

# Fractals in Cubic Graphs & Hamiltonian Cycles

*VMI, March 8 2010*

Stephen Lucas

Department of Mathematics and Statistics

James Madison University, Harrisonburg VA

Thanks to: Vladimir Ejov, Jerzy Filar, Jessica Nelson, Giang Nguyen, Peter Zograf



# Outline

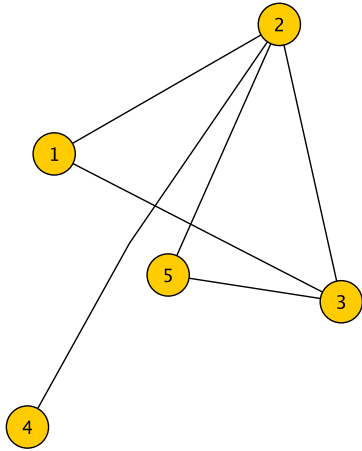
- Graphs as Matrices.
- The fractals.
- Proofs.
- The Hamiltonian Cycle Problem
- The HCP as a Polynomial Problem

# Graphs Definitions

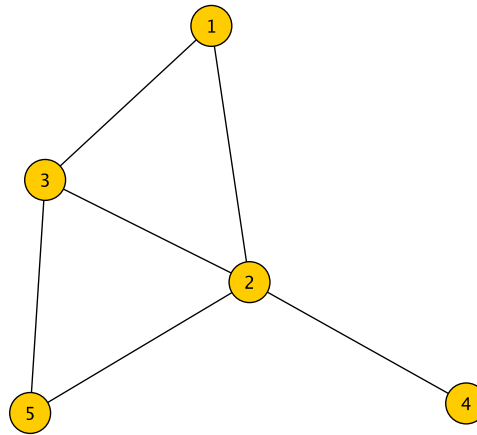
- A graph is a collection of points (nodes, vertices) joined by lines (edges) where location doesn't matter.

# Graphs Definitions

- A graph is a collection of points (nodes, vertices) joined by lines (edges) where location doesn't matter. For example



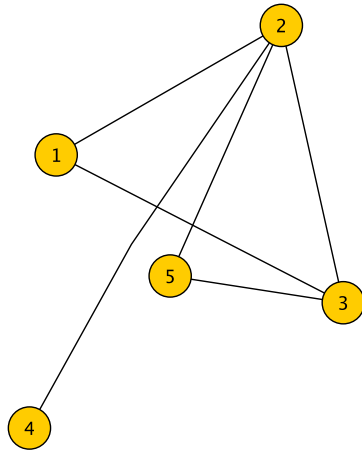
and



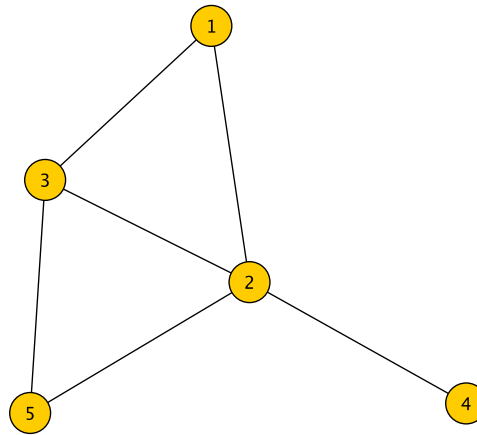
are the same graph.

# Graphs Definitions

- A graph is a collection of points (nodes, vertices) joined by lines (edges) where location doesn't matter. For example



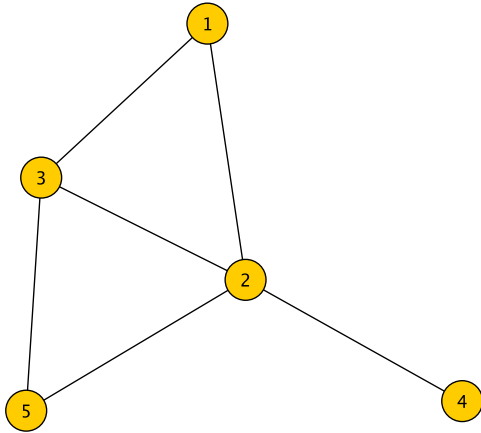
and



are the same graph.

- Some graphs include loops (join a vertex to itself), multiple edges (more than one edges join a pair of vertices), or direction (arrows not lines).

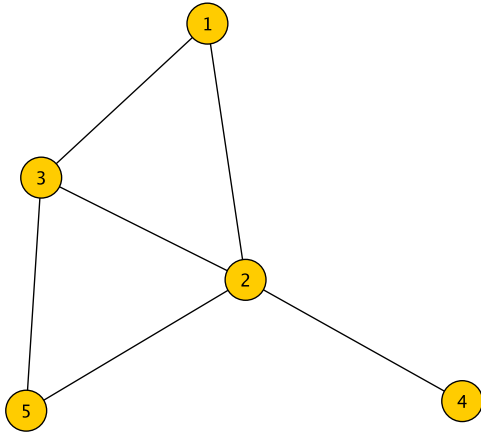
# Graphs as Matrices



A graph  $G$  has an associated adjacency matrix  $A$ , where

$$a_{ij} = \begin{cases} 1, & \text{if an edge joins vertices } i, j, \\ 0, & \text{otherwise.} \end{cases}$$

# Graphs as Matrices



A graph  $G$  has an associated adjacency matrix  $A$ , where

$$a_{ij} = \begin{cases} 1, & \text{if an edge joins vertices } i, j, \\ 0, & \text{otherwise.} \end{cases}$$

In this case,  $A = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \end{pmatrix}$ .

# A Numerical Experiment

Find the adjacency matrices of **all** cubic graphs (each vertex has three edges) with a given number of vertices. For each graph's matrix:



# A Numerical Experiment

Find the adjacency matrices of **all** cubic graphs (each vertex has three edges) with a given number of vertices. For each graph's matrix:

- Divide the matrix by 3, *stochastic matrix*

# A Numerical Experiment

Find the adjacency matrices of **all** cubic graphs (each vertex has three edges) with a given number of vertices. For each graph's matrix:

- Divide the matrix by 3, *stochastic matrix*
- Find its eigenvalues,

# A Numerical Experiment

Find the adjacency matrices of **all** cubic graphs (each vertex has three edges) with a given number of vertices. For each graph's matrix:

- Divide the matrix by 3, *stochastic matrix*
- Find its eigenvalues,
- Take their exponential, *otherwise mean zero*

# A Numerical Experiment

Find the adjacency matrices of **all** cubic graphs (each vertex has three edges) with a given number of vertices. For each graph's matrix:

- Divide the matrix by 3, *stochastic matrix*
- Find its eigenvalues,
- Take their exponential, *otherwise mean zero*
- Find their mean and variance, *for statistical analysis*

# A Numerical Experiment

Find the adjacency matrices of **all** cubic graphs (each vertex has three edges) with a given number of vertices. For each graph's matrix:

- Divide the matrix by 3, *stochastic matrix*
- Find its eigenvalues,
- Take their exponential, *otherwise mean zero*
- Find their mean and variance, *for statistical analysis*
- Plot a single dot of mean versus variance.

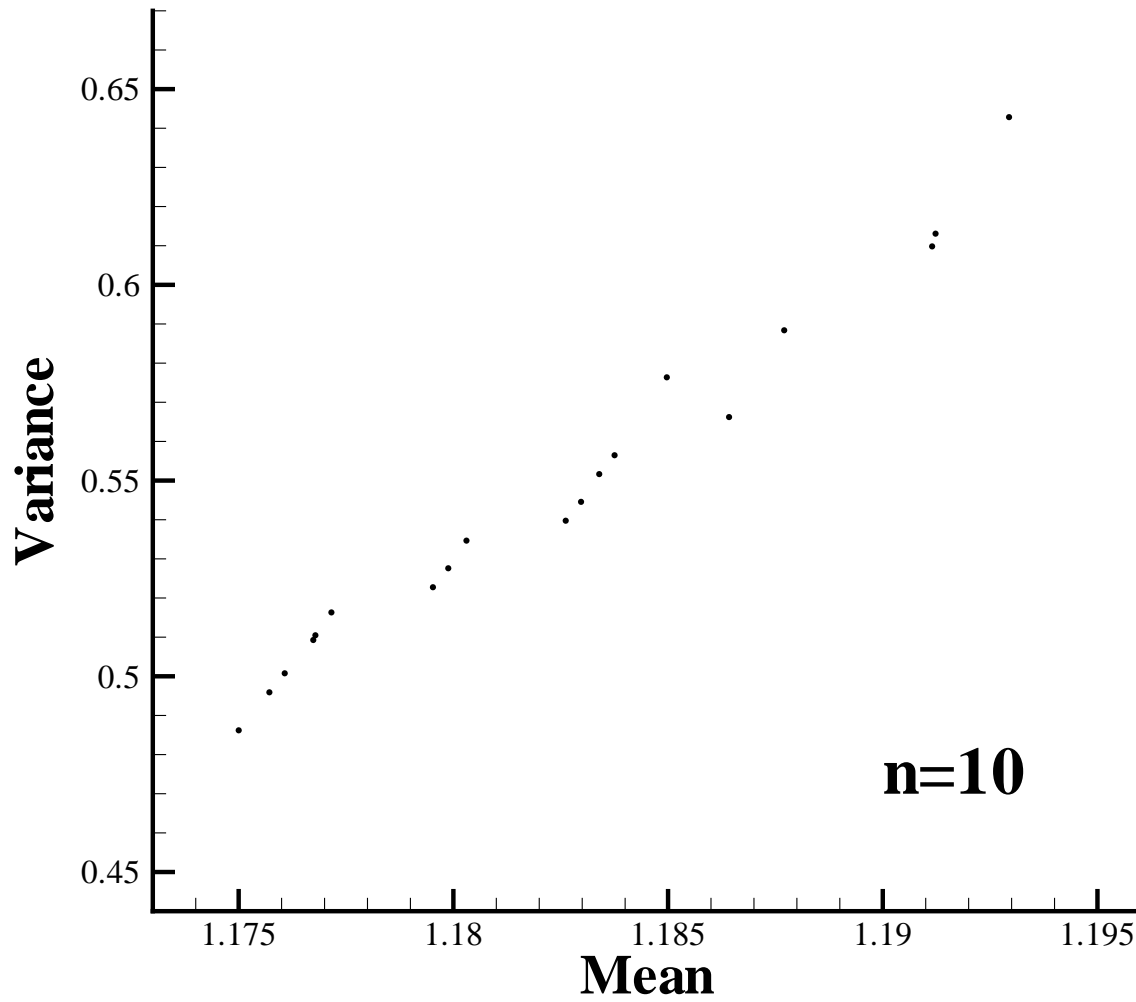
# A Numerical Experiment

Find the adjacency matrices of **all** cubic graphs (each vertex has three edges) with a given number of vertices. For each graph's matrix:

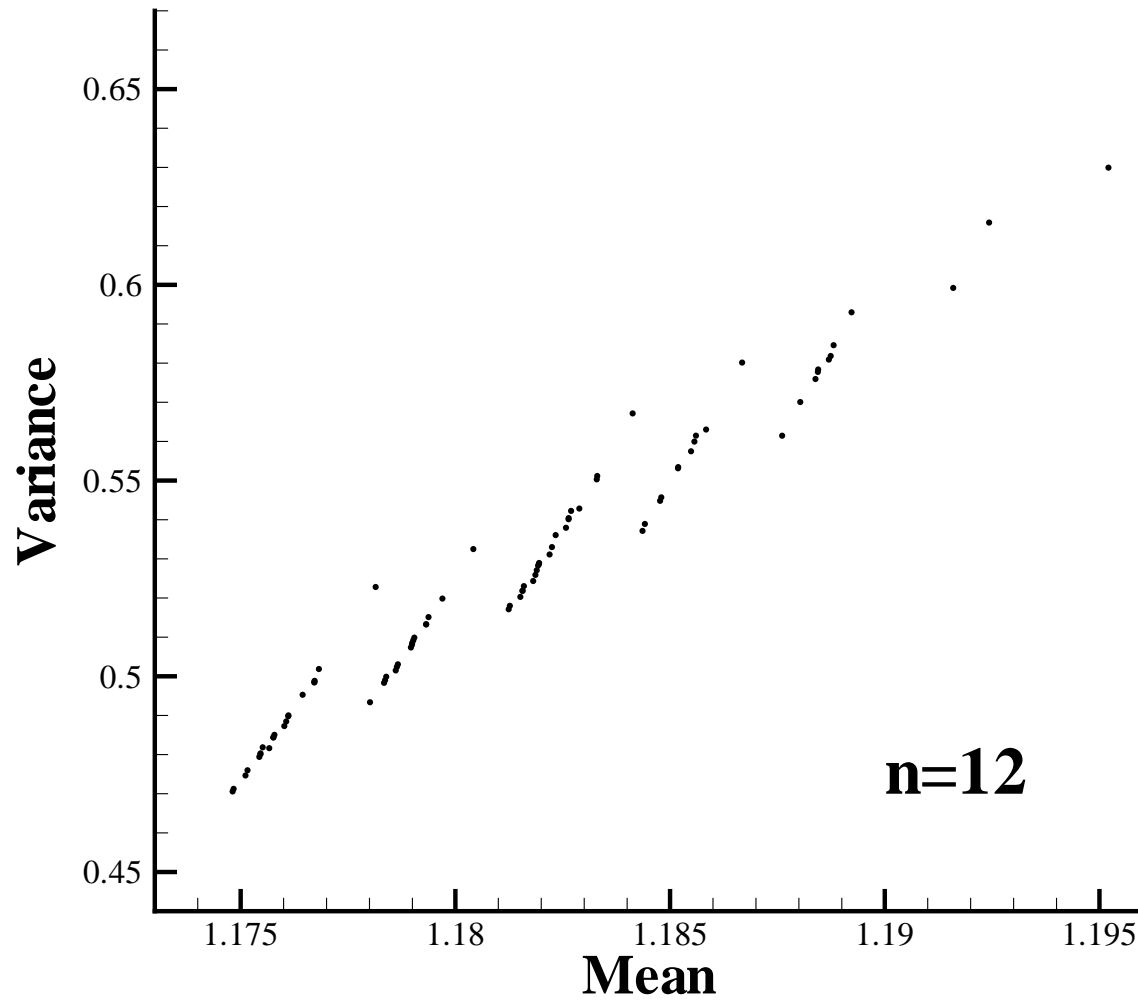
- Divide the matrix by 3, *stochastic matrix*
- Find its eigenvalues,
- Take their exponential, *otherwise mean zero*
- Find their mean and variance, *for statistical analysis*
- Plot a single dot of mean versus variance.

