Spectral theory on combinatorial and quantum graphs

Topic 1: The Ubiquitous Laplacian

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Just what is a Laplacian, and why are Laplacians ubiquitous?

I. *The simplest and most symmetric second-order differential.*

- Linear partial differential equations can be converted to normal forms with a change of variables. The leading term is:

$$\sum_{i,j} \frac{\partial}{\partial_i} A_{ij}(x) \frac{\partial}{\partial_i} u$$

where we may assume that A is symmetric. By diagonalizing A and enforcing invariance under symmetries, we find that A is a multiple of the identity.

What about a surface or manifold?

The essence of a manifold is that it looks locally like Euclidean space. In fact, if you single out a given point, you can find coordinates, called *Fermi coordinates*, in which the metric tensor at that spot becomes the identity, just like for Euclidean space. Of course, it does this only momentarily. Think, for example of the sphere with spherical coordinates θ, ϕ for which

$$x = rsin\theta \cos\phi$$
$$y = rsin\theta \sin\phi$$
$$x = r\cos\theta$$

As we know, fixing $r = 1$, the arc length and Laplacian look like:

$$ds^2 = d\theta^2 + \sin^2\theta d\phi^2$$

$$\Delta = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{\partial^2}{\partial\phi^2},$$

but on the equator, where $\sin\theta = 1$ and its derivative is zero, we obtain the familiar Laplacian as the unweighted sum of the second derivatives with respect to an orthogonal coordinate system.

The weak, or quadratic form

- If you ask what the *Laplace-Beltrami* operator looks like in general coordinates, and you work hard enough, from this you find

$$\Delta_{LB} f := \sum_{ij} \frac{1}{\sqrt{g}} \partial_i g^{ij} \sqrt{g} \partial_i f$$

The weak, or quadratic form

- However, there is a simpler way, when you define the Laplacian by its weak form,

$$(f, g) \to \int \nabla f \cdot \overline{\nabla g} \, dVol$$

By partial integration, if allowed, the latter term contains the Laplacian

$$\int \nabla f \cdot \overline{\nabla g} \, dVol = \int f(-\Delta)\overline{g} \, dVol + \mathrm{B.T.}$$

but the weak form requires less regularity.

The weak, or quadratic form

$$(f, g) \to \int \nabla f \cdot \overline{\nabla g}\, dVol$$

It suffices to consider

$$f \to \mathcal{E}(f) := \int |\nabla f|^2\, dVol.$$

by polarization:

$$\int \nabla f \cdot \overline{\nabla g} = \frac{1}{4}\Big(\mathcal{E}(f+g) - \mathcal{E}(f-g) + i\mathcal{E}(f+ig) - i\mathcal{E}(f-ig)\Big)$$

The weak, or quadratic form

- Verification exercise: Check by partial integration that

$$\int |\nabla f|^2 \, dVol = \int \overline{f}(-\Delta_{LB} f) \, d\mathrm{Vol} + \text{possible boundary contribs.}$$

The usual Laplace-Beltrami operator on, for example a closed manifold (no boundary), is defined by using the Friedrichs extension from a suitable dense set of test functions f. Cf. the lectures by Hatem Najar.

II. *The generator of the simplest probabilistic process*.

The normalized Gaussian probability distribution:

$$P(x,y,t) := \frac{1}{(\pi 4t)^{\frac{d}{2}}} \exp(-|x-y|^2/4t).$$

By convolution, the functions P define a one-parameter semigroup, i.e., for any bounded, continuous function f, $[\mathbb{P}_t f](x) := \int P(x,y,t) f(y) dy$ has the following properties:

1. $lim_{t \to 0} \mathbb{P}_t = \mathbb{I}$
2. $\mathbb{P}_t \mathbb{P}_s = \mathbb{P}_s \mathbb{P}_t = \mathbb{P}_{t+s}$.

II. *The generator of the simplest probabilistic process*.

In semigroup theory, the *infinitesimal generator* refers to its derivative at $t = 0$, which turns out to be ...you guessed it, the Laplacian. For all $t > 0$, P satisfies the heat equation, $\frac{\partial P(x,y,t)}{\partial t} = \Delta_x P(x,y,t) = \Delta_y P(x,y,t)$.

- Verification exercise: Check that P satisfies the heat equation and that $\mathbb{P}_t$ provides the general solution for the initial-value problem for the heat equation on Euclidean space.

III. The Laplacian measures how a function differs from its averages.

- *A basic question of analysis: How does a quantity compare with its average value?*
- *Subharmonic functions*: f(x) always less than its average over balls centered at x. *Superharmonic* refers to the opposite inequality. A harmonic function is both sub- and superharmonic.

