc)
print("Lambda_1 after Vaccination  = %r" % max(g_vacc
    .eig))

t = g.copy()
v = [6,7,0]
print("Nodes to Vaccinize = %r" % v)
t.remove_nodes_from(v)
print("Lambda_1 after Vaccination  = %r" % max(nx.
    linalg.adjacency_spectrum(t)))

'''
Output:
Nodes to Vaccinize = [6, 7, 5]
Lambda_1 after Vaccination  = (1.7320508075688774+0j)
Nodes to Vaccinize = [6, 7, 0]
Lambda_1 after Vaccination  = (1+0j)
'''
```

2. ________ out of **(15 points)**: Given random variables x, y, w, z, **prove or disprove** the following statements about their conditional independence ($\perp$) relationships (see the lecture on D-separation and example below; if you decide to disprove the stmt, then a counter-example of a DAG will suffice):

(a) ________ out of **(0 points)**: Example: $(x \perp y, w | z) \implies (x \perp y | z)$

Proof:

$$p(x, y|z) = \sum_w p(x, y, w|z) = \sum_w p(x|z)p(y, w|z) =$$
$$p(x|z) \sum_w p(y, w|z) = p(x|z)p(y|z)$$

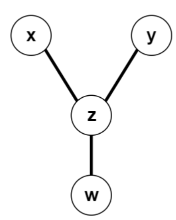
(b) ________ out of **(6 points)**: $(x \perp y, z) \& (x, y \perp w | z) \implies (x \perp w | z)$

(c) ________ out of **(9 points)**: $(x \perp y, z) \& (x \perp y | w) \implies (x \perp y | z, w)$

Ans:

(a) Proved.

(b) **TPT:** $(x \perp y, z) \& (x, y \perp w | z) \implies (x \perp w | z)$



$$x \perp y, z \implies P(x|y, z) = P(x) \qquad (1)$$
$$x, y \perp w | z \implies P(x, y|w, z) = P(x, y|z) \qquad (2)$$

Now,

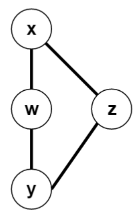
$$\begin{aligned} P(x|w, z) &= \sum_y P(x, y|w, z) && \text{Introducing sum over 'y'} \\ &= \sum_y P(x, y|z) && \text{from (1)} \\ &= P(x|z) && \text{from (2)} \end{aligned}$$

$\therefore x \perp w | z$

(c) **TPT:** $(x \perp y, z) \& (x \perp y | w) \implies (x \perp y | z, w)$

$$x \perp y, z \implies P(x|y, z) = P(x) \tag{1}$$
$$x \perp y | w \implies P(x|y, w) = P(x|w) \tag{2}$$

Now consider the following graph -



In above graph, the second condition does not hold True, as not all paths from x to y go through w $(x - z - y)$.

$\therefore$ *Disproved.*

3. ______ out of (**15 points**): Suppose you need to design an efficient algorithm for analysizing random walks of an undirected simple graph G. Let A be its adjacency matrix with Singular Valude Decomposition (SVD) $A = U\Lambda U^t$.

   (a) ______ out of **(5 points)**: Prove that the power matrix $A^k = U\Lambda^k U^t$.

   (b) ______ out of **(10 points)**: Devise an efficient algorithm to compute A^k for different values of k. What is its Big-O complexity?

Ans:
Random walks on Undirected Simple Graphs.
$A =$ Adj Matrix
$A = U\Lambda U^t$

A is a symmetric matrix $\implies A = A^T$.
Also, A is a positive, semi-definite matrix $\implies$ all λ_i are real and $\lambda_i \geq 0$

(a) Prove: $A^k = U\Lambda^k U^t$

As U and U^T are orthonormal matrices, (SVD property)
$\therefore U * U^T = I$ (Also $U^T * U = I$).

For $k = 2$,

$$\begin{aligned} A^2 = A * A &= U\Lambda U^T * U\Lambda U^T \\ &= U\Lambda I \Lambda U^T \\ \therefore A^2 &= U\Lambda^2 U^T \end{aligned}$$

Similarly for $k = 3$,

$$\begin{aligned} A^3 = A^2 * A &= U\Lambda^2 U^T * U\Lambda U^T \\ &= U\Lambda^2 I \Lambda U^T \\ \therefore A^3 &= U\Lambda^3 U^T \end{aligned}$$

By induction, we can say that -
$A^k = U\Lambda^k U^t$

(b) A pseudo code for the algorithm is as follows -

Listing 2: An efficient algorithm to compute A^k

```
# A is a n*n matrix
def power_mat(A, k):
        if k is even:
                a_square = A*A
                return pow(2,k/2) * a_square
        else:
                return pow(2,(k-1)/2) * A
```

As A is a symmetric square matrix, and it represents an undirected simple graph (with no cycles or self loops), we can mathematically see that, powers of A are scalar multiples of either A or A^2.