$n$	$\#G$
10	19
12	85
14	509
16	4060

$$n = 10$$

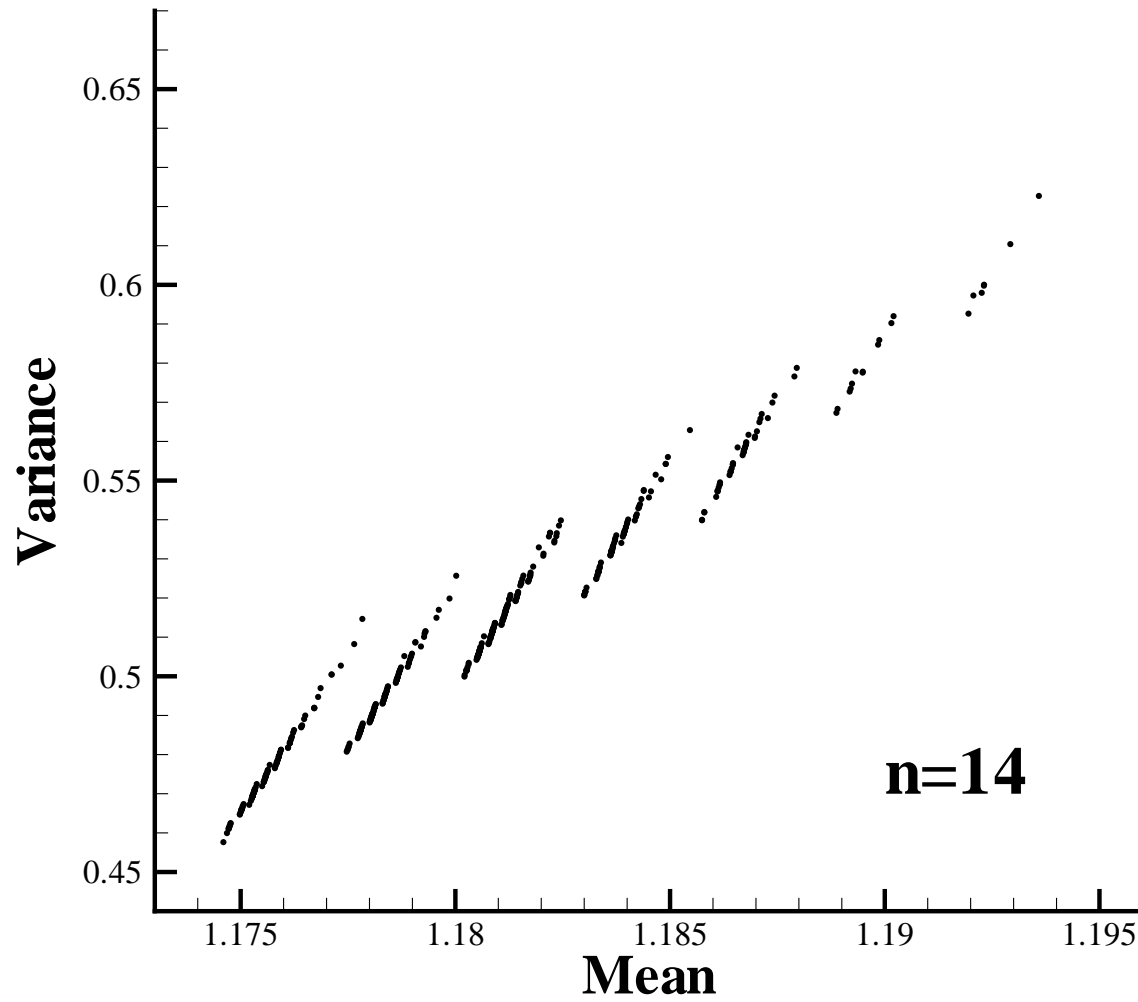


$$n = 12$$

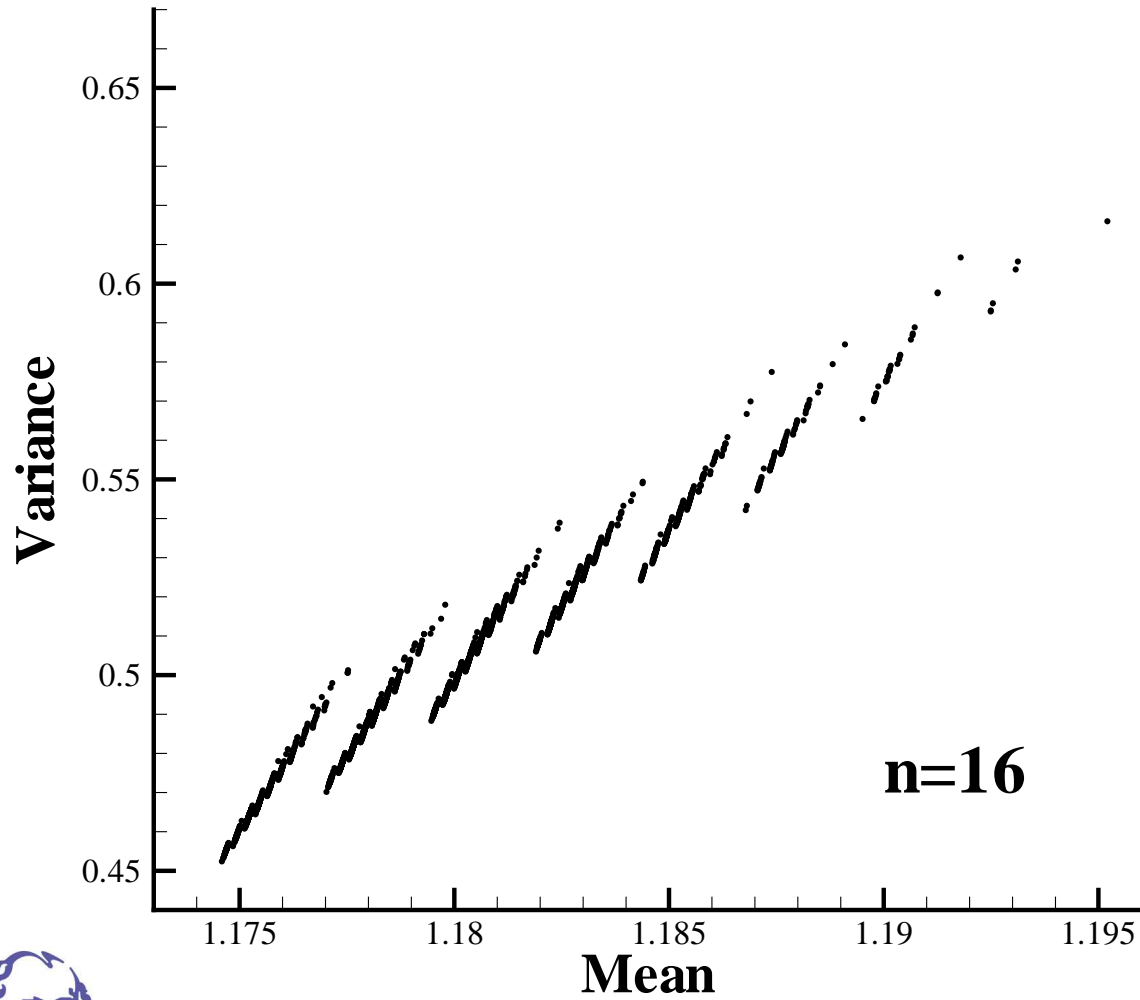




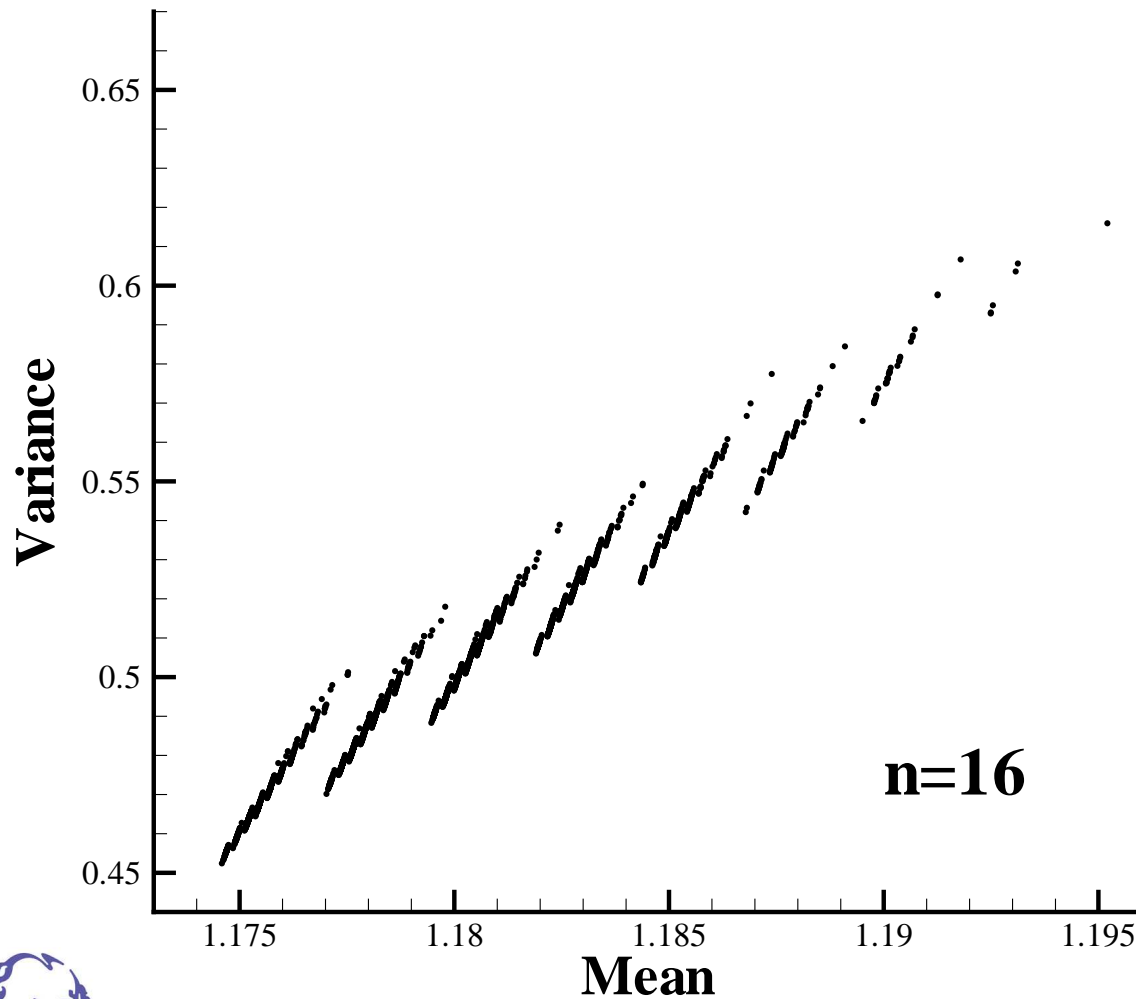
$$n = 14$$



$n = 16$

