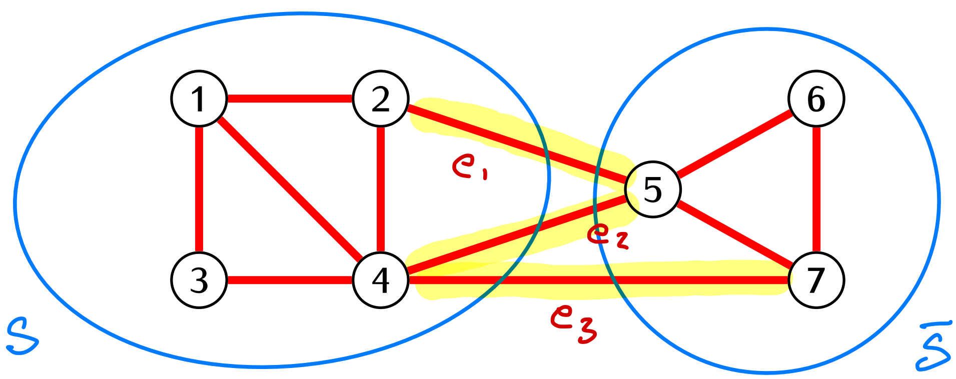
Notation. If S is a finite set then

$$|S| := (\text{the number of elements of } S)$$

Definition

Let G be a graph with the set of vertices V. Let $S \subseteq V$ and let $\overline{S} = V \setminus S$. Then

$$E(S, \overline{S}) = \begin{pmatrix} \text{the set of edges of } G \\ \text{with one end in } S \\ \text{and the other end is } \overline{S} \end{pmatrix}$$



$E(S, \overline{S}) = \{e_1, e_2, e_3\}$

$|E(S, \overline{S})| = 3$

Partitioning problem. For a given connected graph with the set of vertices $V = 1, \dots, N$ and a given number $1 \leq k \leq N$ find $S \subseteq V$ such that $|S| = k$ and that $E(S, \overline{S})$ is as small as possible.

Definition

Let G be a graph with vertices $V = \{1, \ldots, N\}$, and let $S \subseteq V$. The *selector vector* of S is the vector $\mathbf{v}_S \in \mathbb{R}^N$ given by

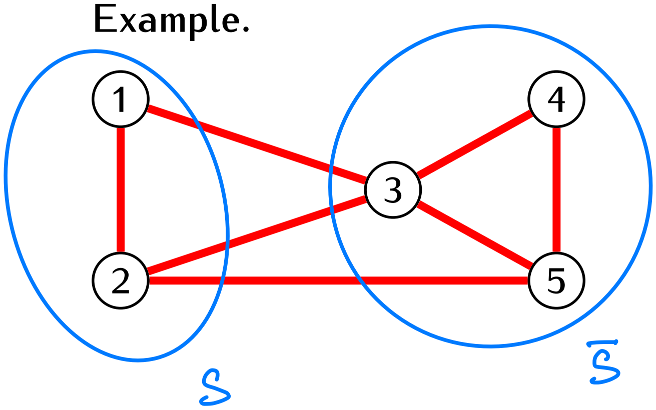
$$\mathbf{v}_S = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} \quad \text{where} \quad x_i = \begin{cases} 1 & \text{if } i \in S \\ -1 & \text{if } i \in \overline{S} \end{cases}$$

Proposition

Let G be a graph with vertices $V = \{1, \ldots, N\}$, and let L be the Laplacian of G. For $S \subseteq V$ we have:

$$|E(S, \overline{S})| = \frac{1}{4} \cdot \mathbf{v}_S^T L \mathbf{v}_S$$

Example.



