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FINDING A HAMILTONIAN CYCLE USING THE CHEBYSHEV POLYNOMIALS

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Abstract: We present an algorithm of finding the Hamiltonian cycle in a general undirected graph by minimization of an appropriately chosen functional. This functional depends on the characteristic polynomial of the graph Laplacian matrix and attains its minimum at the characteristic polynomial of the Laplacian matrix of the Hamiltonian cycle.

Keywords: Hamiltonian cycle, Chebyshev polynomial, minimization of functional

MSC: 65N15, 65M15, 65F08

1. Introduction

The problem of finding a Hamiltonian cycle in a general undirected graph is one of the basic optimization tasks and has a wide application not only in logistics, but also in some modern fields, such as computer graphics or microchip construction [3]. However, it belongs to the so-called NP-complete problems [2] and finding an algorithm that could solve NP-complete problems in polynomial time is one of the seven Millennium Prize Problems [1]. In graph theory, there exists a number of sufficient conditions guaranteeing that a given graph is Hamiltonian (i.e. contains a Hamiltonian cycle). These conditions are most often based on some properties of the graph, such as the sum of degrees of non-adjacent vertices or the minimum degree of the graph [4]. In this contribution we apply a different (numerical) approach: The characteristic polynomial of the Laplacian matrix (one may also choose the adjacency matrix) of an undirected graph formed by a single Hamiltonian cycle is related to some Chebyshev polynomial of the first kind. Whereas linearly constrained minimization problem have already been employed for finding a Hamiltonian cycle (e.g. [5]) we use the properties of Chebyshev polynomials and present the algorithm consisting in finding a Hamiltonian cycle by minimization of an appropriately chosen nonlinear functional.

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2. Graph, its representation and basic properties

By graph G we consider an ordered pair $G = (V, E)$, where

$$\begin{aligned} V &= V(G) = \{v_1, v_2, \dots, v_n\} \\ &\text{is a set of vertices of graph } G \text{ and} \\ E &= E(G) = \{e_1, e_2, \dots, e_m\} \subseteq \binom{V}{2}, \quad e_j = \{v_k, v_l\}, \quad k \neq l, \\ &\text{is a set of edges of the graph } G. \end{aligned}$$

We denote by $B \in \{0, 1\}^{n \times m}$ the incidence matrix of G satisfying $B_{ij} = 1$ if $v_i \in e_j$ and $B_{ij} = 0$ if $v_i \notin e_j$. Arbitrary set of edges can be represented by the vector $\vec{w} \in \{0, 1\}^{m \times 1}$, which is a characteristic vector of the set $W \subseteq E$ satisfying $w_i = 1$ if $e_i \in W$ and $w_i = 0$ otherwise.

Using this notation we may define the *vertex-disjoint cycle cover* \vec{w} of the graph G being any set of edges satisfying

$$\begin{aligned} \vec{w} &\in \{0, 1\}^{m \times 1}, & (1) \\ \mathbf{1}_m^T \vec{w} &= n, & (2) \\ B\vec{w} &= 2 \cdot \mathbf{1}_n, & (3) \end{aligned}$$

where $\mathbf{1}_n = (1, 1, \dots, 1)^T \in \mathbb{R}^n$. While the second condition ensures the cycle cover contains n edges, the third one guarantees that each vertex coincides with exactly 2 edges.

Further, let $W \subseteq E$ be any set of edges and let $\vec{w} \in \{0, 1\}^{m \times 1}$ be its representation. If we denote by $\text{diag}(\vec{w}) \in \{0, 1\}^{m \times m}$ a diagonal matrix with the vector \vec{w} on its main diagonal, then

$$L(\vec{w}) = 4I - B \text{diag}(\vec{w}) B^T \quad (4)$$

is the Laplacian matrix of the graph induced by the set W . Consequently, if $\text{diag}(\vec{w}) = I$, then $L = 4I - BB^T$ is the Laplacian matrix of the graph G .

The least-squares solution of the system $B\vec{w} = 2 \cdot \mathbf{1}_n$ is defined using the Moore–Penrose pseudo-inverse of the matrix B (see e.g. [8]) as follows

$$\vec{w}_{LS} = B^\dagger(2 \cdot \mathbf{1}_n) = 2 \cdot B^\dagger \mathbf{1}_n. \quad (5)$$

The following lemma provides a characterization of the distribution of all vertex-disjoint cycle covers: they all lie on the same sphere with the center at \vec{w}_{LS} and radius equal to $\sqrt{n - \|\vec{w}_{LS}\|^2}$.