After computing powers of A upto A^8 for some random examples, it was observed that if k is even, then $A^k = 2^{k/2} * A^2$.
Otherwise (when k is odd), $A^k = 2^{(k-1)/2} * A$.

If k is even, then we have to compute $A*A$, which is a matrix multiplication of nxn size matrix. So the overall complexity of the algorithm is $O(n^{2.371})$ (using Strassen's modified algorithm for matrix multiplication).
But as $k \to n$, the general algorithm will have a complexity of $O(n^{3.371})$, but the algorithm presented above will requires the same amount of time.

4. ________ out of (**10 points**): Let G be an undirected complete bi-partitie graph. Prove that if λ is an eigenvalue of its adjacency matrix then $-\lambda$ is also its eigenvalue. Hint: Assume that after the permutation of rows and columns, the adjacency matrux is of the form:

$$A = \begin{pmatrix} 0 & B \\ B^t & 0 \end{pmatrix}$$

Ans:
G: Undirected Complete Bi-partite graph
A: Adjacency matrix
For a complete undirected bi-partite graph G ($K_{m,n}$), the adjacency matrix would look like -

$$A = \begin{pmatrix} 0 & B \\ B^t & 0 \end{pmatrix}$$

The dimensions of B would be (m, n).

As told in lecture on graph spectra (Lecture #08), the graph spectra for such a graph is $= \pm\sqrt{m * n}$.
with all others eigenvalues zero except λ_{max} and λ_{min}.

Let's assume we have λ as one eigenvalue of A.
Now, as G is undirected bi-partite, all the eigenvalues must sum up to zero. ($Trace(A) = 0$).
$\therefore$ The sum of the rest of the eigenvalues must be equal to $-\lambda$.

As the two elements in adjacency matrix A are symmetric (B and B^T), we can see that there will be two distinct eigenvalues, and the rest will be zero.
Now, as one of the eigenvalues is λ (fixed because of our assumption), there remains only one other distinct value. And as the eigenvalues should sum up to zero, it has to be $-\lambda$.

5. ______ out of (**20 points**): Consider the following training examples:

Instance	x_1	x_2	x_3	class, y
1	T	T	T	+
2	T	T	T	+
3	F	F	T	+
4	F	T	F	-
5	T	F	T	-
6	T	F	F	-
7	F	F	F	-
8	F	T	F	-

(a) ______ out of **(10 points)**: You will be using a naïve Bayes classifier for this question. Given a test example with attributes $x_1 = T$, $x_2 = T$, and $x_3 = F$, which class will be assigned to this test example? Show your work clearly.

(b) ______ out of **(10 points)**: Repeat the question in part (a) using the following Bayesian Belief network as the classifier:

$$x_3 \to x_2 \to y \to x_1$$

Ans:

(a) $x : x_1, x_2, x_3$ $\qquad n = 8$
$y : +, -$
$P(x_1 = T, x_2 = T, x_3 = F, y = +) =?$
Let's assume value of y to be $+$.

$$P(y = +) = 3/8 = 0.375$$
$$P(y = -) = 5/8 = 0.625$$

$$\begin{aligned} P(x_1 = T, y = +) &= P(y = +) * P(x_1 = T|y = +) \\ &= 0.375 * 2/3 = 0.250 \end{aligned}$$

$$\begin{aligned} P(x_2 = T, y = +) &= P(y = +) * P(x_2 = T|y = +) \\ &= 0.375 * 2/3 = 0.250 \end{aligned}$$

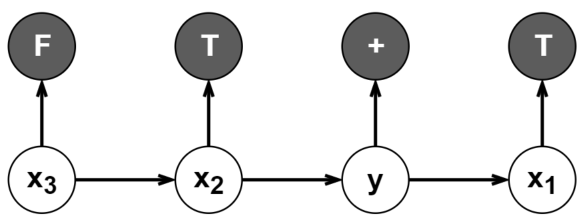
$$\begin{aligned} P(x_3 = T, y = +) &= P(y = +) * P(x_3 = F|y = +) \\ &= 0.375 * 0 = 0 \end{aligned}$$

Now, the probability of observed data = 1.
