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Lecture 11 : Spectral graph theory

We introduce basic spectral graph theory today.

We will use it in analyzing random walks and in other interesting applications.

Eigenvalues and eigenvectors

Given an $n \times n$ matrix A, a nonzero vector v is an eigenvector of A if $Av = \lambda v$ for some scalar λ, which is called an eigenvalue associated with the eigenvector v.

The set of eigenvalues of A is given by the set of solutions to $\det(A - \lambda I) = 0$, the characteristic polynomial.

For an λ with $\det(A - \lambda I) = 0$, any vector $v \neq 0$ in the kernel/nullspace of $A - \lambda I$ is an associated eigenvector.

Real symmetric matrices

Our starting point of spectral graph theory is the following spectral theorem for real symmetric matrices.

Theorem. Let A be an $n \times n$ real symmetric matrix. Then there is an orthonormal basis of $\mathbb{R}^n$ consisting of eigenvectors of A, and the corresponding eigenvalues are real numbers.

We will not prove this theorem; see e.g. the book "algebraic graph theory" by Godsil and Royle.

The above theorem applies to the adjacency matrices of undirected graphs, but not for directed graphs.

This is the main reason that spectral graph theory is much more developed for undirected graphs.

Let $v_1, v_2, \ldots, v_n \in \mathbb{R}^n$ be the orthonormal basis of eigenvectors guaranteed by the above spectral theorem, with corresponding eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$.

Let V be the $n \times n$ matrix with the i-th column being v_n, i.e. $V = \begin{bmatrix} | & | & & | \\ v_1 & v_2 & \cdots & v_n \\ | & | & & | \end{bmatrix}$.

Let D be the $n \times n$ diagonal matrix with the (i,i)-th entry being λ_i, i.e. $D = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix}$.

Then the conditions $Av_i = \lambda_i v_i \ \forall 1 \leq i \leq n$ can be compactly written as $AV = VD$.

Since the columns in V form an orthonormal basis, we have $V^T V = I$ and thus $V^{-1} = V^T$.

So, we can rewrite $AV = VD$ as $A = VDV^{-1} = VDV^T = \begin{bmatrix} | & & | \\ v_1 & \cdots & v_n \\ | & & | \end{bmatrix} \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} \begin{bmatrix} - & v_1 & - \\ & \vdots & \\ - & v_n & - \end{bmatrix}$.

This representation is very convenient in computations.

Powers of matrices

To compute A^k, we observe that it is just $A^k = (VDV^T)^k = (VDV^T)(VDV^T)\cdots(VDV^T) = VD^kV^T$ as $V^TV = I$.

Since D is a diagonal matrix, D^k is easy to compute, i.e. $D = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix}$, $D^k = \begin{bmatrix} \lambda_1^k & & & \\ & \lambda_2^k & & \\ & & \ddots & \\ & & & \lambda_n^k \end{bmatrix}$.

This is very useful in analyzing random walks, as P^t is the transition matrix of the random walk after t steps where P is the transition matrix in one step.

We will use the eigenvalues of the transition matrix to bound the mixing time in a couple of lectures.

Eigen-decomposition

Since $v_1, \dots, v_n$ form an orthonormal basis, any $x \in \mathbb{R}^n$ can be written as $c_1v_1 + c_2v_2 + \dots + c_nv_n$.

By orthonormality, $\langle x, v_i \rangle = \langle c_1v_1 + \cdots + c_nv_n, v_i \rangle = c_1\langle v_1, v_i \rangle + \dots + c_i\langle v_i, v_i \rangle + \dots + c_n\langle v_n, v_i \rangle = c_i$.

Therefore,

$$\begin{aligned} x &= \langle x, v_1 \rangle v_1 + \langle x, v_2 \rangle v_2 + \dots + \langle x, v_n \rangle v_n \\ &= v_1v_1^T x + v_2v_2^T x + \dots + v_nv_n^T x \\ &= (v_1v_1^T + v_2v_2^T + \dots + v_nv_n^T)\, x .. \end{aligned}$$

This is true for all x, and hence $v_1v_1^T + v_2v_2^T + \dots + v_nv_n^T = I$.

