# Random Graph theory

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## 1 Basics of Graph Theory

- A graph $G$ is a pair of sets $G = (V, E)$ where $V$ is a set of vertices, $E$ is a set of edges, and $e \in E$ can be written as $e = (x, y)$ with $x, y \in V$.
- It is comon to represent a graph by *drawing*. Each vertex $v \in V$ is represented as a point in the plane, while edges are lines connecting pairs of points.

There are a number of special graphs, which we will only mention.

- A graph with $n$ nodes is **complete** (denoted by $K_n$) if every node forms an edge with every other node.
- A **cycle graph** (denoted by $C_n$) is a graph that consists of nodes connected in a closed chain. The degree of each vertex is 2.
- A **tree** is a connected graph with no cycles.

The following theorem will get you started with the basics of graph theory.

**Theorem 1.1 First theorem of graph theory**

A finite graph $G$ has an even number of vertices with odd **degree** (i.e. the number of edges incident to it).

*Proof.* Since each edge connects 2 nodes,

$$2|E| = \sum_{v \in V} deg(v) = \sum_{\substack{v \in V \\ deg(v) \text{ even}}} deg(v) + \sum_{\substack{u \in V \\ deg(u) \text{ odd}}} deg(u) \implies \left( \sum_{\substack{u \in V \\ deg(u) \text{ odd}}} deg(u) \right) \text{ is even.}$$

If the sum is even, and each summand is odd, then there must be an even number of summands. □

## 2 Sharp Threshold for Connectivity in Erdos-Renyi Graph Model

Most materials for this section note is taken from [1, 4]. First some background:

- We use $G(n,p)$ to denote an undirected (Erdos-Renyi) graph with $n$ nodes and probability of forming an edge $p(n)$.
- Each edge forms with probability $p \in (0,1)$ **independently** of other edges.
- An graph is **connected** if there is a path between any 2 pairs of nodes.
- When $p = p(n)$ is a function of $n$, we may be interested in the behavior of $G(n,p(n))$ as $n \to \infty$.

## 2.1 Warm-up

**Q1. What is the probability that a vertex is isolated in $G(n,p)$? Ans:** A given node $i$ cannot form an edge with each of the remaining $n-1$ nodes. Thus the probability is $(1-p)^{n-1}$.

**Q2. What is the probability that node 1 and node 2 are both isolated? Ans:** Let $I_1, I_2$ be the indicator that node 1 and node 2 are isolated. Then $P(I_1 \cap I_2) = P(I_1)P(I_2 \mid I_1) = (1-p)^{n-1} * (1-p)^{n-2} = (1-p)^{2n-3}$.

**Q3. What is the probability that a group of $k$ nodes do not connect to the rest of the $n-k$ nodes? Ans:** There are $\binom{n}{k}$ number of ways to choose $k$ vertices. Each of these cannot form an edge with the remaining $n-k$ nodes independently with probability $(1-p)^{n-k}$. So overall we have $(1-p)^{(n-k)k}$.

**Theorem 2.1 Erdos-Renyi 1961**

Consider a graph $g \sim G(n,p(n))$ where $p(n) = \lambda \frac{\ln(n)}{n}$. Then as $n \to \infty$,

$$P(g \text{ connected}) \to 0 \quad \text{if } \lambda < 1$$
$$P(g \text{ connected}) \to 1 \quad \text{if } \lambda > 1$$

*Proof.* Suppose $\lambda < 1$. Since $P(\text{connected}) = 1 - P(\text{disconnected})$, we will show $P(\text{disconnected}) \to 1$ by showing that **there is at least 1 isolated node**. Define

- $X_n$ to be a random variable that counts the number of isolated nodes
- $I_i$ to be a (Bernoulli) indicator random variable such that $I_i = 1$ when node $i$ is isolated and is 0 otherwise
- Let $p = p(n)$ and $q = q(n) = (1-p(n))^{n-1}$ be the probability of a node being isolated

