

## Erratum: Graph theory based approach to identify phase transitions in condensed matter [Phys. Rev. B **111**, 054116 (2025)]

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Due to an oversight, we forgot to write an explicit introduction to how the graphs are constructed from multiparticle systems in our paper. We used fully labeled graphs on a common vertex set, with adjacency matrices arranged so that the rows and columns correspond to the same ordering of the vertices. Within our settings, the graphs are fully connected, and the edge weights are set to the Euclidean distances between the corresponding particles. According to Sec. 8.1.2 of Ref. [1], the cut distance between two graphs in our settings is given by the cut norm of the difference of their adjacency matrices, which is exactly the approach we adopt.

Apart from the above, we would also like to clarify a point in our paper which is not an error but could potentially cause confusion. We present the Frobenius inner product  $\langle A^T, X \rangle_F$  as the trace taking form of  $\text{Tr}(AX)$  in our paper, and it is standard terminology of the optimization field. The aim of Eq. (3) in our paper is to perform a trial update along the original gradient  $A$  prior to the formation of  $W_0 = GX^T - XG^T$  expressly. Here  $A$  can also be replaced by  $W_0$  without performing anything to the subsequent iterations or the eventual output of  $|A|_{\infty \rightarrow 1}$ . Moreover, both  $(I + \frac{\tau}{2}W)^{-1}(I - \frac{\tau}{2}W)$  and  $(I - \frac{\tau}{2}W)^{-1}(I + \frac{\tau}{2}W)$  are correct expressions for the Cayley transform in Eqs. (3) and (6), and the only difference between them is the sign of  $\tau$ . As long as  $W^T = -W$  holds, each update will stay on the Stiefel manifold, thereby ensuring both the correctness and convergence of the iteration. Furthermore, in the code implementation [2,3], we used the trick of extending  $A \in \mathbb{R}^{N \times N}$  and  $X \in \mathbb{R}^{N \times p}$  to square matrices  $\mathfrak{A}$  and  $\mathfrak{X}$  in  $\mathbb{R}^{(N+1) \times (N+1)}$ , respectively, and expressing the objective function as taking the strict trace of a square matrix.

In detail,  $\mathfrak{A} = \begin{pmatrix} A & -A\mathbf{1} \\ -\mathbf{1}^T A & \mathbf{1}^T A\mathbf{1} \end{pmatrix}$ , where  $\mathbf{1}$  denotes a column vector of all ones. The matrix  $\mathfrak{A}$  has the same cut norm as  $A$ , and the sum of the entries in each row and each column is zero [4]. For  $X$ , a new variable  $\mathcal{X} \in \mathbb{R}^{p \times n}$  with  $n = 2(N+1)$  is introduced, subject to the constraint  $\mathcal{X}^T \mathcal{X} = I_n$ . The matrix  $\mathcal{X}$  can be horizontally partitioned into two blocks as  $\mathcal{X} = [U, V]$ , where  $U, V \in \mathbb{R}^{p \times (N+1)}$ , and we define  $\mathfrak{X} = U^T V$ . After extension, the objective function becomes  $\text{Tr}(\mathfrak{A}^T \mathfrak{X})$ , and the feasible domain (Stiefel manifold) changes from  $M_{N,p} = \{X \in \mathbb{R}^{N \times p} : X^T X = I_p\}$  (mistakenly written as  $M_{n,p}$  in our original paper due to a typo) to  $M_{p,n} = \{\mathcal{X} \in \mathbb{R}^{p \times n} : \mathcal{X}^T \mathcal{X} = I_n, n = 2(N+1)\}$ . Obviously,  $\mathcal{X}$  is the iterative variable on the Stiefel manifold, while  $\mathfrak{X}$  is used for the objective function.

In the Grothendieck inequality  $|A|_{\square} \leq |A|_{\infty \rightarrow 1} \leq K_G |A|_{\square}$ , the Grothendieck constant  $K_G$  can be amplified to a safe upper bound of 4, resulting in a new inequation  $|\mathfrak{A}|_{\square} \leq |\mathfrak{A}|_{\infty \rightarrow 1} \leq 4|\mathfrak{A}|_{\square}$ . Alon and Naor proved that the bound on the right-hand side can be attained when the row and column sums of  $\mathfrak{A}$  are zero, and that the constant 4 is tight [4]. Therefore one can consider  $|A|_{\square} \sim |A|_{\infty \rightarrow 1}/K_G \sim |\mathfrak{A}|_{\infty \rightarrow 1}/4$  and take  $|\mathfrak{A}|_{\square} = |\mathfrak{A}|_{\infty \rightarrow 1}/4$ . Since the extended matrix satisfies  $\mathfrak{A} = \mathfrak{A}^T$ , the gradient associated with Eq. (2) in our paper can also be written as  $G = \mathfrak{A} + \mathfrak{A}^T - \mathcal{X}(\mathcal{X}^T \mathfrak{A} + \mathfrak{A}^T \mathcal{X}) = 2[\mathfrak{A} - \mathcal{X}(\mathcal{X}^T \mathfrak{A} + \mathfrak{A}^T \mathcal{X})/2]$  after substituting  $A$  with  $\mathfrak{A}$  and  $X$  with  $\mathcal{X}$ . We emphasize that it is equally correct to write the gradient  $G$  either with or without the factor of 2. The difference simply reflects whether the factor of 2 is absorbed into the gradient itself or into the Cayley transform, and this does not affect the correctness or convergence of the optimization process.

We stress that it is purely for programming and computational convenience and is not central to the theoretical foundation [4,5]. It is also reflected in the original code, which was archived on Zenodo [2] at the time of publication and used for all computational results reported in our paper. We have also synchronized the code on GitHub [3], along with detailed documentation.

These clarifications do not affect the scientific merit or the conclusions of our paper in any way. We apologize for the confusion this may have caused.

- [1] L. Lovász, *Large Networks and Graph Limits* (American Mathematical Soc., Providence, Rhode Island, 2012), Vol. 60.
- [2] <https://doi.org/10.5281/zenodo.14843065>
- [3] [https://github.com/anwanguow/graph\\_phase\\_transition](https://github.com/anwanguow/graph_phase_transition)
- [4] N. Alon and A. Naor, Approximating the cut-norm via grothendieck's inequality, in *Proceedings of the Thirty-sixth Annual ACM Symposium on Theory of Computing* (ACM Press, New York, NY, 2004), pp. 72–80.
- [5] Z. Wen and W. Yin, A feasible method for optimization with orthogonality constraints, *Math. Program.* **142**, 397 (2013).