$|E(S,\overline{S})| = 3$

$$v_S = \begin{array}{c} \begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \\ -1 \end{bmatrix} \end{array} \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array}$$

$$v_S^T L v_S = \begin{bmatrix} 1 & 1 & -1 & -1 & -1 \end{bmatrix} \cdot \begin{array}{c|c} & \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} & \begin{bmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 3 & -1 & 0 & -1 \\ -1 & -1 & 4 & -1 & -1 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & -1 & -1 & -1 & 3 \end{bmatrix} \end{array} \cdot \begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \\ -1 \end{bmatrix}$$

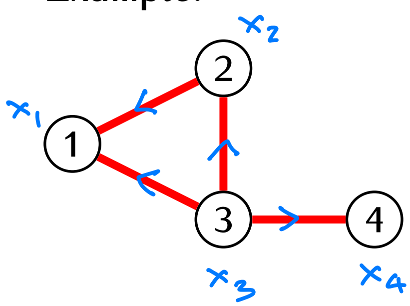
$$= \begin{bmatrix} 1 & 1 & -1 & -1 & -1 \end{bmatrix} \cdot \begin{bmatrix} 2 \\ 4 \\ -4 \\ 0 \\ -2 \end{bmatrix} = 2 + 4 + 4 + 0 + 2$$

$$= 12 = 4 \cdot |E(S,\overline{S})|$$

Notation. If i, j are vertices in a graph then we will write $i \sim j$ if there is an edge joining i and j.

> **Lemma**
>
> Let G be a graph with vertices $V = \{1, \dots, N\}$, and let L be the Laplacian of G. For any vector $\mathbf{v} = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix}$ we have
>
> $$\mathbf{v}^T L \mathbf{v} = \sum_{\substack{i<j \\ i\sim j}} (x_i - x_j)^2$$

Example.



$$v = \begin{array}{c} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \end{array} \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array}$$

$$v^T L v = (x_1 - x_2)^2 + (x_1 - x_3)^2 + (x_2 - x_3)^2 + (x_3 - x_4)^2$$

<u>Recall:</u>

1) $L = B \cdot B^T$ where B = the edge incidence matrix of B with some orientation of edges:

$$B = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} e_1 & e_2 & e_3 & e_4 \end{array} \\ \begin{bmatrix} 1 & 0 & 1 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & -1 & 1 \\ 0 & 0 & 0 & -1 \end{bmatrix} \end{array}$$

2) $$B^T \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{array}{c} e_1 \\ e_2 \\ e_3 \\ e_4 \end{array} \begin{bmatrix} x_1 - x_2 \\ x_2 - x_3 \\ x_1 - x_3 \\ x_3 - x_4 \end{bmatrix}$$

Proof of Lemma.

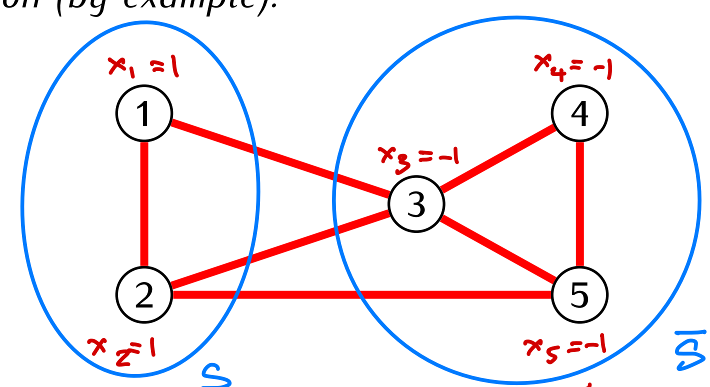
Let B - the edge incidence matrix of G with edges oriented as follows: $i \bullet\!\!\longleftarrow\!\!\bullet\, j$ if $i < j$.