Multiplying both sides by A, we get

$$\begin{aligned} Ax &= A(v_1v_1^T + v_2v_2^T + \dots + v_nv_n^T)\, x \\ &= (\lambda_1 v_1v_1^T + \lambda_2 v_2v_2^T + \dots + \lambda_n v_nv_n^T)\, x . \end{aligned}$$

Thus, $A = \lambda_1 v_1v_1^T + \dots + \lambda_n v_nv_n^T$.

Finally, we claim that $A^{-1} = \frac{1}{\lambda_1} v_1v_1^T + \frac{1}{\lambda_2} v_2v_2^T + \dots + \frac{1}{\lambda_n} v_nv_n^T$ if $\lambda_i \neq 0$ for all i.

because $(\lambda_1 v_1v_1^T + \dots + \lambda_n v_nv_n^T)(\frac{1}{\lambda_1} v_1v_1^T + \dots + \frac{1}{\lambda_n} v_nv_n^T) = v_1v_1^T + \dots + v_nv_n^T = I$.

Later on, we will use this idea to define the "pseudo-inverse" of a matrix A, when A is not of full rank.

Positive semidefinite matrices

This is an important definition, an analog of a matrix being non-negative.

Fact Let A be a real symmetric matrix. The following statements are equivalent.

① A is positive semidefinite, i.e. all eigenvalues of A are non-negative.

② For any $x \in \mathbb{R}^n$, we have $x^TAx \geq 0$, i.e. all quadratic forms are non-negative.

③ $A = U^TU$ for some matrix $U \in \mathbb{R}^{n \times n}$.

Proof Recall that a real symmetric matrix A can be written as VDV^T

③ $A = U^T U$ for some matrix $U \in \mathbb{R}^{n\times n}$.

Proof Recall that a real symmetric matrix A can be written as VDV^T.

① ⇒ ③ Since all eigenvalues are non-negative, we can write $A = (VD^{\frac{1}{2}})(D^{\frac{1}{2}}V^T)$ where $D^{\frac{1}{2}}$ is the $n\times n$ diagonal matrix with $D_{i,i} = \sqrt{\lambda_i}$.

Therefore, by letting $U = VD^{\frac{1}{2}}$, we see that A can be written as UU^T.

③ ⇒ ② $x^T A x = x^T U U^T x = \langle U^T x, U^T x \rangle = \|U^T x\|_2^2 \geq 0$ for any $x \in \mathbb{R}^n$.

② ⇒ ① We prove the contrapositive, ¬① ⇒ ¬②.

If v is an eigenvector with negative eigenvalue, then $v^T A v = \lambda v^T v = \lambda \|v\|_2^2 < 0$. □

We will use the notation $A \succcurlyeq 0$ for A is a positive semidefinite matrix.

This is the basic of "semidefinite programming", a powerful generalization of linear programming.

Unfortunately, we will not be able to see it in this course.

Trace = sum of eigenvalues

Fact Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of A. Then, $\sum_{i=1}^{n} \lambda_i = \text{trace}(A)$ where trace of A is defined as the sum of diagonal entries of A.

Proof Consider $\det(\lambda I - A)$.

Its roots are the eigenvalues of A, and so $\det(\lambda I - A) = (\lambda-\lambda_1)(\lambda-\lambda_2)\cdots(\lambda-\lambda_n)$.

Note that the coefficients of $\lambda^{n-1} = -\sum_{i=1}^{n} \lambda_i$.

On the other hand, $\det(\lambda I - A) = \det \begin{pmatrix} \lambda - a_{11} & -a_{12} & \cdots & -a_{1n} \\ -a_{22} & \lambda - a_{22} & & -a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ -a_{n1} & -a_{n2} & \cdots & \lambda - a_{nn} \end{pmatrix}$.

By the (expansion) definition of the determinant, the coefficient of λ^{n-1} only appears in the term $(\lambda - a_{11})(\lambda - a_{22})\ldots(\lambda - a_{nn})$, which is $-\sum_{i=1}^{n} a_{ii}$.

