Minimizing Sign Changes Rowwise: Consecutive Ones Property and Beyond

Dominique Fortin and Ider Tseveendorj

Abstract A 0–1 matrix where in each row the 1s occur consecutively is said to have the consecutive 1s property. Since this property is scarcely fulfilled in real problems and since it is non-deterministic polynomial time (NP)-hard to find the *nearest* arrangement to the property, we give a quadratic assignment formulation for optimizing the *distance* to the property. The formulation carries over the sign case with $0, +1, -1$ matrix entries. We discuss and compare this exact approach, for both signed and unsigned cases, with spectral approaches based on bisection instead.

Keywords 0–1 matrices · Consecutive 1s property · Consecutive sign property · Trigraph · QAP · Hoffman–Wielandt · Gilmore–Lawler

1 Introduction

A 0–1 matrix where in, say each row, the 1s occur consecutively is said to have the consecutive 1s property (C1P). This property and its approximations have numerous applications in clustering, seriation, and at a low-level data storage for compacting sparse matrices. Testing this property holds in polynomial time; however, it scarcely happens for real-life cases, thus methods that approximate, in some sense, the property have been proposed: upto an approximation factor [6], with respect to spectral ordering [1, 18, 10], number and distance of consecutive intervals of 1s [16], within an ordered set of matrices [17], etc. Most approaches lead quickly to non-deterministic polynomial time (NP)-hard optimization problems. In this chapter, we give a raw formulation leading to a quadratic assignment problem (QAP) an NP-hard problem too; unlike previous spectral approximations that relate the C1P

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optimization problem to bisection (through the Laplacian of underlied correlation and its second (Fiedler) eigenvector to force convexity), the QAP formulation is exact and does not enforce convexity.

The QAP approach allows a straigthforward generalization to consecutive $-1, 0, +1$ entries (C±P for consecutive sign property), no matter the ordering among consecutive values. It brings up new connections with the sign change counting function [12], as a signed generalization of the counting function [14, 20], both playing a prominent role for improving a local solution in global optimization.

Since there is no methodological difference with maximizing the number of transitions instead, it relates our study to studies, to name a few, in mathematical physics: the six vertex model under boundary wall condition and the alternating sign matrices [9, 22]; in graph theory: a *trigraph* [2, 7, 8] has a signed vertex–vertex adjacency matrix. Bearing in mind the consecutive sign property, we mainly follow the lead of minimization, despite it deserves studying the six vertex model or the trigraph case, under further constraints on the transitions within a row.

The chapter is organized as follows: Sect. 2 provides the basic formulation for minimizing the number of transitions between 1s and 0s along either dimension of matrices; in Sect. 3, we review bounding schemes for an enumerative approach in both actual and spectral domains; in Sect. 4, we suggest a way to deal with the signed case by recoursing to the average in spite of Schur convexity. The remaining sections provide a thorough discussion of NP-hardness (Sect. 5), of experiments for moderate-size matrices either signed or unsigned (Sect. 6) and of the comparison between the circular and the standard shift case (Sect. 7).

2 Consecutive Ones Approximation

2.1 Minimizing Transitions

For a sparse $n \times m$ matrix A, let us consider the problem of minimizing the number of transitions between valid and void entries in a per row basis; values do not matter so that we assume the matrix binary with a 1 for valid entry and 0 otherwise. Denote the identity matrix I and the circular shift by one column matrix S_c, using Toeplitz matrix:

$$I - S_c = \begin{bmatrix} 1 & 0 & \dots & -1 \\ -1 & 1 & 0 & \dots \\ & & \dots & \\ 0 & \dots & -1 & 1 \end{bmatrix},$$

then the total number of circular column transitions is $\|A(I - S_c)\|^2$ using standard dot product for matrices, namely, $(A, B) = (\text{Vect}\,(A), \text{Vect}\,(B))$. The squared norm accounts for both ± 1 differences between consecutive columns. Let $Y \in \Pi_m$ be an unknown column permutation matrix minimizing the total number of circular column transitions; define $\#C(A, Y) = \|AY(I - S_c)\|^2$, then we have to optimize $\min\#C(A, Y)$ over column permutations $Y \in \Pi_m$. It is straightforward to set it as a QAP since