Lemma 1. *Let $\vec{w} \in \{0, 1\}^m$ be a vertex-disjoint cycle cover, then*

$$\|\vec{w} - \vec{w}_{LS}\|^2 = n - \|\vec{w}_{LS}\|^2. \quad (6)$$

Proof. One can find the proof in [6]. □

3. Definition of the solution space

In this chapter we describe how we chose the solution space in which the minimum of the functional will be searched. At first let us consider any undirected graph containing two different Hamiltonian cycles (cf. Figure 1).

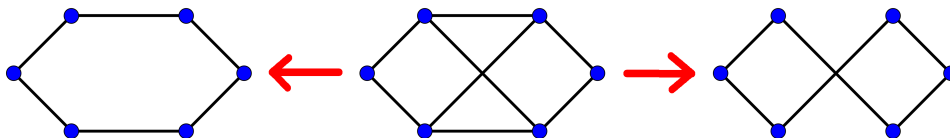


Figure 1: Graph with two Hamiltonian cycles

Consequently, the Laplacian matrices of the subgraphs induced by these Hamiltonian cycles have the following form

$$L_A = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ -1 & 0 & 0 & 0 & -1 & 2 \end{pmatrix}, \quad L_B = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & -1 \\ -1 & 2 & 0 & 0 & -1 & 0 \\ 0 & 0 & 2 & -1 & 0 & -1 \\ 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & -1 & 0 & -1 & 2 & 0 \\ -1 & 0 & -1 & 0 & 0 & 2 \end{pmatrix}.$$

We observe that we can obtain one matrix from the other one simply by simultaneous permutation of columns and rows, i.e. $L_A = PL_B P^T$ for some permutation matrix P . Hence, both matrices share a common characteristic polynomial. In this case it has a form

$$p_A(x) = p_B(x) = x^6 - 12x^5 + 54x^4 - 112x^3 + 105x^2 - 36x. \quad (7)$$

If the Laplacian matrix of the n -cycle is tridiagonal with another two -1 in the corners, we call it in the *standard form* (cf. matrix L_A).

Lemma 2. *Let L_n be the Laplacian matrix of the n -cycle in the standard form and $j = n/2$ for n even or $j = (n + 1)/2$ for n odd. Then the eigenvectors and eigenvalues of the matrix L_n have the following form:*

$$\begin{aligned} \vec{u}_{k,1} &= \left[\cos\left(1 \frac{k\pi}{n}\right), \cos\left(3 \frac{k\pi}{n}\right), \dots, \cos\left((2n-1) \frac{k\pi}{n}\right) \right]^T, \quad k = 0, 1, \dots, j-1, \\ \vec{u}_{k,2} &= \left[\sin\left(1 \frac{k\pi}{n}\right), \sin\left(3 \frac{k\pi}{n}\right), \dots, \sin\left((2n-1) \frac{k\pi}{n}\right) \right]^T, \quad k = 1, 2, \dots, n-j, \end{aligned}$$

$$\lambda_k = 4 \sin^2 \left(\frac{k\pi}{n} \right), \quad k = 0, 1, \dots, n-j.$$

In this notation vectors $\vec{u}_{k,1}$ and $\vec{u}_{k,2}$ are two linearly independent eigenvectors that correspond to the eigenvalue λ_k , for all suitable k .

Proof. The proof results immediately from the identities

$$\begin{aligned} -\cos \left((i-2) \frac{k\pi}{n} \right) + 2 \cos \left(i \frac{k\pi}{n} \right) - \cos \left((i+2) \frac{k\pi}{n} \right) \\ = 4 \sin^2 \left(\frac{k\pi}{n} \right) \cdot \cos \left(i \frac{k\pi}{n} \right), \end{aligned} \quad (8)$$

$$\begin{aligned} -\sin \left((i-2) \frac{k\pi}{n} \right) + 2 \sin \left(i \frac{k\pi}{n} \right) - \sin \left((i+2) \frac{k\pi}{n} \right) \\ = 4 \sin^2 \left(\frac{k\pi}{n} \right) \cdot \sin \left(i \frac{k\pi}{n} \right). \end{aligned} \quad (9)$$

□

Remark 3. In Lemma 2 for $\lambda_0 = 0$ we obtain a single eigenvector $\vec{u}_{0,1} = \mathbf{1}_n$. When n is even and $j = n/2$ then since $\vec{u}_{j,1} = [0, 0, \dots, 0]^T$ for eigenvalue $\lambda_j = 4$ only a single eigenvector $\vec{u}_{j,2} = [1, -1, 1, \dots, -1]^T$ is obtained as well. If we want to consider all eigenvalues λ_k with their multiplicities then instead of the upper bound $k = n - j$ we simply take $k = n - 1$ and use the fact that $\lambda_k = \lambda_{n-k}$.