We want to show $P(X_n > 0) \to 1$, or equivalently, $P(X_n = 0) \to 0$. To get a bound on $P(X_n = 0)$, we observe:

$$\begin{aligned}
\text{Var}(X_n) &= E\left(X_n - E(X_n)\right) \\
&= P(X_n = 0)(0 - E(X_n)^2 + P(X_n = 1)(1 - E(X_n))^2 + \ldots \\
&\geq P(X_n = 0)E(X_n)^2.
\end{aligned}$$

Thus

$$\frac{\text{Var}(X_n)}{E(X_n)^2} \geq P(X_n = 0). \tag{2.1}$$

We will now calculate $\text{Var}(X_n)$ and $E(X_n)$ explicitly to show that the left hand side of (2.1) goes to 0. By

linearity of expectation and applying definition of indicators,

$$E(X_n) = E\left(\sum_{i=1}^{n} I_i\right) = \sum_{i=1}^{n} E(I_i) = \sum_{i=1}^{n} P(I_i) = nq.$$

Since indicators $I_i$ are **not independent** (why?), we use equation (1.10) in your book [3]:

$$\begin{aligned}
\mathrm{Var}(X_n) &= \mathrm{Var}\left(\sum_{i=1}^{n} I_i\right) = \sum_{i=1}^{n} \mathrm{Var}(I_i) + \sum_{i=1}^{n}\sum_{j\neq i} \mathrm{Cov}(I_i, I_j) \\
&= \sum_{i=1}^{n} q(1-q) + \sum_{i=1}^{n}\sum_{j\neq i} [E(I_i I_j) - E(I_i)E(I_j)] \quad (\text{since Var(Bernoulli)} = p(1-p)) \\
&= nq(1-q) + \sum_{i=1}^{n}\sum_{j\neq i} [P(I_i \cap I_j) - P(I_i)P(I_j)] \\
&= nq(1-q) + \sum_{i=1}^{n}\sum_{j\neq i} \left[(1-p)^{n-1}(1-p)^{n-2} - (1-p)^{n-1}(1-p)^{n-1}\right] \\
&= nq(1-q) + \sum_{i=1}^{n}\sum_{j\neq i} \left[\frac{q^2}{1-p} - q^2\right] \\
&= nq(1-q) + n(n-1)q^2\frac{p}{1-p}.
\end{aligned}$$

Thus

$$\frac{\mathrm{Var}(X_n)}{E(X_n)^2} = \frac{nq(1-q) + n(n-1)q^2\frac{p}{1-p}}{(nq)^2} = \frac{1-q}{nq} + \frac{n-1}{n}\frac{p}{1-p}.$$

We will now show these terms approach 0 as $n \to \infty$, then eq (2.1) will give us what we need. The first term is dominated by $nq$, and

$$\begin{aligned}
\lim_{n\to\infty} nq &= \lim_{n\to\infty} n(1-p)^{n-1} = \lim_{n\to\infty} \exp\{\ln(n) + (n-1)\ln(1-p)\} \\
&= \lim_{n\to\infty} \exp\left\{\ln(n) + (n-1)\ln\left(1 - \frac{\lambda\ln(n)}{n}\right)\right\} \\
&\approx \lim_{n\to\infty} \exp\left\{\ln(n) - \lambda\frac{n-1}{n}\ln(n)\right\} \quad \left(\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \ldots \approx x + O(x^2) \text{ for small } x\right) \\
&= \lim_{n\to\infty} \exp\left\{\ln(n)\left(1 - \lambda\frac{n-1}{n}\right)\right\} \\
&= \infty \qquad (\text{since } \lambda < 1 \text{ and } n \to \infty)
\end{aligned}$$

For the second term, observe that $p = \lambda\frac{\ln(n)}{n} \to 0$ as $n \to \infty$. So $\frac{p}{1-p} \to 0$ as well. This completes the case for $\lambda < 1$.

