LINEAR ALGEBRA AND VECTOR ANALYSIS

MATH 22B

Unit 18: Spectra

Seminar

18.1. If you hit a drum, you hear eigenvalues of its Laplacian. An actual drum is a finite network of fibres. The sound we hear when hitting the drum is made of spectra of the eigenvalues of a **Laplacian matrix** defined by the network. You remember the Laplacian matrix from last semester, when we defined the discrete gradient d, the discrete divergence d^* and formed the Laplacian $L = d^* d$. We even computed some spectra already then.

18.2. Mark Kac asked in 1966 whether one can hear the shape of a drum. [1] [2] This problem is still not solved for convex drums. A drum is a planar region with piecewise smooth boundary for which the line between two arbitrary points is contained in the drum.

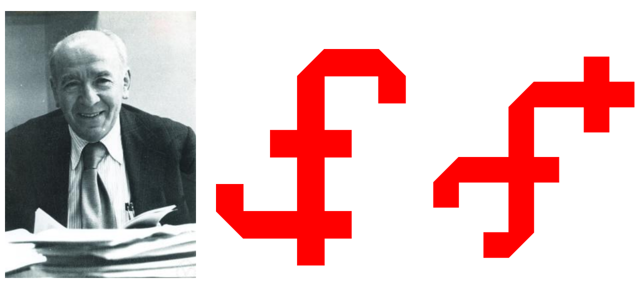

Figure 1. Mark Kac asked in 1966 whether one can hear the shape of a drum. Carolyn Gordon, David Webb and Scott Wolpert found in 1992 the first non-isometric isospectral domains. They are shown to the right.

18.3. Instead of looking at actual drums, we can look at a small finite network and compute the eigenvalues of the Laplacian matrix L associated to this network. It is defined as follows. L is a $n \times n$ matrix if there are n nodes. If node i is connected to node j, let $L_{ij} = L_{ji} = -1$, otherwise put a zero. In the diagonal,place $L_{ii} = d(i)$, where $d(i)$ is the number of neighbors of the node i.

[1] M. Kac, Can One Hear the Shape of a Drum?, American Mathematical Monthly, 73, 1966, page 1-23

[2] C. Gordon, D.L. Webb and S. Wolpert, One can not hear the shape of a drum, Bull. Amer. Math. Soc. 27 (1992), page 134-138

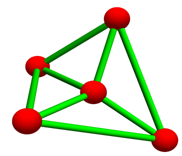

FIGURE 2. A small drum with 5 nodes.

18.4. For a wheel graph with 5 nodes, we have

$$\begin{bmatrix} 4 & -1 & -1 & -1 & -1 \\ -1 & 3 & -1 & 0 & -1 \\ -1 & -1 & 3 & -1 & 0 \\ -1 & 0 & -1 & 3 & -1 \\ -1 & -1 & 0 & -1 & 3 \end{bmatrix}$$

There are two eigenvalues 5 with eigenvectors $[-2, 0, 1, 0, 1]$ and $[-2, 1, 0, 1, 0]$ and two eigenvalues 3 with eigenvectors $[0, -1, 0, 1, 0]$ and $[0, 0, -1, 0, 1]$. Finally, there is the eigenvalue 0 with eigenvector $[1, 1, 1, 1, 1]$.

18.5. Here are two isospectral networks.

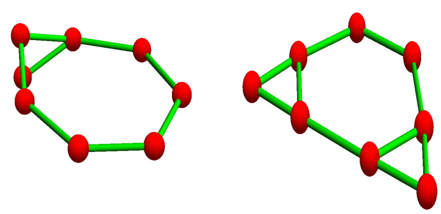

FIGURE 3. An example of a cospectral pair for the Laplace operator L_0 given by W. Hamers and E. Spence in 2004. Both have 8 nodes.

18.6. What are the properties of the Laplacian L?

Problem A: The Laplacian L of a network always has an eigenvalue 0.

Hint. Remember the lecture last week.

18.7. We can write $L = d^*d$, where d is a $m \times n$ matrix, where m is the number of edges and n the number of nodes.

Problem B: Any matrix L of the form $L = A^*A$ has real eigenvalues.

Hint. Use a theorem.