Therefore, $\sum_{i=1}^{n} \lambda_i = \sum_{i=1}^{n} a_{ii} = \text{trace}(A)$. □

Graph spectrum

Spectral graph theory relates the combinatorial properties of a graph to the eigenvalues and eigenvectors of its associated matrix (e.g. adjacency matrix, Laplacian matrix).

Let's look at some examples and compute their spectrums.

Complete graph What is the spectrum of a complete graph K_n?

If G is a complete graph, then $A(G) = J - I$, where J denotes the all-one matrix.

Any vector is an eigenvector of I with eigenvalue 1.

Hence the eigenvalues of A are one less than that of J.

Since J is of rank 1, there are $n-1$ eigenvalues of 0.

The all-one vector is an eigenvector of J with eigenvalue n.

So, A has one eigenvalue of $n-1$, and $n-1$ eigenvalues of -1.

This is an example with the largest eigenvalue gap between the largest eigenvalue and the second largest.

Complete bipartite graph What is the spectrum of a complete bipartite graph $K_{m,n}$?

The adjacency matrix of $K_{m,n}$ looks like this: $\begin{array}{cc} \begin{matrix} m\{ \\ n\{ \end{matrix} & \begin{bmatrix} 0 & \boxed{1} \\ \boxed{1} & 0 \end{bmatrix} \\ & \underbrace{\quad}_{m}\underbrace{\quad}_{n} \end{array}$.

It is of rank 2, so there are $n+m-2$ eigenvalues of 0, and two non-zero eigenvalues λ_1, λ_2.

As $\sum_{i=1}^{n+m} \lambda_i = \text{trace}(A) = 0$, we have $\lambda_1 = -\lambda_2$. Let this value be k.

Thus, $\det(\lambda I - A) = \lambda^{n+m} - k^2 \lambda^{n+m-2}$.

To determine k, we use the (expansion) definition of determinant of $\begin{pmatrix} \lambda & & \boxed{-1} \\ & \lambda \quad \lambda & \\ \boxed{-1} & & \ddots \quad \lambda \end{pmatrix}$.

Any term that contributes to λ^{n+m-2} must have $n+m-2$ diagonal entries,

and the remaining two entries must be $-a_{ij}$ and $-a_{ji}$ for some i, j.

There are totally mn such terms, where the sign of each term is -1.

So, $k^2 = mn$, and thus $k = \sqrt{mn}$.

To conclude, there are $n+m-2$ eigenvalues of 0, and one eigenvalue of $\sqrt{mn}$, and one of $-\sqrt{mn}$.

Bipartite graphs We can characterize bipartite graphs by the spectrums.

Claim If G is a bipartite graph and λ is an eigenvalue of $A(G)$ with multiplicity k,

then $-\lambda$ is an eigenvalue of $A(G)$ with multiplicity k.

Proof If G is a bipartite graph, then we can permute the rows and columns of $A(G)$ to

obtain the form $A(G) = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}$.

Suppose $u = \begin{pmatrix} x \\ y \end{pmatrix}$ is an eigenvector of $A(G)$ with eigenvalue λ.

Then $\begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix}$ which implies $B^T x = \lambda y$ and $By = \lambda x$.

Then $\begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix}$ which implies $B^T x = \lambda y$ and $By = \lambda x$.

This implies that $\begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}\begin{pmatrix} x \\ -y \end{pmatrix} = \begin{pmatrix} -By \\ B^T x \end{pmatrix} = \begin{pmatrix} -\lambda x \\ \lambda y \end{pmatrix} = -\lambda \begin{pmatrix} x \\ -y \end{pmatrix}$,

and thus $\begin{pmatrix} x \\ -y \end{pmatrix}$ is an eigenvector of $A(G)$ with eigenvalue $-\lambda$.

k linearly independent eigenvectors with eigenvalue λ would give k linearly independent with eigenvalue $-\lambda$, hence the claim. □

The above result shows that the spectrum of a bipartite graph is symmetric around the origin. We now prove that the converse is also true.