We have:

$$
\begin{aligned}
v^T L v &= v^T B B^T v \\
&= (B^T v)^T B^T v \\
&= \underset{\substack{\uparrow \\ \text{dot product}}}{(B^T v) \bullet (B^T v)} \\
&= \begin{bmatrix} x_i - x_j \\ \vdots \\ \\ \end{bmatrix} \bullet \begin{bmatrix} x_i - x_j \\ \\ \\ \end{bmatrix} \leftarrow \text{for } i<j,\ i \sim j \\
&= \sum_{\substack{i \sim j \\ i < j}} (x_i - x_j)^2
\end{aligned}
$$

Proof of Proposition (by example).

$$
v_S = \begin{array}{c} \begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \\ -1 \end{bmatrix} \end{array} \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array}
$$



$(x_i - x_j)^2 = 0$ if i and j are both in S or in $\bar{S}$

$(x_i - x_j)^2 = 2^2 = 4$ if $i \in S$ and $j \in \bar{S}$ or $i \in \bar{S}$ and $j \in S$

<u>By Lemma:</u> $\displaystyle v_S^T \cdot L \cdot v_S = \sum_{\substack{i<j \\ i \sim j}} (x_i - x_j)^2 = \sum_{\substack{i<j \\ i \sim j \\ i,j \text{ are in different groups}}} 4 = 4 \cdot |E(S, \bar{S})|$

<u>So:</u> $|E(S, \bar{S})| = \frac{1}{4} v_S^T L v_S$

Partitioning problem restated:

Given a connected graph with vertices $\{1, 2, \dots, N\}$ and Laplacian L find a vector $v = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} \in \mathbb{R}^N$ such that:

hard → [(1) $x_i = \pm 1$ for $i = 1, 2, \dots, N$

(2) $\sum_i x_i = k - (N-k)$ (equivalently: $v \cdot \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} = k - (N-k)$) dot product

(3) $v^T L v$ is the the smallest possible.

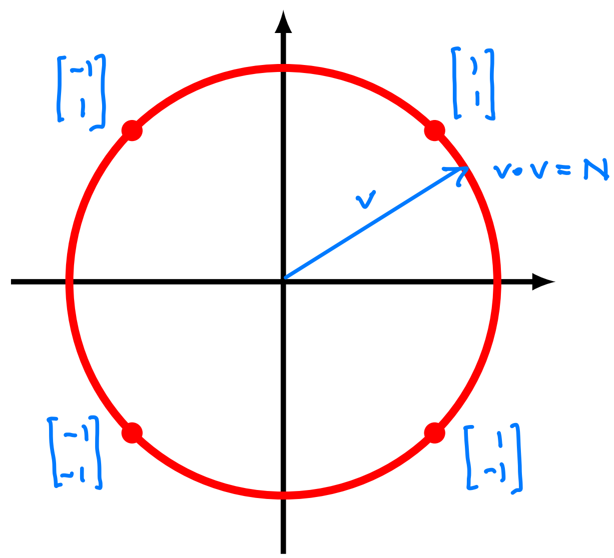
Relaxation:

Find a vector $v = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} \in \mathbb{R}^N$ such that:

(1') $v \cdot v = N$

(2) $v \cdot \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} = k - (N-k)$

(3) $v^T L v$ is the smallest possible.



Note:

Let v_P = a solution of the partitioning problem

v_R = a solution of the relaxed problem

Then

1) $v_P^T L v_P \geqslant v_R^T L v_R$

2) we can use v_R to get an approximated solution of the partitioning problem

Preparation: Eigenvectors of the Laplacian of a graph

Let G be a connected graph with N vertices and L be the Laplacian of G.

1) Since L is a symmetric matrix, it has N orthonormal eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_N$.

orthonormal:

$$u_i \cdot u_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

Let

$$\begin{aligned}
\lambda_1 &= \text{eigenvalue corresponding to } \mathbf{u}_1 \\
\lambda_2 &= \text{eigenvalue corresponding to } \mathbf{u}_2 \\
\dots \quad & \dots \quad \dots \quad \dots \quad \dots \quad \dots \quad \dots \\
\lambda_N &= \text{eigenvalue corresponding to } \mathbf{u}_N
\end{aligned}$$

We can assume that $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_N$.

