Polcovar: Software for Computing the Mean and Variance of Subgraph Counts in Random Graphs

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Abstract

The mean and variance of the number of appearances of a given subgraph $H$ in an Erdős–Rényi random graph over $n$ nodes are rational polynomials in $n$ [2]. We present a piece of software named Polcovar (from polynomial and covariance) that computes the exact rational coefficients of these polynomials in function of $H$.

1 Introduction

Large networks can be characterised by the number of times specific subgraphs appear in them. For instance, the number of triangles measures the clustering in a network and the number of wedges (i.e. 2-stars / 2-paths) characterises the inequality of the degree distribution. Even the number of vertices and edges in a graph can be characterised in this way as the number of times the complete graphs on one and two nodes appear as subgraphs. To assess whether a graph contains many or few subgraphs for its size, the subgraph count must be compared to the expected subgraph count in random graphs. To do this, we must know the distribution of subgraph counts. Under mild conditions which are valid for all examples given above, the subgraph count becomes normal in the large graph limit. Consequently, the distribution of subgraph counts is characterised by its mean and average. Expressions for the mean and variance of subgraph counts are given in [2], and are always rational polynomials in the number of nodes $n$ of the network. In this paper, we present Matlab software for computing the exact coefficients rational of these polynomials, as their expressions are usually too unwieldy to be computed by hand.

2 Subgraph Counts

We consider a random graph $G$ on $n$ nodes distributed according to the Erdős–Rényi model with parameter $p$, i.e., each edge in $G$ exists with probability $p$ [1]. Let $H = (W, F)$ be a pattern, i.e. a small graph with $k = |W|$ vertices and
\[ l = |F| \text{ edges, and } c_H \text{ the number of times this pattern appears as a subgraph of } G. \] The mean of variance of \( c_H \) are then given by the following expressions \[2\]:

\[
\begin{align*}
\mathbb{E}[c_H] &= \frac{n!}{|\text{Aut}(H)|} p^{-l} \\
\text{Var}[c_H] &= \sum_J \left( \frac{n!|V(J)|}{|\text{Aut'}(J)|} p^{-|E(J)|} \right) - \mathbb{E}[c_H]^2
\end{align*}
\]

where \( n! \) is the falling factorial, the sum is over all graphs \( J \) containing two differently colored copies of \( H \) (which might overlap), \( \text{Aut}(H) \) is the automorphism group of the graph \( H \), and \( \text{Aut'}(J) \) is the group of automorphisms of \( J \) that preserve the edges of the underlying distinct copies of \( H \).

Although the normal limit for \( n \to \infty \) is only true when the graph \( H \) is strictly balanced, the expressions for the mean and variance are always correct. Note also that they are true exactly for any \( n \), not just in the large \( n \) limit.

Alternatively, the following expression can be used, which gives the same result. It is this expression that we implement in our code.

\[
\text{Var}[c_H] = -\mathbb{E}[c_H]^2 + \frac{1}{\text{Aut}(H)^2} \sum_{i=0}^{k} \frac{n^{2k-i}}{i!(k-i)!^2} \sum_{P,Q} p^{-m(P,Q)}
\]

where the inner sum is over all pairs of \( k \)-permutations, and \( m(P,Q) \) denotes the number of edges in the overlay of \( H \) permuted by \( P \) and \( H \) permuted by \( Q \) which share \( i \) nodes.

### 3 Special Cases

For specific small graphs \( H \), we get the following exact results.

#### 3.1 Node Count

Taking \( H \) as the graph with one node gives the number of nodes. Plugging this graph into the general form expression gives \( \mathbb{E}[c_H] = n \) and \( \text{Var}[c_H] = 0 \). In other words, the number of nodes is always exactly \( n \), as expected.

#### 3.2 Edge Count

Edges are always independent of each other and therefore the binomial approximation for the number of edges \( m = c_H \) is exact.

\[
\begin{align*}
\mathbb{E}[m] &= \frac{1}{p} \binom{n}{2} = \frac{n(n-1)}{2p} \\
\text{Var}[m] &= \frac{n(n-1)}{8} \text{ when } p = 1/2
\end{align*}
\]

\(^1\text{defined as } n! = n(n-1) \cdots (n-i+1)\)
These expressions can be derived both by the general form we gave above, and by the fact that the number of edges is a binomial distribution.

### 3.3 Triangle Count

In a random $n$-graph with parameter $p = 1/2$, the number of triangles $t$ has mean and variance given by

$$
E[t] = \frac{1}{8} \binom{n}{3}
$$

$$
\text{Var}[t] = \frac{1}{128} n^4 - \frac{11}{384} n^3 + \frac{1}{32} n^2 - \frac{1}{96} n
$$

The expressions follow from the general form given below.

### 3.4 Wedge Count

The number $s$ of wedges (i.e., pairs of edges sharing one endpoint, also known as 2-stars or 2-paths) has the following distributions when $p = 1/2$:

$$
E[s] = \frac{n^3}{8}
$$

$$
\text{Var}[s] = \frac{1}{8} n^4 - \frac{19}{32} n^3 + \frac{29}{32} n^2 - \frac{7}{16} n
$$

The expressions follow from the general form given below.