Claim. If the nonzero eigenvalues occur in pairs λ_i, λ_j with $\lambda_i = -\lambda_j$, then G is bipartite.

Proof. Let k be an odd number.

Then $\sum_{i=1}^{n} \lambda_i^k = 0$, by the symmetry of the spectrum.

Note that $\lambda_1^k, \lambda_2^k, \ldots, \lambda_n^k$ are the eigenvalues of A^k, because if $Au = \lambda u$ then $A^k u = \lambda^k u$.

So, we have $\text{trace}(A^k) = \sum_{i=1}^{n} \lambda_i^k = 0$.

Observe that $A^k_{i,j}$ is the number of length k walks from i to j in G (by induction).

If G has an odd cycle of length k, then $A^k_{ii} > 0$ for some i and $\text{trace}(A^k) > 0$.

So, since $\text{trace}(A^k) = 0$, G must have no odd cycles and thus bipartite. □

Laplacian Matrices

Given an undirected graph G, the Laplacian matrix $L(G)$ is defined as $D(G) - A(G)$, where

$D(G) = \begin{pmatrix} d_1 & & 0 \\ & d_2 & \\ 0 & & \ddots \; d_n \end{pmatrix}$ is a diagonal matrix with d_i = degree of vertex i in G.

When G is a regular graph, then $D = \begin{pmatrix} d & & 0 \\ & d & \\ 0 & & \ddots \; d \end{pmatrix}$ and $L = D - A$. Any eigenvector of A with eigenvalue λ is an eigenvector of L with eigenvalue with eigenvalue $d - \lambda$, and vice versa.

So, in this case the spectrums of the adjacency matrix and the Laplacian matrix are basically equivalent, but when G is non-regular it may not be easy to relate their eigenvalues.

Let's try to understand more about the spectrum of the Laplacian matrices.

Let $\vec{1}$ be the all-one vector. Then it can be easily checked that $L\vec{1} = 0$.

So L has 0 as an eigenvalue.

Can L have a smaller eigenvalue?

Let $e = ij$ be an edge in G.

Then it can be verified that
$$L(G) = L(G-e) + \underbrace{\begin{array}{c|cc} & i & j \\ \hline i & 1 & -1 \\ j & -1 & 1 \end{array}}_{\text{call this } L_e} = L(G-e) + L_e = L(G-e) + \begin{array}{c|c} i & 1 \\ j & -1 \end{array} \begin{array}{cc} i & j \\ \hline 1 & -1 \end{array}$$

Let $e = ij$. Let b_e be the column vector with the i-th position $= +1$ and the j-th position $= -1$, and 0 otherwise.

By induction, we can write $L(G) = \sum_{e \in E} L_e = \sum_{e = ij \in G} b_e b_e^T$.

Let $B = \begin{pmatrix} | & | & & | \\ b_1 & b_2 & \cdots & b_m \\ | & | & & | \end{pmatrix}$ be the matrix whose columns are $\{ b_e \mid e \in G \}$. Then $L = BB^T$.

This shows that L is positive semidefinite, and thus 0 is the smallest eigenvalue.

Connectedness

Claim A graph is connected if and only if 0 is an eigenvalue of $L(G)$ with multiplicity 1.

Proof If G is disconnected, then the vertex set can be partitioned into two sets S_1 and S_2 such that there are no edges between them. Then $L(G) = \begin{pmatrix} L(G_1) & 0 \\ 0 & L(G_2) \end{pmatrix}$ and so $\begin{pmatrix} 1 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$ are both eigenvectors of $L(G)$ with eigenvalue 0, hence multiplicity ≥ 2.

If G is connected, consider $x^T L x = x^T \left(\sum_{e \in G} L_e \right) x = x^T \left(\sum_{e \in G} b_e b_e^T \right) x = \sum_{e = ij \in G} (x_i - x_j)^2 \geq 0$

If x is an eigenvector with eigenvalue 0, then $Lx = 0$ and thus $x^T L x = 0$.