III. *The Laplacian measures how a function differs from its averages.*

Suppose that a sufficiently smooth function f is defined on some Euclidean set. Let us define its average over nearby spheres of radius r as

$$F(x,r) := \langle f \rangle_{\mathbb{S}_r(x)} = \frac{1}{d\,\omega_d\,r^{d-1}} \int_{|y-x|=r} f(y) d^{d-1}y, \tag{1.5}$$

where the volume of the $d-1$-dimensional sphere of radius r has been expressed in terms of the volume of the unit ball in d dimensions,

$$\omega_d := \frac{\pi^{\frac{d}{2}}}{\Gamma\left(1+\frac{d}{2}\right)}.$$

III. *The Laplacian measures how a function differs from its averages*.

For now x is simply fixed. If f is continuous at x, then clearly $F(x, 0) = f(x)$. But how do the two quantities deviate from each other when $r > 0$? We can differentiate with respect to r as follows. First rewrite $F(x, r)$ as an integral over the unit sphere, as

$$F(x,r) = \frac{1}{d\ \omega_d} \int_{\mathbb{S}^{d-1}} f(x + r\alpha) d^{d-1}\alpha, \tag{1.6}$$

because of which

$$\begin{aligned} \frac{\partial F(x,r)}{\partial r} &= \frac{1}{d\ \omega_d} \int_{\mathbb{S}^{d-1}} \alpha \cdot \nabla f(x + r\alpha) d^{d-1}\alpha \\ &= \frac{1}{d\ \omega_d\, r^{d-1}} \int_{|y-x|=r} n \cdot \nabla f(y) d^{d-1} y \\ &= \left(\frac{r}{d}\right) \frac{1}{\omega_d\, r^d} \int_{|y-x|\le r} \nabla \cdot \nabla f(y) d^d y, \end{aligned}$$

III. *The Laplacian measures how a function differs from its averages*.

- *In words: The Laplacian of a function f at x measures the rate at which nearby averages of f increase as you move away from x.*
- *This point of view makes no reference to differentiation!*
- *While we won't develop the subject here, this gives one a way to define Laplacians on abstract measure spaces.*

Spectral theory on combinatorial and quantum graphs

Topic 2: The Ubiquitous Notion of a Graph

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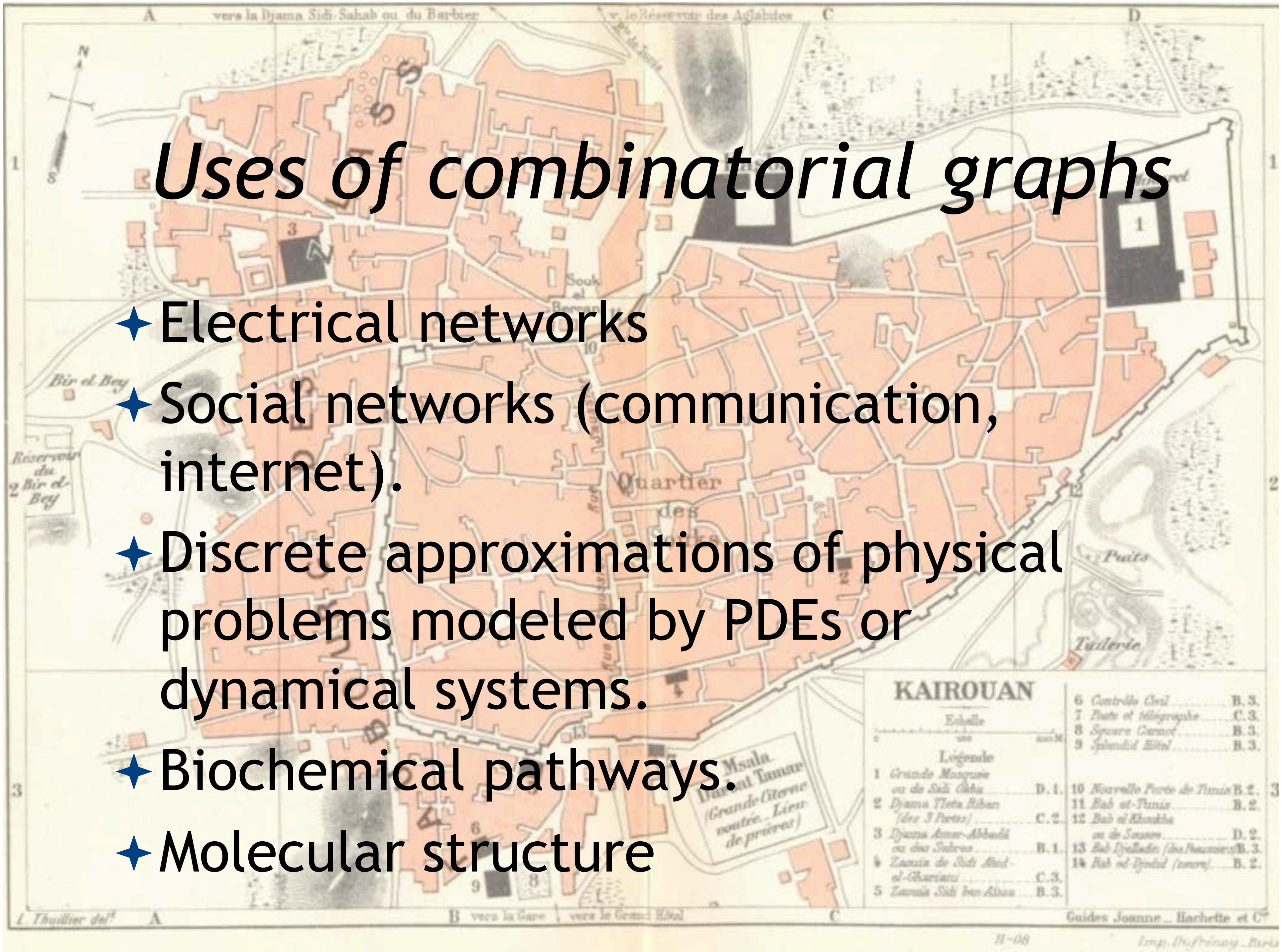
Just what is a graph, and why are graphs ubiquitous?