$$\begin{aligned}\#C(A, Y) &= (AY(I - S_c), AY(I - S_c)) = (A^t AY, Y(I - S_c)(I - S_c)^t) \\ &= \mathrm{QAP}(Y; A^t A, T_m)\end{aligned}$$

one of the most difficult problem in combinatorial optimization whose traveling salesperson problem (TSP) is a special case. By analogy, we could minimize the number of circular row transitions over row permutations $X \in \Pi_n$,

$$\begin{aligned}\#R(A, X) &= ((I - S_c)^t XA, (I - S_c)^t XA) = ((I - S_c)(I - S_c)^t X, XAA^t) \\ &= \mathrm{QAP}(X; T_n, AA^t)\end{aligned}$$

where

$$T_n = \begin{bmatrix} 2 & -1 & \dots & -1 \\ -1 & 2 & -1 & \dots \\ & & \dots & \\ -1 & \dots & -1 & 2 \end{bmatrix},$$

a Toeplitz matrix with neat eigenvalues $2(1 - \cos\frac{2k\pi}{n})$ for $k = 0, n - 1$. Minimizing in both dimensions at the same time is twice involved since

$$\begin{aligned}\#R(A, X) + \#C(A, Y) = {} & ((I - S_c)^t XAY, (I - S_c)^t XAY) \\ & + (XAY(I - S_c), XAY(I - S_c)) \\ & \text{s.t. } X \in \Pi_n, \quad Y \in \Pi_m\end{aligned}$$

since $XX^t = I_n$ and $YY^t = I_m$, respectively.

Solving QAP is hard in general, only a few cases are known to be polynomially solvable see Sect. 5, therefore, we have to recourse to a Branch and Bound (B&B) scheme in order to prove optimality of relaxed problem:

$$\begin{aligned}&\min\mathrm{QAP}(X; T_n, AA^t) \\ &\text{s.t. } X \in \mathcal{E}_n\end{aligned}$$

where $\mathcal{E}_n$ stands for doubly-stochastic matrices, a nice domain described by linear constraints $Xe = e$ and $X^t e = e$ for the all 1s vector e. Notice the harness involved with the squaring in the n^2 unknown entries in X while the dimension is merely n. See Sect. 6 for small-sized experiments.

Table 1 Eigenvalues of Toeplitz matrices for different shifts

Type	Shift	Eigenvalues	
Circular	$s \geq 1$	$2(1 - \cos \frac{2sk\pi}{n})$	$k = 0 \cdots n-1$
Standard	1	$2(1 - \cos \frac{k\pi}{n})$	$k = 0 \cdots n-1$
Standard n even	2	$2(1 - \cos \frac{k\pi}{n}), 2(1 - \cos \frac{(k+1)\pi}{n+1})$	$k = 0, 2, \cdots n-2$
Standard n odd	2	$0, 2(1 - \cos \frac{(k-1)\pi}{n}), 2(1 - \cos \frac{k\pi}{n+1})$	$k = 2, 4 \cdots n-1$

If we count transitions without wrapping the matrix then circular shift is replaced by standard shift S and T_n has four corners modified:

$$I - S = \begin{bmatrix} 1 & 0 & \dots & 0 \\ -1 & 1 & 0 & \dots \\ & & \dots & \\ \dots & & & 1 \\ 0 & \dots & & -1 \end{bmatrix}$$

$$T_n = \begin{bmatrix} 1 & -1 & \dots & 0 \\ -1 & 2 & -1 & \dots \\ & & \dots & \\ \dots & -1 & 2 & -1 \\ 0 & \dots & -1 & 1 \end{bmatrix},$$

a Toeplitz matrix whose eigenvectors and eigenvalues are analytically known as a function of the dimension n [21]. Both circular and standard shifts extends to transitions between columns/rows at distances > 1 leading to symmetric semidefinite programming (SDP) Toeplitz matrices with off-diagonals at the same distance apart (whose eigenvectors and eigenvalues are analytically known as a function of the dimension n too [11]) (Table 1).

