大学共同利用機関法人 情報・システム研究機構
統計数理研究所
The Institute of Statistical Mathematics

Graph theoretic methods for Data Visualization.

I. Pairwise Display and the `PairViz` `R` package

Wayne Oldford   based on joint work with Catherine Hurley

WATERLOO | MATHEMATICS
STATISTICS AND ACTUARIAL SCIENCE

2011 年度の統計数理研究所共同研究集会
「データ解析環境Rの整備と利用」

Tutorial B1

WATERLOO

The problem

- Can we automatically, yet meaningfully, layout complex statistical displays?
- Can we navigate high dimensional structure in a useful yet controlled way?
- Answer: Yes

  graph theory provides framework,
  Statistics adds meaning.

Radial axes

7 variates:

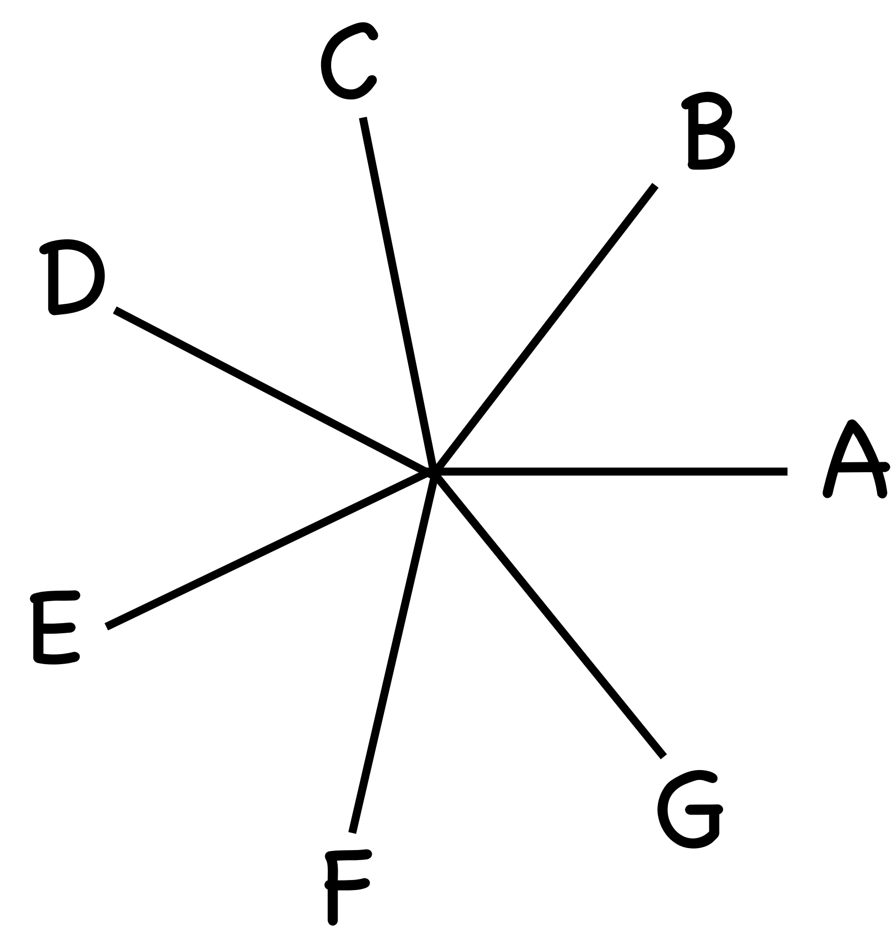
A, B, C, D, E, F, G

Radial axes

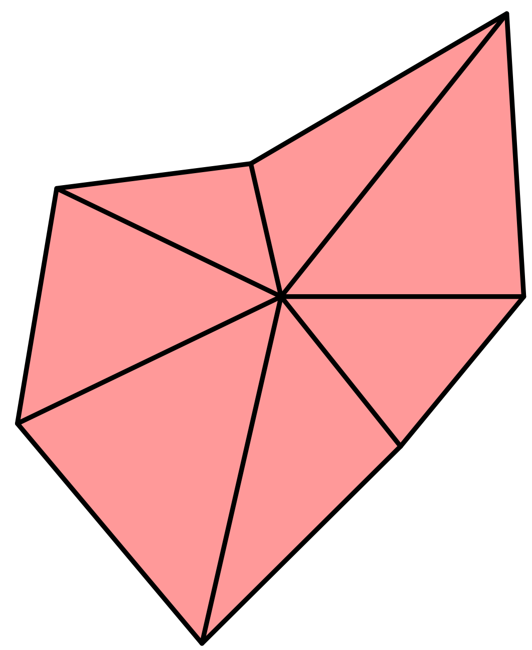
7 variates:

A, B, C, D, E, F, G

Arrange axes as equiangular radii:



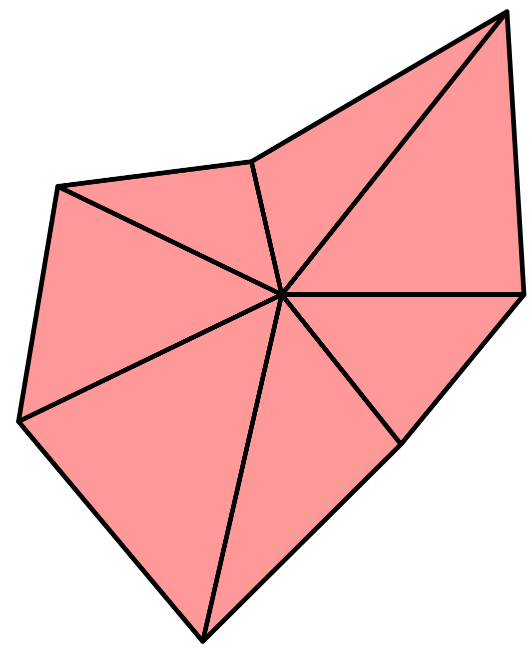
Radial axes



Length of each radius is proportional to (scaled) variate value for that case.

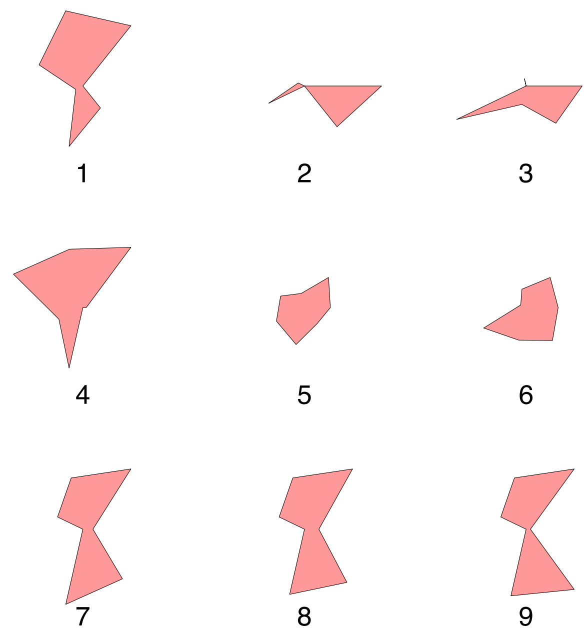
Have a "star-shaped" glyph for each case.

Radial axes:



- Compare cases by shape of glyph,

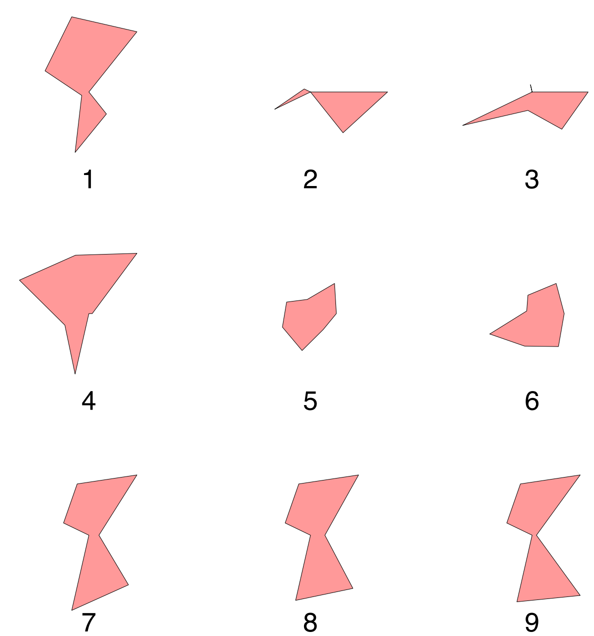
Radial axes:



- Compare cases by shape of glyph, here 9 cases in 7 dimensions
- Visually cluster high dimensional data by shape:

{7,8,9,1} {2,3} {4} {5,6} ?

Radial axes:

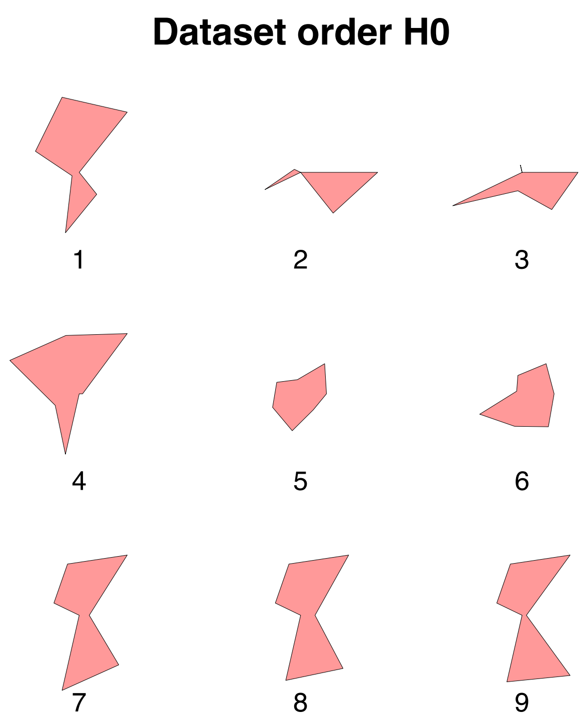


- Compare cases by shape of glyph, here 9 cases in 7 dimensions
- Visually cluster high dimensional data by shape:

  {7,8,9,1} {2,3} {4} {5,6} ?

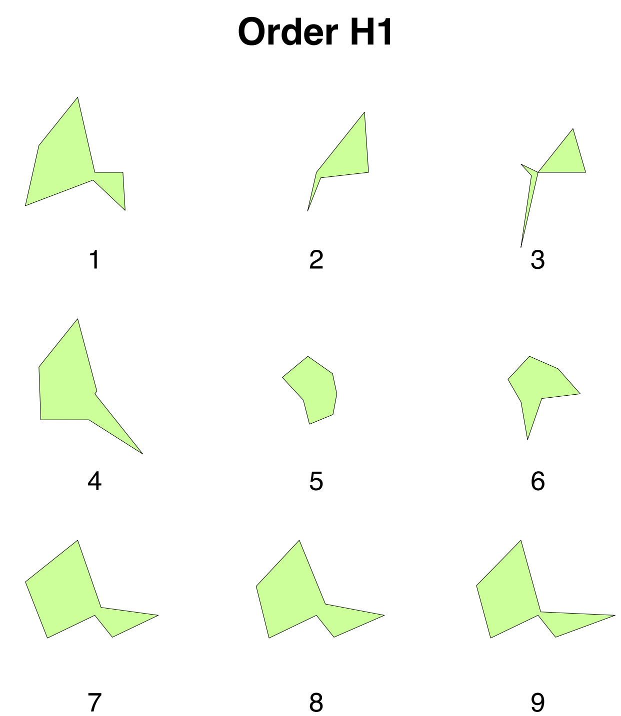
- What if the variables were assigned in a different order?