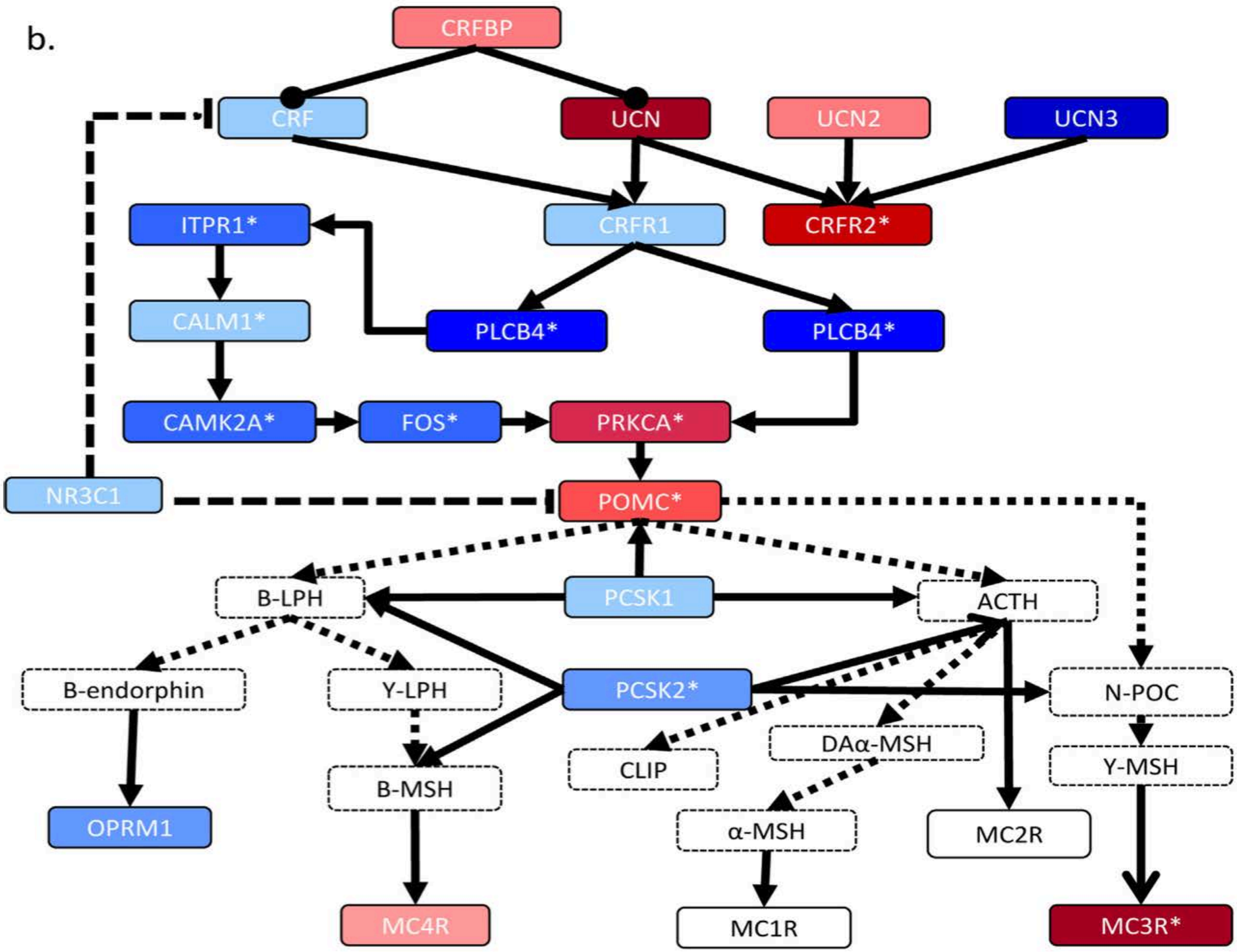
Combinatorial graphs

- Sets of n “vertices” and m edges, with $m \le n(n-1)$. (Or $n(n-1)/2$ if we don’t “orient” the edges).
- There is a vertex space isomorphic to C^n and an edge space isomorphic to C^m.
- A matrix can be used to efficiently describe which edges connect to which vertices.