**Part II.** Now suppose $\lambda > 1$. We want to show $P(\text{connected}) \to 1$, or equivalently $P(\text{disconnected}) \to 0$. A graph is disconnected if there is a subgraph of $k$ nodes that does not connect to any of the other $n-k$ nodes

(draw a picture). By symmetry, we only have to consider $k \in \{1,2,...\lfloor n/2 \rfloor\}$. So

$$
\begin{aligned}
P(\text{disconnected}) &= \bigcup_{k=1}^{\lfloor n/2 \rfloor} P(\text{some set of } k \text{ nodes not connected to the rest}) \\
&\leq \sum_{k=1}^{\lfloor n/2 \rfloor} P(\text{some set of } k \text{ nodes not connected to the rest}) \quad \text{(inclusion-exclusion picture)} \\
&= \sum_{k=1}^{\lfloor n/2 \rfloor} \binom{n}{k} \left[(1-p)^{(n-k)}\right]^k \\
&\leq \sum_{k=1}^{\lfloor n/2 \rfloor} \binom{n}{k} e^{-p(n-k)k} \quad \left(e^{-x} = 1 - x + \frac{x^2}{2} - ... \approx 1 - x + O(x^2) \text{ for small } x\right) \\
&= \sum_{k=1}^{\lfloor n/2 \rfloor} \binom{n}{k} \exp\left\{\frac{-\lambda \ln(n)(n-k)k}{n}\right\} \\
&= \sum_{k=1}^{\lfloor n/2 \rfloor} \binom{n}{k} n^{\frac{-\lambda}{n}(n-k)k} \\
&= \sum_{k=1}^{n^*} \binom{n}{k} n^{\frac{-\lambda}{n}(n-k)k} + \sum_{k=n^*+1}^{\lfloor n/2 \rfloor} \binom{n}{k} n^{\frac{-\lambda}{n}(n-k)k} \quad \left(\text{Choose } n^* s.t. \frac{\lambda(n-n^*)}{n} > 1 \iff n^* = \lfloor n(1-\frac{1}{\lambda}) \rfloor\right)
\end{aligned}
$$

For the first term,

$$
\begin{aligned}
\sum_{k=1}^{n^*} \binom{n}{k} n^{\frac{-\lambda}{n}(n-k)k} &\leq \sum_{k=1}^{n^*} n^k n^{\frac{-\lambda}{n}(n-k)k} = \sum_{k=1}^{n^*} \left[n^{1-\frac{\lambda}{n}(n-k)}\right]^k \\
&\leq \sum_{k=1}^{n^*} \left[n^{1-\frac{\lambda}{n}(n-n^*)}\right]^k \qquad \text{(judiciously bound inner } k \text{ with something bigger)} \\
&= \sum_{k=1}^{n^*} r^k \qquad \left(\text{define } r = n^{1-\frac{\lambda}{n}(n-n^*)}\right) \\
&= \left(\sum_{k=0}^{n^*} r^k\right) - 1 \\
&= \frac{r}{1-r} \qquad \left(\text{geometric series. } r < 1 \text{ since } 1 - \frac{\lambda}{n}(n-n^*) < 0\right) \\
&= \frac{1}{n^{\frac{\lambda}{n}(n-n^*)-1} - 1} \\
&\longrightarrow 0 \qquad \text{(since } n \to \infty \text{ and exponent} > 0)
\end{aligned}
$$

For the second term, we use a better bound than before (see homework):