On the other hand, eigenvalues of AA^t and A^tA are derived from singular values of A since $\sigma = UAV$ for orthogonal matrices U, V yields diagonalization $\sigma^2 = UAVV^tA^tU^t = UAA^tU^t$ while $\sigma^2 = V^tA^tU^tUAV = V^tA^tAV$.

Let $\bar{A} = E_{nm} - A$, the complement of A for the $n \times m$ all 1s matrix E_{nm}; since the role played by 0s is the same as the 1s. It suggests to add the number of transitions in the complement $\#C(\bar{A}, Y) = \|\bar{A}Y(I - S_c)\|^2$. Using properties of permutation matrices $E_{nm}^t E_{nm} = nE_{mm} = E_m$, where a single index is a shortcut for square case, $E_mY = E_m$ and $Y^tE_m = E_m$ then,

$$\begin{aligned} \#C(A, Y) + \#C(\bar{A}, Y) &= 2(A^tAY, YT) - ((\Delta + \Delta^t)Y, YT) + n(E_m, T_m) \\ &= 2\mathrm{QAP}(Y; A^tA, T_m) - \mathrm{QAP}(Y; \Delta + \Delta^t, T_m) + n(E_m, T_m), \end{aligned}$$

a kind of Laplacian for the *column degrees* $(\Delta + \Delta^t)/2 = (E_{nm}^t\, A + A^t\, E_{nm})/2$.

2.2 Maximizing Correlation

Define the in correlation as the product A^tA, another approach aims at maximizing the cumulated correlations after permutation, i.e., $((AY)^t(AY)U_m) = ((AY)^t(AY)L_m)$ for the all 1s $m \times m$ upper (respectively lower) triangular matrix U_m (respectively L_m). Using symmetry and properties of permutation matrices, we get

$$\begin{aligned}\mathrm{QAP}(Y; A^tA, U_m) + \mathrm{QAP}(Y; A^tA, L_m) &= (A^tAY, YE_m) + (A^tAY, YI_m)\\ &= (A^tAE_m, Y) + (A^tA, I_m)\\ &= \mathrm{LAP}(Y; A^tAE_m) + \mathrm{diag}(\Delta),\end{aligned}$$

a linear assignment problem with m equivalent solutions. Therefore, the intuitive correlation maximizing does not lead to a valid formulation.

3 Branch and Bound

For either correlation matrix F (AA^t and A^tA), let us consider a partial assignment, w.l.o.g. $X = \begin{bmatrix} X^{11} & 0 \\ 0 & X^{22}\end{bmatrix}$, where X^{22} stands for the unassigned indices, then the problem rewrites:

$$\begin{aligned}\mathrm{QAP}(X; T_n, F) = \mathrm{QAP}(X^{22}; T_n^{22}, F^{22}) + (T^{11}X^{11}, X^{11}F^{11})\\ + 2(T_n^{21}X^{11}F^{12}, X^{22}),\end{aligned}$$

where we used symmetry of both block submatrices $F^{21} = F^{12^t}$ and $T_n^{21} = T_n^{12^t}$. The second term is a constant and the last term is a linear assignment problem $\mathrm{LAP}(X^{22}; T_n^{21}X^{11}F^{12})$ since X^{11} is fully specified. The subproblem in first term may be bounded in various ways.

3.1 Spectral Bound

In Sect. 2.1, we gave the spectral bound for $\mathrm{QAP}(X^{22}; T_n^{22}, F^{22})$ at the root of the enumeration tree; however, deeper in the tree when some columns are assigned, the Toeplitz shift matrix shrinks to unassigned indices. For standard shift, since a fixed index symmetrically cancels a -1, it splits in three different patterns according to the diagonal corners diag([1, . . ., 1]), diag([1, . . ., 2]), diag([2, . . ., 2]) with possibly isolated eigenvalues (of value 1 or 2). The kernel method in [11, 21]) directly applies on corresponding diagonal discrepancies, namely, for size n, eigenvalues are $2(1 - \cos(\theta))$ with necessary conditions:

$$\begin{aligned}
\operatorname{diag}([1,\ldots,1]) &: \sin(\theta)(\sin((n-1)\theta) - 2\sin(n\theta) + \sin((n+1)\theta)) = 0 \\
&\qquad \theta = \frac{k\pi}{n}, \quad k = 0..n-1, \\
\operatorname{diag}([2,\ldots,2]) &: \sin((n+1)\theta) = 0 \\
&\qquad \theta = \frac{k\pi}{n+1}, \quad k = 1..n, \\
\operatorname{diag}([1,\ldots,2]) &: \sin(\theta)(\sin((n+1)\theta - \sin(n\theta)) = 0 \\
&\qquad \theta = \frac{k\pi}{2n+1}, \quad k = 1,3,5\ldots 2n-1
\end{aligned}$$

For circular shift, however, the number of patterns increases unless the antidiagonals -1s corners are fixed, in which case it reduces to the standard shift patterns. Despite tractable, an analytical expression for circular eigenvalues is more involved.

The overall time complexity is $O(n^3)$ since singular value decomposition (SVD) requires very few sweeps of n^3 complexity each, the same complexity as linear assignment by, say hungarian method. Define $\lambda(T_n^{22}, F^{22}) \leq \mathrm{QAP}(X^{22}; T_n^{22}, F^{22})$ as the corresponding spectral bound using Hoffman–Wielandt (Lidskii–Mirsky–Wielandt) inequalities:

$$(\lambda \nearrow (A), \lambda \searrow (B)) \leq (AU, UB) \leq (\lambda \nearrow (A), \lambda \nearrow (B))$$

for, respectively, ascending $\nearrow$, descending $\searrow$ orderings, then the whole bound simplifies to

$$\begin{aligned}
&\lambda(T_n^{22}, F^{22}) = (\lambda \nearrow (T_n^{22}), \lambda \searrow (F^{22})) + (T_n^{11} X^{11}, X^{11} F^{11}) \\
&\lambda(T_n^{22}, F^{22}) + 2\mathrm{minLAP}(X^{22}; T_n^{21} X^{11} F^{12}) \leq \mathrm{QAP}(X; T_n, F).
\end{aligned}$$

3.2 *Gilmore–Lawler Bound*

Every candidate assignment $x_{ij} = 1 \in X^{22}$ leads to a linear relaxation (see [19] and references therein) of $\mathrm{QAP}(X^{22}; T_n^{22}, F^{22})$

$$\begin{aligned}
\mathrm{LAP}^{ij} &\equiv (A^{ij} X^{22}) \\
A_{kl}^{ij} &= {T_n^{22}}_{ik} {F^{22}}_{jl}, \quad \text{for all } k \neq i, \text{for all } l \neq j.
\end{aligned}$$

By virtue of Hardy–Littlewood–Pólya (H.L.P. for short [13]), values of $l_{ij} = \mathrm{minLAP}^{ij}$ for all i, j are easily retrieved by sorting rows in both matrices (negative entries in T_n^{22} are not actually a deal for which we can add E then subtract the constant to get the result):

$$l_{ij} = (T_{i.}^{22} \searrow, F_{j.}^{22} \nearrow).$$

Let $\mathcal{L}$ be the result for all such LAPs, then the whole bounding becomes:

$$\begin{aligned}&\mathrm{LAP}(X^{22}; T_n, F, \mathcal{L}) = (\mathcal{L} + \mathrm{diag}(T_n^{22} \otimes F^{22}) + 2(T_n^{21} X^{11} F^{12}, X^{22}),\\&(T_n X^{11}, X^{11} F^{11}) + \mathrm{minLAP}(X^{22}; T_n, F, \mathcal{L}) \leq \mathrm{QAP}(X; T_n, F),\end{aligned}$$

where $\mathrm{diag}(T_n^{22} \otimes F^{22})$ is assumed matrixified conformably with $\mathcal{L}$ (precisely in $n \times n$ row major order).