Uses of combinatorial graphs



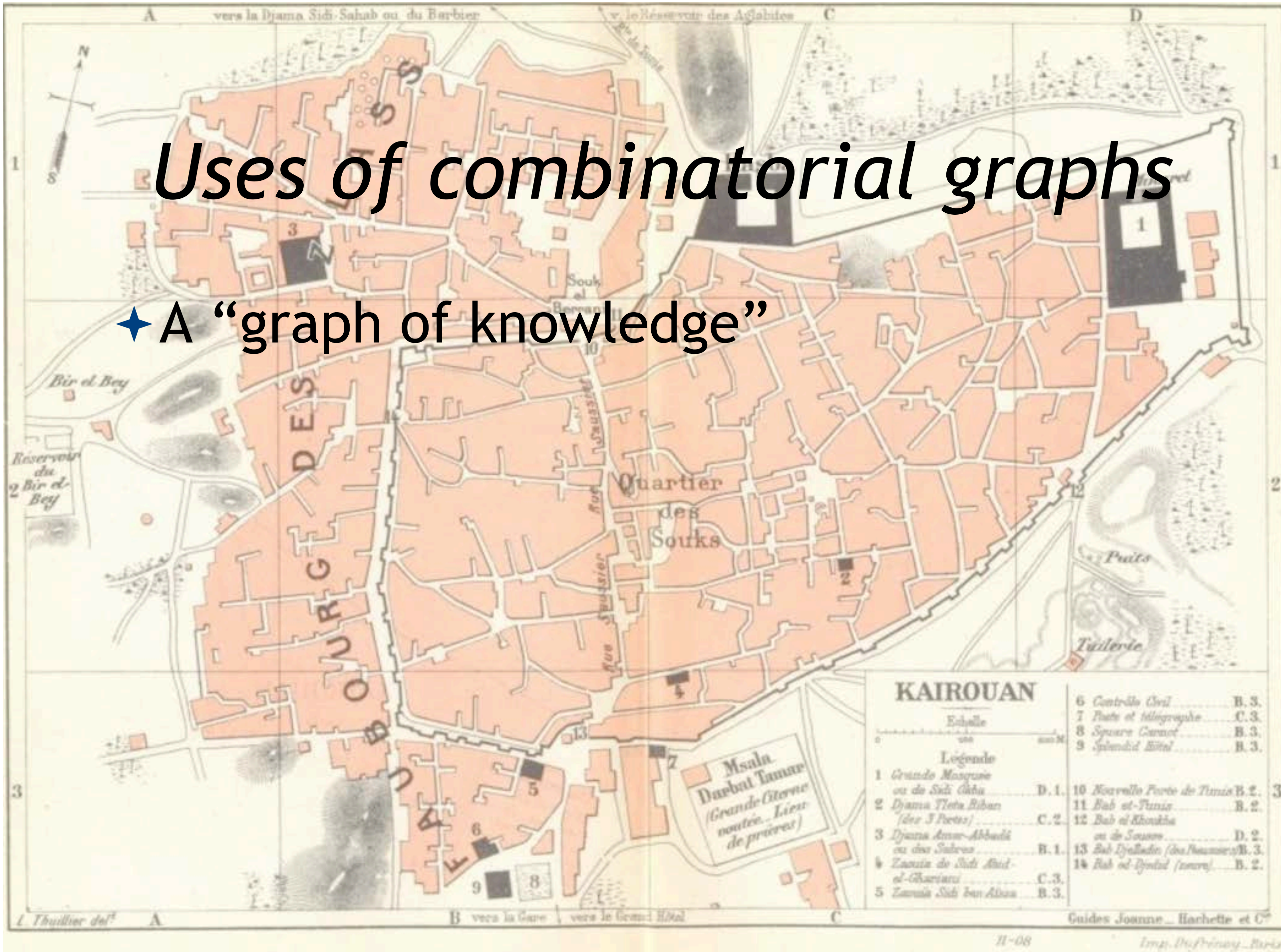
- Electrical networks
- Social networks (communication, internet).
- Discrete approximations of physical problems modeled by PDEs or dynamical systems.
- Biochemical pathways.
- Molecular structure