$$\binom{n}{k} < \left(\frac{ek}{k}\right)^k.$$

Thus

$$\begin{aligned}
\sum_{k=n^*+1}^{\lfloor n/2\rfloor}\binom{n}{k}n^{\frac{-\lambda}{n}(n-k)k} &< \sum_{k=n^*+1}^{\lfloor n/2\rfloor}\left(\frac{en}{k}\right)^k n^{\frac{-\lambda(n-k)k}{n}} = \sum_{k=n^*+1}^{\lfloor n/2\rfloor}\left[\frac{en^{1-\frac{\lambda(n-k)}{n}}}{k}\right]^k \\
&\leq \sum_{k=n^*+1}^{\lfloor n/2\rfloor}\left[\frac{en^{1-\frac{\lambda(n-\frac{n}{2})}{n}}}{n^*+1}\right]^k \qquad \text{(bound inner } k \text{ with something from above)} \\
&= \sum_{k=n^*+1}^{\lfloor n/2\rfloor}\left[\frac{en^{1-\frac{\lambda}{2}}}{n(1-\frac{1}{\lambda})+1}\right]^k \leq \sum_{k=n^*+1}^{\lfloor n/2\rfloor}\left[\frac{en^{\frac{-\lambda}{2}}}{1-\frac{1}{\lambda}}\right]^k \\
&\leq \sum_{k=n^*+1}^{\lfloor n/2\rfloor} r^k \qquad \left(r=\frac{en^{\frac{-\lambda}{2}}}{1-\frac{1}{\lambda}}, 0<r<1 \text{ for large } n\right) \\
&\leq \sum_{k=n^*+1}^{\infty} r^k = \sum_{k=0}^{\infty} r^k - \sum_{k=n^*+1}^{n^*} r^k \\
&= \frac{1}{1-r} - \frac{1-r^{n^*+1}}{1-r} \qquad \left(\text{finite geometric series } \sum_{k=0}^{m} r^k = \frac{1-r^{m+1}}{1-r}\right) \\
&= \frac{r^{n^*+1}}{1-r} \longrightarrow 0 \qquad \text{since } n^* \to \infty.
\end{aligned}$$

□

# 3 Clustering graphs

Sometimes it is useful to **cluster** a graph, which lumps a graph's nodes into several groups so that there are much more edges within groups than between groups. There are many algorithms to do this (e.g. K-means, hierarchical), which is not our focus. Rather, we will combine random graph theory with (discrete time) Markov chains to define a new distance measure that can be used together with various clustering algorithms. Most material is based on [7].

## 3.1 Euclidean distance for clustering in k-means algorithm

Clustering algorithms require some measures of similarity (i.e. distance) between 2 nodes. One common distance measure is the Euclidean distance: $d(\mathbf{x},\mathbf{y}) = \sqrt{\sum_i (x_i - y_i)^2}$. This defines the traditional k-means and hierarchical clustering algorithms.

**(review) k-means algorithm:**

(1) Randomly initialize $k$ cluster centers $c_1, \ldots c_k$.

(2) Assign each node to some cluster based on the smallest **Euclidean distance** to each cluster center $c_i$.

(3) Update center location $c_1, \ldots, c_k$ by computing the means of the nodes in the cluster.

(4) Repeat 2 and 3 until assignments no longer change

## 3.2 Random Walk and Euclidean Commute Time (ETC) Distance

We setup a Markov chain as follows:

- Consider a connected **weighted graph** with $N$ nodes where each edge connecting nodes $i$ and $j$ has a weight $w_{ij} > 0$ that is symmetric $w_{ij} = w_{ji}$.
- Let each node of a graph be a state in a Markov chain.
- For node $i$, the probability of jumping to an adjacent node $j$ is $p_{ij} = \frac{a_{ij}}{a_{i\cdot}}$ where $a_{i\cdot} = \sum_j a_{ij}$. Hence large $w_{ij}$ values means easier communication through the edge.
- Connectivity implies the Markov chain is irreducible.

Based on this Markov chain, we define 2 important quantities:

- Starting at state $i$, the **average first passage time**

$$\begin{cases} m(k|k) = 0 \\ m(k|i) = 1 + \sum_{j=1}^{N} p_{ij} m(k|j) \quad \text{if } i \neq k. \end{cases} \tag{3.1}$$

  is the average number of steps a random walker needs to enter state $k$.

- Starting at state $i$, the **average commute time**

$$n(i,j) = m(j|i) + m(i|j)$$

  is the number of steps a random walker take to enter $j \neq i$ for the first time, then go back to $i$. One can show that this function is a distance measure.

$\sqrt{n(i,j)}$ is called the **Euclidean Commute Time (ETC) Distance**. Intuitively, $n(i,j)$ decreases when 2 nodes are highly connected, or when the length of any path decrease. The fact that it takes "connectivity" between nodes into account sets it apart from shortest path distances.