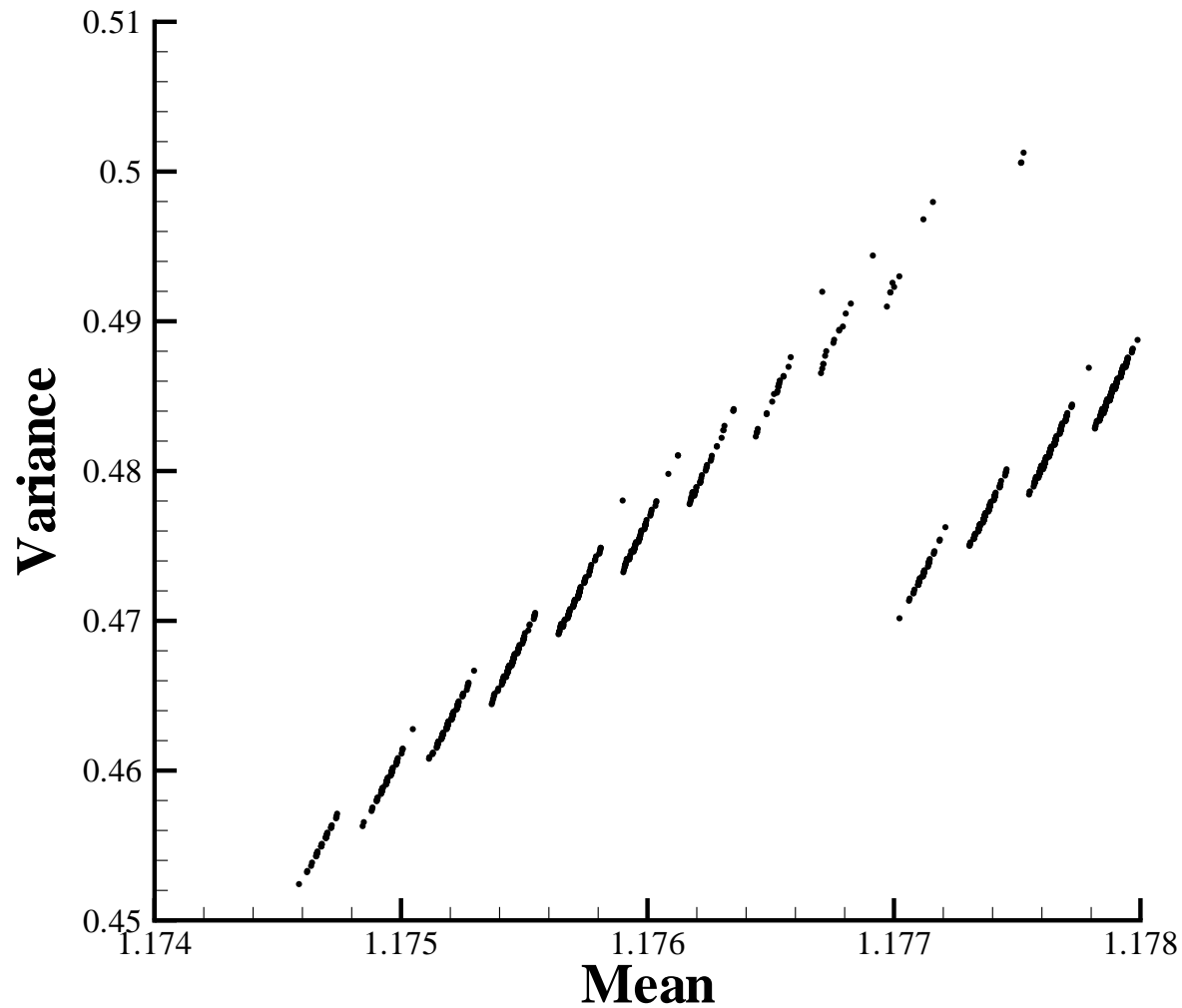


$$n = 16$$

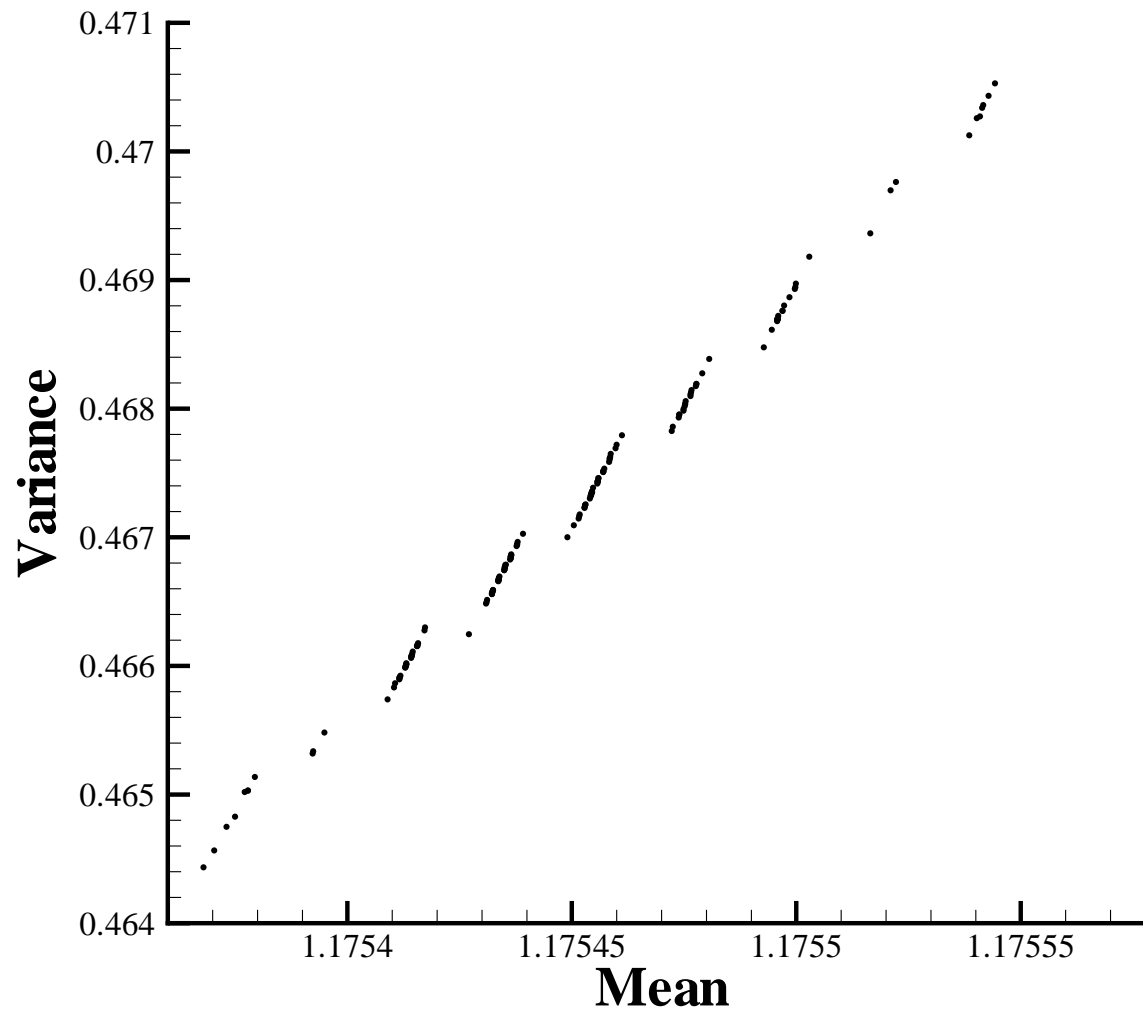


Data appears to be straight lines, with roughly the same slope and distance between them. Call them “**filars**” (Dictionary meaning: threadlike).