Radial axes: order effect

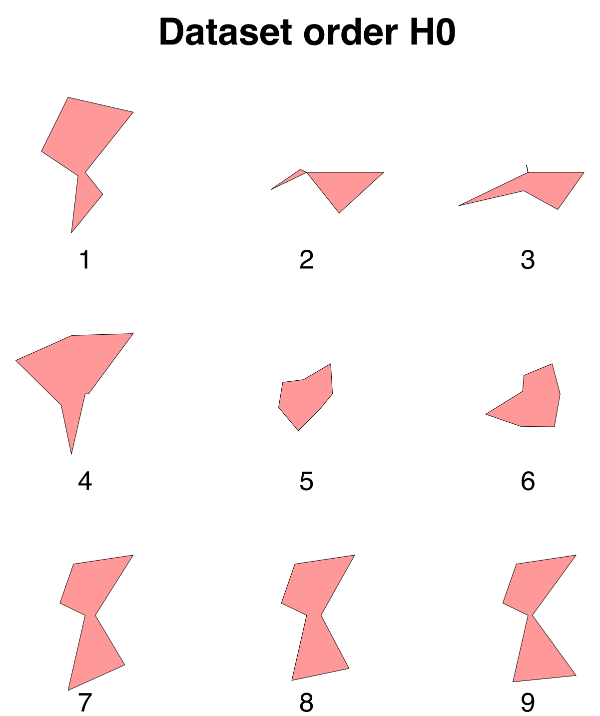


{7,8,9,1} {2,3} {4} {5,6} ?

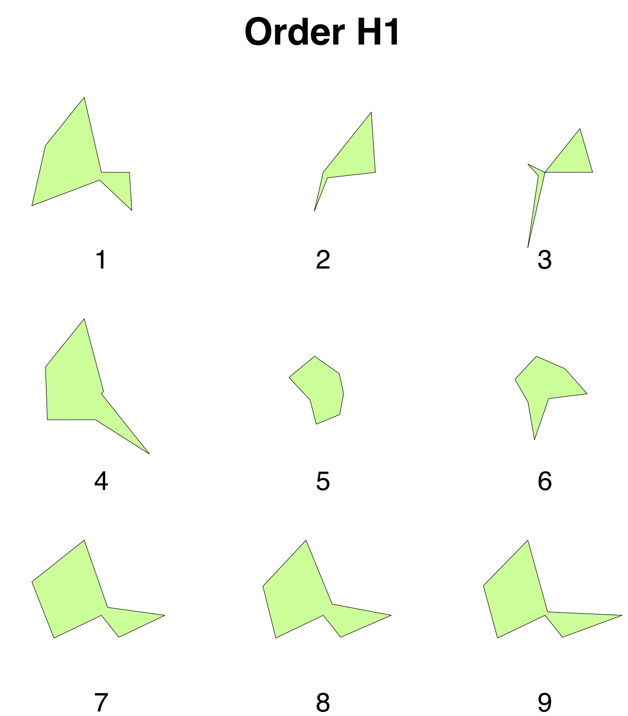
{7,8,9,1} {2,3} {4} {5} {6} ?



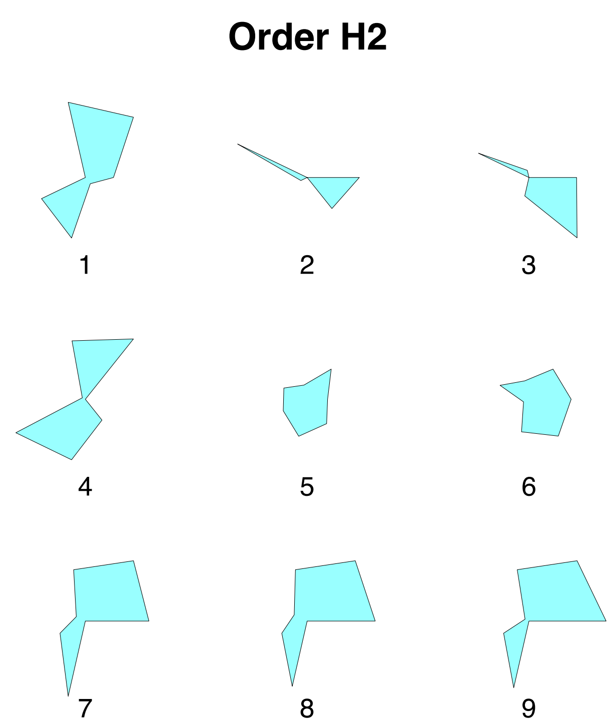
Radial axes: order effect



{7,8,9,1} {2,3} {4} {5,6} ?



{7,8,9,1} {2,3} {4} {5} {6} ?

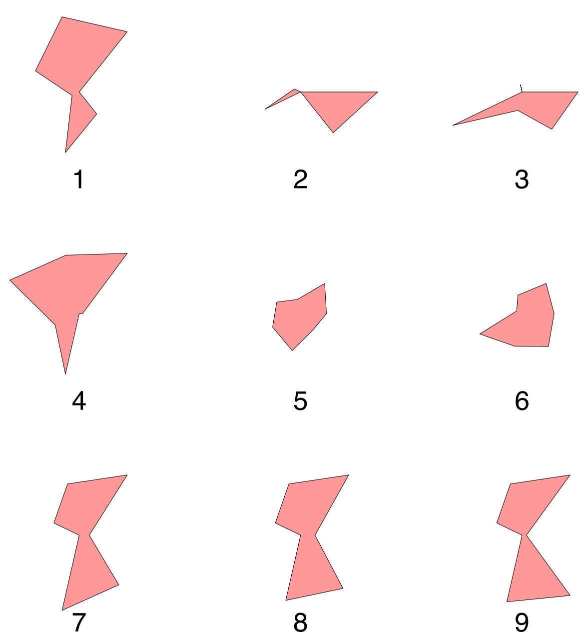


{1,4} {2,3} {5,6} {7,8,9} ?

Radial axes: order effect

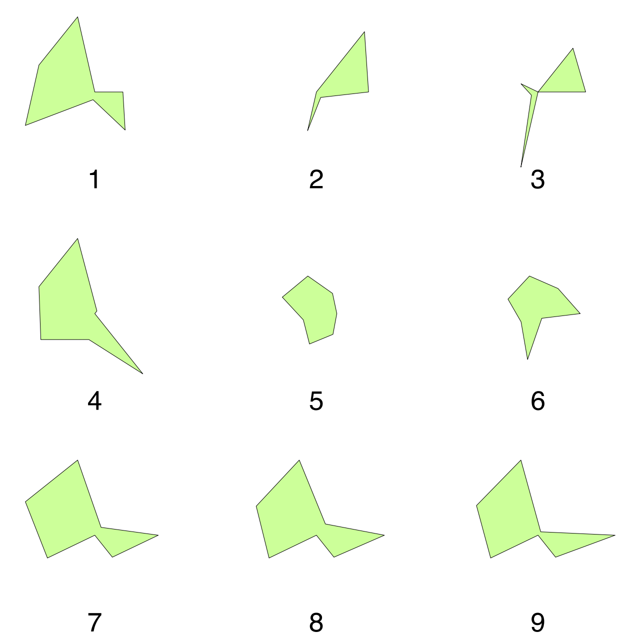
… different orders = different visual effect

Dataset order H0



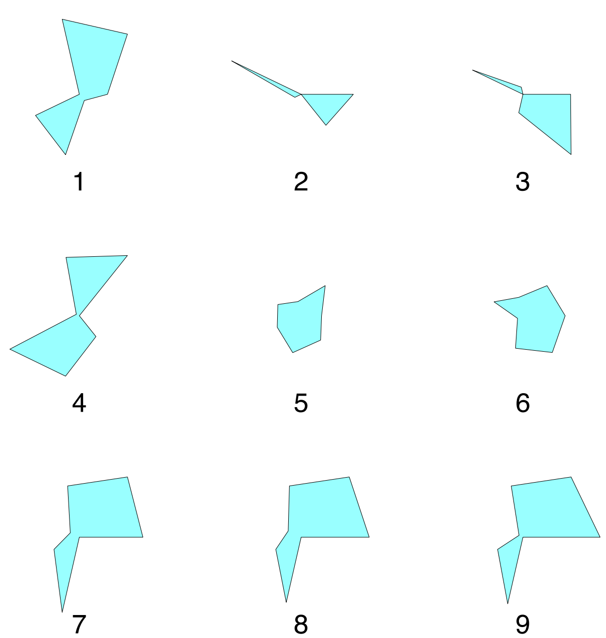
{7,8,9,1} {2,3} {4} {5,6} ?

Order H1



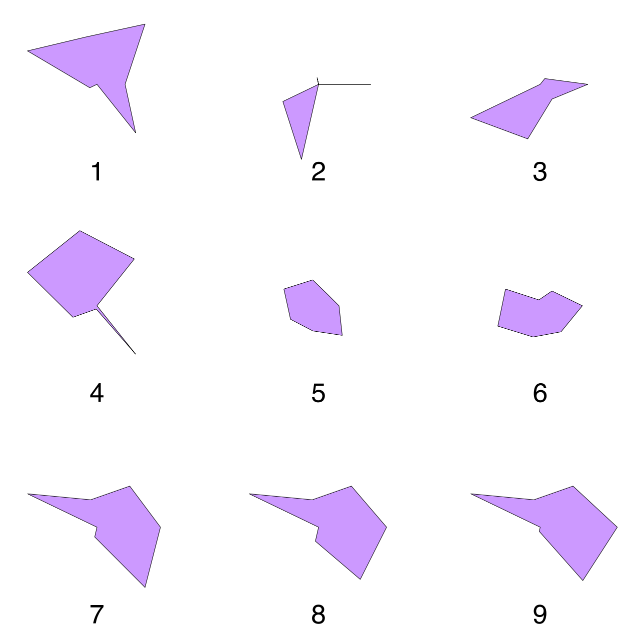
{7,8,9,1} {2,3} {4} {5} {6} ?

Order H2



{1,4} {2,3} {5,6} {7,8,9} ?