2) $\lambda_i \geq 0$ for $i = 1, \dots, N$ (since L can be written in the form BB^T for some matrix B).

3) Since G connected, we have $\lambda_1 = 0$ and $\lambda_i > 0$ for $i = 2, \dots, N$.

4) We can take

$$\mathbf{u}_1 = \frac{1}{\sqrt{N}} \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

Solution of the relaxed problem

Let $0 = \lambda_1 < \lambda_2 \leq \ldots \leq \lambda_N$ - eigenvalues of L

$\frac{1}{\sqrt{N}}\begin{bmatrix}1\\ \vdots\\ 1\end{bmatrix} = u_1 \quad u_2 \quad \cdots \quad u_N$ - corresponding orthonormal eigenvectors

Take $v \in \mathbb{R}^N$ that satisfies the conditions (1'), (2), (3)

Since $\{u_1, \ldots, u_N\}$ is a basis of $\mathbb{R}^N$ we have:

$$v = \sum_i c_i u_i \qquad \text{for some } c_i \in \mathbb{R}$$

Condition (1') gives:

$$N = v \cdot v = \left(\sum_i c_i u_i\right)\left(\sum_i c_i u_i\right) = \sum_{ij} c_i c_j (u_i \cdot u_j) \underset{\text{by orthonormality of } \{u_1, \ldots, u_N\}}{=} \sum_i c_i^2$$

Condition (2) gives:

$$k - (N-k) = v \cdot \begin{bmatrix}1\\ \vdots\\ 1\end{bmatrix} = \left(\sum_i c_i u_i\right)\cdot\begin{bmatrix}1\\ \vdots\\ 1\end{bmatrix} = \sum_i c_i \left(u_i \cdot \begin{bmatrix}1\\ \vdots\\ 1\end{bmatrix}\right) \underset{\text{since } u_i \cdot \begin{bmatrix}1\\ \vdots\\ 1\end{bmatrix} = 0 \text{ for } i>1}{=} c_1 \cdot \frac{N}{\sqrt{N}} = c_1\sqrt{N}$$

Thus: $c_1 = \dfrac{k-(N-k)}{\sqrt{N}}$

Condition (3):

$$v^T L v = \left(\sum_i c_i u_i\right)^T L \left(\sum_i c_i u_i\right) = \left(\sum_i c_i u_i\right)^T \left(\sum_i c_i L u_i\right) \underset{u_i \text{ is an eigenvector of } L \text{ corresp. to } \lambda_i}{=} \left(\sum_i c_i u_i\right)^T \left(\sum_i c_i \lambda_i u_i\right)$$

$$= \sum_{ij} c_i c_j \lambda_j (u_i \cdot u_j) \underset{\text{by orthonormality of } \{u_1, \ldots, u_N\}}{=} \sum_i c_i^2 \lambda_i \underset{\lambda_1 = 0}{=} c_1^2 \cdot 0 + (c_2^2 \cdot \lambda_2 + c_3^2 \lambda_3 + \ldots + c_N^2 \lambda_N)$$

$$\underset{\lambda_2 \leq \lambda_3 \leq \ldots \leq \lambda_N}{\geq} c_1^2 \cdot 0 + (c_2^2 \cdot \lambda_2 + c_3^2 \lambda_2 + \ldots + c_N^2 \cdot \lambda_2)$$

$$= c_1^2 \cdot 0 + (c_2^2 + c_3^2 + \ldots + c_N^2)\lambda_2 = w^T L w$$

for $w = c_1 u_1 + d u_2$

where $d = \sqrt{c_2^2 + \ldots + c_N^2}$

Upshot: To get a vector $v \in \mathbb{R}^N$ that satisfies (1'), (2), (3) we need to take:

$$v = c u_1 + d u_2$$

where:

$$c = \frac{k - (N-k)}{\sqrt{N}}, \qquad c^2 + d^2 = N \quad (\text{or } d^2 = N - c^2)$$