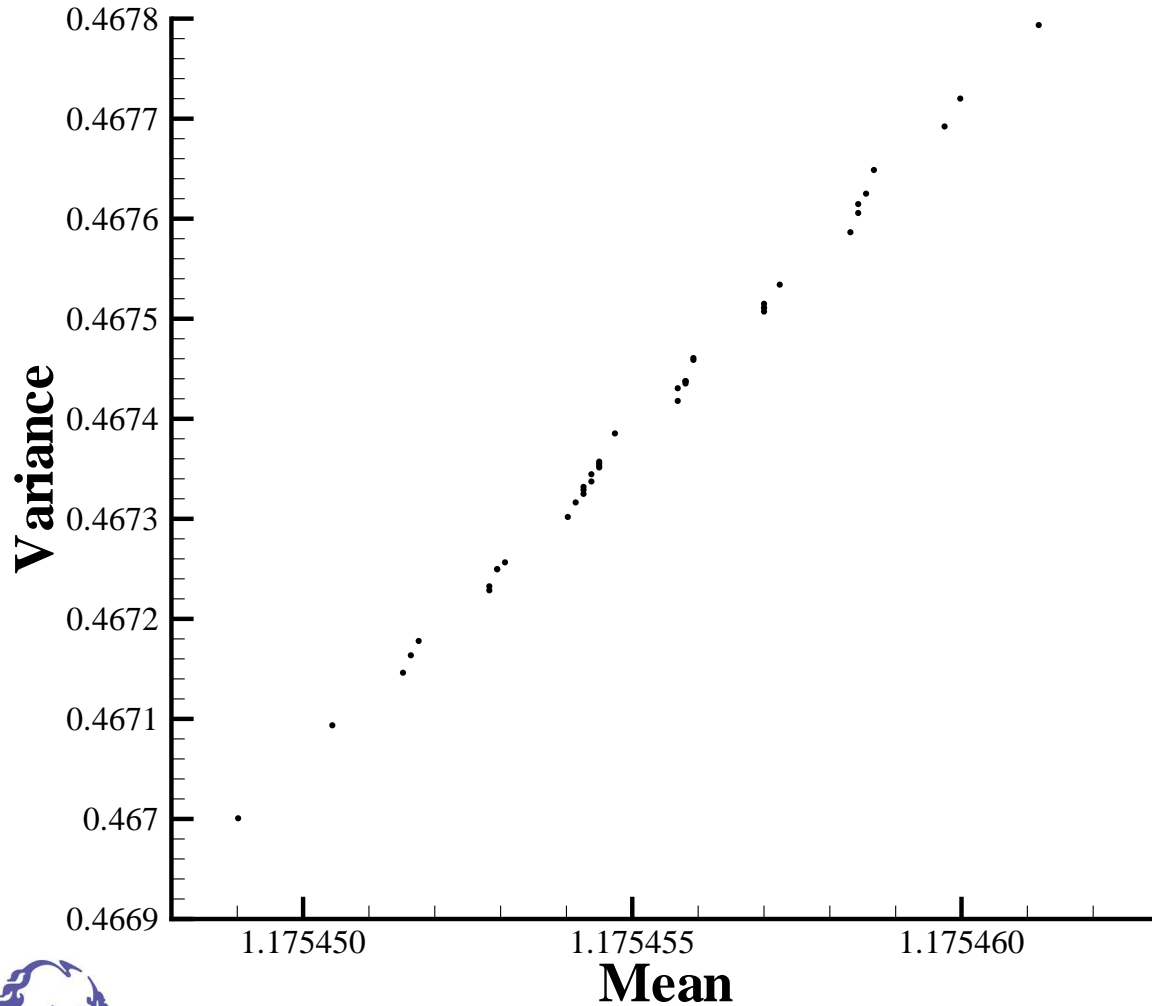
# $n = 16$ , Zoom in on Leftmost Filar



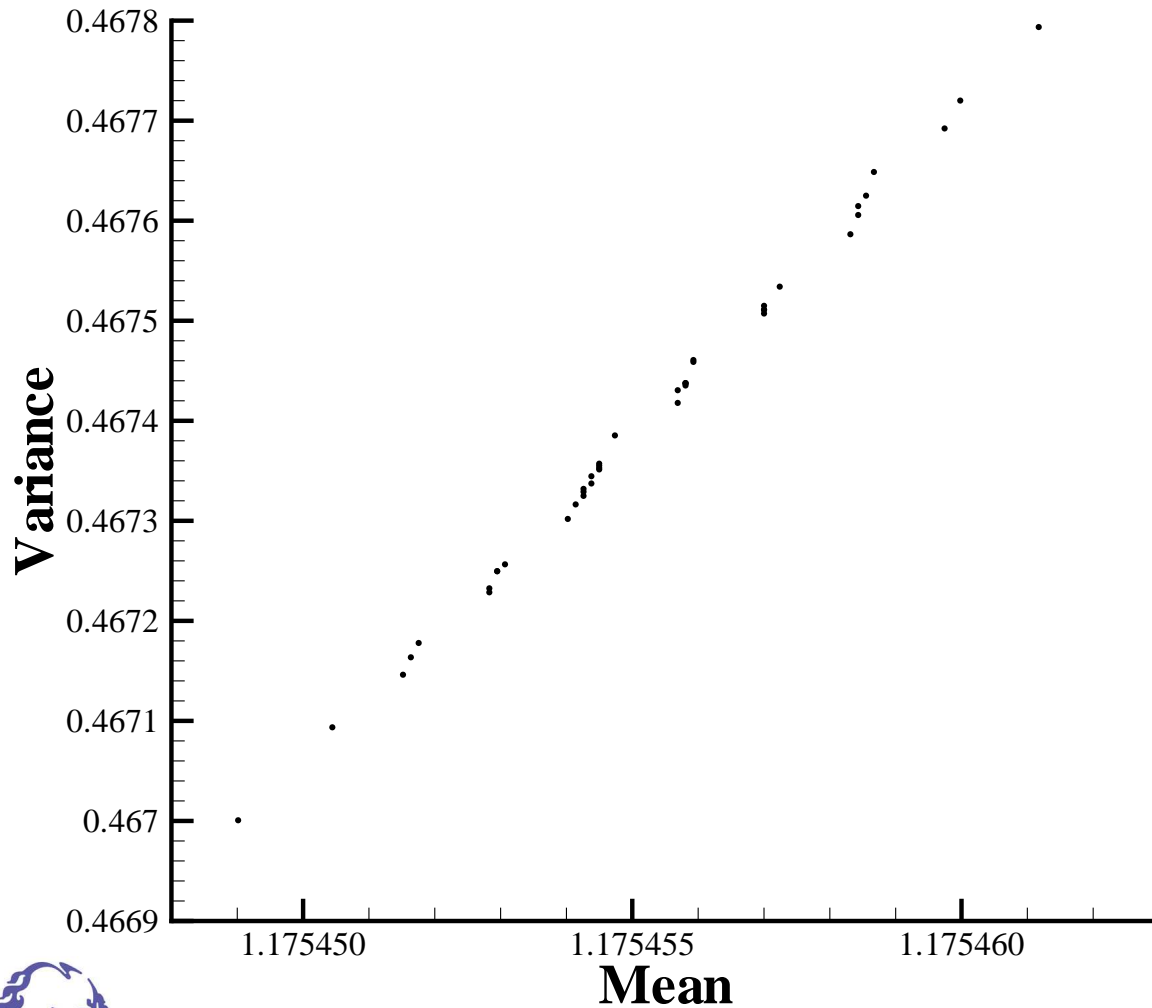
# $n = 16$ , Zoom in on 4th Subfilar of 1st Filar



# $n = 16$ , Zoom in on 5th Subsubfilar of 4th Subfilar of 1st Filar

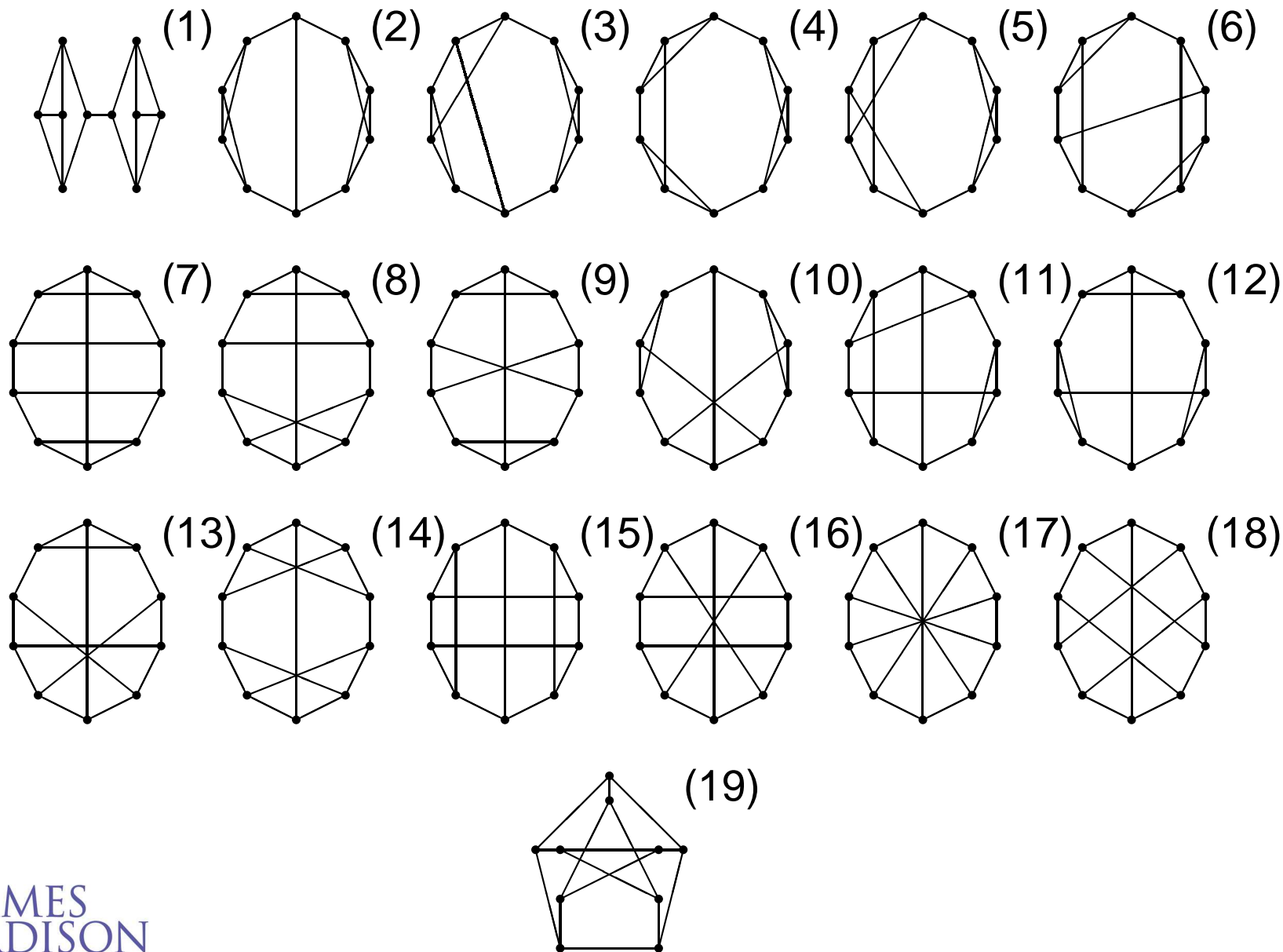


# $n = 16$ , Zoom in on 5th Subsubfilar of 4th Subfilar of 1st Filar



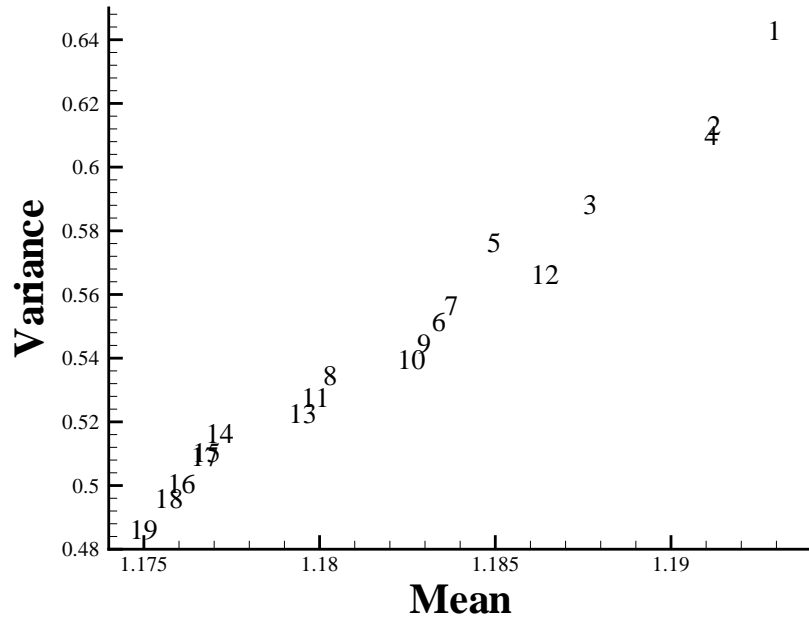
Appears to be a fractal structure.

# Ten Vertex Cubic Graphs in Detail

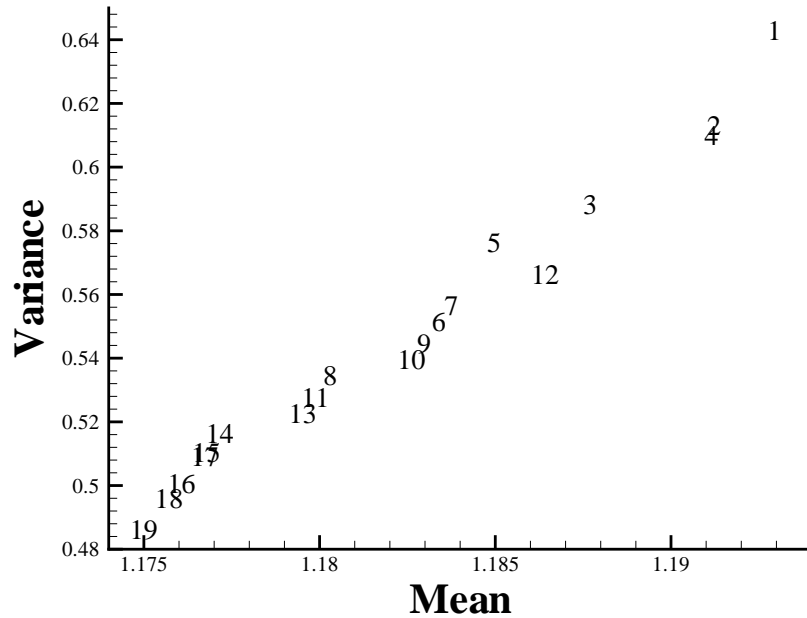




# $n = 10$ with Labels

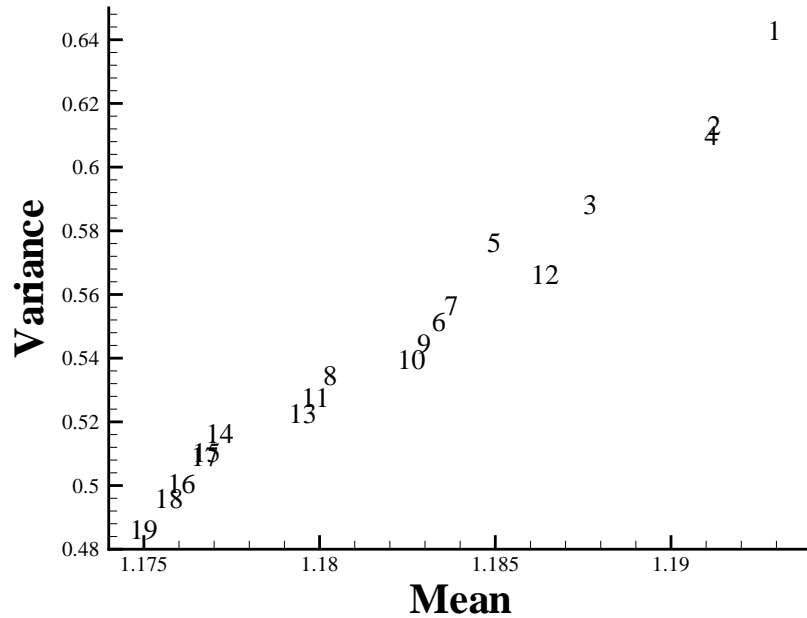


# $n = 10$ with Labels



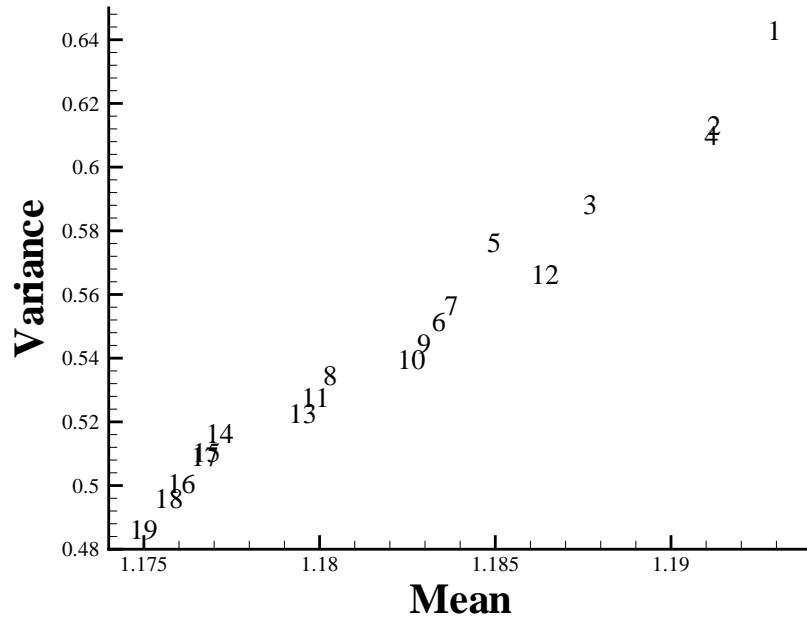
Graphs 19,18,16,17,15,14 have no subcycles of length 3,