For given $n \geq 3$ the following lemma provides an expression for the characteristic polynomial of the Laplacian matrix of n -cycle (c.f. Table 1).

Lemma 4. Let $n \in \mathbb{N}, n \geq 3$ be given, then the characteristic polynomial of the Laplacian matrix of n -cycle has a form

$$S_n(x) = 2 \cdot \left(T_n \left(\frac{x}{2} - 1 \right) - (-1)^n \right), \quad (10)$$

where $T_n(x)$ is the Chebyshev polynomial of the first kind.

Proof. We show that $\lambda_k, k = 0, 1, \dots, n-1$, from Lemma 2 (with their multiplicity) are roots of S_n . Hence, let us evaluate $S_n(\lambda_k)$ for $k = 0, 1, \dots, n-1$:

$$\begin{aligned} S_n(\lambda_k) &= 2 \left(T_n \left(\frac{\lambda_k}{2} - 1 \right) - (-1)^n \right) = 2 \left(T_n \left(2 \sin^2 \left(\frac{k\pi}{n} \right) - 1 \right) - (-1)^n \right) \\ &= 2 \left(T_n \left(-\cos \left(2 \frac{k\pi}{n} \right) \right) - (-1)^n \right) = 2(-1)^n \left(T_n \left(\cos \left(2 \frac{k\pi}{n} \right) \right) - 1 \right) \\ &= 2(-1)^n \left(\cos(2k\pi) - 1 \right) = 2(-1)^n (1 - 1) = 0, \end{aligned} \quad (11)$$

where we used the property $T_n(\cos \alpha) = \cos(n\alpha)$ and the parity of the Chebyshev polynomials (cf. [7]).

We shall also evaluate $S'_n(\lambda_k)$ for $k = 0, 1, \dots, n-1$:

$$\begin{aligned} S'_n(\lambda_k) &= 2T'_n\left(\frac{\lambda_k}{2} - 1\right) = 2nU_{n-1}\left(\frac{\lambda_k}{2} - 1\right) = 2nU_{n-1}\left(-\cos\left(2\frac{k\pi}{n}\right)\right) \\ &= 2n(-1)^{n-1}U_{n-1}\left(\cos\left(2\frac{k\pi}{n}\right)\right) = 2n(-1)^{n-1}\frac{\sin(2k\pi)}{\sin 2\frac{k\pi}{n}} = 0, \end{aligned} \quad (12)$$

for all considered k except $k = 0$ and $k = n/2$. For $\lambda_0 = 0$ and $\lambda_{n/2} = 4$ (for n even) we obtain $S'_n(0) = 2nU_{n-1}(-1) = 2n^2(-1)^{n-1}$ and $S'_n(4) = 2nU_{n-1}(1) = 2n^2$. This corresponds to Lemma 2, since the multiplicity of the root $\lambda_0 = 0$ and $\lambda_{n/2} = 4$ (for n even) is always equal to one. Here we have also employed the properties of the Chebyshev polynomials of the second kind: $T'_n(x) = nU_{n-1}(x)$ and $U_n(\cos \alpha) = \frac{\sin(n+1)\alpha}{\sin \alpha}$ (cf. [7]). \square

n	$T_n(x)$	$S_n(x)$
3	$4x^3 - 3x$	$x^3 - 6x^2 + 9x$
4	$8x^4 - 8x^2 + 1$	$x^4 - 8x^3 + 20x^2 - 16x$
5	$16x^5 - 20x^3 + 5x$	$x^5 - 10x^4 + 35x^3 - 50x^2 + 25x$
6	$32x^6 - 48x^4 + 18x^2 - 1$	$x^6 - 12x^5 + 54x^4 - 112x^3 + 105x^2 - 36x$
7	$64x^7 - 112x^5 + 56x^3 - 7x$	$x^7 - 14x^6 + 77x^5 - 210x^4 + 294x^3 - 196x^2 + 49x$
\vdots	\vdots	\vdots

Table 1: Comparison of polynomials $T_n(x)$ and $S_n(x)$.