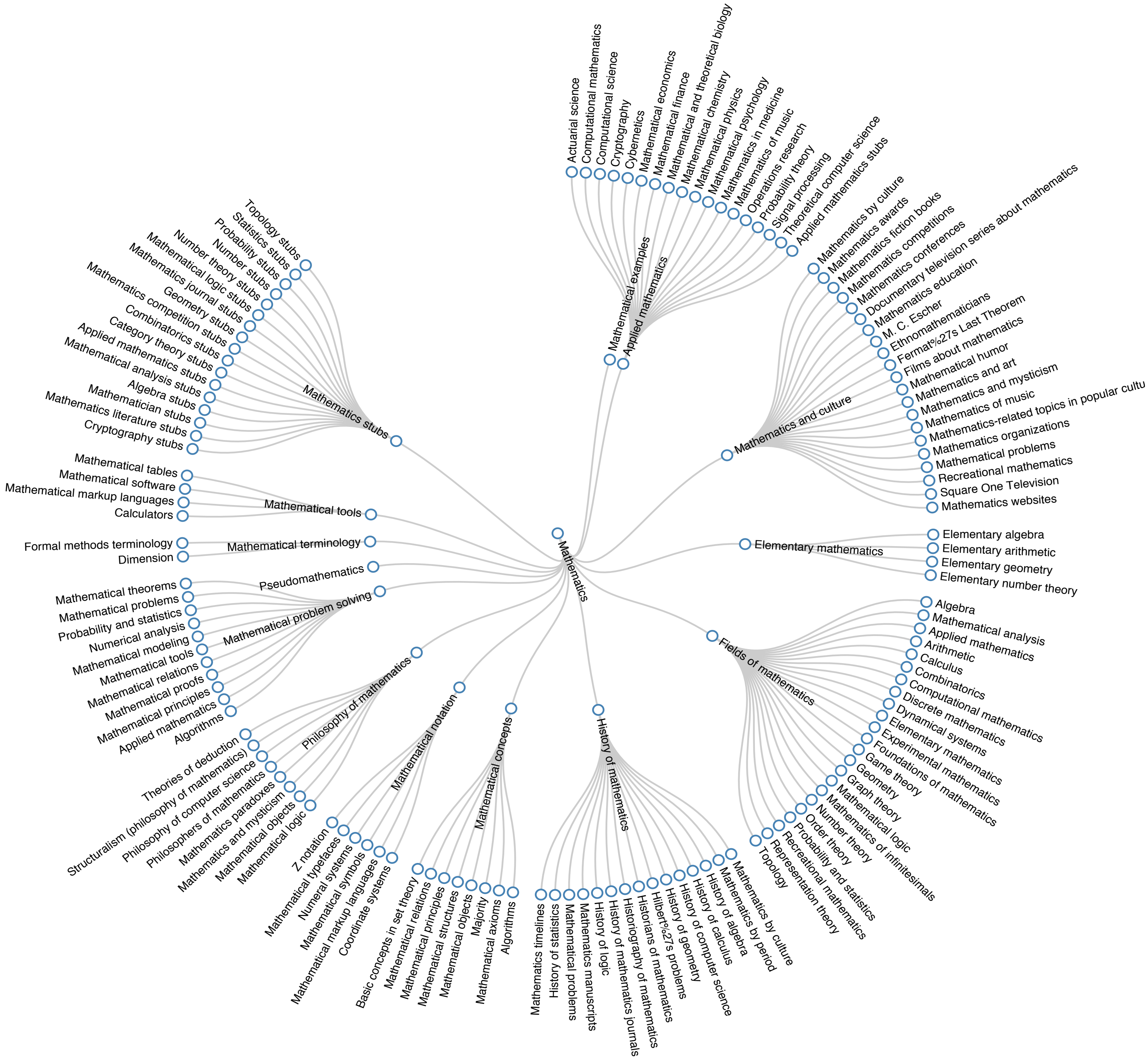


From Constance Harrell et al., Psychoneuroendocrinology 62 (2015) 252–264.

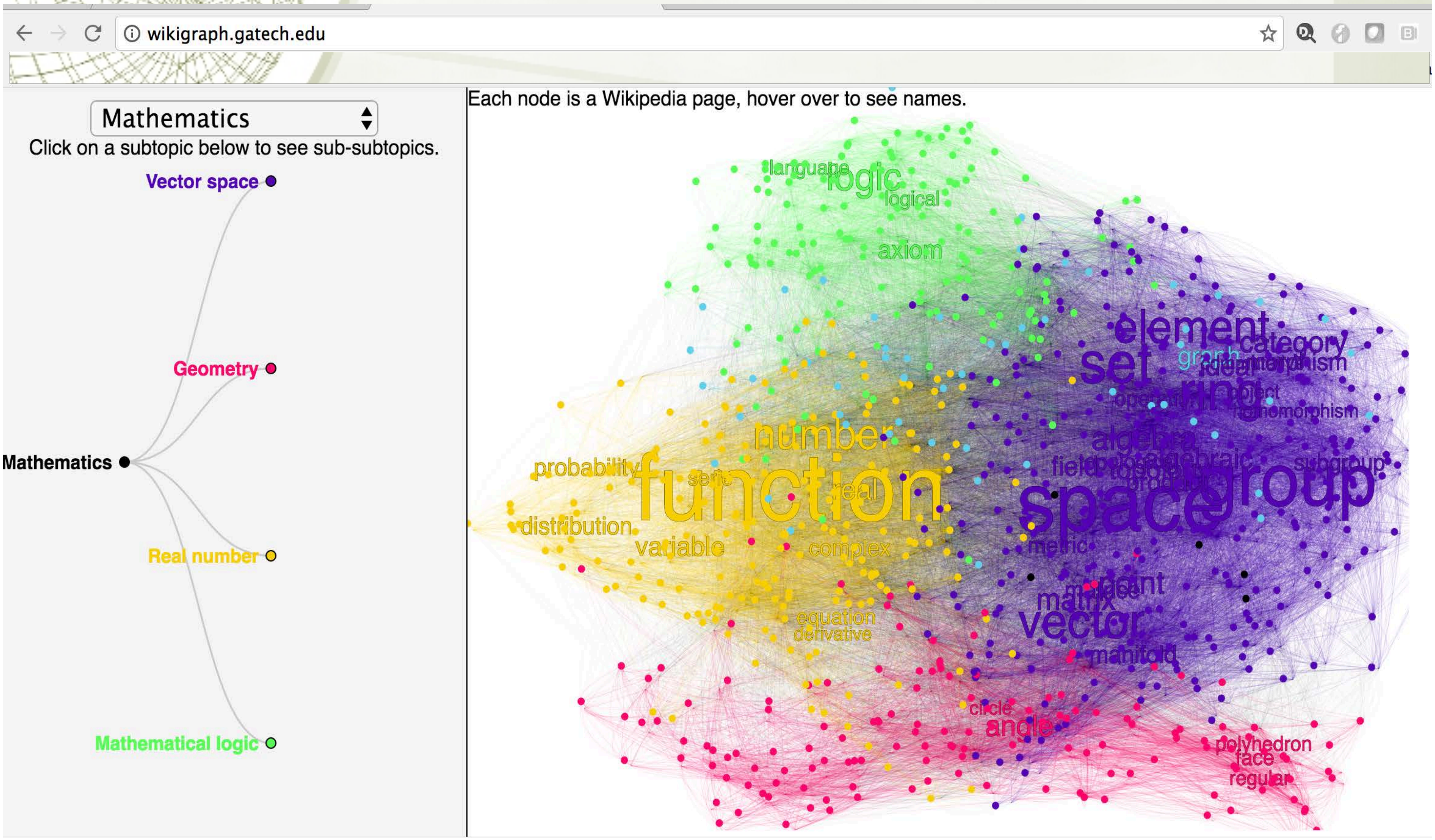
Uses of combinatorial graphs

- A "graph of knowledge"