# $n = 10$ with Labels



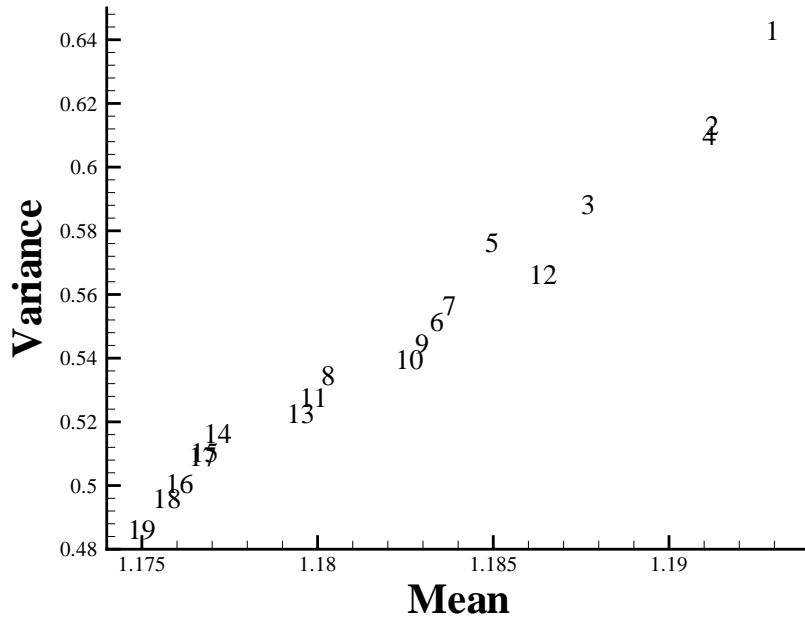
Graphs 19,18,16,17,15,14 have no subcycles of length 3,  
Graphs 13,11,8 have 1 subcycle of length 3,

# $n = 10$ with Labels



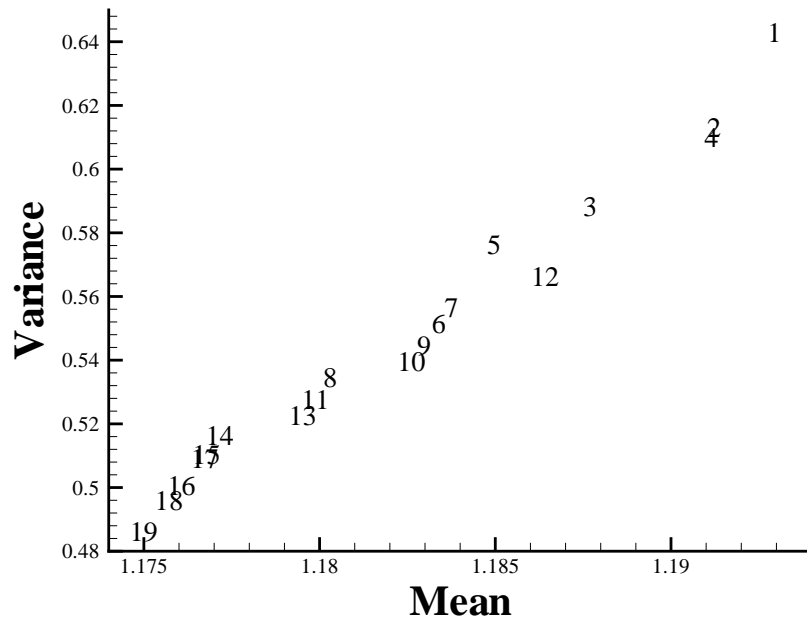
Graphs 19,18,16,17,15,14 have no subcycles of length 3,  
Graphs 13,11,8 have 1 subcycle of length 3,  
Graphs 10,9,6,7,5 have 2 subcycles of length 3,

# $n = 10$ with Labels



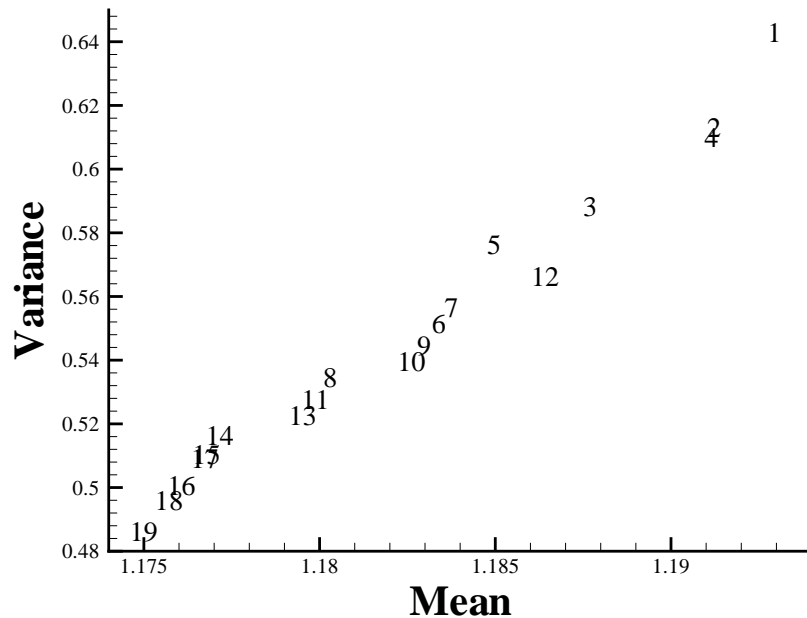
Graphs 19,18,16,17,15,14 have no subcycles of length 3,  
Graphs 13,11,8 have 1 subcycle of length 3,  
Graphs 10,9,6,7,5 have 2 subcycles of length 3,  
Graphs 12,3 have 3 subcycles of length 3, and

# $n = 10$ with Labels



Graphs 19,18,16,17,15,14 have no subcycles of length 3,  
Graphs 13,11,8 have 1 subcycle of length 3,  
Graphs 10,9,6,7,5 have 2 subcycles of length 3,  
Graphs 12,3 have 3 subcycles of length 3, and  
Graphs 4,2,1 have 4 subcycles of length 3.

# $n = 10$ with Labels



Graphs 19,18,16,17,15,14 have no subcycles of length 3,

Graphs 13,11,8 have 1 subcycle of length 3,

Graphs 10,9,6,7,5 have 2 subcycles of length 3,

Graphs 12,3 have 3 subcycles of length 3, and

Graphs 4,2,1 have 4 subcycles of length 3.

Graphs 17,15 have the same number of subcycles of length 4.

# Clustering Into Filars

- $\text{tr}(A^j) = \sum_{i=1}^n \lambda_i^j$ , and the  $(k, k)$ th element of  $A^j$  is the number of closed walks starting and finishing at vertex  $k$  of length  $j$ .



# Clustering Into Filars

- $\text{tr}(A^j) = \sum_{i=1}^n \lambda_i^j$ , and the  $(k, k)$ th element of  $A^j$  is the number of closed walks starting and finishing at vertex  $k$  of length  $j$ .
- The mean of the exponentials of the eigenvalues of  $A/3$  is

$$\mu = \frac{1}{n} \sum_{i=1}^n \exp(\lambda_i) = \frac{1}{n} \sum_{i=1}^n \sum_{j=0}^{\infty} \frac{\lambda_i^j}{j!} = \frac{1}{n} \sum_{j=0}^{\infty} \frac{1}{j!} \sum_{i=1}^n \lambda_i^j = \frac{1}{n} \sum_{j=0}^{\infty} \frac{\text{tr}(A^j)}{3^j j!}.$$

# Clustering Into Filars

•  $\text{tr}(A^j) = \sum_{i=1}^n \lambda_i^j$ , and the  $(k, k)$ th element of  $A^j$  is the number of closed walks starting and finishing at vertex  $k$  of length  $j$ .

• The mean of the exponentials of the eigenvalues of  $A/3$  is

$$\mu = \frac{1}{n} \sum_{i=1}^n \exp(\lambda_i) = \frac{1}{n} \sum_{i=1}^n \sum_{j=0}^{\infty} \frac{\lambda_i^j}{j!} = \frac{1}{n} \sum_{j=0}^{\infty} \frac{1}{j!} \sum_{i=1}^n \lambda_i^j = \frac{1}{n} \sum_{j=0}^{\infty} \frac{\text{tr}(A^j)}{3^j j!}.$$

• For all cubic graphs,  $\text{tr}(A^0) = n$ ,  $\text{tr}(A^1) = 0$  and  $\text{tr}(A^2) = 3n$ , so

$$\mu = \frac{7}{6} + \frac{1}{n} \sum_{j=3}^{\infty} \frac{\text{tr}(A^j)}{3^j j!}.$$

# Clustering Into Filars

- $\text{tr}(A^j) = \sum_{i=1}^n \lambda_i^j$ , and the  $(k, k)$ th element of  $A^j$  is the number of closed walks starting and finishing at vertex  $k$  of length  $j$ .

- The mean of the exponentials of the eigenvalues of  $A/3$  is

$$\mu = \frac{1}{n} \sum_{i=1}^n \exp(\lambda_i) = \frac{1}{n} \sum_{i=1}^n \sum_{j=0}^{\infty} \frac{\lambda_i^j}{j!} = \frac{1}{n} \sum_{j=0}^{\infty} \frac{1}{j!} \sum_{i=1}^n \lambda_i^j = \frac{1}{n} \sum_{j=0}^{\infty} \frac{\text{tr}(A^j)}{3^j j!}.$$

- For all cubic graphs,  $\text{tr}(A^0) = n$ ,  $\text{tr}(A^1) = 0$  and  $\text{tr}(A^2) = 3n$ , so

$$\mu = \frac{7}{6} + \frac{1}{n} \sum_{j=3}^{\infty} \frac{\text{tr}(A^j)}{3^j j!}.$$

- Number of closed walks of increasing length separate graphs in different filars, subfilars, etc.

# (Roughly) Filars as Straight Lines

$$\text{Similarly, } s^2 = \frac{1}{n-1} \left( \sum_{j=0}^{\infty} \frac{2^j \text{tr}(A^j)}{3^j j!} - n\mu^2 \right).$$

# (Roughly) Filars as Straight Lines

$$\text{Similarly, } s^2 = \frac{1}{n-1} \left( \sum_{j=0}^{\infty} \frac{2^j \text{tr}(A^j)}{3^j j!} - n\mu^2 \right).$$

Assume we move from graph  $A$  with mean  $\mu_A$  to graph  $B$  with mean  $\mu_B$  where  $\text{tr}(B^j) = \text{tr}(A^j)$  for all  $j \neq k$  and  $\text{tr}(B^k) = \text{tr}(A^k) + \delta$ .

# (Roughly) Filars as Straight Lines

$$\text{Similarly, } s^2 = \frac{1}{n-1} \left( \sum_{j=0}^{\infty} \frac{2^j \text{tr}(A^j)}{3^j j!} - n\mu^2 \right).$$

Assume we move from graph  $A$  with mean  $\mu_A$  to graph  $B$  with mean  $\mu_B$  where  $\text{tr}(B^j) = \text{tr}(A^j)$  for all  $j \neq k$  and  $\text{tr}(B^k) = \text{tr}(A^k) + \delta$ .

Then  $\mu_B = \mu_A + \frac{\delta}{n3^k k!}$ , and

$$s_B^2 = s_A^2 + \frac{\delta 2^k}{(n-1)3^k k!} - \frac{2\delta\mu_A}{(n-1)3^k k!} - \frac{\delta^2}{n(n-1)3^{2k} (k!)^2}.$$

# (Roughly) Filars as Straight Lines

$$\text{Similarly, } s^2 = \frac{1}{n-1} \left( \sum_{j=0}^{\infty} \frac{2^j \text{tr}(A^j)}{3^j j!} - n\mu^2 \right).$$

Assume we move from graph  $A$  with mean  $\mu_A$  to graph  $B$  with mean  $\mu_B$  where  $\text{tr}(B^j) = \text{tr}(A^j)$  for all  $j \neq k$  and  $\text{tr}(B^k) = \text{tr}(A^k) + \delta$ .