For $x^T L x = \sum_{e = ij \in G} (x_i - x_j)^2 = 0$, we must have $x_i = x_j$ for every edge $ij \in E$.

Since G is connected, it implies that $x = c \cdot \vec{1}$ for some c, i.e. a multiple of $\vec{1}$.

Hence, the eigenvalue 0 has multiplicity one. □

Actually, the proof can be used to prove the following (exercise).

Claim The Laplacian matrix $L(G)$ has 0 as its eigenvalue with multiplicity k if and only if the graph G has k connected components.

Generalizations

So far we have just used the graph spectrum to deduce some simple properties of the graph, such as bipartiteness or connectedness, which are easy to deduce by other methods (e.g. BFS).

But the nice thing about these spectral characterizations is that they can be generalized nontrivially:

- λ_2 is "small" iff the graph is "close" to disconnected (i.e. existence of a "sparse" cut).
- λ_k is "small" iff the graph is "close" to having k connected components (i.e. k disjoint "sparse" cuts).
- α_n is "close" to $-\alpha_1$ (adjacency matrix) iff the graph has a Component "close" to bipartite.

We will prove the first item and mention the next two items next time.

Rayleigh Quotient

The main tool in relating eigenvalues and eigenvectors to optimization problem is the Rayleigh quotient,

which is defined as $\frac{x^TAx}{x^Tx} = \frac{\sum_{i,j} a_{ij} x_i x_j}{\sum_i x_i^2}$

Let A be a real symmetric matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$, and orthonormal eigenvectors $v_1, v_2, \ldots, v_n$.

Claim $\lambda_1 = \max_x \frac{x^TAx}{x^Tx}$

proof Let $x = c_1v_1 + c_2v_2 + \ldots + c_nv_n$, as $v_1, \ldots, v_n$ form a basis

Then
$$x^TAx = (c_1v_1 + \ldots + c_nv_n)^T A (c_1v_1 + \ldots + c_nv_n)$$
$$= (c_1v_1 + \ldots + c_nv_n)^T (c_1\lambda_1v_1 + c_2\lambda_2v_2 + \ldots + c_n\lambda_nv_n)$$
$$= \sum_{i=1}^n c_i^2 \lambda_i \quad \text{(because } v_1, \ldots, v_n \text{ are orthonormal)}$$

Similarly, $x^Tx = (c_1v_1 + \ldots + c_nv_n)^T(c_1v_1 + \ldots + c_nv_n) = \sum_{i=1}^n c_i^2$.

So, $\frac{x^TAx}{x^Tx} = \frac{\sum_{i=1}^n c_i^2\lambda_i}{\sum_{i=1}^n c_i^2} \leq \frac{\lambda_1 \sum_{i=1}^n c_i^2}{\sum_{i=1}^n c_i^2} = \lambda_1$.

Since v_1 attains the maximum, the claim follows. □

This can be extended to characterize other eigenvalues.

Let T_k be the set of vectors that are orthogonal to $v_1, v_2, \ldots, v_{k-1}$.

Claim $\lambda_k = \max_{x \in T_k} \frac{x^TAx}{x^Tx}$

proof Let $x \in T_k$. Write $x = c_1v_1 + \ldots + c_nv_n$.

Recall that $c_i = \langle x, v_i \rangle$. Since $x \in T_k$, we have $c_1 = c_2 = \ldots = c_{k-1} = 0$.

Then, $\frac{x^TAx}{x^Tx} = \frac{\sum_{i=k}^n c_i^2\lambda_i}{\sum_{i=k}^n c_i^2} \leq \frac{\lambda_k \sum_{i=k}^n c_i^2}{\sum_{i=k}^n c_i^2} = \lambda_k$.

Since $v_k \in T_k$ and $\frac{v_k^TAv_k}{v_k^Tv_k} = \lambda_k$, the claim follows. □

The above result gives a characterization of λ_k, but it requires the knowledge of the previous eigenvectors.

The result below gives a characterization without knowing the eigenvectors, and is more useful in giving bounds on eigenvalues.

