Random Graph theory

Benjamin Chu

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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 and E is a set of edges where $e \in E$ can be written as $e = (x, y)$ where $x, y \in V$.
- 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. $\square$

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:

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

Thus

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

We will now calculate $\mathrm{Var}(X_n)$ 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

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

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 $k \in \{1, 2, \ldots \lfloor n/2 \rfloor\}$. So

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

For the first term,

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

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

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

Thus

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

□

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 distance metric 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:

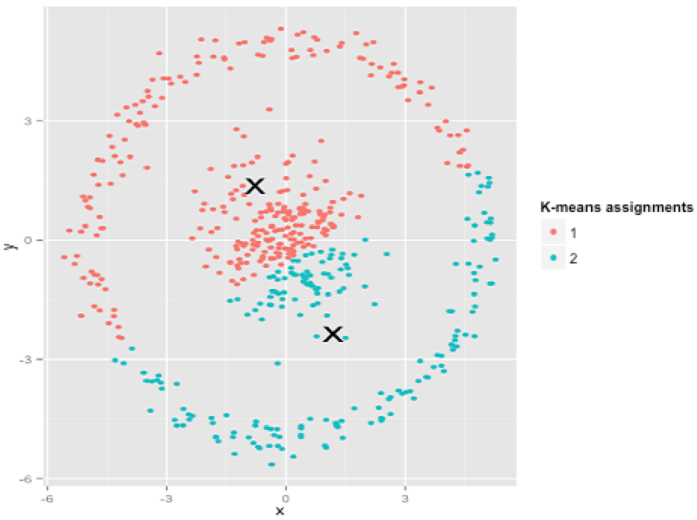
(1) Randomly initialize k cluster centers $c_1, \ldots c_k$.

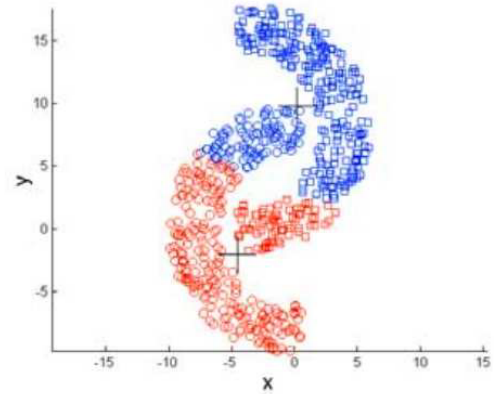
(2) Assign each node to some cluster based on the smallest **Euclidean distance** to each cluster center c_i.

(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

It is well known that k-means often fail because the Euclidean distance implicitly assumes data has Gaussian shape. Some examples that it fails:





Figures from

- `https://stats.stackexchange.com/questions/133656/how-to-understand-the-drawbacks-of-k-means`
- `http://i-systems.github.io/HSE545/machine%20learning%20all/05%20Clustering/iSystems_01_K-means_Clustering.html`

3.2 Random Walk on a Graph is a Markov chain

Markov chain setup:

- 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 3 important quantities:

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

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

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

- Starting at state i, the **average first passage cost**

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

  is the average cost incurred by the random walker to enter state k. $c(j|i)$ is the cost of transitioning from i to j. Note $m(k|i)$ is a special case of $o(k|i)$ where all $c(j|i) = 1$.

- Starting at 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 is a metric.

Intuition: $n(i,j)$ 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 Euclidean Commute Time (ETC) Distance

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

3.4 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 $\mathbf{p}_1, \ldots, \mathbf{p}_k$ where each $\mathbf{p}_i$ is a node.

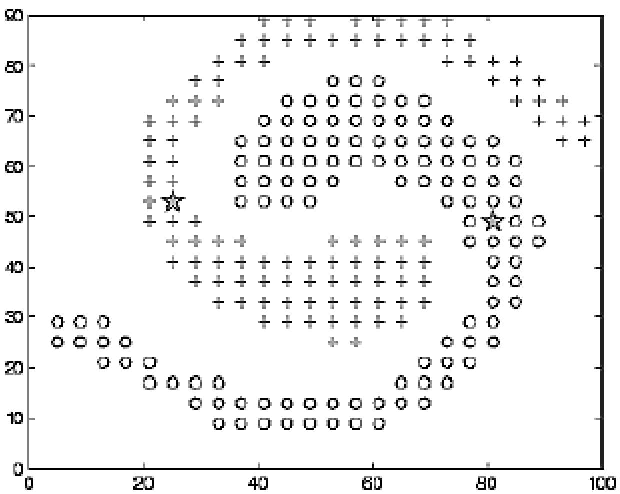
(3) Assign each node $\mathbf{x}_i$ to the nearest cluster C_l by finding which of $\mathbf{p}_1, \ldots, \mathbf{p}_k$ is closest to $\mathbf{x}_i$, where closeness is measured by the ETC distance: $\text{dist}(\mathbf{x}_i, \mathbf{p}_j) = n(i, j)^2$

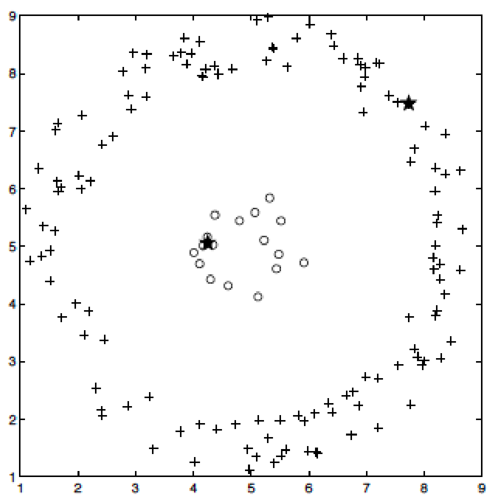
(4) Recompute new cluster centers $\mathbf{p}_1, \ldots, \mathbf{p}_k$ so by minimizing the within-cluster distance:

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

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

This gives the following clustering result:





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

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 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.

In Ramsey theory, this corresponds to the value $R(3,3)$. Similarly, $R(3,4)$ is the minimal number of nodes to guarantee a red triangle or green square. 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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