$\therefore P(x_1 = T, x_2 = T, x_3 = F) = 1$

$$\begin{aligned}
P(y = +|x_1 = T, x_2 = T, x_3 = F) &= \frac{P(x_1 = T, x_2 = T, x_3 = F, y = +)}{P(x_1 = T, x_2 = T, x_3 = F)} \\
&= P(y = +) * P(x_1 = T, x_2 = T, x_3 = F|y = +) \\
&= P(y = +) * P(x_1 = T|y = +) * \\
&\quad P(x_2 = T|y = +) * P(x_3 = F|y = +) \\
&= 0.375 * 0.250 * 0.250 * 0 \\
&= 0
\end{aligned}$$

$\therefore P(y = +|T, T, F) = 0$
$\therefore P(y = -|T, T, F) = 1$
$\therefore$ Classify as $y =' -'$.

(b) $P(y|x_3 = F, x_2 = T, x_1 = T) =?$



Let $X : x_3 = F, x_2 = T, x_1 = T$
We know that $P(X) = 1$, as it is observed.

Now,

$$\begin{aligned}
P(y = +|X) &= \frac{P(y = +, X)}{P(X)} \\
&= P(x_3 = F)P(x_2 = T|x_3 = F)P(y = +|x_2 = T)P(x_1 = T|y = +) \\
&= 4/8 * 2/4 * 2/4 * 2/3 = 1/12 \\
&= 0.0833
\end{aligned}$$

$$\begin{aligned}
P(y = -|X) &= \frac{P(y = -, X}{X} \\
&= P(x_3 = F)P(x_2 = T|x_3 = F)P(y = -|x_2 = T)P(x_1 = T|y = -) \\
&= 4/8 * 2/4 * 2/4 * 2/5 = 1/20 \\
&= 0.05
\end{aligned}$$

As $P(y = +|X) > P(y = -|X)$, classify as '+'.

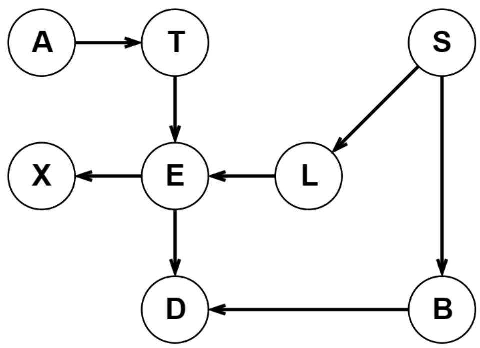
6. ________ out of (**10 points**): Show the key steps of the Junction Tree algorithm for the following DAG (Note: No need to show the details of the last step, i.e., the Belief Propagation inference step):

$$A \to T \to E \to D; S \to L \to E \to X; S \to B \to D$$

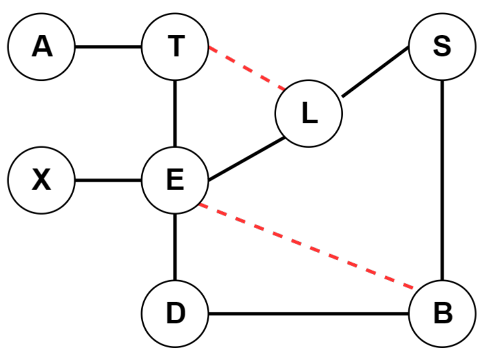
Ans:

Junction Tree Algorithm

(a) Start with DAG

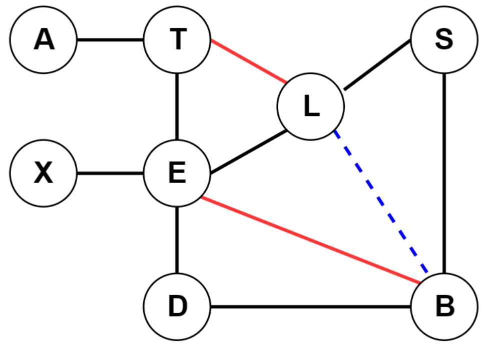


(b) Convert DAG $\to$ Undirected Graph (with Moralization)



(c) Triangulation

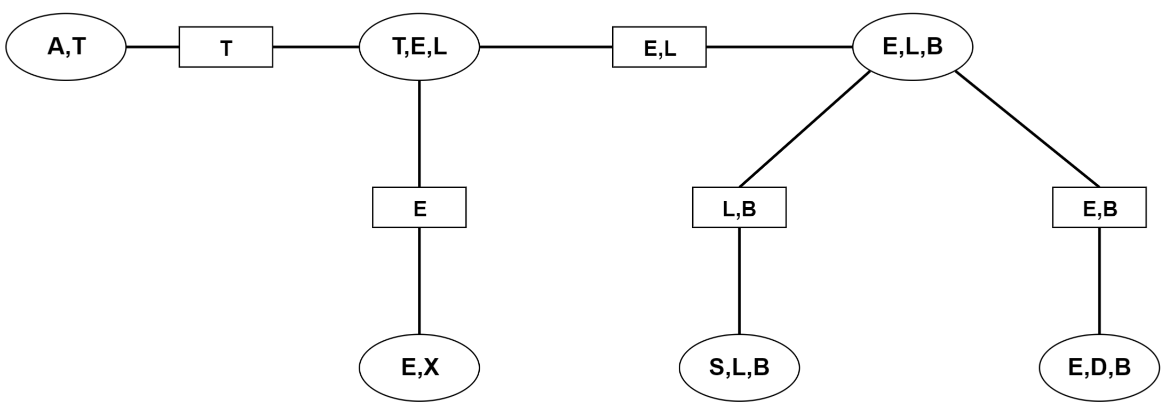
Cycle with more than 3 nodes $= S - B - E - L - S$
Converted to a triangle by adding edge $B - L$.