Then  $\mu_B = \mu_A + \frac{\delta}{n3^k k!}$ , and

$$s_B^2 = s_A^2 + \frac{\delta 2^k}{(n-1)3^k k!} - \frac{2\delta\mu_A}{(n-1)3^k k!} - \frac{\delta^2}{n(n-1)3^{2k}(k!)^2}.$$

When moving from graphs  $A$  to  $B$ ,  $\mu$  increases by  $\delta/(n3^k k!)$  and  $s^2$  increases by  $\delta(2^k - 2\mu)/((n-1)3^k k!)$ .

# (Roughly) Filars as Straight Lines

$$\text{Similarly, } s^2 = \frac{1}{n-1} \left( \sum_{j=0}^{\infty} \frac{2^j \text{tr}(A^j)}{3^j j!} - n\mu^2 \right).$$

Assume we move from graph  $A$  with mean  $\mu_A$  to graph  $B$  with mean  $\mu_B$  where  $\text{tr}(B^j) = \text{tr}(A^j)$  for all  $j \neq k$  and  $\text{tr}(B^k) = \text{tr}(A^k) + \delta$ .

Then  $\mu_B = \mu_A + \frac{\delta}{n3^k k!}$ , and

$$s_B^2 = s_A^2 + \frac{\delta 2^k}{(n-1)3^k k!} - \frac{2\delta\mu_A}{(n-1)3^k k!} - \frac{\delta^2}{n(n-1)3^{2k}(k!)^2}.$$

When moving from graphs  $A$  to  $B$ ,  $\mu$  increases by  $\delta/(n3^k k!)$  and  $s^2$  increases by  $\delta(2^k - 2\mu)/((n-1)3^k k!)$ .

Now  $\mu$  only changes over a very small range. So the ratio ( $s^2$  increase/ $\mu$  increase) equals  $(n/(n-1))(2^k - 2\mu)$ .



# More Formal Derivation

The Ihara-Selberg trace formula for regular graphs of degree  $q + 1$  can be written as

$$\frac{1}{n} \sum_{i=1}^n e^{t\lambda_i} = \frac{q+1}{2\pi} \int_{-2\sqrt{q}}^{2\sqrt{q}} e^{st} \frac{\sqrt{4q-x^2}}{(q+1)^2-x^2} dx + \frac{1}{n} \sum_{\gamma} \sum_{k=1}^{\infty} \frac{l(\gamma)}{2^{kl(\gamma)/2}} I_{kl(\gamma)}(2\sqrt{qt}),$$

where  $\gamma$  runs over all oriented primitive closed geodesics, and  $l(\gamma)$  is the length of  $\gamma$ .

# More Formal Derivation

The Ihara-Selberg trace formula for regular graphs of degree  $q + 1$  can be written as

$$\frac{1}{n} \sum_{i=1}^n e^{t\lambda_i} = \frac{q+1}{2\pi} \int_{-2\sqrt{q}}^{2\sqrt{q}} e^{st} \frac{\sqrt{4q-x^2}}{(q+1)^2-x^2} dx + \frac{1}{n} \sum_{\gamma} \sum_{k=1}^{\infty} \frac{l(\gamma)}{2^{kl(\gamma)/2}} I_{kl(\gamma)}(2\sqrt{q}t),$$

where  $\gamma$  runs over all oriented primitive closed geodesics, and  $l(\gamma)$  is the length of  $\gamma$ . Letting  $n_l$  be the number of geodesics of length  $l$ , and setting

$$q = 2, \quad \frac{1}{n} \sum_{i=1}^n e^{t\lambda_i} = J(t) + \frac{2}{n} \sum_{l=3}^{\infty} l n_l F_l(t),$$

$$\text{where } J(t) = \frac{3}{2\pi} \int_{-2\sqrt{2}}^{2\sqrt{2}} e^{tx} \frac{\sqrt{8-x^2}}{9-x^2} dx \text{ and } F_l(t) = \sum_{k=1}^{\infty} \frac{I_{kl}(2\sqrt{2}t)}{2^{kl/2}}.$$

# More Formal Derivation

The Ihara-Selberg trace formula for regular graphs of degree  $q + 1$  can be written as

$$\frac{1}{n} \sum_{i=1}^n e^{t\lambda_i} = \frac{q+1}{2\pi} \int_{-2\sqrt{q}}^{2\sqrt{q}} e^{st} \frac{\sqrt{4q-x^2}}{(q+1)^2-x^2} dx + \frac{1}{n} \sum_{\gamma} \sum_{k=1}^{\infty} \frac{l(\gamma)}{2^{kl(\gamma)/2}} I_{kl(\gamma)}(2\sqrt{q}t),$$

where  $\gamma$  runs over all oriented primitive closed geodesics, and  $l(\gamma)$  is the length of  $\gamma$ . Letting  $n_l$  be the number of geodesics of length  $l$ , and setting

$$q = 2, \quad \frac{1}{n} \sum_{i=1}^n e^{t\lambda_i} = J(t) + \frac{2}{n} \sum_{l=3}^{\infty} l n_l F_l(t),$$

where  $J(t) = \frac{3}{2\pi} \int_{-2\sqrt{2}}^{2\sqrt{2}} e^{tx} \frac{\sqrt{8-x^2}}{9-x^2} dx$  and  $F_l(t) = \sum_{k=1}^{\infty} \frac{I_{kl}(2\sqrt{2}t)}{2^{kl/2}}$ .

Note that  $I_m(z) \approx \frac{1}{m!} \left(\frac{z}{2}\right)^m$  as  $m \rightarrow \infty$  and  $0 < z \ll \sqrt{m+1}$ .

# Mean and Variance

$$\mu = \frac{1}{n} \sum_{i=1}^n e^{\lambda_i/3} = J(1/3) + \frac{2}{n} \sum_{l=3}^{\infty} l n_l F_l(1/3),$$

# Mean and Variance

$$\mu = \frac{1}{n} \sum_{i=1}^n e^{\lambda_i/3} = J(1/3) + \frac{2}{n} \sum_{l=3}^{\infty} \ln_l F_l(1/3),$$

$$\sigma^2 = \frac{1}{n} \sum_{i=1}^n \left( e^{\lambda_i/3} - \mu \right)^2 = \frac{1}{n} \sum_{i=1}^n e^{2\lambda_i/3} - \mu^2$$

# Mean and Variance

$$\mu = \frac{1}{n} \sum_{i=1}^n e^{\lambda_i/3} = J(1/3) + \frac{2}{n} \sum_{l=3}^{\infty} \ln_l F_l(1/3),$$

$$\begin{aligned} \sigma &= \frac{1}{n} \sum_{i=1}^n \left( e^{\lambda_i/3} - \mu \right)^2 = \frac{1}{n} \sum_{i=1}^n e^{2\lambda_i/3} - \mu^2 \\ &= \left( J(2/3) - J(1/3)^2 \right) + \frac{2}{n} \sum_{l=3}^{\infty} \ln_l \left( F_l(2/3) - 2J(1/3)F_l(1/3) \right) \\ &\quad + \left( \frac{2}{n} \sum_{l=3}^{\infty} \ln_l F_l(1/3) \right)^2. \end{aligned}$$

# Mean and Variance

$$\mu = \frac{1}{n} \sum_{i=1}^n e^{\lambda_i/3} = J(1/3) + \frac{2}{n} \sum_{l=3}^{\infty} l n_l F_l(1/3),$$

$$\begin{aligned} \sigma &= \frac{1}{n} \sum_{i=1}^n \left( e^{\lambda_i/3} - \mu \right)^2 = \frac{1}{n} \sum_{i=1}^n e^{2\lambda_i/3} - \mu^2 \\ &= \left( J(2/3) - J(1/3)^2 \right) + \frac{2}{n} \sum_{l=3}^{\infty} l n_l \left( F_l(2/3) - 2J(1/3)F_l(1/3) \right) \\ &\quad + \left( \frac{2}{n} \sum_{l=3}^{\infty} l n_l F_l(1/3) \right)^2. \end{aligned}$$

Ignoring the (small) quadratic term, a change  $\delta_l$  to  $n_l$  changes  $\mu$  by  $2lF_l(1/3)\delta_l/n$  and  $\sigma$  by  $2l(F_l(2/3) - 2J(1/3)F_l(1/3))\delta_l/n$  – each filar is a straight line.

# Hamiltonian Cycles

- A Hamiltonian cycle is a closed path that only enters and exits each vertex exactly once.



# Hamiltonian Cycles

- A Hamiltonian cycle is a closed path that only enters and exits each vertex exactly once.
- Given a graph, the amount of work required to find Hamiltonian cycles (or even prove they don't exist) appears to be exponential.

# Hamiltonian Cycles

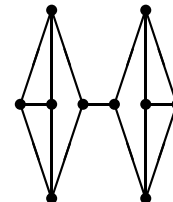
- A Hamiltonian cycle is a closed path that only enters and exits each vertex exactly once.
- Given a graph, the amount of work required to find Hamiltonian cycles (or even prove they don't exist) appears to be exponential.
- Given a proposed Hamiltonian cycle, it's easy to prove if it is correct. This is typical of **NP-Complete** problems.

# Hamiltonian Cycles

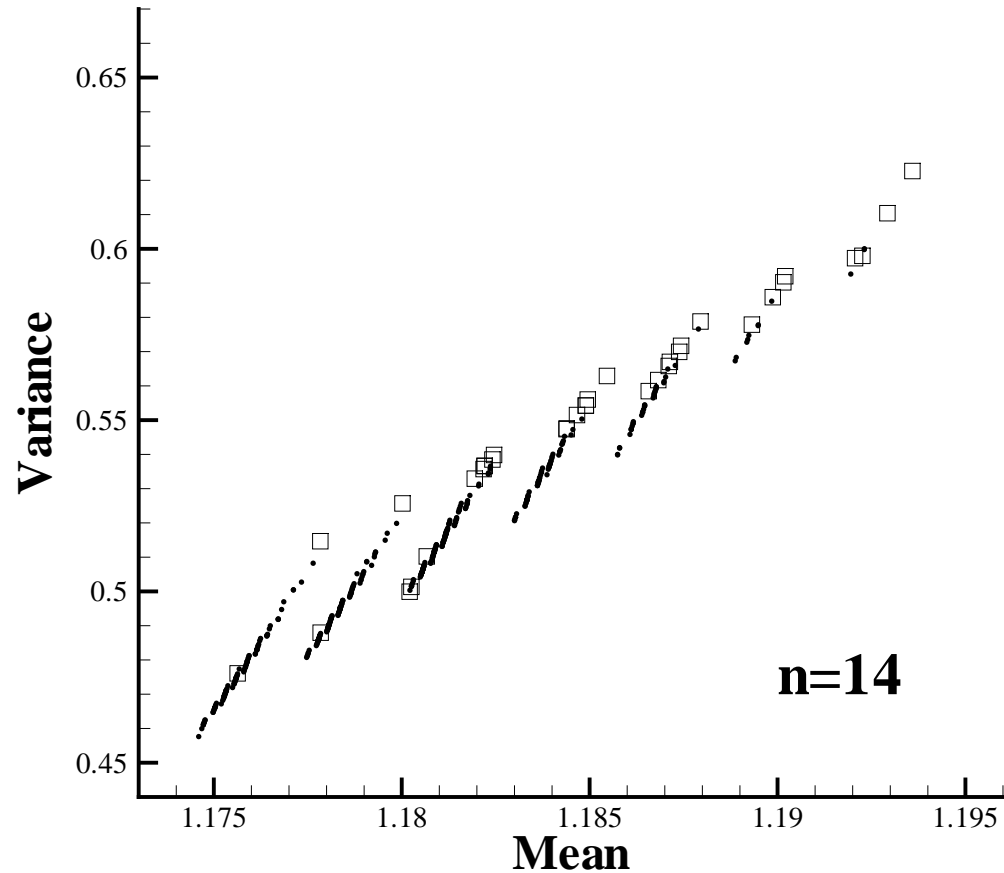
- A Hamiltonian cycle is a closed path that only enters and exits each vertex exactly once.
- Given a graph, the amount of work required to find Hamiltonian cycles (or even prove they don't exist) appears to be exponential.
- Given a proposed Hamiltonian cycle, it's easy to prove if it is correct. This is typical of **NP-Complete** problems.
- Even the Hamiltonian cycle problem on cubic graphs is NP-Complete.

# Hamiltonian Cycles

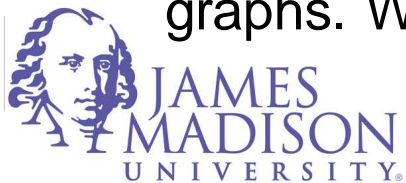
- A Hamiltonian cycle is a closed path that only enters and exits each vertex exactly once.
- Given a graph, the amount of work required to find Hamiltonian cycles (or even prove they don't exist) appears to be exponential.
- Given a proposed Hamiltonian cycle, it's easy to prove if it is correct. This is typical of **NP-Complete** problems.
- Even the Hamiltonian cycle problem on cubic graphs is NP-Complete.
- A bridge graph is one that can be split in pieces by removing an edge (or vertex). This can be established in polynomial time, and a bridge graph is clearly not Hamiltonian.