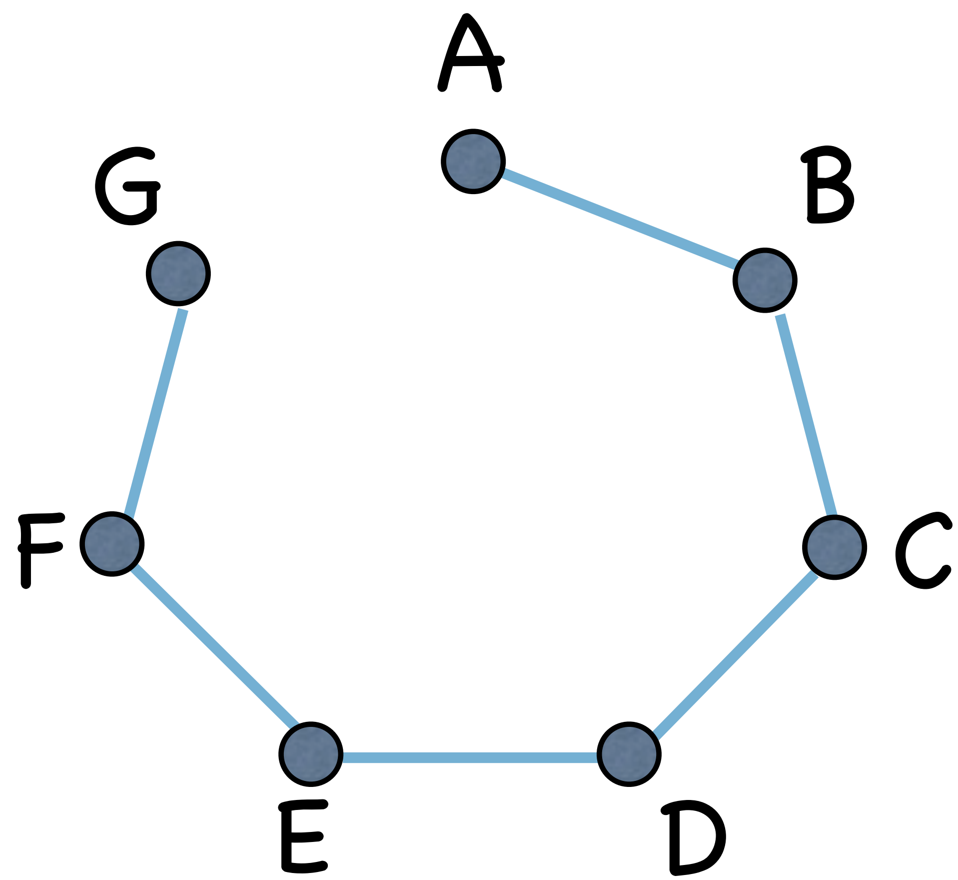
Order H3



{1} {2} {3} {4} {5} {6} {7,8,9} ?

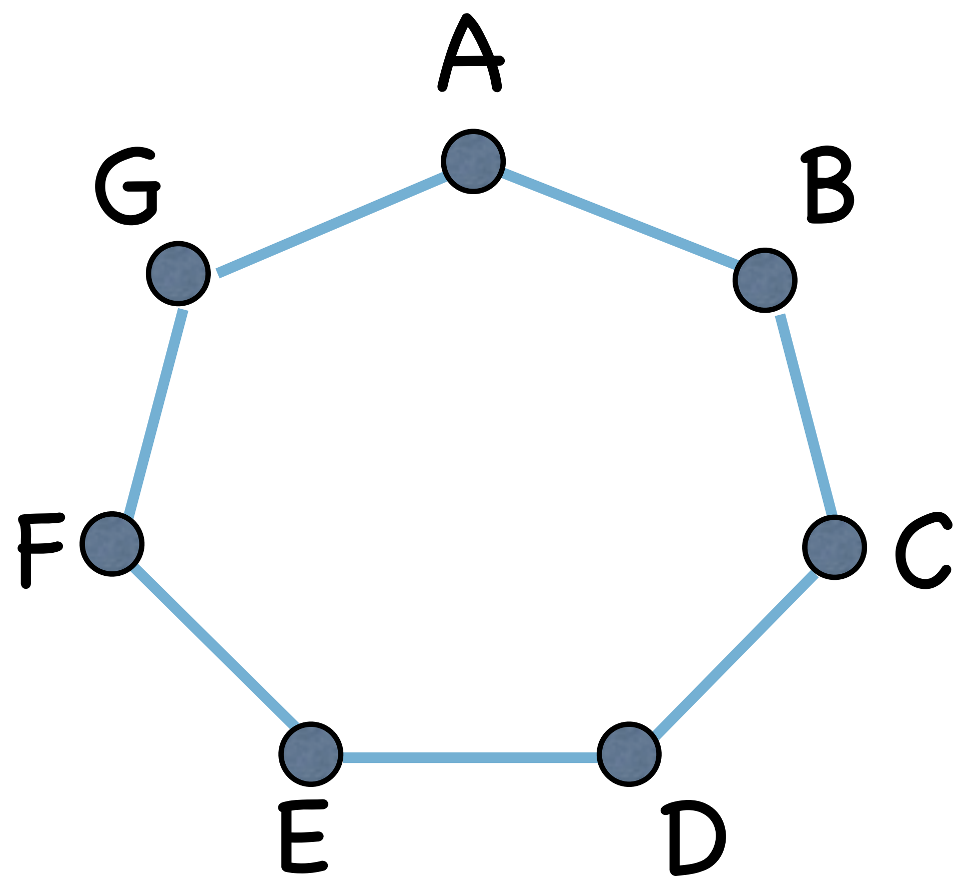
Radial axes: reduced order effect

A variate ordering = Hamiltonian path



Radial axes: reduced order effect

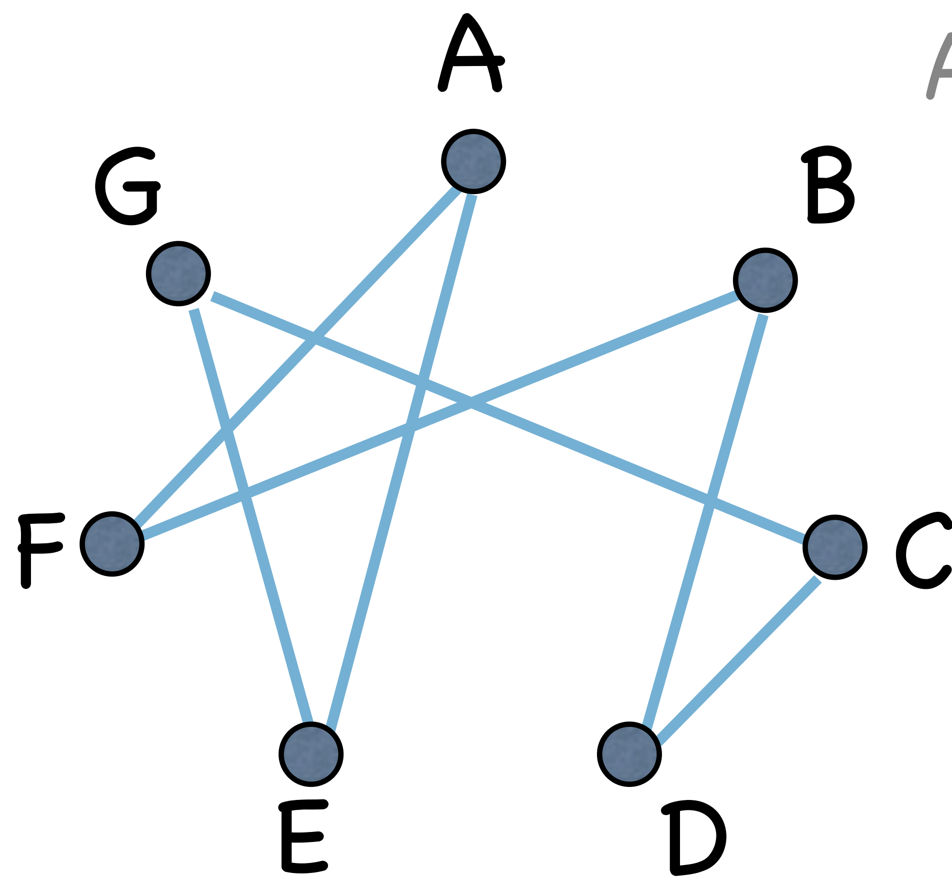
A variate ordering = Hamiltonian cycle or tour



Radial axes: reduced order effect

A variate ordering = Hamiltonian cycle or tour

There are **lots** of Hamiltonians to choose ...

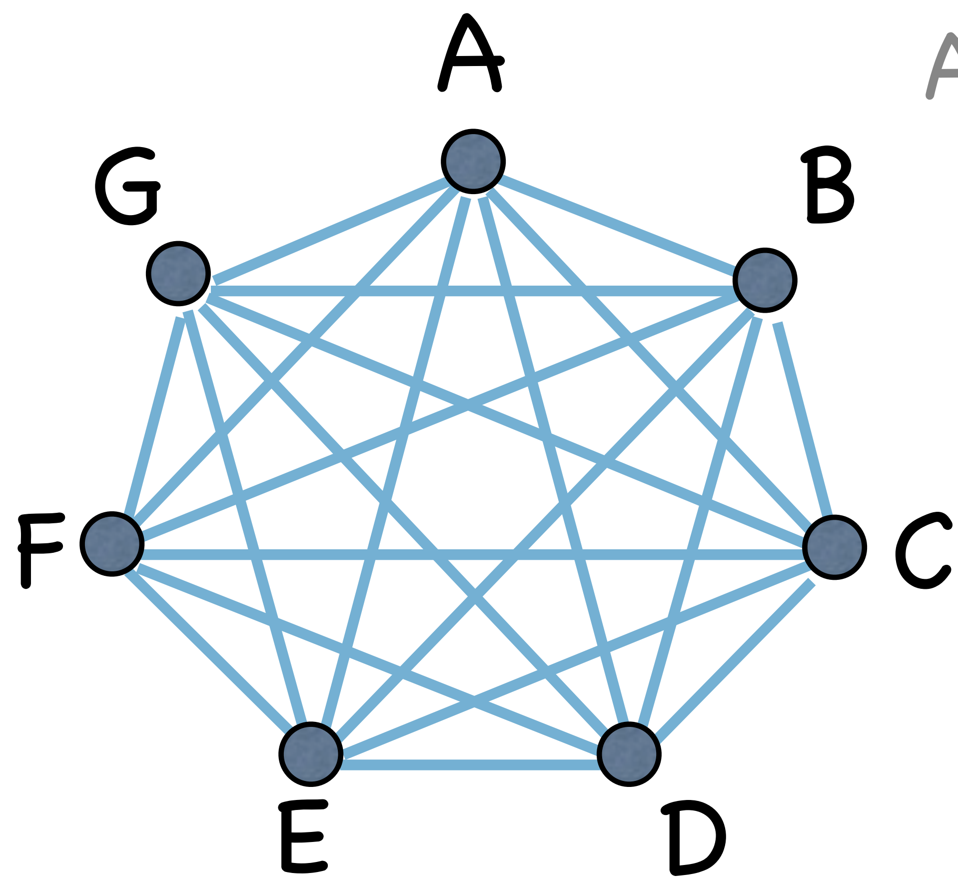


A Hamiltonian visits every node on the complete graph K_7

Radial axes: reduced order effect

A variate ordering = Hamiltonian cycle or tour

There are **lots** of Hamiltonians to choose ...