This gives:

$$d^2 = N - c^2 = N - \frac{(k-(N-k))^2}{N} \underset{\uparrow \text{check}}{=} \frac{4k(N-k)}{N}$$

$$d = \pm\sqrt{\frac{4k(N-k)}{N}}$$

We obtain:

1) The solution of the relaxed partitioning problem is given by the vector

$$v_R = \underbrace{\frac{k-(N-k)}{\sqrt{N}}}_{c} \cdot \underbrace{\frac{1}{\sqrt{N}} \cdot \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}}_{u_1} \underbrace{\pm \sqrt{\frac{4k(N-k)}{N}}}_{d} \cdot u_2$$

2) For this vector we have:

$$v_R^T L v_R = c \cdot 0 + d^2 \cdot \lambda_2 = \frac{4k(N-k)}{N} \cdot \lambda_2$$

Theorem

Let G be a graph with N vertices, and let λ_2 be the second smallest eigenvalue of the Laplacian of G. Then for any set S of vertices of G we have

$$|E(S, \bar{S})| \geq \frac{|S| \cdot |\bar{S}|}{N} \cdot \lambda_2$$

Proof: Assume that $|S| = k$.

Let v_S = the selector vector for the set S

v_R = the solution of the relaxed partitioning problem

We have:

$$|E(S,\bar{S})| = \frac{1}{4} v_S^T L v_S \geqslant \frac{1}{4} v_R^T L v_R = \frac{1}{4} \frac{4k(N-k)}{N} \cdot \lambda_2$$

$$= \frac{|S| \cdot |\bar{S}|}{N} \cdot \lambda_2$$

Definition

Let G be a graph. The second smallest eigenvalue λ_2 of the Laplacian of G is called the *algebraic connectivity* of G.

Back to the partitioning problem

Recall: Given a connected graph with the set of vertices $V = \{1, 2, \dots, N\}$ and $0 < k < N$ we want to find $S \subseteq V$ such that $|S| = k$ and $|E(S, \overline{S})|$ is as small as possible (equivalently: $\mathbf{v}_S^T L \mathbf{v}_S$ is as small as possible).

Approximated solution:

1) Compute v_R = the solution of the relaxed problem

2) Take the set $S \subseteq V$ such that the selector vector v_S is the closest to v_R.

Recall: $\underbrace{\mathrm{dist}(v_R, v_S)}_{\text{distance between vectors}} = \| v_R - v_S \| = \sqrt{(v_R - v_S)\cdot(v_R - v_S)}$

$$= \sqrt{\underbrace{v_R \cdot v_R}_{N} - 2 v_R \cdot v_S + \underbrace{v_S \cdot v_S}_{N}}$$

$$= \sqrt{2N - v_R \cdot v_S}$$

Thus $\mathrm{dist}(v_R, v_S)$ is the smallest when $v_R \cdot v_S$ is the largest.

Recall: $v_R = c u_1 + d u_2 \qquad u_1 = \frac{1}{\sqrt{N}}\begin{bmatrix}1\\ \vdots \\ 1\end{bmatrix}$, u_2 - eigenvector of L corresponding to λ_2

$$v_R \cdot v_S = \underbrace{c \cdot \frac{1}{\sqrt{N}} \cdot \begin{bmatrix}1\\ \vdots \\ 1\end{bmatrix} \cdot v_S}_{= \frac{c}{\sqrt{N}} \cdot (k - (N-k))} + d \cdot u_2 \cdot v_S \qquad d = \pm \sqrt{\frac{4k(N-k)}{N}}$$

(does not depend on S)

Thus we want $d \cdot u_2 \cdot v_S$ to be as large as possible

Note:

1) if $d > 0$ then $d \cdot u_2 \cdot v_S$ is the biggest if entries of v_S equal to 1 correspond to the k largest entries of u_2.