Since the equation (3) has in general infinitely many solutions (e.g. 2-factors) we denote by $\mathcal{H} \subset \mathbb{R}^{m \times 1}$ the set of all its solutions. Each vector $\vec{z} \in \mathcal{H}$ can then be expressed in a form

$$\vec{z} = \vec{z}_0 + \sum_{j=1}^{m-n} \beta_j \cdot \vec{z}_j, \quad (13)$$

where \vec{z}_0 is any solution of equation (3) and $\text{span}(\{\vec{z}_j\}_{j=1}^{m-n})$ is the nullspace of B .

Remark 5. We consider $\vec{z}_0 = x_{LS}$ being the least-square solution of the equation (3) and $\{\vec{z}_j\}_{j=1}^{m-n}$ form the orthonormal basis.

Let $\vec{z} \in \mathcal{H}$ be any vector, then in virtue of (4) we define the matrices:

$$L(\vec{z}) = 4 \cdot I - B \cdot \text{diag}(\vec{z}) \cdot B^T. \quad (14)$$

The set of matrices $\mathcal{L} = \{L(\vec{z}), \vec{z} \in \mathcal{H}\}$ then has the same dimension as \mathcal{H} and any matrix $L \in \mathcal{L}$ can be expressed in a form $L = L_0 + \sum_{i=1}^{m-n} \beta_i \cdot L_i$ with $L_i = -B \cdot \text{diag}(\vec{z}_i) \cdot B^T$ and $L_0 = 4 \cdot I - B \cdot \text{diag}(\vec{z}_0) \cdot B^T$.

For each $L \in \mathcal{L}$ we shall compute its characteristic polynomial

$$p_L(x) = \det(x \cdot I - L) \quad (15)$$

and obtain the set of (admissible) polynomials $\mathcal{P} = \{p_L(x), L \in \mathcal{L}\}$. Consequently, if the graph G contains the Hamiltonian cycle, then $S_n(x) \in \mathcal{P}$. Hence, we shall try to find a functional $F: \mathcal{P} \rightarrow \mathbb{R}$ so that there holds:

$$S_n = \arg \min_{p \in \mathcal{P}} F(p). \quad (16)$$

Thus, the whole problem is reduced to finding the minimum of the functional F . Moreover, since

$$\min_{p \in \mathcal{P}} F(p) = \min_{L \in \mathcal{L}} F(p_L(x)) = \min_{L \in \mathcal{L}} F(\det(x \cdot I - L)), \quad (17)$$

it suffices to find a proper matrix $L = L_0 + \sum_{i=1}^{m-n} \beta_i \cdot L_i$, i.e. a proper coefficients β_i , $i = 1, 2, \dots, m - n$.

4. Definition of functionals and their derivatives

4.1. Coordinate functional

One possible choice of the functional consists in expressing any polynomial $p \in \mathcal{P}$ in the basis formed by polynomials S_i , $1 \leq i \leq n$, i.e. $p = \sum_{i=1}^n \alpha_i \cdot S_i$. Since the minimum of the desired functional should be reached at $p = S_n$, i.e. $\alpha_i = 0$ for $i = 1, 2, \dots, n - 1$, we choose

$$F_c(p) = \sum_{i=1}^{n-1} \alpha_i^2 = \sum_{i=1}^{n-1} \alpha_i^2(p). \quad (18)$$

In what follows, we would like to find out, how the coefficients α_i depend on the polynomial p . We apply the discrete orthogonality of the Chebyshev polynomials (cf. [7]):

$$\sum_{k=0}^{n-1} T_i(x_k) T_j(x_k) = \begin{cases} 0 & \text{if } i \neq j, \\ n & \text{if } i = j = 0, \\ n/2 & \text{if } i = j \neq 0, \end{cases} \quad (19)$$

where $0 \leq i, j < n$ and x_k are Chebyshev's nodes of $T_n(x)$. Then there holds