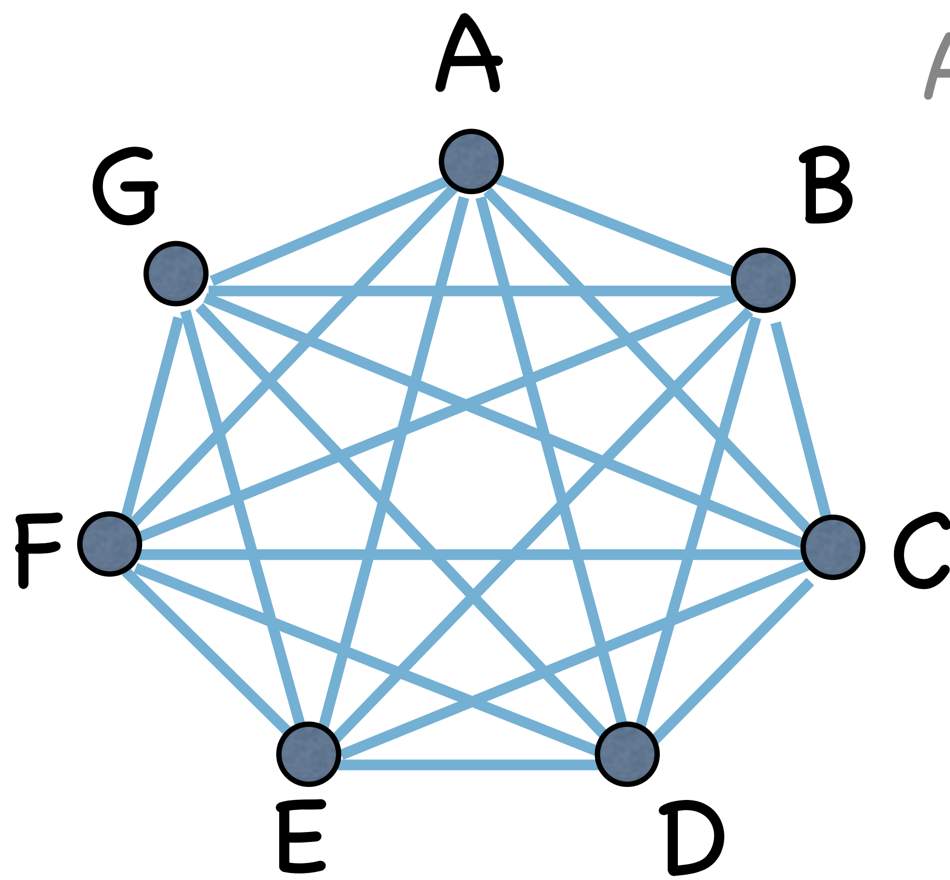
A Hamiltonian visits every node on the complete graph K_7

An Eulerian Tour visits every edge once (nodes possibly many times)

Radial axes: reduced order effect

A variate ordering = Hamiltonian cycle or tour

There are **lots** of Hamiltonians to choose ...



A Hamiltonian visits every node on the complete graph K_7

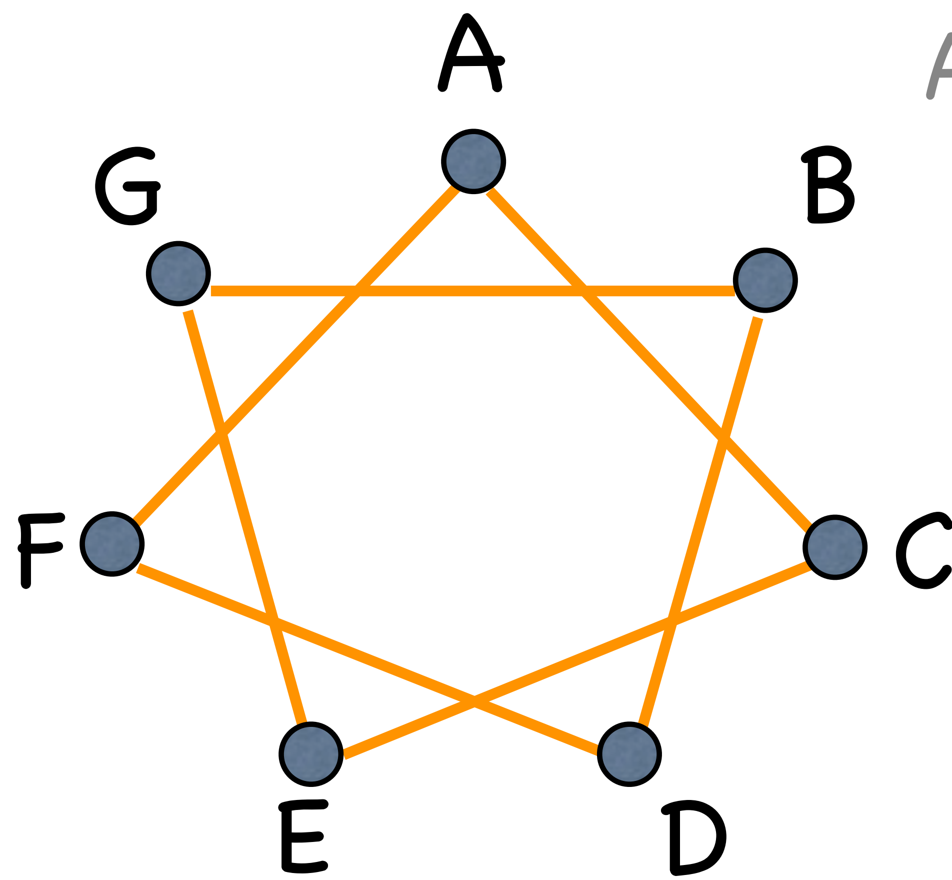
An Eulerian Tour visits every edge once (nodes possibly many times)

Non-(edge)-intersecting Hamiltonian tours whose union is the entire graph, is called a Hamiltonian Decomposition.

Radial axes: reduced order effect

A variate ordering = Hamiltonian cycle or tour

There are **lots** of Hamiltonians to choose ...



A Hamiltonian visits every node on the complete graph K_7

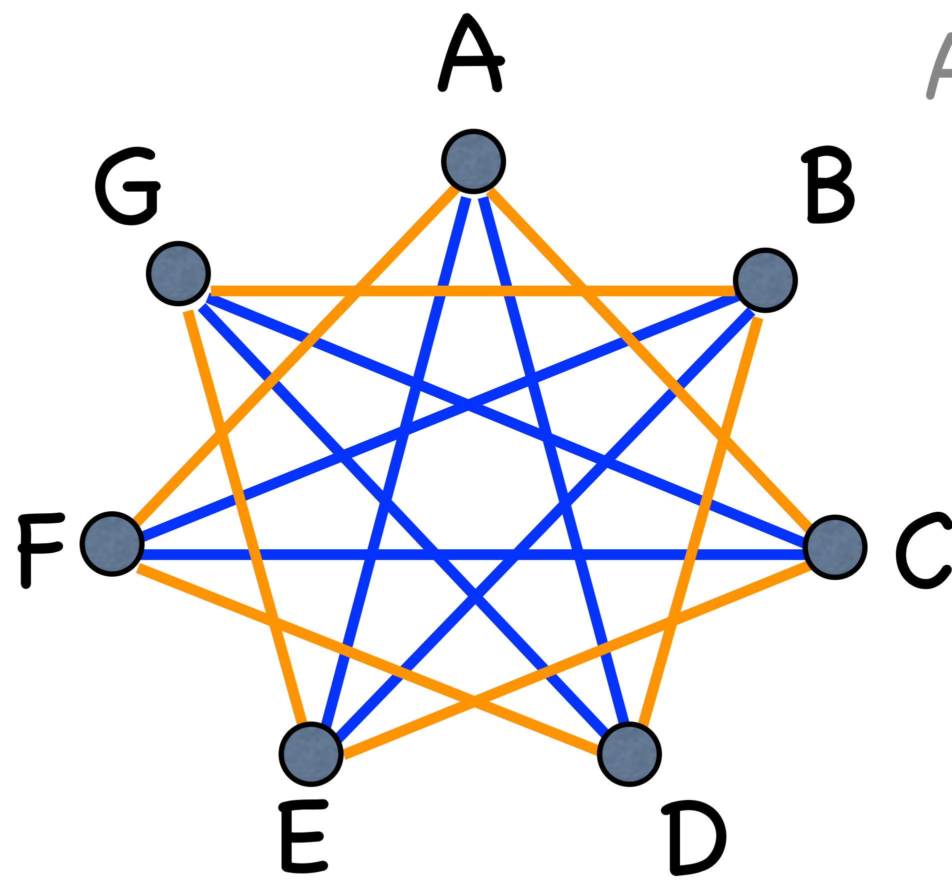
An Eulerian Tour visits every edge once (nodes possibly many times)

Non-(edge)-intersecting Hamiltonian tours whose union is the entire graph, is called a Hamiltonian Decomposition.

Radial axes: reduced order effect

A variate ordering = Hamiltonian cycle or tour

There are **lots** of Hamiltonians to choose ...



A Hamiltonian visits every node on the complete graph K_7

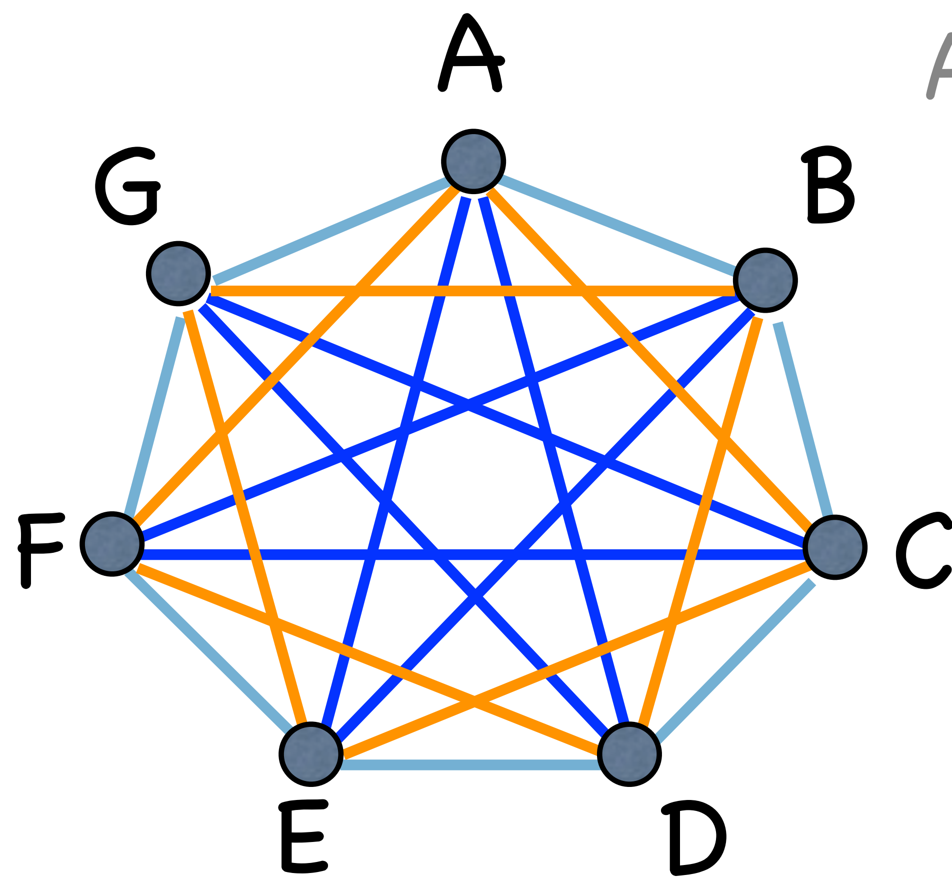
An Eulerian Tour visits every edge once (nodes possibly many times)

Non-(edge)-intersecting Hamiltonian tours whose union is the entire graph, is called a Hamiltonian Decomposition.

Radial axes: reduced order effect

A variate ordering = Hamiltonian cycle or tour

There are **lots** of Hamiltonians to choose ...