Courant-Fischer Theorem $\lambda_k = \max_{\substack{S \subseteq R^n \\ \dim(S)=k}} \min_{x \in S} \frac{x^T A x}{x^T x} = \min_{\substack{S \subseteq R^n \\ \dim(S)=n-k+1}} \max_{x \in S} \frac{x^T A x}{x^T x}$

Proof (optional) We first consider the max-min term.

Let S_k be the k-dimensional subspace spanned by $v_1, \ldots, v_k$, i.e. $\{x \mid x = c_1 v_1 + \ldots + c_k v_k$ for some $c_1, \ldots, c_k\}$.

For any $x \in S_k$, $\frac{x^T A x}{x^T x} = \frac{(c_1 v_1 + \ldots + c_k v_k)^T A (c_1 v_1 + \ldots + c_k v_k)}{(c_1 v_1 + \ldots + c_k v_k)^T (c_1 v_1 + \ldots + c_k v_k)} = \frac{\sum_{i=1}^k c_i^2 \lambda_i}{\sum_{i=1}^k c_i^2} \geq \frac{\lambda_k \sum_{i=1}^k c_i^2}{\sum_{i=1}^k c_i^2} = \lambda_k$.

So, $\max_{\substack{S \subseteq R \\ \dim(S)=k}} \min_{x \in S} \frac{x^T A x}{x^T x} \geq \min_{x \in S_k} \frac{x^T A x}{x^T x} \geq \lambda_k$.

To prove that the maximum cannot be greater that λ_k, observe that any k-dimensional subspace must intersect the n-k+1 dimensional subspace T_k spanned by $\{v_k, v_{k+1}, \ldots, v_n\}$.

For any $x \in T_k$, $\frac{x^T A x}{x^T x} = \frac{\sum_{i=k}^n c_i^2 \lambda_i}{\sum_{i=k}^n c_i^2} \leq \lambda_k$.

So, $\max_{\substack{S \subseteq R \\ \dim(S)=k}} \min_{x \in S} \frac{x^T A x}{x^T x} \leq \max_{\substack{S \subseteq R \\ \dim(S)=k}} \min_{x \in S \cap T_k} \frac{x^T A x}{x^T x} \leq \lambda_k$. □

First Eigenvalue

Let A be the adjacency matrix of an undirected graph. Let α_1 be its largest eigenvalue.

Claim $\alpha_1 \leq d_{max}$, where d_{max} denotes the maximum degree in G.

Proof Let v_1 be an eigenvector with eigenvalue λ_1.

Let j be the vertex with $v_1(j) \geq v_1(i)$ for all i.

$\alpha_1 v_1(j) = (A v_1)(j) = \sum_{i: ij \in E(G)} v_1(i) \leq \sum_{i: ij \in E(G)} v_1(j) = \deg(j) v_1(j) \leq d_{max} v_1(j)$.

Therefore, $\alpha_1 \leq d_{max}$. □

In fact, if $\lambda_1 = d_{max}$, then the above inequalities must hold as equalities, i.e. $v_1(i) = v_1(j)$ for every neighbor i of j and $\deg(j) = d_{max}$. It implies that when G is connected and $\lambda_1 = d_{max}$, then G must be d_{max}-regular and the eigenvalue λ_1 is of multiplicity 1, since the eigenvectors for λ_1 must be of the form $c \cdot \vec{1}$ for some constant c.

The Perron-Frobenius theorem for non-negative matrices tell us more about the first eigenvalue.

Theorem Let G be a connected undirected graph. Then

① the first eigenvalue is of multiplicity one.

② $|\alpha_i| \leq \alpha_1$ for all i.

③ all entries of the first eigenvector are non-zero and have the same sign.

We will not prove it in class See Chapter 8 of Godsil-Royle for proofs.

References

You are referred to the course notes on "spectral graph theory" by Dan Spielman for more background.

The book "Algebraic graph theory" by Godsil and Royle is also a good reference.

The course notes "graph partitioning and expanders" by Luca Trevisan is closely related and well written.