### 3.5 Other Patterns

For the number $q$ of squares we get:

$$
E[q] = \frac{1}{128} n^4 - \frac{3}{64} n^3 + \frac{1}{128} n^2 - \frac{3}{64} n
$$

$$
\text{Var}[q] = \frac{1}{512} n^6 - \frac{5}{256} n^5 + \frac{161}{2048} n^4 - \frac{163}{1024} n^3 + \frac{327}{2048} n^2 - \frac{63}{1024} n
$$

For the number $c_H$ of 4-cliques we get:

$$
E[c_H] = \frac{1}{1536} n^4 - \frac{1}{256} n^3 + \frac{11}{1536} n^2 - \frac{1}{256} n
$$

$$
\text{Var}[c_H] = \frac{1}{32768} n^6 - \frac{17}{98304} n^5 + \frac{19}{49152} n^4 - \frac{73}{98304} n^3 + \frac{115}{98304} n^2 - \frac{11}{16384} n
$$

### 4 Proof Outline

A complete proof can be found in [2]. We here outline the proof as a starting point. The total number of possible subgraphs $H$ in a graph with $n$ vertices is

$$
\frac{n^k}{|\text{Aut}(H)|}
$$
Define the random variables $x_i \in \{0, 1\}$ to denote the presence or absence of each possible pattern $i$. Then,

$$c_H = \sum x_i.$$ 

The expected value of each $x_i$ is given by

$$E[x_i] = p^{-i}.$$ 

Thus, the expected value of $c_H$ can be expressed as

$$E[c_H] = E[\sum x_i] = \sum E[x_i] = \frac{n_k}{|\text{Aut}(H)|} p^{-i}.$$ 

To compute the variance we exploit the fact that the variance equals the expected value of the square minus the square of the expected value:

$$\text{Var}[c_H] = E[c_H^2] - E[c_H]^2 = E[(\sum x_i)(\sum x_i)] - E[c_H]^2 = E[\sum x_i x_j] - E[c_H]^2 = \sum E[x_i x_j] - E[c_H]^2.$$ 

Then, each possible pair corresponds to one possible pattern graph $J$, of which the possible number is $\frac{|V(J)|}{|\text{Aut}(J)|}$, and each exists with independently with probability $p^{-|E(J)|}$. From this follows the given expression.

## 5 Extension to Covariances

The method can be extended to covariances between the count statistics of different patterns. As an example:

$$\text{Cov}[c_{\text{edge}}, c_{\text{triangle}}] = \frac{1}{32} n^3 - \frac{3}{32} n^2 + \frac{1}{16} n$$

## 6 The Software

Our code is written in the programming language Matlab, and contains two entry points, the function `polcovar_mu()` that computes the mean and the function `polcovar_sigma()` that computes the variance or covariance.

```matlab
r = polcovar_mu(H);
r = polcovar_sigma(H1, H2);
```
The input graphs $H$ must be given as $k \times k$ adjacency matrices. The function `polcovar_sigma()` expects two graphs $H_1$ and $H_2$ and returns the covariance of their subgraph counts. To compute the variance, pass the same adjacency matrix as both arguments. All input matrices must be symmetric 0/1 matrices with zero diagonals. All computations are valid for Erdős–Rényi graphs with $p = 1/2$.

The return values are rational polynomials in form of $2 \times (m + 1)$ matrices, where $m$ is the degree, coded in the following way:

$$
\begin{bmatrix}
a_m & a_{m-1} & \cdots & a_1 & a_0 \\
b_m & b_{m-1} & \cdots & b_1 & b_0
\end{bmatrix}
$$

representing the following rational polynomial in $n$:

$$P_r(n) = \sum_{i=0}^{m} \frac{a_i}{b_i} n^i$$

All fractions $a_i / b_i$ are returned in simplified form.

### 6.1 Example

The following example uses Polcovar to compute the mean and standard deviation of the number of triangles in a random graph with 1,000,000 nodes.

```matlab
% Adjacency matrix of a triangle
H = [ 0 1 1; 1 0 1; 1 1 0]

% Compute polynomials
r_mu = polcovar_mu(H)
r_sigma = polcovar_sigma(H, H)

% Evaluate polynomials for a graph with 1,000,000 nodes
n = 1000000
mu = polyval(r_mu(1,:) ./ r_mu(2,:), n)
sigma = polyval(r_sigma(1,:) ./ r_sigma(2,:), n)
sigma_stddev = sqrt(sigma)
```

This will compute that a random graph with 1,000,000 nodes can be expected to contain $2.0833 \times 10^{16} \pm 8.8388 \times 10^{10}$ triangles.

### Acknowledgements

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References

[1] Paul Erdős and Alfréd Rényi. On random graphs I. *Publ. Math. Debrecen*, 6:290–297, 1959.

[2] Andrzej Ruciński. When are small subgraphs of a random graph normally distributed? *Prob. Th. Rel. Fields*, 78:1–10, 1988.