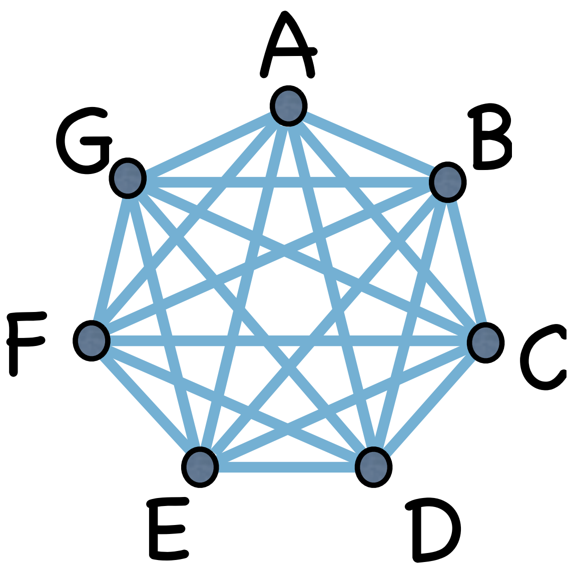
A Hamiltonian visits every node on the complete graph K_7

An Eulerian Tour visits every edge once (nodes possibly many times)

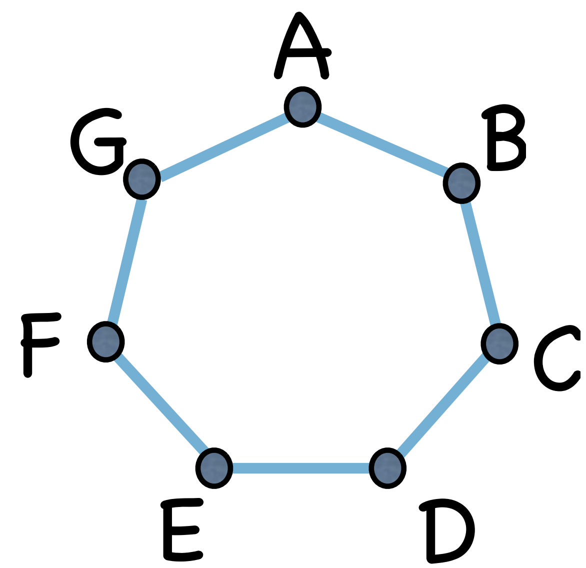
Non-(edge)-intersecting Hamiltonian tours whose union is the entire graph, is called a Hamiltonian Decomposition.