The overall time complexity is $O(n^2 \log n)$ for building $\mathcal{L}$ and $O(n^3)$ for final LAP. Notice that sorting, all but diagonal entries, simplifies to extracting maximum and second maximum to give $l_{ij} = -\max F_{i.}^{22} - \max_2 F_{i.}^{22}$ or $l_{ij} = -\max F_{i.}^{22}$ depending on either row in T_n^{22}, so that complexity shrinks to $O(n^2)$ for building $\mathcal{L}$ indeed.

4 Consecutive Signs Approximation

The QAP formulation carries over the signed version provided transitions between opposite signs never occurs contiguously; otherwise, the transition accounts for 2 instead of 1 as required. To circumvent this defect, we may apply to the ground set $\{0, +1, -1\}$ the three permutations, identity, left shift $\{+1, -1, 0\}$, and right shift $\{-1, 0, +1\}$ to yield a multiobjective problem. As usual for multiobjective problems, taking the mean of all three QAPs (Schur convexity) helps in searching the optimal solution, despite the average is accurate only at optimum. The sum of all three QAPs amounts to a single QAP so that the formulation for C1P directly applies at the expense of an actual counting at each integral node in the B&B enumeration.

5 About Problem Hardness

Testing consecutive ones property is known to be polynomial and a PC-tree storing all permutations fulfilling the property results when true; however, if the property fails then we only have a tree having prime nodes to deal with QAP formulation.

On the other hand, if the C1P is fulfilled then correlation matrix (either AA^t or $A^t A$) may be reordered through overlapping sets such that it is monotone anti-Monge (see Robinson property [3]). Since, Toeplitz matrices T are clearly benevolent [4] for the underlied Toeplitz function $f(1) = -1 <= 0 = f(j)$ for all $j \neq 0, 1$, then under the C1P, the monotone anti-Monge-benevolent Toeplitz QAP polynomially solvable case applies. Otherwise, either correlation matrix fails to fulfill anti-Monge monotone property and despite Toeplitz is benevolent, minimizing the number of transitions is NP-hard by reduction from the Hamming TSP [18] as soon as there is more than one row. It completes the panel of negative result for QAP easy solvable cases to the case of non-anti-Monge monotone-Toeplitz benevolent pair [4]. Moreover, it yields another direct hardness proof by reduction from the NP-complete even–odd partition problem, after converting each 1 in the matrix by a sequence 10 and each 0 by a sequence 01 to guarantee evenness while the number of transitions is doubled after unshuffling the overall sequence. Most generalizations like $(k - \delta)$C1P, for instance, leads to NP-hard problems [5].

Unlike other spectral approaches, ours does not force any convexity and straightforwardly generalizes to 3D dissimilarity data [17]: in real applications, very oftenly the objects indexing a dissimilarity $\mathcal{D}$ are measured with respect to some human predefined criterion so that there is a set of dissimilarities $\mathcal{D} = \{D_1, \ldots, D_K\}$ associated with each *measurable* criterion in $[1, k]$. Correspondingly, the minimization of the weighted number of transitions rewrites as a weighted maximization of correlations:

$$\#R(\mathcal{A}, X) = \sum_{k=1}^{K} w_k \mathrm{QAP}(X; T_n, A_k A_k^t).$$

6 Experiments

For a maximum of 1000 B&B nodes, the history of enumeration for Gilmore–Lawler bounds and Hoffman–Wielandt (spectral) bounds, showed in minimizing case, that the spectral lower bound happens to be far below than Gilmore–Lawler lower bound, despite the Toeplitz structure gives eigenvalues for free. Many subproblems in the history have a negative Hoffman–Wielandt lower spectral bound due to the remaining assignment part while the number of transitions is obviously nonnegative!