## 3.3 Computation of Euclidean Commute Time (ETC) Distance

### 3.3.1 Closed form solution involving pseudoinverse

Define

- The **adjacency matrix** $\mathbf{A} = (a_{ij})$ where $a_{ij} = w_{ij}$ if node $i$ is connected to $j$, otherwise $a_{ij} = 0$
- $\mathbf{D} = \text{diag}(a_{i\cdot})$ where $a_{i\cdot} = \sum_j a_{ij}$
- The **Laplacian matrix** of the graph is $\mathbf{L} = \mathbf{D} - \mathbf{A}$

Note the Laplacian $\mathbf{L}$ is not full rank because $\mathbf{1}$ (vector of 1s) is in its null space. Hence the following theorem involves a pseudoinverse $\mathbf{L}^+$:

**Theorem 3.1 Computaton of average commute time $n(i,j)$**

We can compute average commute time between nodes $i$ and $j$ by:

$$n(i,j) = V_G(\mathbf{e}_i - \mathbf{e}_j)^t \mathbf{L}^+ (\mathbf{e}_i - \mathbf{e}_j)$$

where $\mathbf{L}^+$ is the Moore-Penrose pseudoinverse of $\mathbf{L}, V_G = \sum_{i,j} a_{ij}$ is the volume of the graph, and $\mathbf{e}_i$'s are the standard basis vectors that is 0 everywhere and is 1 at position $i$.

*Proof.* See appendix of [2]. □

Observe that:

(1) $\mathbf{L}^+$ is symmetric since $\mathbf{L}$ is.

(2) $\mathbf{L}^+$ is positive semidefinite, since $\mathbf{L}$ psd $\iff$ $\mathbf{L}^+$ psd, and $\mathbf{L}$ is psd since it is diagonally dominant.

Here (1) + (2) above implies that $\mathbf{L}^+$ defines an inner product between $\mathbf{x}$ and $\mathbf{y}$ as $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^t \mathbf{L}^+ \mathbf{y}$ in $\mathbb{R}^n$. This induces a norm: $||\mathbf{x}|| = (\mathbf{x}^t \mathbf{L}^+ \mathbf{x})^{1/2}$. Therefore, the quantity $[n(i,j)]^{1/2}$ is called the **Euclidean Commute Time** (ETC) **Distance**.

### 3.3.2 Closed form formula for pseudoinverse

One way to compute the pseudoinverse is to do $\mathbf{L}^+ = (\mathbf{L} - \mathbf{1}\mathbf{1}^y/n)^{-1} - \mathbf{1}\mathbf{1}^t/n$ via sparse (low rank) Cholesky factorization [2] (homework). For large graphs, [7] suggests Markov chain Monte Carlo.

### 3.3.3 Iterative methods for ETC distance

An alternative is to use iterative methods. Using a more familiar notation, we observe that the recursive relation for $m(k|i)$ in equation (3.1) can be interpreted as a matrix-matrix multiplication:

$$m_{ik} = \sum_{j=1}^{N} p_{ij} m_{jk} + 1 \iff \mathbf{M}^{(n+1)} = \mathbf{P}\mathbf{M}^{(n)} + \left(\mathbf{1}\mathbf{1}^t - diag(\mathbf{1})\right) \tag{3.2}$$

If the degree for each node is small, then $\mathbf{P}$ is a sparse matrix, so the multiplication $\mathbf{P}\mathbf{M}^{(n)}$ is linear in the number of non-zero entries. The programming illustrations below uses 50 iterations to estimate $\mathbf{M}$, which appears to be sufficient for the problems tested.

## 3.4 Revised k-means clustering using ETC Distance

(1) Connect each node to its $h$ nearest neighbors, then add the edges of a minimum spanning tree. Then add weights $w_{ij}$ using your favorite method (e.g. inverse Euclidean distance).