2) if $d < 0$ then $d \cdot u_2 \cdot v_S$ is the biggest if entries of v_S equal to 1 correspond to the k smallest entries of u_2.

The spectral partitioning algorithm

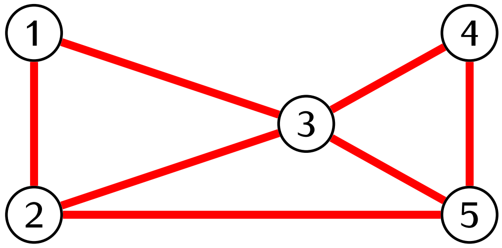
Recall: Given a connected graph with the set of vertices $V = \{1, 2, \ldots, N\}$ and $0 < k < N$ we want to find $S \subseteq V$ such that $|E(S, \overline{S})|$ is as small as possible.

Approximated solution:

1. Compute the Laplacian L of the graph.
2. Compute the eigenvector of L corresponding to the second smallest eigenvalue λ_2:
$$\mathbf{u}_2 = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix}$$
3. Let
$$\begin{aligned} S_+ &= \{i_1, \ldots, i_k\} \subseteq V \\ S_- &= \{j_1, \ldots, j_k\} \subseteq V \end{aligned}$$
such that
   - $x_{i_1}, \ldots, x_{i_k}$ are the largest entries of $\mathbf{u}_2$
   - $x_{j_1}, \ldots, x_{j_k}$ are the smallest entries of $\mathbf{u}_2$.

   If $x_{i_1} + \cdots + x_{i_k} \geq -(x_{j_1} + \cdots + x_{j_k})$ take $S = S_+$. Otherwise take $S = S_-$.

Example.



$$L = \begin{bmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 3 & -1 & 0 & -1 \\ -1 & -1 & 4 & -1 & -1 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & -1 & -1 & -1 & 3 \end{bmatrix}$$

Eigenvalues of L :

$$\lambda_1 = 0 \;, \quad \underbrace{\lambda_1 = 1.586}_{} \;, \quad \lambda_3 = 4.14 \;, \quad \lambda_2 = 5$$

$$u_1 = \begin{array}{cc} \begin{bmatrix} 0.653 \\ 0.271 \\ 0 \\ -0.653 \\ -0.271 \end{bmatrix} & \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \end{array}$$

Definition

Let G be a graph with the set of vertices V. The *Cheeger constant* of G is the number

$$h(G) = \min\left\{\frac{|E(S,\overline{S})|}{|S|} \;\middle|\; S \subseteq V,\ 1 \leq |S| \leq \frac{|V|}{2}\right\}$$

Corollary

If λ_2 is the algebraic connectivity a graph G then

$$h(G) \geq \tfrac{1}{2}\lambda_2$$

Proof: We had: if $S \subseteq V$ then

$$|E(S,\overline{S})| \geq \frac{|S| \cdot |\overline{S}|}{|V|} \cdot \lambda_2$$

so:

$$\frac{|E(S,\overline{S})|}{|S|} \geq \frac{|\overline{S}|}{|V|} \cdot \lambda_2$$

If $|S| \leq \frac{|V|}{2}$ then $|\overline{S}| \geq \frac{|V|}{2}$ so:

$$|E(S,\overline{S})| \geq \frac{|\overline{S}|}{|V|} \cdot \lambda_2 \geq \frac{|V|}{2|V|} \cdot \lambda_2 = \frac{1}{2}\lambda_2$$

for all S such that $|S| \leq \frac{|V|}{2}$

We get: $h(G) = \min\left\{ |E(S,\overline{S})| \;\middle|\; |S| \leq \frac{|V|}{2} \right\} \geq \frac{1}{2}\lambda_2$

Theorem (Cheeger inequality)

If λ_2 is the algebraic connectivity of a graph G then

$$\sqrt{2\lambda_2 d_{\max}} \geq h(G)$$

where $d_{\max}$ is the maximal degree of a vertex of G.