Mathematics
Applied mathematics
Actuarial science
Computational mathematics
Computational science
Cryptography
Cybernetics
Mathematical economics
Mathematical finance
Mathematical and theoretical biology
Mathematical chemistry
Mathematical physics
Mathematical psychology
Mathematics in medicine
Mathematics of music
Operations research
Probability theory
Signal processing
Theoretical computer science
Applied mathematics stubs
Mathematical examples
Mathematics and culture
Mathematics by culture
Mathematics awards
Mathematics fiction books
Mathematics competitions
Mathematics conferences
Documentary television series about mathematics
Mathematics education
M. C. Escher
Ethnomathematicians
Fermat%27s Last Theorem
Films about mathematics
Mathematical humor
Mathematics and art
Mathematics and mysticism
Mathematics of music
Mathematics-related topics in popular cultu
Mathematics organizations
Mathematical problems
Recreational mathematics
Square One Television
Mathematics websites
Elementary mathematics
Elementary algebra
Elementary arithmetic
Elementary geometry
Elementary number theory
Fields of mathematics
Algebra
Mathematical analysis
Applied mathematics
Arithmetic
Calculus
Combinatorics
Computational mathematics
Discrete mathematics
Dynamical systems
Elementary mathematics
Experimental mathematics
Foundations of mathematics
Game theory
Geometry
Graph theory
Mathematical logic
Mathematics of infinitesimals
Number theory
Order theory
Probability and statistics
Recreational mathematics
Representation theory
Topology
History of mathematics
Mathematics timelines
History of statistics
Mathematical problems
Mathematics manuscripts
History of logic
History of mathematics journals
Historiography of mathematics
Historians of mathematics
Hilbert%27s problems
History of geometry
History of computer science
History of calculus
History of algebra
Mathematics by period
Mathematics by culture
Mathematical concepts
Basic concepts in set theory
Mathematical relations
Mathematical principles
Mathematical structures
Mathematical objects
Majority
Mathematical axioms
Algorithms
Mathematical notation
Z notation
Mathematical typefaces
Numeral systems
Mathematical symbols
Mathematical markup languages
Coordinate systems
Philosophy of mathematics
Theories of deduction
Structuralism (philosophy of mathematics)
Philosophy of computer science
Philosophers of mathematics
Mathematics paradoxes
Mathematics and mysticism
Mathematical objects
Mathematical logic
Mathematical problem solving
Mathematical theorems
Mathematical problems
Probability and statistics
Numerical analysis
Mathematical modeling
Mathematical tools
Mathematical relations
Mathematical proofs
Mathematical principles
Applied mathematics
Algorithms
Pseudomathematics
Mathematical terminology
Formal methods terminology
Dimension
Mathematical tools
Mathematical tables
Mathematical software
Mathematical markup languages
Calculators
Mathematics stubs
Topology stubs
Statistics stubs
Probability stubs
Number stubs
Number theory stubs
Mathematical logic stubs
Mathematics journal stubs
Geometry stubs
Mathematics competition stubs
Combinatorics stubs
Category theory stubs
Applied mathematics stubs
Mathematical analysis stubs
Algebra stubs
Mathematician stubs
Mathematics literature stubs
Cryptography stubs

Wikigraph – a project of P. Laban



“Standard” combinatorial graphs

- Finite. $m, n < \infty$.
- Connected.
- Undirected.
- Loop-free.
- Unweighted.

Matrices describing graphs

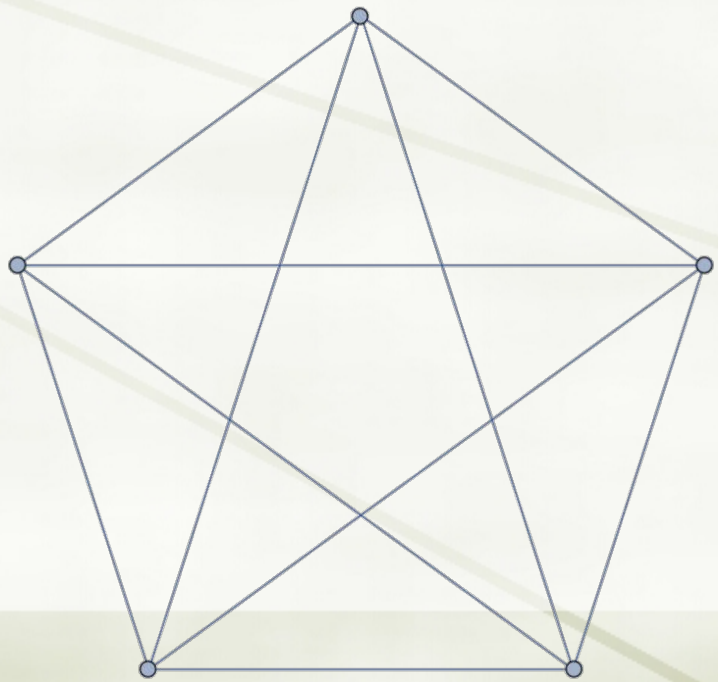
- The $n \times n$ *adjacency matrix* specifies which vertices are connected to which other vertices.
- The $n \times m$ *incidence matrix* specifies which vertices attach to a given edge.
- The $m \times n$ *discrete gradient* specifies how *oriented* edges attach to the vertices.