Radial axes: reduced order effect

An Eulerian

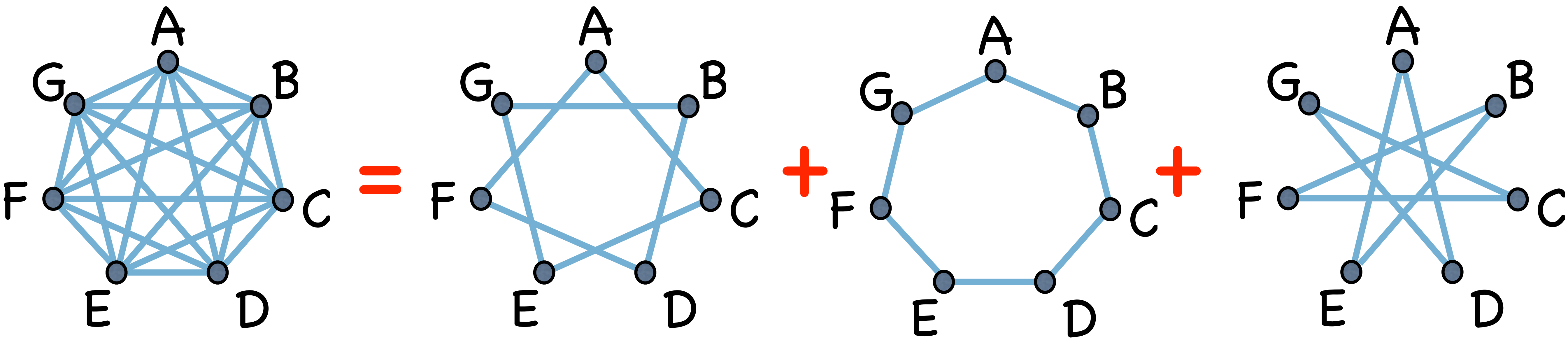


A Hamiltonian



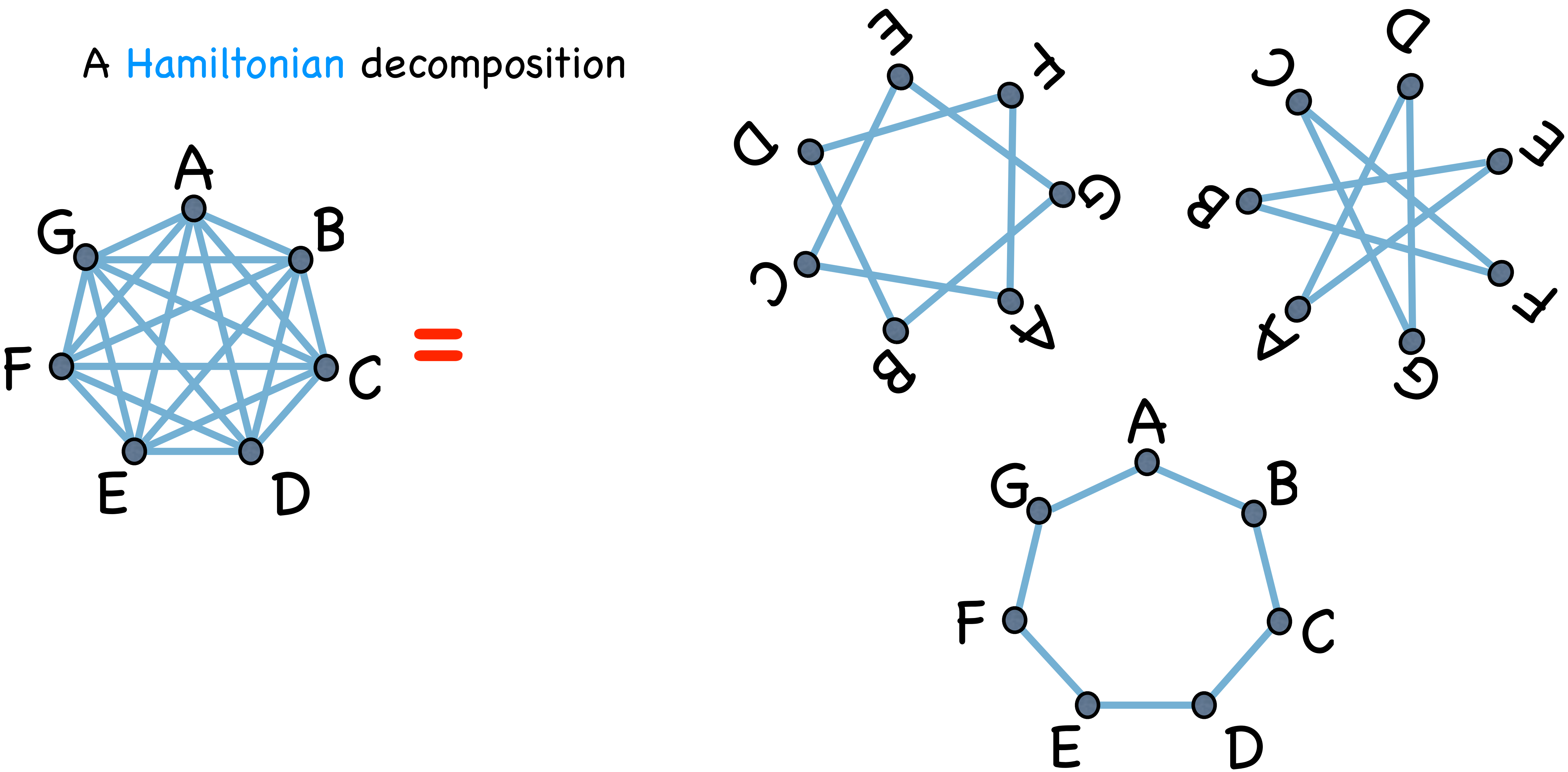
Radial axes: reduced order effect

A Hamiltonian decomposition



Radial axes: reduced order effect

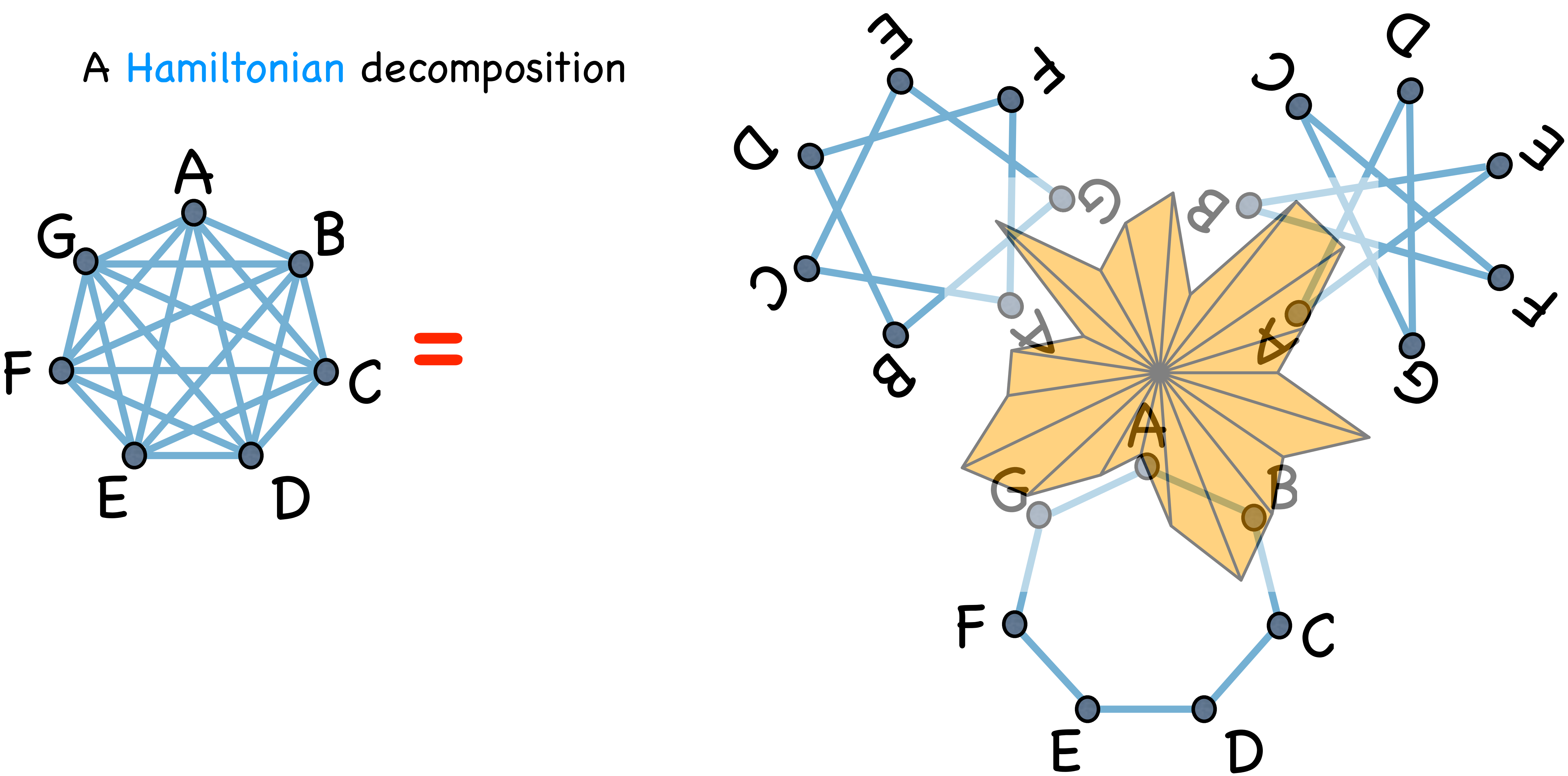
A Hamiltonian decomposition



– Which when assembled form an Eulerian cycle composed of Hamiltonians

Radial axes: reduced order effect

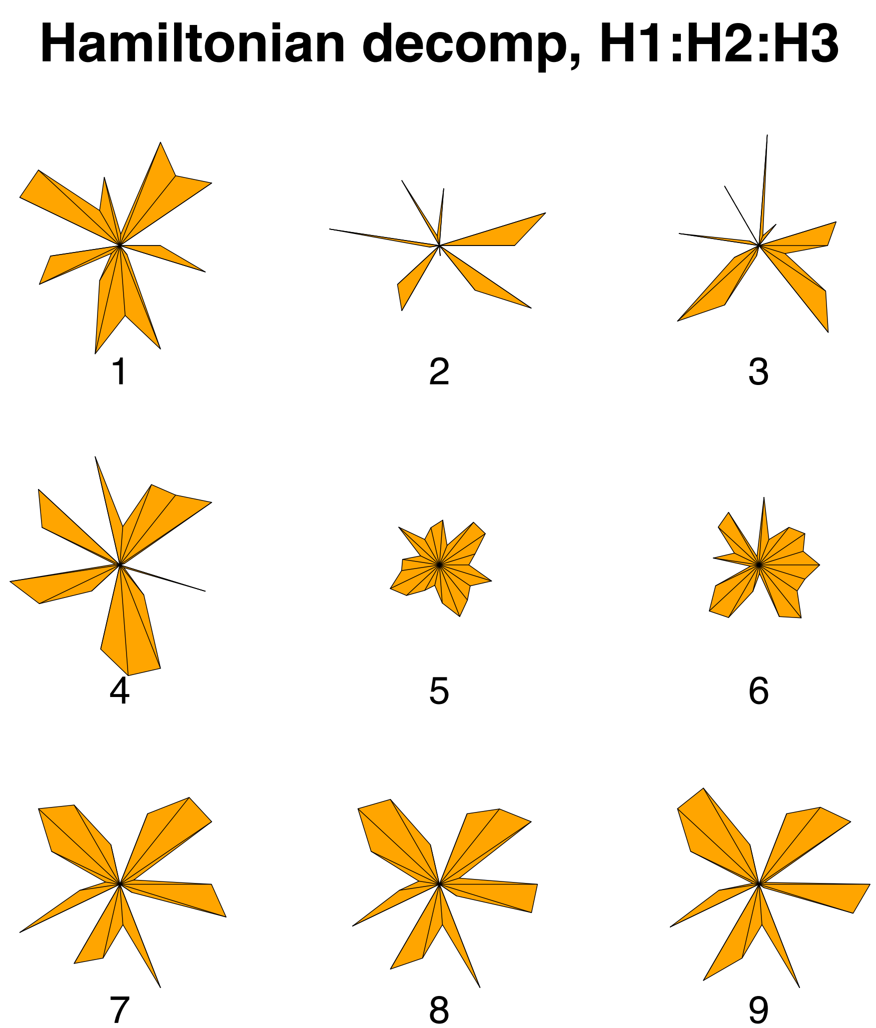
A Hamiltonian decomposition



- Which when assembled form an Eulerian cycle composed of Hamiltonians
- Could build a glyph from these cycles (21 radii instead of 7)

Radial axes: reduced order effect

A Hamiltonian decomposition

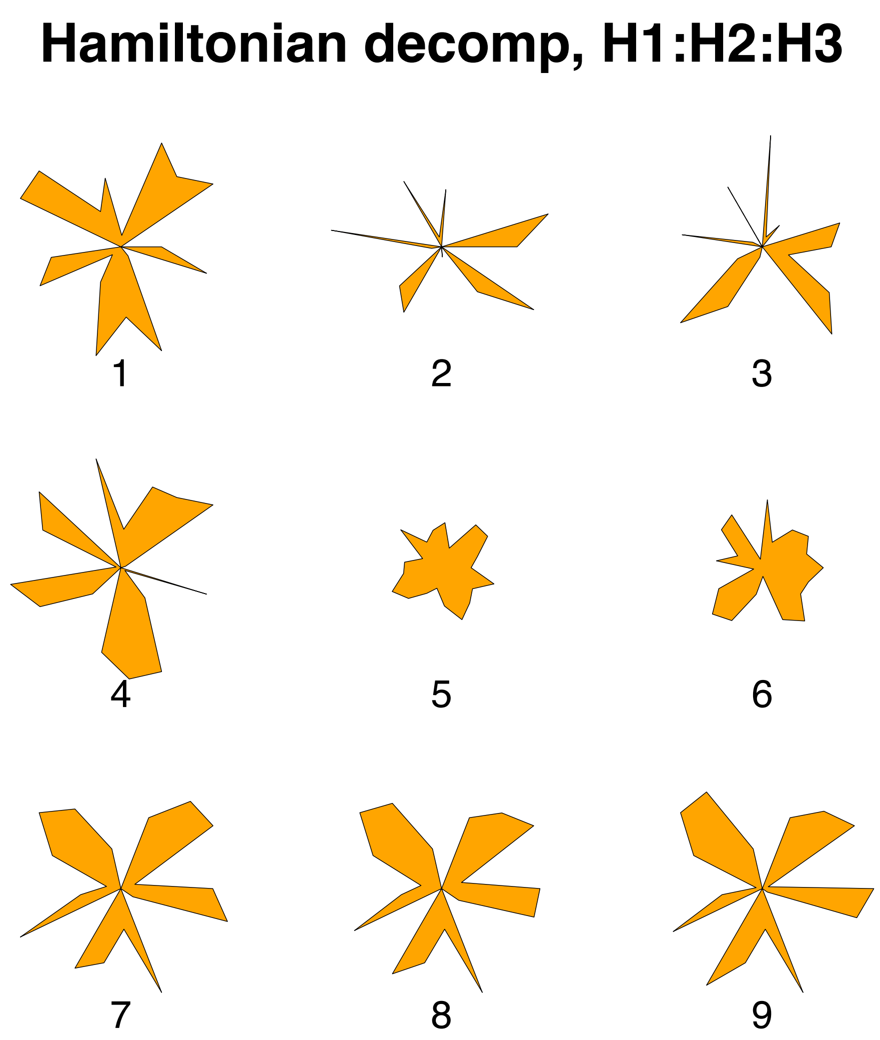


- Could build a glyph from these cycles (21 radii instead of 7)