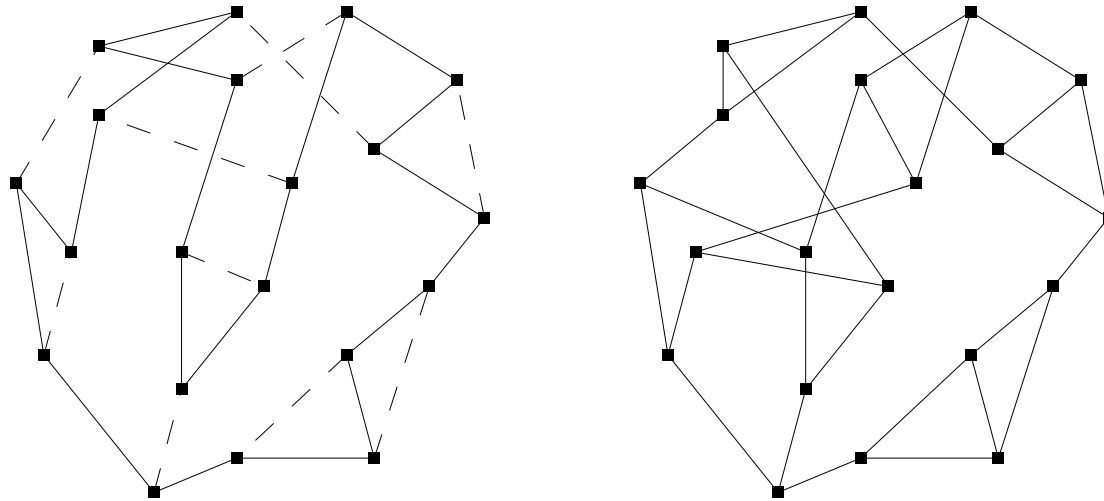
# Hamiltonian Cycles and Cubic Graph Filars



Most non-Hamiltonian graphs are at the ends of filars, and are **bridge** graphs. What is the relationship between bridge graphs and their position in a filar?



# Eigenanalysis Inadequate



These twenty vertex cubic graphs are co-spectral (have the same eigenvalues), the one on the left has Hamiltonian cycles, the one on the right does not.

# A Conjecture

Robinson and Wormald proved that *almost all* regular graphs are Hamiltonian.

# A Conjecture

Robinson and Wormald proved that *almost all* regular graphs are Hamiltonian.

Graph Size	Number Cubic	Number Non-H	Ratio Non-H/Cubic	Number Cubic Bridge	Ratio Bridge/Non-H
10	19	2	0.1053	1	0.5000
12	85	5	0.0588	4	0.8000
14	509	35	0.0688	29	0.8286
16	4 060	219	0.0539	186	0.8493
18	41 301	1 666	0.0403	1 435	0.8613
20	510 490	14 498	0.0284	12 671	0.8740
22	7 319 447	148 790	0.0203	131 820	0.8859
24	117 940 535	1 768 732	0.0150	1 590 900	0.8995



# A Conjecture

Robinson and Wormald proved that *almost all* regular graphs are Hamiltonian.

Graph Size	Number Cubic	Number Non-H	Ratio Non-H/Cubic	Number Bridge	Ratio Bridge/Non-H
10	19	2	0.1053	1	0.5000
12	85	5	0.0588	4	0.8000
14	509	35	0.0688	29	0.8286
16	4 060	219	0.0539	186	0.8493
18	41 301	1 666	0.0403	1 435	0.8613
20	510 490	14 498	0.0284	12 671	0.8740
22	7 319 447	148 790	0.0203	131 820	0.8859
24	117 940 535	1 768 732	0.0150	1 590 900	0.8995

Conjecture (Filar, Haythorpe & Nguyen):

Almost all regular non-Hamiltonian graphs are bridge graphs.

# A Property of Hamiltonian Cycles

- A *directed* graph  $G$  has an adjacency matrix  $A$ , where

$$a_{ij} = \begin{cases} 1, & \text{if an arrow joins vertex } i \text{ to vertex } j, \\ 0, & \text{otherwise.} \end{cases}$$

# A Property of Hamiltonian Cycles

- A *directed* graph  $G$  has an adjacency matrix  $A$ , where

$$a_{ij} = \begin{cases} 1, & \text{if an arrow joins vertex } i \text{ to vertex } j, \\ 0, & \text{otherwise.} \end{cases}$$

- A Hamiltonian Cycle is a directed subgraph with the original  $n$  vertices and  $n$  selected edges – one leaving each vertex. So its adjacency matrix is a permutation matrix ( $I$  with row swaps).

# A Property of Hamiltonian Cycles

- A directed graph  $G$  has an adjacency matrix  $A$ , where

$$a_{ij} = \begin{cases} 1, & \text{if an arrow joins vertex } i \text{ to vertex } j, \\ 0, & \text{otherwise.} \end{cases}$$

- A Hamiltonian Cycle is a directed subgraph with the original  $n$  vertices and  $n$  selected edges – one leaving each vertex. So its adjacency matrix is a permutation matrix ( $I$  with row swaps).

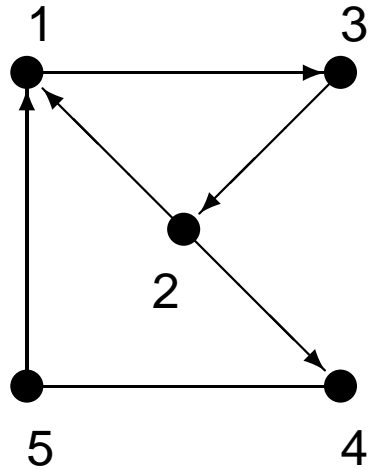
**Theorem:** *An  $n \times n$  permutation matrix is the adjacency matrix of some Hamiltonian cyclic graph on  $n$  vertices if and only if its characteristic polynomial is  $\lambda^n - 1 = 0$ .*

# A System of Polynomial Equations

The *modified adjacency matrix* of a graph places the variable  $x_{ij}$  at row  $i$  column  $j$  if there is a (directed) edge.

# A System of Polynomial Equations

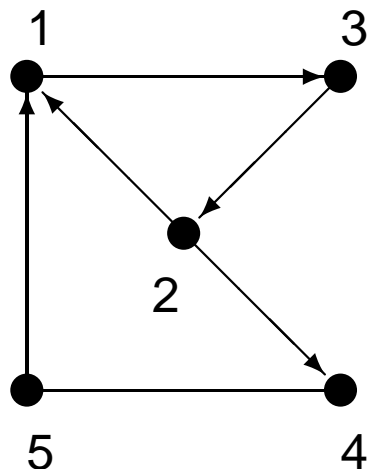
The *modified adjacency matrix* of a graph places the variable  $x_{ij}$  at row  $i$  column  $j$  if there is a (directed) edge. For example



$$X = \begin{pmatrix} 0 & 0 & x_{1,3} & 0 & 0 \\ x_{2,1} & 0 & 0 & x_{2,4} & 0 \\ 0 & x_{3,2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & x_{4,5} \\ x_{5,1} & 0 & 0 & x_{5,4} & 0 \end{pmatrix}.$$

# A System of Polynomial Equations

The *modified adjacency matrix* of a graph places the variable  $x_{ij}$  at row  $i$  column  $j$  if there is a (directed) edge. For example



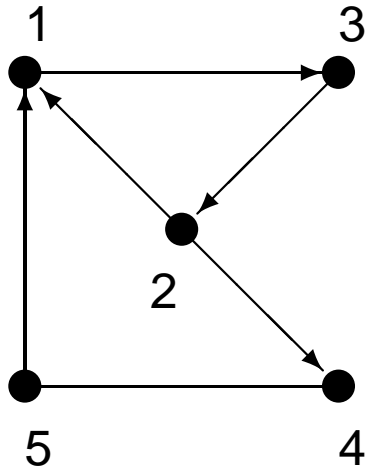
$$X = \begin{pmatrix} 0 & 0 & x_{1,3} & 0 & 0 \\ x_{2,1} & 0 & 0 & x_{2,4} & 0 \\ 0 & x_{3,2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & x_{4,5} \\ x_{5,1} & 0 & 0 & x_{5,4} & 0 \end{pmatrix}.$$

A Hamiltonian cycle is equivalent to the solution of the system of polynomial equations ( $x_{ij} = 1$  if (directed) edge is in Hamiltonian cycle)

$$\begin{cases} x_{ij}(1 - x_{ij}) = 0 \text{ for all } (i, j) \in E, \\ \sum_j x_{ij} - 1 = 0, \text{ for all } i, \\ \sum_i x_{ij} - 1 = 0 \text{ for all } j, \\ \det(\lambda I - X) - \lambda^n + 1 = 0, \end{cases}$$

# A System of Polynomial Equations

The *modified adjacency matrix* of a graph places the variable  $x_{ij}$  at row  $i$  column  $j$  if there is a (directed) edge. For example



$$X = \begin{pmatrix} 0 & 0 & x_{1,3} & 0 & 0 \\ x_{2,1} & 0 & 0 & x_{2,4} & 0 \\ 0 & x_{3,2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & x_{4,5} \\ x_{5,1} & 0 & 0 & x_{5,4} & 0 \end{pmatrix}.$$

A Hamiltonian cycle is equivalent to the solution of the system of polynomial equations ( $x_{ij} = 1$  if (directed) edge is in Hamiltonian cycle)

$$\begin{cases} x_{ij}(1 - x_{ij}) = 0 \text{ for all } (i, j) \in E, \\ \sum_j x_{ij} - 1 = 0, \text{ for all } i, \\ \sum_i x_{ij} - 1 = 0 \text{ for all } j, \\ \det(\lambda I - X) - \lambda^n + 1 = 0, \end{cases}$$



# Solution Method

Can be solved (symbolically) using Gröbner bases, as applied using Buchberger's algorithm.

# Solution Method

Can be solved (symbolically) using Gröbner bases, as applied using Buchberger's algorithm. For example (Maple),

```
with(grobner):ff:=[x13*(1-x13),x21*(1-x21),x24*(1-x24),  
x32*(1-x32),x45*(1-x45),x51*(1-x51),x54*(1-x54),x21+x51-1,  
x32-1,x13-1,x24+x54-1,x45-1,x13-1,x21+x24-1,x32-1,x45-1,  
x51+x54-1,x45*x54,x21*x32*x13,x21*x32*x13*x45*x54-x51*x32*  
x13*x24*x45+1];  
gbasis(ff,[x13,x21,x24,x32,x45,x51,x54])
```

# Solution Method

Can be solved (symbolically) using Gröbner bases, as applied using Buchberger's algorithm. For example (Maple),

```
with(grobner):ff:=[x13*(1-x13),x21*(1-x21),x24*(1-x24),  
x32*(1-x32),x45*(1-x45),x51*(1-x51),x54*(1-x54),x21+x51-1,  
x32-1,x13-1,x24+x54-1,x45-1,x13-1,x21+x24-1,x32-1,x45-1,  
x51+x54-1,x45*x54,x21*x32*x13,x21*x32*x13*x45*x54-x51*x32*  
x13*x24*x45+1];
```

```
gbasis(ff,[x13,x21,x24,x32,x45,x51,x54])
```

which returns

```
gbasis=[x13-1,x21,x24-1,x32-1,x45-1,x51-1,x54]
```

# Solution Method

Can be solved (symbolically) using Gröbner bases, as applied using Buchberger's algorithm. For example (Maple),

```
with(grobner):ff:=[x13*(1-x13),x21*(1-x21),x24*(1-x24),  
x32*(1-x32),x45*(1-x45),x51*(1-x51),x54*(1-x54),x21+x51-1,  
x32-1,x13-1,x24+x54-1,x45-1,x13-1,x21+x24-1,x32-1,x45-1,  
x51+x54-1,x45*x54,x21*x32*x13,x21*x32*x13*x45*x54-x51*x32*  
x13*x24*x45+1];  
gbasis(ff,[x13,x21,x24,x32,x45,x51,x54])
```

which returns

```
gbasis=[x13-1,x21,x24-1,x32-1,x45-1,x51-1,x54]
```

and implies  $x_{13} = 1$ ,  $x_{21} = 0$ ,  $x_{24} = 1$ ,  $x_{32} = 1$ ,  $x_{45} = 1$ ,  $x_{51} = 1$  and  $x_{54} = 0$ , so the Hamiltonian cycle 1-3-2-4-5-1.