Complete graph

```
MatrixForm[CompleteAdj[5]]
```

$$\begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

```
AdjacencyGraph[%]
```

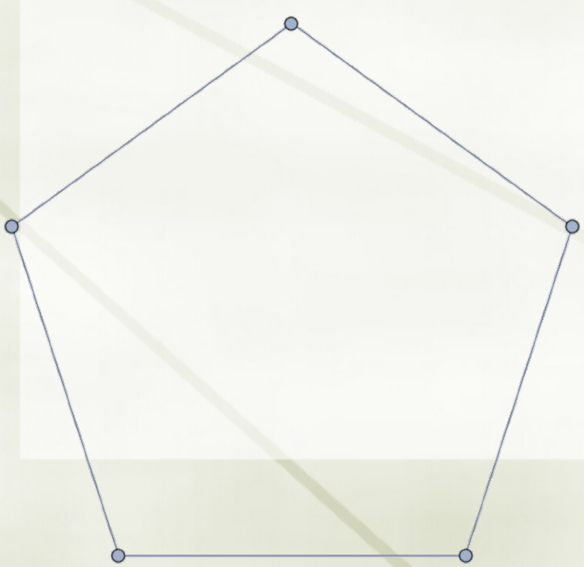


Ring and star

```
MatrixForm[RingAdj[5]]
```

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}$$

```
AdjacencyGraph[%]
```



```
MatrixForm[StarAdj[5]]
```

$$\begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

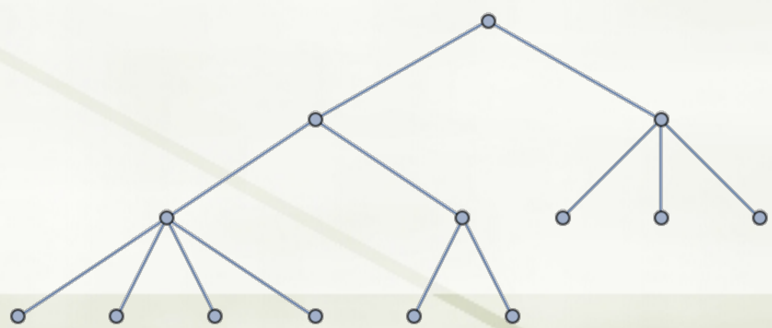
```
AdjacencyGraph[%]
```

Tree

```
MatrixForm[Tree[{2, 2, 3, 4, 2}]]
```

$$\begin{pmatrix}
0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}$$

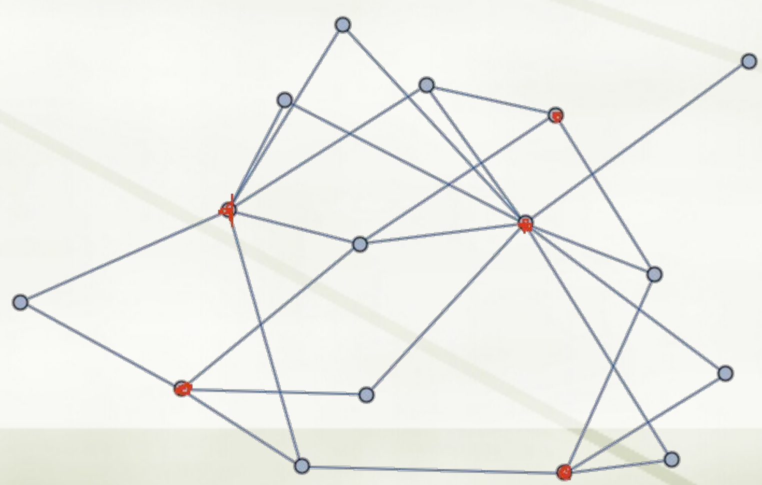
```
AdjacencyGraph[%]
```



Bipartite

A classic problem in graph theory is to determine how many labels, or “colors,” are necessary for the vertices, so that no two vertices with the same label are connected. A bipartite graph is one where only two labels are necessary.

```
AdjacencyGraph[RandBipAdj[.5, 5, 16]]
```