$$\begin{aligned}
\sum_{k=0}^{n-1} p(y_k) T_j(x_k) &= \sum_{k=0}^{n-1} \left(\sum_{i=1}^n \alpha_i S_i(y_k) \right) T_j(x_k) \\
&= 2 \sum_{k=0}^{n-1} \sum_{i=1}^n \alpha_i \left(T_i \left(\frac{y_k}{2} - 1 \right) - (-1)^i \right) T_j(x_k) \\
&= 2 \sum_{i=1}^n \alpha_i \sum_{k=0}^{n-1} T_i(x_k) T_j(x_k) - 2 \sum_{i=1}^n \alpha_i (-1)^i \sum_{k=0}^{n-1} T_j(x_k) \\
&= 2 \sum_{i=1}^n \alpha_i \left(\frac{n}{2} \delta_{ij} \right) - 2 \sum_{i=1}^n \alpha_i (-1)^i \cdot 0 = n \cdot \alpha_j, \tag{20}
\end{aligned}$$

where $y_k = 2(x_k + 1)$. Hence $\alpha_j = \frac{1}{n} \sum_{k=0}^{n-1} p(y_k) T_j(x_k)$.

Since all polynomials p depend on the choice of the vector $(\beta_1, \beta_2, \dots, \beta_{m-n})$, we need to compute the derivative of F with respect to β_i :

$$\frac{\partial F_c}{\partial \beta_i} = \frac{\partial}{\partial \beta_i} \sum_{j=1}^{n-1} \alpha_j^2 = 2 \sum_{j=1}^{n-1} \alpha_j \cdot \frac{\partial \alpha_j}{\partial \beta_i}, \tag{21}$$

$$\frac{\partial \alpha_j}{\partial \beta_i} = \frac{1}{n} \sum_{k=0}^{n-1} T_j(x_k) \frac{\partial}{\partial \beta_i} p(y_k), \tag{22}$$

$$\frac{\partial p(y_k)}{\partial \beta_i} = \frac{\partial}{\partial \beta_i} \det \left(y_k I - L_0 - \sum_{j=1}^{m-n} \beta_j \cdot L_j \right). \tag{23}$$

If we now denote $R_k = y_k I - L_0 - \sum_{j=1}^{m-n} \beta_j \cdot L_j$, we may apply Jacobi's formula $(\det A(x))' = \text{tr}(\text{adj } A(x) \cdot A'(x))$ and obtain:

$$\frac{\partial p(y_k)}{\partial \beta_i} = \text{tr}(\text{adj } R_k \cdot (-L_i)) = -\det R_k \cdot \text{tr}(R_k^{-1} \cdot L_i), \tag{24}$$

for nonsingular matrix R_k .

4.2. Integral functional

Since the polynomials S_n are defined using Chebyshev's polynomials, they solve the following (Chebyshev's) differential equation (cf. [7]):

$$x(4-x)y'' + (2-x)y' + n^2y = -2n^2(-1)^n, \tag{25}$$

$$y(0) = 0, \quad y(4) = 2(1 - (-1)^n). \tag{26}$$

If we transfer the boundary condition and transform the equation into the divergent form we obtain the following quadratic functional:

$$F_{in}(p) = \int_0^4 \sqrt{x(4-x)} (p')^2 - \frac{n^2}{\sqrt{x(4-x)}} p^2 + 2 f_n(x) p \, dx, \quad (27)$$

where $f_n(x) = \frac{(2-x)(n^2-1)}{\sqrt{x(4-x)}}$ for n odd and $f_n(x) = \frac{-2n^2}{\sqrt{x(4-x)}}$ for n even.

Remark 6. To evaluate integrals containing $\sqrt{1-x^2}$ on the interval $(-1, 1)$ one can apply the Chebyshev-Gauss quadrature rules:

$$\int_{-1}^1 \frac{f(x)}{\sqrt{1-x^2}} dx \approx \sum_{k=1}^n w_k f(x_k), \quad \int_{-1}^1 g(x) \sqrt{1-x^2} dx \approx \sum_{k=1}^n \hat{w}_k g(\hat{x}_k),$$

where x_k are roots of $T_n(x)$ and $w_k = \frac{\pi}{n}$, while \hat{x}_k are roots of $T'_{n+1}(x)$ and $\hat{w}_k = \frac{\pi}{n+1} \sin^2\left(\frac{\pi k}{n+1}\right)$. These formulas are exact for polynomials up to order $2n-1$ and when we transform them on the interval $[0, 4]$, we obtain the following expressions:

$$\int_0^4 \frac{p^2(y)}{\sqrt{y(4-y)}} dy = 2\pi \left[\sum_{i=1}^n \alpha_i^2 + 2 \left(\sum_{i=1}^n \alpha_i (-1)^i \right)^2 \right], \quad (28)$$