As for eigenvalues of subproblems, the corresponding Toeplitz matrix decomposes into a principal diagonal matrix fulfilling the standard case from upper left corner $\begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$ to lower right corner $\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$ while the remaining matrix simplifies to a smaller circular Toeplitz case along one pair of 0s on symmetric entries at upper and lower diagonals. W.l.o.g. assume they occur at entries $(1, 2)$, $(2, 1)$, then applying the row and column permutations $[2, 3, \ldots, n, 1]$ yields a standard shift case with diagonal corners equal to 2, like in standard subproblems. Notice that, due to this observation, we need no facet defining inequalities for sum of hermitian matrices [15] and directly retrieve the eigenvalues of subproblems instead.

Due to these spectral observations, we do not report the history of enumeration for bounds and the examples below were rerun with the Gilmore–Lawler bound solely.

It is worth noticing that the standard count associated with the circular count is not monotonic; it may happen in the enumeration that standard count may be better than the next standard count associated to the next circular incumbent (upto 1 or 2 transitions); however, we always obtain the best standard incumbent from the best circular incumbent. Finally, for all experiments we never succeed in closing the gap within the node limit; however, the index of the best incumbent remains far from the node limit so that we are in the common situation where the optimum is very likely but the proof of optimality is hopeless due to the huge number of nodes remaining.

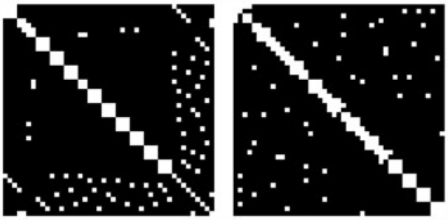

Fig. 1 MANN_a9 quadratic assignment problem (QAP; min, start, max) circular (respectively standard) rowwise transitions at (400,0,378)th Branch and Bound (B&B) nodes and value (184,234,378; respectively (176,225,293))

Fig. 2 Johnson8-2-4 quadratic assignment problem (QAP; min, start, max) circular (respectively standard) rowwise transitions at (13,0,8)th Branch and Bound (B&B) nodes and value (280,328,504; respectively (270,310,480))

6.1 C1P on Symmetric Matrices

We borrow from maximum clique Dimacs benchmark, two easy examples for the maximum clique problem that exhibit two opposite behaviors w.r.t. the enumerative procedure.

6.2 C±P on Random Matrix

The lack of dedicated benchmarks for the consecutive sign problem leads us to test the formulation against random matrices. As in Sect. 6.1, we draw the (best min incumbent, original, best max incumbent) in black, white, and gray pixels instead, according to the trivaluation. The enumeration is applied on both a single valuation (Fig. 3) and the averaging approximation (Fig. 4). Clearly, the averaging formulation yields better results for both the circular count and the standard count but unlike the C1P case there is no visual evidence that the best incumbent improves over the original data despite the relative improvements are comparable (see Table 2); however, the visual evidence looks stronger between the best min and max incumbents. Our random examples have a dense number (>60 %) of transitions among the complete

Fig. 3 Random 45×45quadratic assignment problem (QAP; min, start, max) circular (respectively standard) rowwise transitions at (565,0,0)th Branch and Bound (B&B) nodes and value (1174,1348,1343; respectively (1150,1313,1321))

Fig. 4 Random 45×45 average quadratic assignment problem (QAP; min, start, max) circular (resp. standard) rowwise transitions at (141,0,36)th Branch and Bound (B&B) nodes and value (1141,1348,1568) (resp. (1118,1313,1531))

Table 2 Relative improvement of rowwise transitions between original and best incumbent

	Minimize		Maximize	
Example	Circular (%)	Standard (%)	Circular (%)	Standard (%)
C1P (Fig. 1)	21	22	38	23
C1P (Fig. 2)	15	13	44	35
C±P (Fig. 3)	13	12	0	0
C±P (Fig. 4)	15	15	14	14

alternate case, so the best incumbent in standard max case is mostly found at the root of the B&B tree unlike the averaging formulation.

7 Circular Shift versus Standard Shift

Though most real-life applications require standard shift formulation, counting circular transitions makes sense for it is clearly an upper bound for C1P; since the optimization problem is more constrained, the B&B enumeration seems faster when there is a big gap between bounds and slower when the gap is narrow. It always lead in our experiments, to better standard incumbents than the standard formulation.

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