Radial axes glyphs

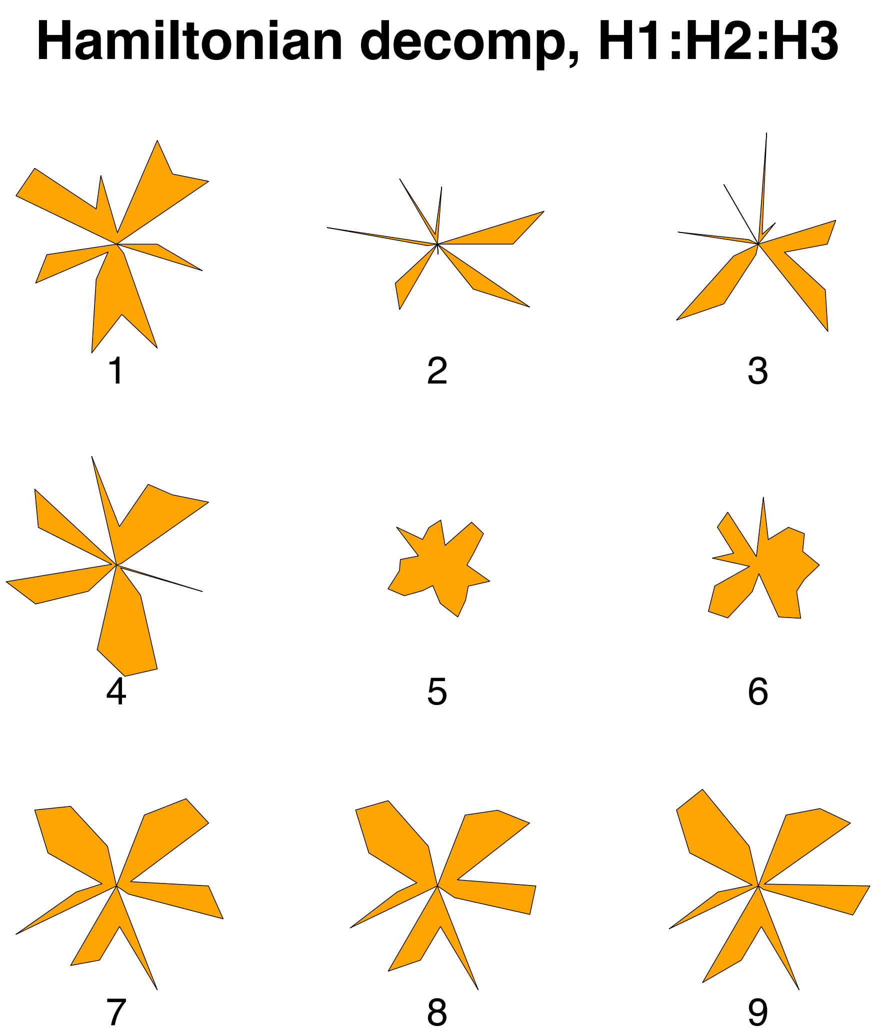
A Hamiltonian decomposition

{1,4} {2,3} {5,6} {7,8,9}

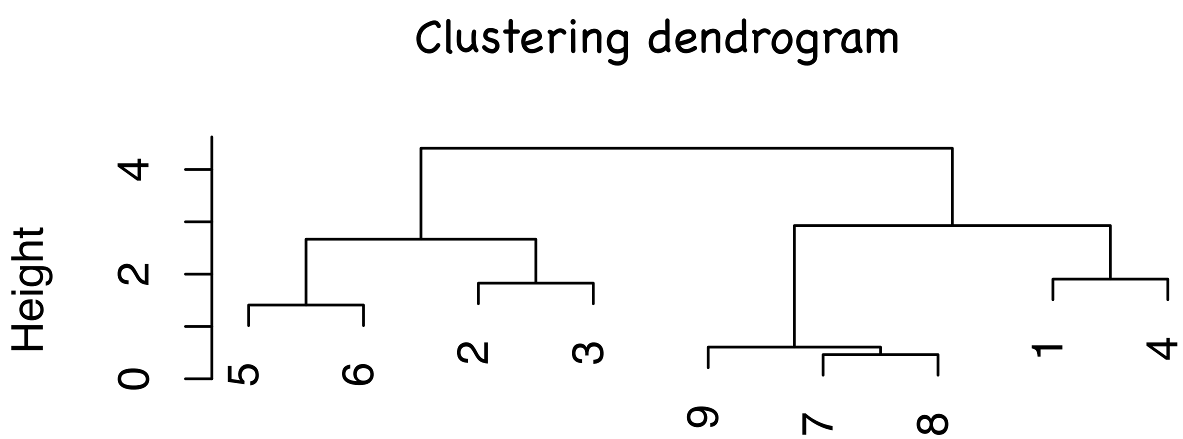


Radial axes glyphs

A Hamiltonian decomposition

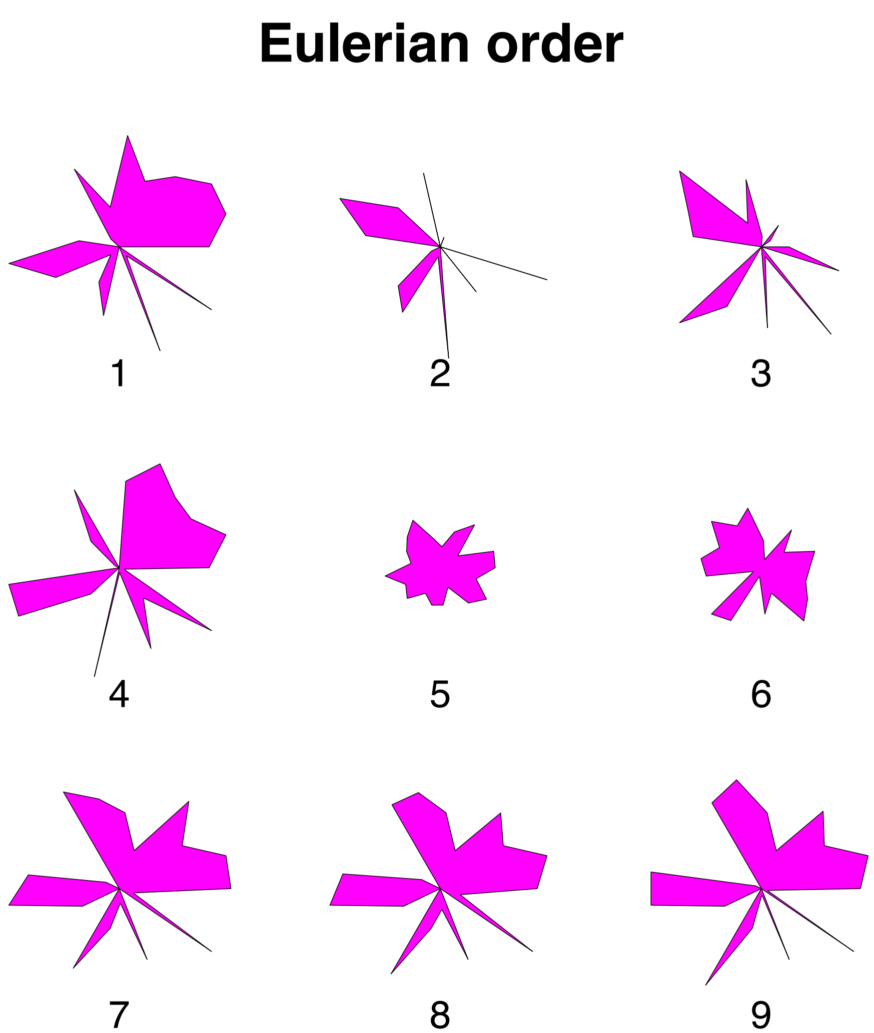


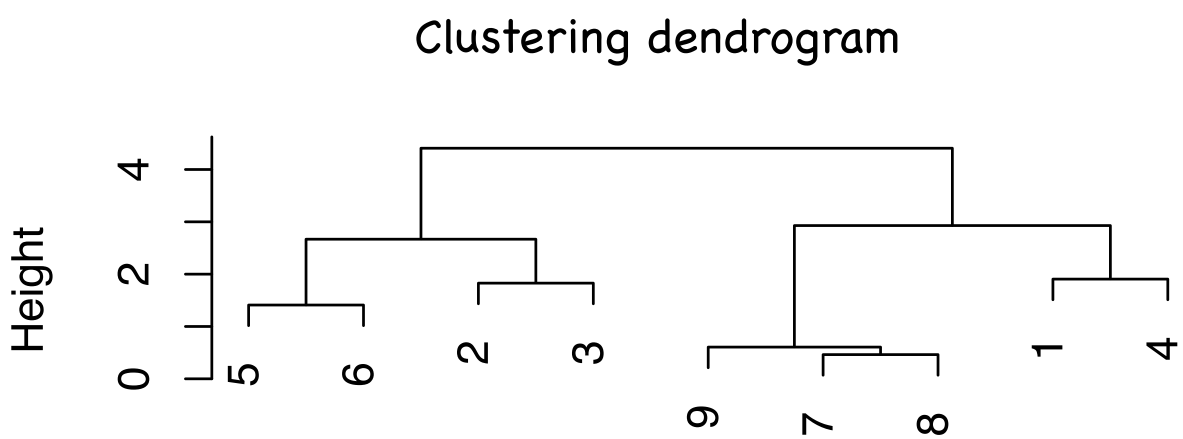
{1,4} {2,3} {5,6} {7,8,9}



Radial axes glyphs

A Greedy Eulerian (maximizing pairwise correlation)

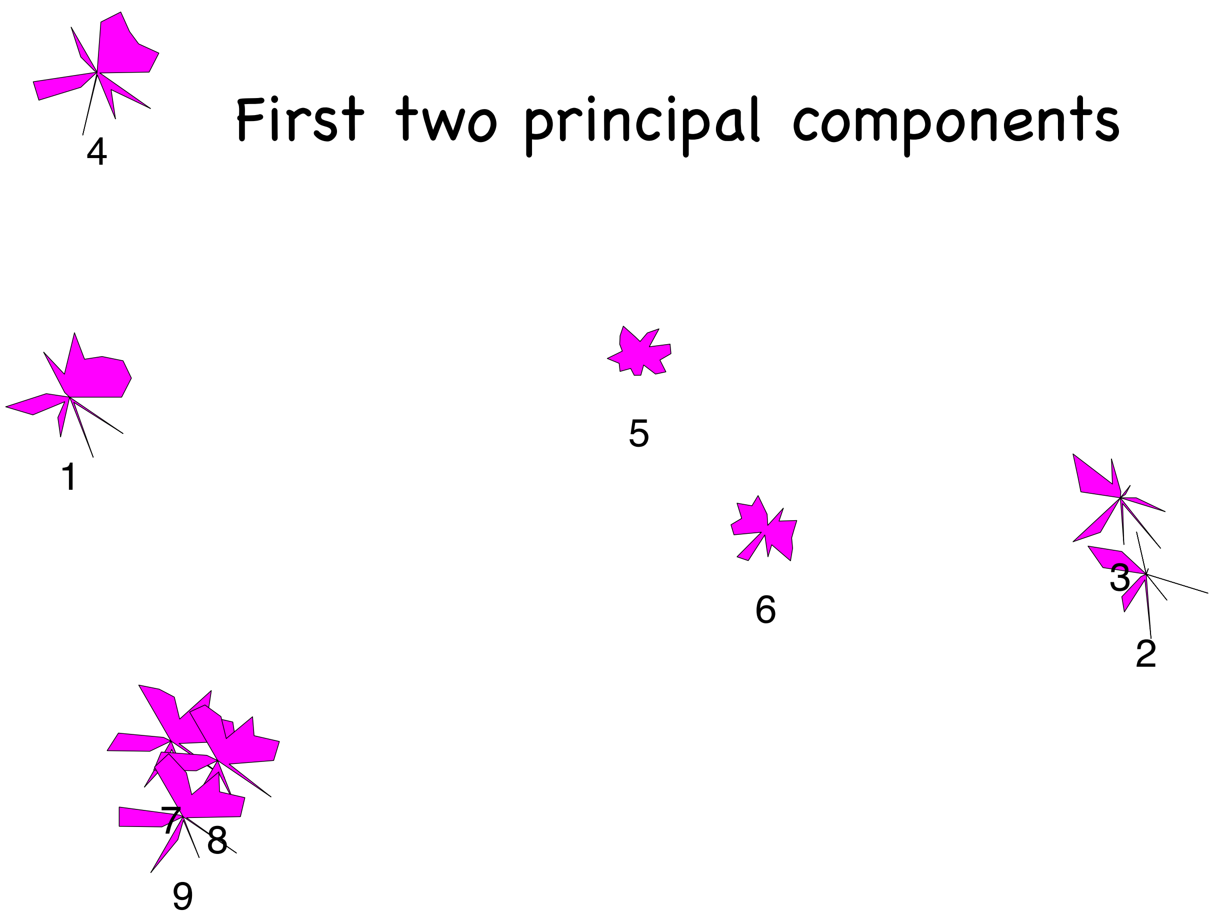




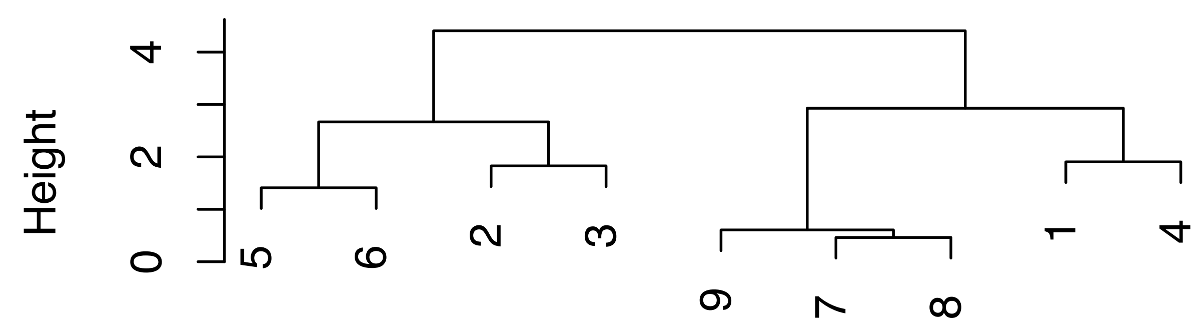
Radial axes glyphs

A Greedy Eulerian (maximizing pairwise correlation)