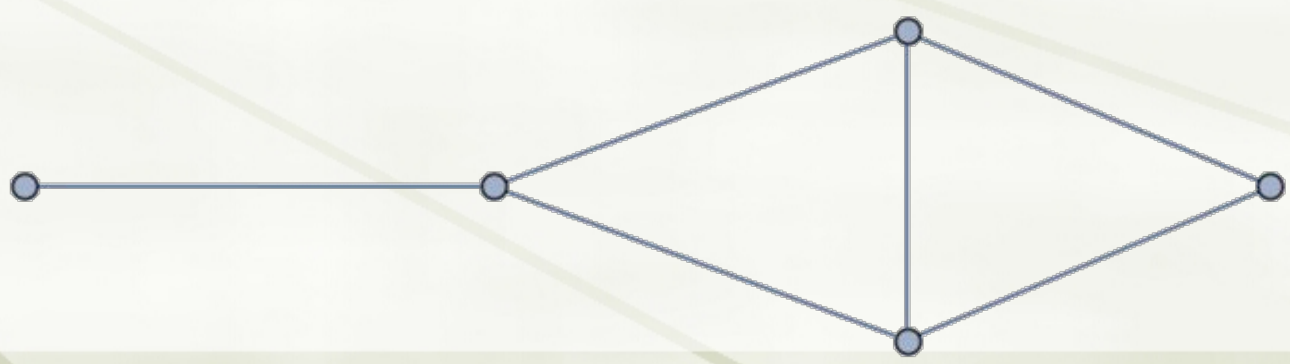


Prof. H's favorite example

```
MatrixForm[FaveAdj]
```

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 & 0 \end{pmatrix}$$

```
AdjacencyGraph[FaveAdj]
```



Prof. H's favorite example

Incidence matrix:

```
MatrixForm[B]
```

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 \end{pmatrix}$$

Prof. H's favorite example

```
MatrixForm[B.Transpose[B]]
```

$$\begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 1 & 3 & 1 & 0 & 1 \\ 0 & 1 & 3 & 1 & 1 \\ 0 & 0 & 1 & 2 & 1 \\ 0 & 1 & 1 & 1 & 3 \end{pmatrix}$$

The diagonal is the set of "degrees" (or valences, i.e., the number of neighbors.

Prof. H's favorite example

```
MatrixForm[B.Transpose[B]]
```

$$\begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 1 & 3 & 1 & 0 & 1 \\ 0 & 1 & 3 & 1 & 1 \\ 0 & 0 & 1 & 2 & 1 \\ 0 & 1 & 1 & 1 & 3 \end{pmatrix} = \text{Deg} + \text{A}$$

Prof. H's favorite example

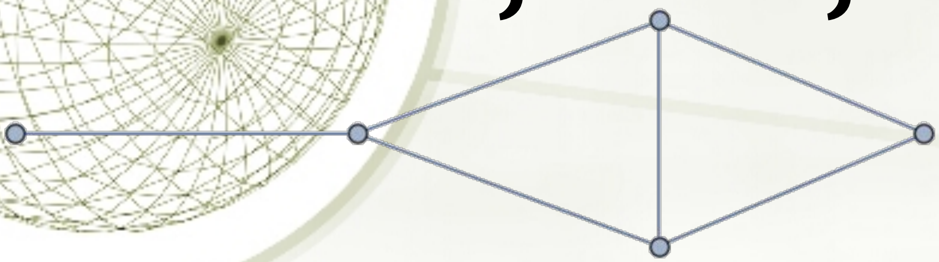
`MatrixForm[Dif]`

Gradient:

$$\begin{pmatrix} -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 0 & 1 \\ 0 & -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

(An arbitrary orientation has been put on the edges)

Prof. H's favorite example



```
MatrixForm[Transpose[Dif].Dif]]
```

$$\begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & -1 \\ 0 & -1 & 3 & -1 & -1 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & -1 & -1 & -1 & 3 \end{pmatrix} = \text{Deg} - \text{A}$$

Prof. H's favorite example

Gradient:

(Both orientations are allowed on the edges.)

```
MatrixForm[FullDif]
```

$$\begin{pmatrix} -1 & 1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & -1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 1 & -1 \end{pmatrix}$$

Prof. H's favorite example

```
MatrixForm[Transpose[FullDif].FullDif]
```

$$\begin{pmatrix} 2 & -2 & 0 & 0 & 0 \\ -2 & 6 & -2 & 0 & -2 \\ 0 & -2 & 6 & -2 & -2 \\ 0 & 0 & -2 & 4 & -2 \\ 0 & -2 & -2 & -2 & 6 \end{pmatrix}$$

(exactly twice the previous caculation, 2 (Deg – A).)

The Laplacian on a graph

- The operator *d*d* is what we will define (up to a sign) as the *graph Laplacian*, $-\Delta = d^*d$. The quadratic form of this is:

$$\begin{aligned}\langle d^* df, f\rangle_{\mathcal{V}} &= \langle df, df\rangle_{\mathcal{E}} \\ &= \sum_{e\in\mathcal{E}} |f(t(e)) - f(s(e))|^2\end{aligned}$$

The Laplacian on a graph

- The operator d^*d is what we will define (up to a sign) as the *graph Laplacian*,

$-\Delta = d^*d$. Notice that

$$-\Delta = \mathrm{Deg} - A$$

- This means that at a vertex v,

$$[-\Delta f](v) = \mathrm{Deg}(v)(f(v) - \langle f \rangle_{w\sim v}).$$

The Laplacian on a graph

- The *renormalized graph Laplacian* of Fan Chung is defined as

  $$\mathrm{Deg}^{-1/2}\,(-\,\Delta)\,\mathrm{Deg}^{-1/2}$$

- This is related by a similarity transformation to

  $$\mathrm{Deg}^{-1}\,[-\,\Delta\, f](v) = f(v) - \langle f\rangle_{w\sim v}.$$

The Laplacian on a graph

- In the next lecture we will discuss quantum graphs, where the edges have the metric structure of intervals.