(d) Find cliques

$$
\begin{aligned}
c_1 &= A, T \\
c_2 &= T, E, L \\
c_3 &= E, X \\
c_4 &= S, L, B \\
c_5 &= E, D, B \\
c_6 &= E, L, B
\end{aligned}
$$

(e) Create a junction tree



7. ______ out of (**15 points**): Using the Maximum Likelihood estimation, find the parameters for the following Bernoulli Trials problem (show all the derivations):
INPUT:

- M iid coin flips: $D = H, H, T, H, ...$
- Model: $p(H) = \theta$ and $p(T) = 1 - \theta$

OUTPUT: θ^*_{ML}

(a) ______ out of **(10 points)**: What is the likelihood function $l(\theta; D) = \log p(D|\theta)$? (Hint: Introduce a random variable x that is equal to 1 if the trial is a Head and it is equal to zero if the trial is a Tail.)

(b) ______ out of **(5 points)**: What is θ^*_{ML}?

Ans:

MLE - Bernoulli trials
i/p: 'M' `i.i.d.` coin flips
$D = H, H, T, H$
model: $P(H) = \theta$ and $P(T) = 1 - \theta$
o/p : θ^*_{ML}

(a) For Bernoulli trials,
$f(x) = p^x * (1-p)^(1-x)$
$x = 0, 1$

Converting $D = H, H, T, H, ... \rightarrow D = x_1, x_2, ..., x_m$
by assuming $x_i = 1$ if $D_i = H$
and $x_i = 0$ if $D_i = T$
$\therefore D_{new} = 1, 1, 0, 1, ...$
Now, based on assumptions above -

$$\begin{aligned} P(\theta|x) &= \theta^{x_1}(1-\theta)^{1-x_1} \ldots \theta^{x_m}(1-\theta)^{1-x_n} \\ &= \theta^{x_1+\ldots+x_m}(i-\theta)^{n-(x_1+\ldots+x_m)} \end{aligned}$$

$$\begin{aligned} \ln L(\theta|x) = \log P(\theta|D) &= \ln\theta \sum_{i=1}^{M} x_i + \ln(1-\theta)(n * \sum_{i=1}^{M} x_i) \\ &= n\bar{x}\ln\theta + n(1-\bar{x})\ln 1 - \theta \end{aligned}$$

(b) To find θ^*_{ML}, taking partial derivative wrt θ, -

$$\frac{\partial \ln L(\theta|x)}{\partial\theta} = n\left(\frac{\bar{x}}{\theta} + \frac{1-\bar{x}}{1-\theta}\right) = 0$$
$$\therefore \frac{\bar{x}}{\theta} = \frac{1-\bar{x}}{1-\theta}$$
$$\therefore \bar{x} - \bar{x}\theta = \theta - \bar{x}\theta$$
$$\therefore \theta^* = \bar{x}$$

Since $x = 0, 1$,
taking average/mean gives us the probability θ for $x = H$,
and $1 - \theta$ for $x = T$.

Intuitively, say for $M = 5$,

$$D = H, H, T, H, T \implies x_i = 1, 1, 0, 1, 0$$
$$P(x = H) = \frac{3}{5} \implies \bar{x} = \frac{\sum_{i=1}^{M} x_i}{M} = \frac{1+1+0+1+0}{5} = \frac{3}{5}$$
$$\text{and } P(x = T) = 1 - \frac{3}{5} = \frac{2}{5} \implies 1 - \bar{x} = \frac{2}{5}$$