(2) Choose number of clusters $k$ and its respective cluster centers $\mathbf{p}_1, ..., \mathbf{p}_k$ where each $\mathbf{p}_i$ is a node.

(3) Assign each node $\mathbf{x}_i$ to the nearest cluster $C_l$ by finding which of $\mathbf{p}_1, ..., \mathbf{p}_k$ is closest to $\mathbf{x}_i$, where closeness is measured as a function of the ETC distance: $\text{dist}(\mathbf{x}_i, \mathbf{p}_j) = n(i,j)^2$

(4) Recompute new cluster centers $\mathbf{p}_1, ..., \mathbf{p}_k$ by minimizing the within-cluster distance:

$$\mathbf{p}_l = \text{argmin}_{\mathbf{x}_j} \left\{ \sum_{\mathbf{x}_k \in C_l} n(k,j)^2 \right\}$$

(5) Repeat (2) and (3) until convergence.

### 3.5 Some simulations

It is well known that K-means algorithm assumes Gaussian clusters with the same variance. Below illustrates 2 scenarios, one where k-means is expected to work, another where k-means is expected to fail. Here the graph is formed by connecting each node to 3 of its nearest neighbors with weight equal to the inverse Euclidean distance. Each node $i$ is connected to node $i+1$ except for the transition node between the 2 clusters. For a better alternative to guarantee connectedness, [7] suggests to add edges from a **minimal spanning tree** (homework).

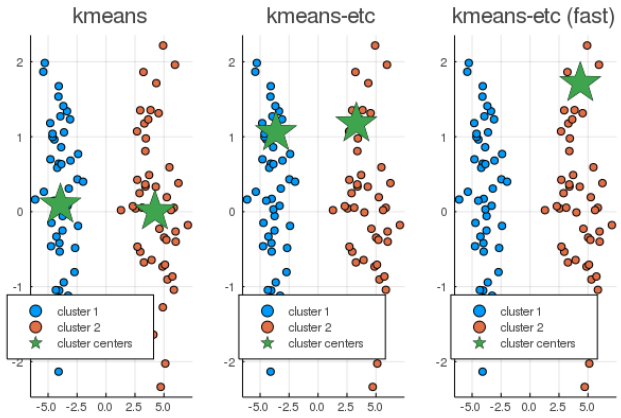



Figure 1: Two unit variance Gaussian clusters with mean -4 and 4.

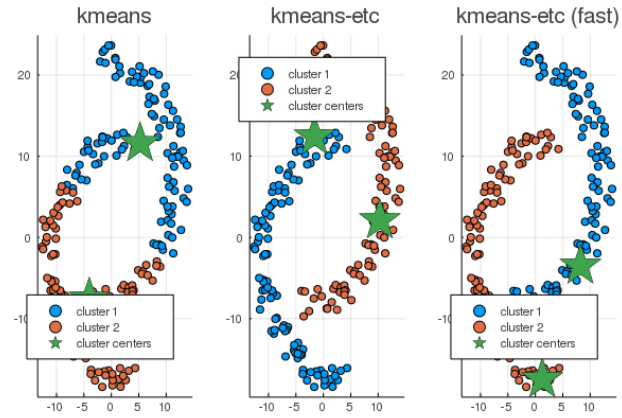
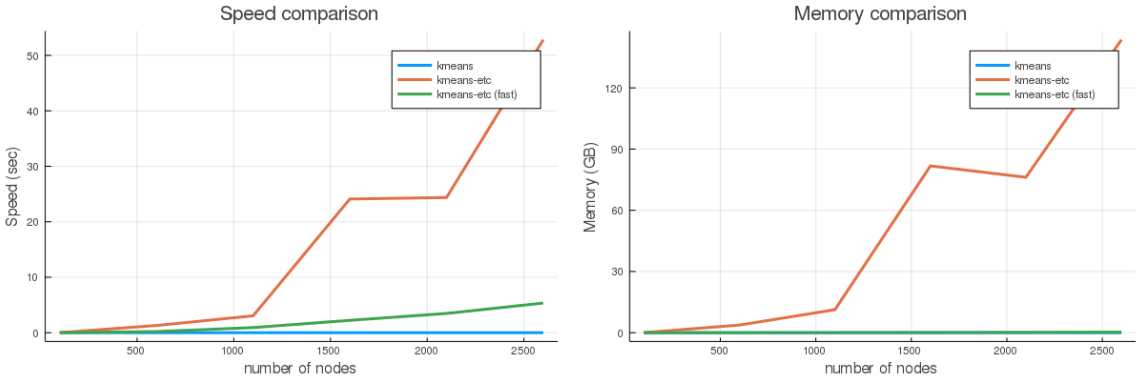