First two principal components



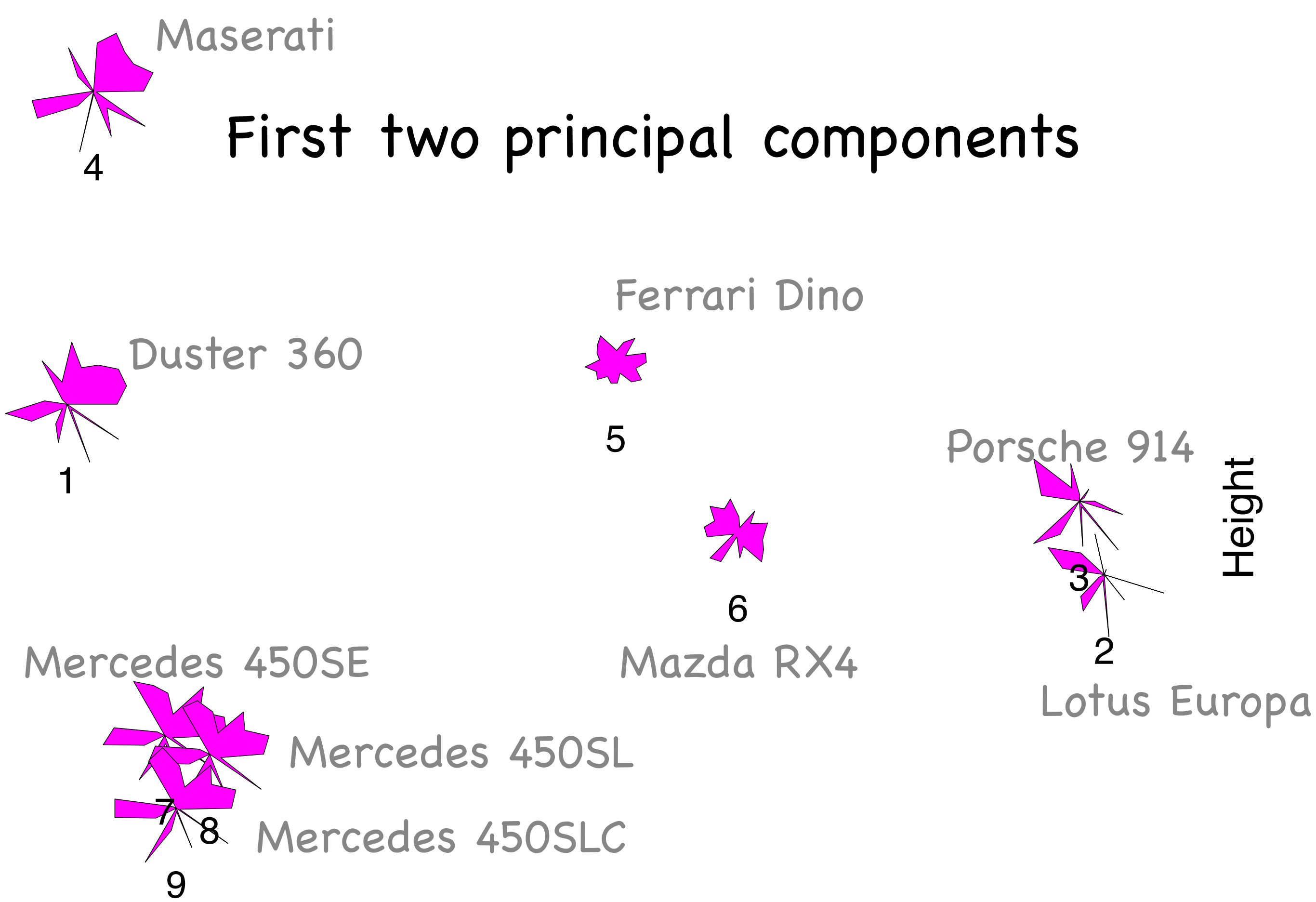
Clustering dendrogram



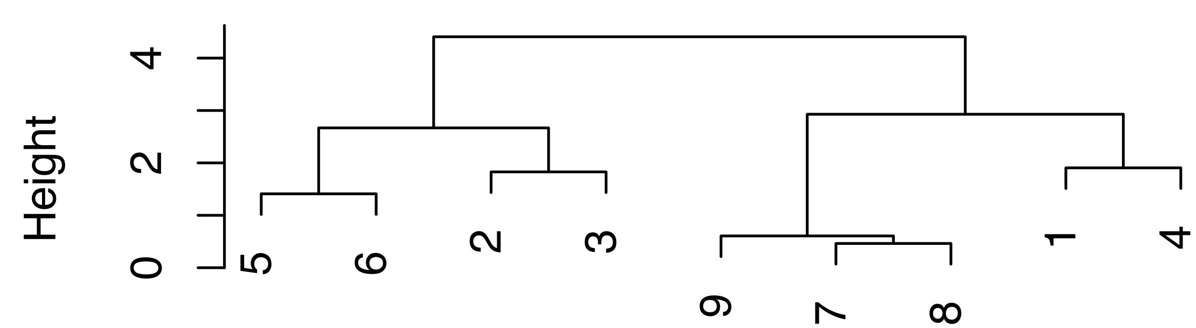
All pairs (Greedy Eulerian or Hamiltonian decomposition) reduce the effect of variable pair patterns, making star glyphs more reliable.

Radial axes glyphs

A Greedy Eulerian (maximizing pairwise correlation)



First two principal components



All pairs (Greedy Eulerian or Hamiltonian decomposition) reduce the effect of variable pair patterns, making star glyphs more reliable.

Radial axes

- Hamiltonian decomposition
  - all pairs of variates appear so no one pair dominates
  - divides glyph into sectors with all variates appearing once in each sector
  - ameliorates well known order effect
  - there are many Hamiltonian decompositions for a complete graph
    - For K_7, two generator decomps.
  - could choose Hamiltonian to maximize some measure on sum of edges (TSP)

Radial axes

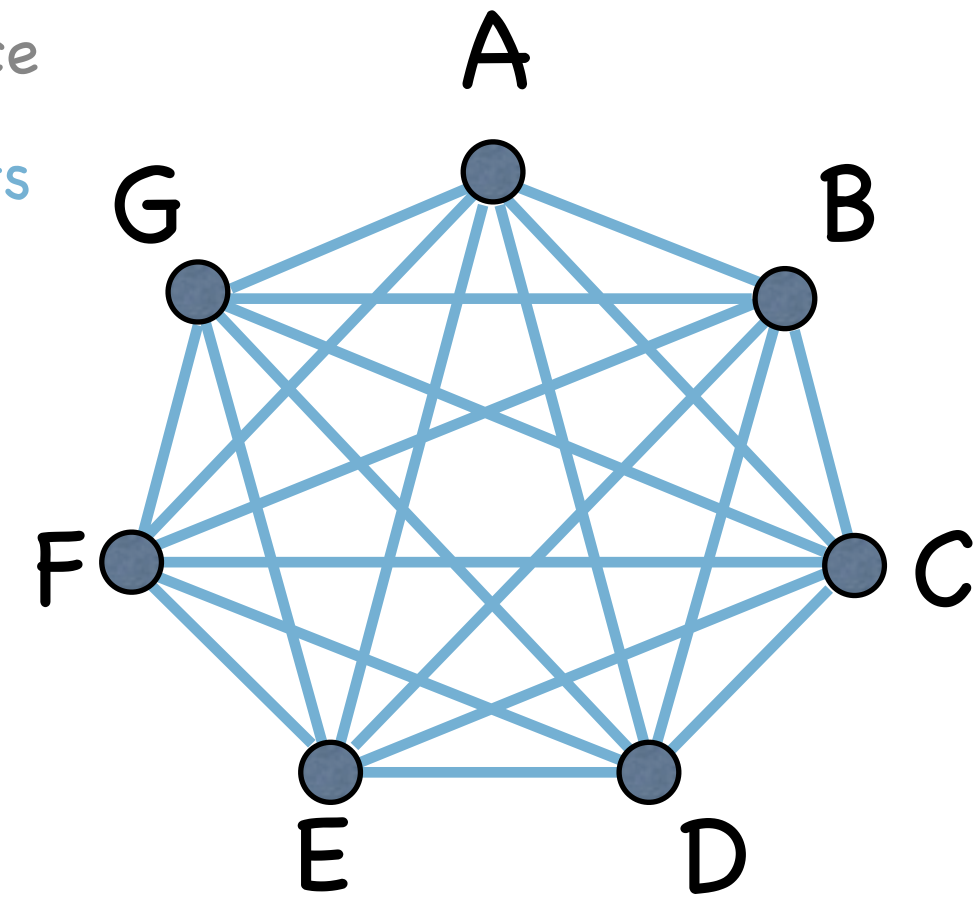
- Eulerian
  - all pairs of variates appear
  - can order pairs (greedy Eulerian)
  - could choose fewer radial axes (early pairs are emphasized).
  - lots of Eulerians

    (e.g. for K_7: 129,976,320;

    $K_{21:}$ > 3.5×10^{184})

More abstractly ...

– Visiting all nodes once would give all objects in some order, a Hamiltonian.



– Visiting all edges once would give all object pairs in some order, an Eulerian.

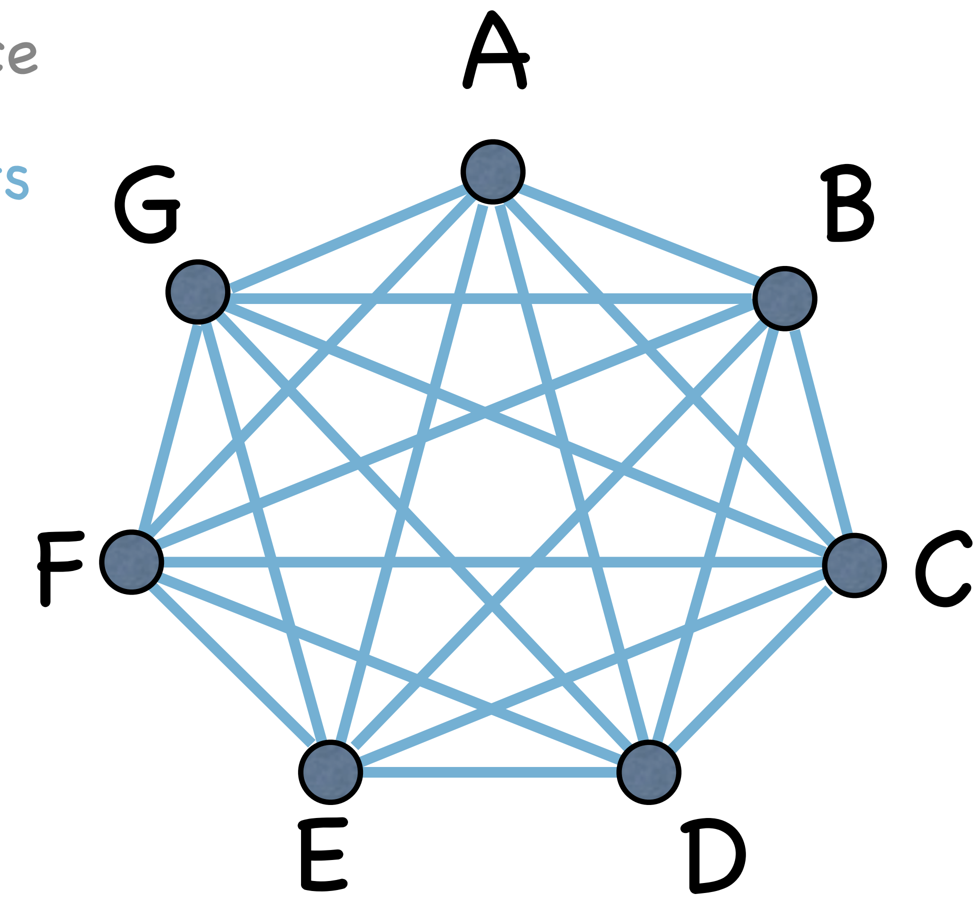
– Visiting all edges via a Hamiltonian Decomposition gives all pairs of objects and distributes the objects so that all appear in a block

– There is still considerable choice on the order of the nodes in a walk within these constraints; possibly accommodate with weights on edges.

More abstractly ...

Order of objects = a walk or tour on the complete graph

- Visiting all nodes once would give all objects in some order, a Hamiltonian.



- Visiting all edges once would give all object pairs in some order, an Eulerian.

- Visiting all edges via a Hamiltonian Decomposition gives all pairs of objects and distributes the objects so that all appear in a block

- There is still considerable choice on the order of the nodes in a walk within these constraints; possibly accommodate with weights on edges.

PairViz demo

Summary

- Graph theory has much to offer
  - map "objects" to nodes
  - map "transitions" or "comparison" to edges
  - add statistically meaningful weights to edges
  - use weights to guide the visual search
  - use Hamiltonians, Eulerians to reduce unintended effects.

- Lots more to explore ... constructions, decompositions, weights, applications, ...

Thank you

Thank you

御清聴ありがとうございました

Questions?

質問はありますか？

Papers

Hurley & Oldford:

Pairwise display of high dimensional information via Eulerian tours and Hamiltonian decompositions (**JCGS, 2010**)

Eulerian tour algorithms for data visualization and the `PairViz` package (**Comp Stats 2011**)

`PairViz` R package ... available on CRAN.