Problem C: Show that $L = A^*A$ has non-negative eigenvalues.

Hint: Here is a start: assume v is an eigenvector of L to the eigenvalue λ then $(v, Lv) = (v, A^*Av) = (Av, Av) = |Av|^2$.

18.8. A matrix is doubly stochastic if all matrix entries are non-negative and each row and each column adds up to 1. Each column vector is then a discrete probability distribution.

Theorem: The inverse g of $1 + L$ is doubly stochastic.

Problem D: Either prove this theorem or look whether you find the theorem.

18.9. Hint: This result follows from the matrix forest theorem which tells that $\det(L + 1)$ is the number of rooted forests in a graph. The entries of g_{ij} can be interpreted as probabilities of forests.

18.10. In the case of the wheel graph before

$$24g = \begin{bmatrix} 8 & 4 & 4 & 4 & 4 \\ 4 & 9 & 4 & 3 & 4 \\ 4 & 4 & 9 & 4 & 3 \\ 4 & 3 & 4 & 9 & 4 \\ 4 & 4 & 3 & 4 & 9 \end{bmatrix} .$$

All rows and columns add up to 24 so that g is stochastic.

18.11. Why are spectra interesting. One reason is Hückel theory.

FIGURE 4. Erich Hueckel devised a method to compute approximate molecular orbital electron systems. Pavel Chebotarev and Elena Shamis proved the matrix forest theorem and also were the first to see that the inverse of $1 + L$ is doubly stochastic.

18.12. The Wikipedia article about Hueckel mentions that Hueckel had a lack of communication skills. But a poem he wrote about Schrödinger shows his humor (it was freely translated by Felix Bloch)

Erwin with his psi can do
Calculations quite a few.
But one thing has not been seen:
Just what does psi really mean?

Homework

This homework is due on 3/12/2019

Problem 18.1 Compute the eigenvalues of the Laplacian of K_n, the complete graph with n nodes.

Problem 18.2 Below is Mathematica code encoding two networks. The **Halbeisen-Hungerbuehler isospectral graphs**. Verify that the Laplacians have the same characteristic Polynomial. What is $\det(L+1)$, the number of rooted forests of the Halbeisen-Hungerbuehler graphs? Check that $(L+1)^{-1}$ is a doubly stochastic matrix.

```
s1=UndirectedGraph[Graph[{71->72,72->73,73->74,74->75,75->76,76->77,77->70,70->71,
  71->73,75->77,77->1,1->2,2->73,75->3,3->4,4->71,72->76,74->5,76->6,70->7,72->8}]];
s2=UndirectedGraph[Graph[{71->72,72->73,73->74,74->75,75->76,76->77,77->70,70->71,
  71->73,75->77,74->1,1->2,2->70,72->3,3->4,4->76,72->76, 71->5,73->6,75->7,77->8}]];
L1=Normal[KirchhoffMatrix[s1]]; L2=Normal[KirchhoffMatrix[s2]];
K1=IdentityMatrix[Length[L1]]+L1;
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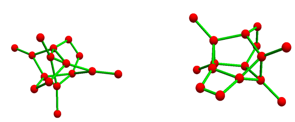

Figure 5. The Halbeisen Hungerbuehler isospectral graphs

Problem 18.3 According to **Hueckel theory**, the eigenvectors of L can help to understand the information about the distribution of electrons in a molecule. Below is an example, where we compute the eigenvalues and eigenvectors of the water molecule. What is the largest eigenvalue of the caffeine molecule? What is the corresponding eigenvector?

```
A=Normal[ChemicalData["Water", "AdjacencyMatrix"]];
L=DiagonalMatrix[Total[A]]-A; Eigensystem[L]
```

Problem 18.4 **Euler's handshake formula** tells that the trace of L is twice the number of edges in the graph of L. Prove this formula.

Problem 18.5 The Pseudo determinant $\mathrm{Det}(L)$ of a matrix L is the product of the non-zero eigenvalues of L. In comparison, the determinant is the product of all the eigenvalues. The Matrix tree theorem tells that $\mathrm{Det}(L)$ with Laplacian L is the number of rooted trees in a graph. Find a formula for the number of rooted trees in a complete graph K_n.

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