Figure 2: Two non-convex clusters.

Below compares scalability of the k-means, k-means using closed form pseudoinverse of ETC distance (kmeans-etc), and k-means using the iterative algorithm to estimate ETC distance (kmeans-etc (fast)). One should not take it too seriously because I did not try very hard to optimize this code.




# 4 Problems

In honor of Ken Lange, you are required to do 2 problems. If you do more I will grade your top 2 problems. Every problem is worth the same number of points. If a problem has subproblems, each subproblem is worth the same number of points.

**Problem 4.1 Bounds of binomial coefficients**

For integers $n$ and $k$, prove the following inequalities

$$\frac{n^k}{k^k} \leq \binom{n}{k} \leq \frac{n^k}{k!} < \left(\frac{ne}{k}\right)^k$$

which is used in part 2 of our sharp threshold proof. For the strict inequality, rewrite $\frac{n^k}{k!} = \left(\frac{n}{k}\right)^k \frac{k^k}{k!}$ and use Taylor expansion on $e^k$.

**Problem 4.2 Verify this unproved claim**

Prove that $\mathbf{L}^+$ in theorem 3.1 can be computed via

$$\mathbf{L}^+ = \left(\mathbf{L} - \frac{\mathbf{1}\mathbf{1}^t}{n}\right)^{-1} + \frac{\mathbf{1}\mathbf{1}^t}{n}$$

where $\mathbf{1}$ is a vector of 1s. This is equation (3) in [2], but it came without a proof.

**Problem 4.3 Mandatory computational problem**

Starting with my code, do one of the computational problems below:

- Compute the pseudoinverse $\mathbf{L}^+$ via sparse (low rank) Cholesky factorization. Recall Cholesky

for $\mathbf{Ax} = \mathbf{b}$ is solved via back substitution: $\mathbf{Ax} = \mathbf{b} \iff \mathbf{LL}^t\mathbf{x} = \mathbf{b} \iff \mathbf{L}^t\mathbf{x} = \mathbf{y}$ and $\mathbf{Ly} = \mathbf{b}$.

- In my code for computing the adjacency matrix $\mathbf{A}$, use your favorite algorithm to add graph edges corresponding to the **minimum spanning tree**. Hopefully this solves most of our stability problem.

**Problem 4.4 Colorings of graphs**

Let $K_z$ be a **complete graph** where all $z \in \mathbb{Z}_+$ nodes forms an edge with every other node. With equal probability, each edge is colored with red or green. Prove that $z = 6$ is the minimal number of nodes needed to guarantee the existance of a **monochromatic triangle** (i.e. triangle with all edges the same color). This type of problem is what Ramsey theory studies, which we almost did.

We have just shown $R(3,3) = 6$. Similarly, $R(3,4)$ is the minimal number of nodes to guarantee a red triangle or green rectangle. Function $R$ obviously generalizes to more colors and shapes. Using Erdos' probabilistic method, Ramsey's theorem (see [6] or theorem 3.3 of [5]) says this number is finite but exponential. This takes us to Erdos' famous quote:

> Suppose aliens invade earth and threaten to obliterate us within a year unless human beings can find $R(5,5)$. We could marshal the world's best minds and fastest computers, and within a year we could probably calculate the value. However, if the aliens demanded $R(6,6)$, we would have no choice but to launch a preemptive attack.

If you want to be famous, find $R(5,5)$.

## References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