$$\int_0^4 \sqrt{y(4-y)} (p'(y))^2 dy = 2\pi \sum_{i=1}^n i^2 \alpha_i^2, \quad (29)$$

$$\int_0^4 f_n(y) p(y) dy = 4\pi n^2 \sum_{i=1}^n (-1)^i \alpha_i, \text{ for } n \text{ even}, \quad (30)$$

$$\int_0^4 f_n(y) p(y) dy = -2\pi(n^2-1)\alpha_1, \text{ for } n \text{ odd}, \quad (31)$$

providing $p(y) = \sum_{i=1}^n \alpha_i S_i(y)$. Consequently, for the functional F_{in} there holds:

$$F_{in}(p) \stackrel{n \text{ even}}{=} -2\pi \left[\sum_{i=1}^n (n^2 - i^2) \alpha_i^2 - 2n^2 \left(1 - \sum_{i=1}^n \alpha_i (-1)^i \right) \sum_{i=1}^n \alpha_i (-1)^i \right], \quad (32)$$

$$F_{in}(p) \stackrel{n \text{ odd}}{=} -2\pi \left[\sum_{i=1}^n (n^2 - i^2) \alpha_i^2 + 2n^2 \left(\sum_{i=1}^n \alpha_i (-1)^i \right)^2 + (n^2 - 1) \alpha_1 \right]. \quad (33)$$

Unfortunately, these functionals failed to be positive and, hence, they do not attain their minimum in $p = S_n$. Therefore, together with the functional F_c (cf. (18)) we consider only functional (28) (functional $F_{in,1}$) and (29) (functional $F_{in,2}$) with the sums ending at $i = n-1$.

5. Numerical experiments

For the minimization we employ the gradient descent method with the backtracking line search driven by the Armijo condition (cf. Figure 2). We consider random graphs with 16 vertices and 18–32 edges containing Hamiltonian cycle. For each kind of graph and for each functional we generate 100 random graphs. The results in Table 2 show numbers of graphs for which the algorithm successfully ended and found the Hamiltonian cycle. If the algorithm failed, it was due to finding a local extremum or exceeding the maximum number of iterations.

functional	16/18	16/20	16/22	16/24	16/26	16/28	16/30	16/32
F_c	93	80	82	70	58	55	54	50
$F_{in,1}$	77	61	63	54	48	35	37	31
$F_{in,2}$	96	88	80	66	63	71	63	62

Table 2: Numerical results for all considered functionals.

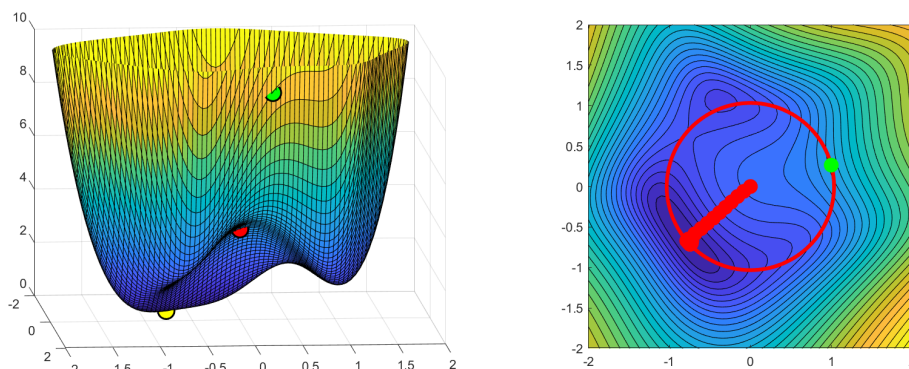


Figure 2: An example of minimization algorithm for the functional F_c and a graph with 7 vertices and 9 edges. The minimum lies on the circle with the center in x_{LS} . The other point on the circle corresponds to the 2-factor of the graph considered.

6. Conclusion

Numerical experiments show that all three functionals contain unwanted local extrema which cause problems during minimization process. It also results from the Table 2 that the more edges a graph has, the more complicated it is to reach the global minimum. Of these three algorithms, algorithm $F_{in,1}$ provided the worst results, probably due to the presence of the oscillation term $(\sum_{i=1}^{n-1} \alpha_i (-1)^i)^2$.

The construction of another (hopefully convex) functional, as well as improvements to the minimization process and different choice of the null space basis of the incidence matrix B will be the subject of the future research.

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