# Solution Method

Can be solved (symbolically) using Gröbner bases, as applied using Buchberger's algorithm. For example (Maple),

```
with(grobner):ff:=[x13*(1-x13),x21*(1-x21),x24*(1-x24),  
x32*(1-x32),x45*(1-x45),x51*(1-x51),x54*(1-x54),x21+x51-1,  
x32-1,x13-1,x24+x54-1,x45-1,x13-1,x21+x24-1,x32-1,x45-1,  
x51+x54-1,x45*x54,x21*x32*x13,x21*x32*x13*x45*x54-x51*x32*  
x13*x24*x45+1];  
gbasis(ff,[x13,x21,x24,x32,x45,x51,x54])
```

which returns

```
gbasis=[x13-1,x21,x24-1,x32-1,x45-1,x51-1,x54]
```

and implies  $x_{13} = 1$ ,  $x_{21} = 0$ ,  $x_{24} = 1$ ,  $x_{32} = 1$ ,  $x_{45} = 1$ ,  $x_{51} = 1$  and  $x_{54} = 0$ , so the Hamiltonian cycle 1-3-2-4-5-1.

But,  $\det(\lambda I - X)$  grows exponentially in number of vertices.

# Using the Symbolic Determinant

**Theorem:** *The product terms making up the symbolic determinant of the modified adjacency matrix represent sets of subcycles on all vertices of a given graph. In addition, a Hamiltonian cycle will be obtained when the path from any vertex visits every other vertex before returning.*

# Using the Symbolic Determinant

**Theorem:** *The product terms making up the symbolic determinant of the modified adjacency matrix represent sets of subcycles on all vertices of a given graph. In addition, a Hamiltonian cycle will be obtained when the path from any vertex visits every other vertex before returning.*

*Proof:* An elementary product from a matrix  $A$  is a product of  $n$  entries from the matrix, exactly one from each row and column.

# Using the Symbolic Determinant

**Theorem:** *The product terms making up the symbolic determinant of the modified adjacency matrix represent sets of subcycles on all vertices of a given graph. In addition, a Hamiltonian cycle will be obtained when the path from any vertex visits every other vertex before returning.*

*Proof:* An elementary product from a matrix  $A$  is a product of  $n$  entries from the matrix, exactly one from each row and column.

Write it as  $a_{1j_1} a_{2j_2} \cdots a_{nj_n}$ ,  $(j_1, j_2, \dots, j_n)$  a permutation of  $(1, 2, \dots, n)$ .



# Using the Symbolic Determinant

**Theorem:** *The product terms making up the symbolic determinant of the modified adjacency matrix represent sets of subcycles on all vertices of a given graph. In addition, a Hamiltonian cycle will be obtained when the path from any vertex visits every other vertex before returning.*

*Proof:* An elementary product from a matrix  $A$  is a product of  $n$  entries from the matrix, exactly one from each row and column.

Write it as  $a_{1j_1} a_{2j_2} \cdots a_{nj_n}$ ,  $(j_1, j_2, \dots, j_n)$  a permutation of  $(1, 2, \dots, n)$ .

A signed elementary product prefixes  $\pm 1$  depending on whether  $(j_1, j_2, \dots, j_n)$  is even or odd.

# Using the Symbolic Determinant

**Theorem:** *The product terms making up the symbolic determinant of the modified adjacency matrix represent sets of subcycles on all vertices of a given graph. In addition, a Hamiltonian cycle will be obtained when the path from any vertex visits every other vertex before returning.*

*Proof:* An elementary product from a matrix  $A$  is a product of  $n$  entries from the matrix, exactly one from each row and column.

Write it as  $a_{1j_1} a_{2j_2} \cdots a_{nj_n}$ ,  $(j_1, j_2, \dots, j_n)$  a permutation of  $(1, 2, \dots, n)$ .

A signed elementary product prefixes  $\pm 1$  depending on whether  $(j_1, j_2, \dots, j_n)$  is even or odd.

$\det(A)$  is the sum of all the signed elementary products from  $A$ .

# Using the Symbolic Determinant

**Theorem:** *The product terms making up the symbolic determinant of the modified adjacency matrix represent sets of subcycles on all vertices of a given graph. In addition, a Hamiltonian cycle will be obtained when the path from any vertex visits every other vertex before returning.*

*Proof:* An elementary product from a matrix  $A$  is a product of  $n$  entries from the matrix, exactly one from each row and column.

Write it as  $a_{1j_1} a_{2j_2} \cdots a_{nj_n}$ ,  $(j_1, j_2, \dots, j_n)$  a permutation of  $(1, 2, \dots, n)$ .

A signed elementary product prefixes  $\pm 1$  depending on whether  $(j_1, j_2, \dots, j_n)$  is even or odd.

$\det(A)$  is the sum of all the signed elementary products from  $A$ .

Applied to a modified adjacency matrix elementary products will involve  $x_{ij}$ 's, so will have exactly one (directed) edge out from each vertex.

# Using the Symbolic Determinant

**Theorem:** *The product terms making up the symbolic determinant of the modified adjacency matrix represent sets of subcycles on all vertices of a given graph. In addition, a Hamiltonian cycle will be obtained when the path from any vertex visits every other vertex before returning.*

*Proof:* An elementary product from a matrix  $A$  is a product of  $n$  entries from the matrix, exactly one from each row and column.

Write it as  $a_{1j_1} a_{2j_2} \cdots a_{nj_n}$ ,  $(j_1, j_2, \dots, j_n)$  a permutation of  $(1, 2, \dots, n)$ .

A signed elementary product prefixes  $\pm 1$  depending on whether  $(j_1, j_2, \dots, j_n)$  is even or odd.

$\det(A)$  is the sum of all the signed elementary products from  $A$ .

Applied to a modified adjacency matrix elementary products will involve  $x_{ij}$ 's, so will have exactly one (directed) edge out from each vertex.

Following these edges from a given vertex forms a subcycle, which may include all vertices. Otherwise, additional subcycles can be formed by starting from a vertex not yet visited.

# Using the Symbolic Determinant

**Theorem:** *The product terms making up the symbolic determinant of the modified adjacency matrix represent sets of subcycles on all vertices of a given graph. In addition, a Hamiltonian cycle will be obtained when the path from any vertex visits every other vertex before returning.*

*Proof:* An elementary product from a matrix  $A$  is a product of  $n$  entries from the matrix, exactly one from each row and column.

Write it as  $a_{1j_1} a_{2j_2} \cdots a_{nj_n}$ ,  $(j_1, j_2, \dots, j_n)$  a permutation of  $(1, 2, \dots, n)$ .

A signed elementary product prefixes  $\pm 1$  depending on whether  $(j_1, j_2, \dots, j_n)$  is even or odd.

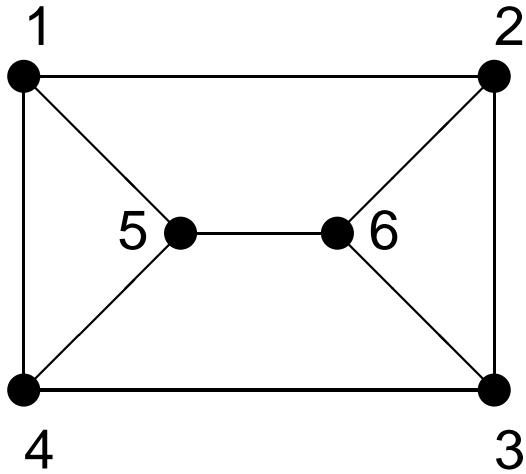
$\det(A)$  is the sum of all the signed elementary products from  $A$ .

Applied to a modified adjacency matrix elementary products will involve  $x_{ij}$ 's, so will have exactly one (directed) edge out from each vertex.

Following these edges from a given vertex forms a subcycle, which may include all vertices. Otherwise, additional subcycles can be formed by starting from a vertex not yet visited.

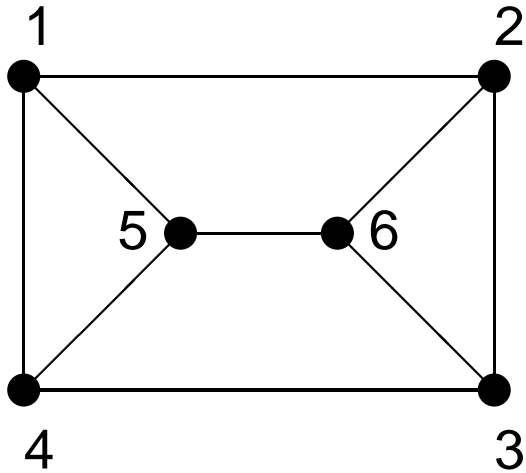
Elementary products can be scanned in linear time, but there are an exponential number of them, and exponential time is required to form them in the symbolic determinant.

# An Example



$$X = \begin{pmatrix} 0 & x_{1,2} & 0 & x_{1,4} & x_{1,5} & 0 \\ x_{2,1} & 0 & x_{2,3} & 0 & 0 & x_{2,6} \\ 0 & x_{3,2} & 0 & x_{3,4} & 0 & x_{3,6} \\ x_{4,1} & 0 & x_{4,3} & 0 & x_{4,5} & 0 \\ x_{5,1} & 0 & 0 & x_{5,4} & 0 & x_{5,6} \\ 0 & x_{6,2} & x_{6,3} & 0 & x_{6,5} & 0 \end{pmatrix}$$

# An Example



$$X = \begin{pmatrix} 0 & x_{1,2} & 0 & x_{1,4} & x_{1,5} & 0 \\ x_{2,1} & 0 & x_{2,3} & 0 & 0 & x_{2,6} \\ 0 & x_{3,2} & 0 & x_{3,4} & 0 & x_{3,6} \\ x_{4,1} & 0 & x_{4,3} & 0 & x_{4,5} & 0 \\ x_{5,1} & 0 & 0 & x_{5,4} & 0 & x_{5,6} \\ 0 & x_{6,2} & x_{6,3} & 0 & x_{6,5} & 0 \end{pmatrix}$$

$$\det(X) =$$

$$\begin{aligned} & x_{54}x_{41}x_{26}x_{15}x_{63}x_{32} + x_{54}x_{41}x_{36}x_{23}x_{15}x_{62} - x_{54}x_{12}x_{41}x_{36}x_{23}x_{65} - \\ & x_{14}x_{51}x_{43}x_{32}x_{26}x_{65} + x_{14}x_{43}x_{32}x_{56}x_{21}x_{65} + x_{34}x_{43}x_{56}x_{21}x_{15}x_{62} - \\ & x_{34}x_{12}x_{43}x_{56}x_{21}x_{65} - x_{34}x_{51}x_{43}x_{26}x_{15}x_{62} + x_{34}x_{12}x_{51}x_{43}x_{26}x_{65} + \\ & x_{54}x_{12}x_{21}x_{36}x_{43}x_{65} + x_{14}x_{51}x_{62}x_{45}x_{36}x_{23} + x_{34}x_{12}x_{63}x_{45}x_{56}x_{21} - \\ & x_{34}x_{12}x_{51}x_{63}x_{45}x_{26} - x_{14}x_{63}x_{32}x_{45}x_{56}x_{21} + x_{14}x_{51}x_{63}x_{32}x_{45}x_{26} - \\ & x_{54}x_{12}x_{21}x_{45}x_{36}x_{63} - x_{14}x_{23}x_{32}x_{56}x_{41}x_{65} - x_{34}x_{23}x_{56}x_{41}x_{15}x_{62} \\ & + x_{34}x_{12}x_{23}x_{56}x_{41}x_{65} - x_{54}x_{21}x_{36}x_{43}x_{15}x_{62} \end{aligned}$$

# Further Work and References

- Fractals in other graphs? (They exist in regular graphs.)
- Prove the bridge graph conjecture, or look at other kinds of graphs.
- Is there a better polynomial form of the HCP?
- GBs for other NP-Complete problems? (Already exact cover = Sudoku)
- The development of Boolean Gröbner Bases techniques.



# Further Work and References

- Fractals in other graphs? (They exist in regular graphs.)
- Prove the bridge graph conjecture, or look at other kinds of graphs.
- Is there a better polynomial form of the HCP?
- GBs for other NP-Complete problems? (Already exact cover = Sudoku)
- The development of Boolean Gröbner Bases techniques.
  - J.L. Nelson, S.K. Lucas, J.A. Filar & V. Ejov, Solving the Hamiltonian Cycle problem using symbolic determinants, *Taiwanese J. Math.* **10** 327-338 (2006).
  - V. Ejov, J.A. Filar, S.K. Lucas & P. Zograf, Clustering of spectra and fractals of regular graphs, *J. Math. Anal. Appl.* **333** 236-246 (2007).
  - V. Ejov, S. Friedland & G.T. Nguyen, A note on the graph's resolvent and the multifilar structure, *Linear Algebra and its Applications* **431** (2009) 1367–1379.
  - E. Arnold, S.K. Lucas & L. Taalman, Gröbner Basis representations of Sudoku, *College Math. J.* **41**(2) 101-111 (2010).