SOLVING AN INVERSE EIGENVALUE PROBLEM WITH TRIPLE CONSTRAINTS ON EIGENVALUES, SINGULAR VALUES, AND DIAGONAL ELEMENTS

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Abstract. An inverse eigenvalue problem usually entails two constraints, one conditioned upon the spectrum and the other on the structure. This paper investigates the problem where triple constraints of eigenvalues, singular values, and diagonal entries are imposed simultaneously. An approach combining an eclectic mix of skills from differential geometry, optimization theory, and analytic gradient flow is employed to prove the solvability of such a problem. The result generalizes the classical Mirsky, Sing-Thompson, and Weyl-Horn theorems concerning the respective majorization relationships between any two of the arrays of main diagonal entries, eigenvalues, and singular values. The existence theory fills a gap in the classical matrix theory. The technique might be useful for exploring other types of existence problems.

Key words. inverse eigenvalue problem, majorization relationships, projected gradient flow, Łojasiewicz gradient inequality, projected Hessian

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1. Introduction.

Inverse eigenvalue problems arise in a remarkable variety of applications. The subject has been studied and applied systematically in system and control theory, geophysics, molecular spectroscopy, particle physics, structure analysis, and many other disciplines. The research efforts in this area are too extensive to enumerate. See, for example, our book [12] for a list of over 400 references and a chapter outlining specific applications to pole assignment problem, applied mechanics, neuron transport, preconditioning, quadrature rules, data mining, molecular structure modeling, and others. The extensive survey [15] and the newly expanded seminal book [18] contain works and more references in the engineering literature. Generally speaking, the basic goal of an inverse eigenvalue problem is to reconstruct the physical parameters of a certain system from the knowledge or desire of its dynamical behavior. Since the dynamical behavior often is governed by the underlying natural frequencies and/or normal modes, the spectral constraints are thus imposed. On the other hand, in order that the resulting model is physically realizable, additional structural constraints must also be imposed upon the construction. See, for example, [13, 21, 26, 30]. The structural constraints also help narrow down the choices of possible solutions and improve the otherwise ill-posedness of an inverse problem. Depending on the application, the structural constraints appear in different forms and, thus, lead to different challenges in inverse eigenvalue problems. One common assumption in the application of inverse problems is that the underlying physical system is somehow representable in terms of matrices [25]. Most of the studies therefore center around eigenvalues problems, and particularly the inverse eigenvalue problems, for matrices.

In recent years, singular values and their inherent properties are also found to play critical roles in the data that a matrix represents. Image compression, dimension reduction, noise removal, and principal component analysis are just a few examples of the wide range of applications of singular value decomposition [38]. A natural outgrowth of the inverse eigenvalue problems is the generalization to inverse singular value problems [5, 29, 40, 42, 43] which we still categorize very early on as a special kind of spectral constraint [7].

Considered in this paper is a new type of inverse eigenvalue problems, demanding all three constraints – eigenvalues, singular values, and diagonals – be satisfied at the same time. To our knowledge, such an inverse problem with two spectral constraints and one structural constraint impose immediate challenges to conventional methods. We propose an approach employing an eclectic mix of skills from analytic gradient dynamics and optimization theory to successfully tackle this otherwise very difficult problem. We establish the theory of solvability as well as provide a method for computation. The technique, innovative in itself, might be useful for applications to other types of existence problems. For example, we can explore the problem with additional prescribed entries at locations other than just the diagonals.

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1.1. Prerequisites. It must be noted first that not all prescribed constraints are feasible. Inherent to all matrices is a universal property that diagonal elements, eigenvalues, and singular values are related in peculiar orders known as the majorization. Specifically, let $\mathbf{d} \in \mathbb{R}^n$ be a real vector with entries arranged in the order $|d_1| \geq \ldots \geq |d_n|$, $\boldsymbol{\sigma} \in \mathbb{R}^n$ be a nonnegative vector with entries in the order $\sigma_1 \geq \ldots \geq \sigma_n \geq 0$, and $\boldsymbol{\lambda} \in \mathbb{C}^n$ be a complex vector whose entries are closed under complex conjugation and are ordered as $|\lambda_1| \geq \ldots \geq |\lambda_n|$. Then $\mathbf{d}$, $\boldsymbol{\lambda}$, and $\boldsymbol{\sigma}$ must comply with the following classical results in matrix theory. Each result characterizes relationships involving a specific sequence of inequalities [31].

THEOREM 1.1. *(Weyl-Horn Theorem [20, 41]) There exists a real matrix $A \in \mathbb{R}^{n\times n}$ with singular values $\boldsymbol{\sigma}$ and eigenvalues $\boldsymbol{\lambda}$ if and only if*

$$\prod_{i=1}^{k} |\lambda_i| \leq \prod_{i=1}^{k} \sigma_i, \quad k = 1, 2, \ldots, n-1, \tag{1.1}$$

and

$$\prod_{i=1}^{n} |\lambda_i| = \prod_{i=1}^{n} \sigma_i. \tag{1.2}$$

THEOREM 1.2. *(Sing-Thompson Theorem [37, 39]) There exists a real matrix $A \in \mathbb{R}^{n\times n}$ with singular values $\boldsymbol{\sigma}$ and main diagonal entries $\mathbf{d}$, possibly in different order, if and only if*

$$\sum_{i=1}^{k} |d_i| \leq \sum_{i=1}^{k} \sigma_i, \quad k = 1, 2, \ldots, n, \tag{1.3}$$

and

$$\sum_{i=1}^{n-1} |d_i| - |d_n| \leq \sum_{i=1}^{n-1} \sigma_i - \sigma_n. \tag{1.4}$$

With regard to the relationship between diagonal entries and eigenvalues, we have two separate results. The first result in its most common form holds for general matrices.

THEOREM 1.3. *(Mirsky Theorem [32]) There exists a real matrix $A \in \mathbb{R}^{n\times n}$ with eigenvalues $\boldsymbol{\lambda}$ and main diagonal entries $\mathbf{d}$, possibly in different order, if and only if*

$$\sum_{i=1}^{n} \lambda_i = \sum_{i=1}^{n} d_i. \tag{1.5}$$

For Hermitian matrices, a more restrictive condition than (1.5) holds, which sometimes is referred to as a majorization from above.

THEOREM 1.4. *(Schur-Horn Theorem [3]) Suppose that entries of $\boldsymbol{\lambda} \in \mathbb{R}^n$ are arranged in the order $\lambda_1 \geq \ldots \geq \lambda_n$ and entries of $\mathbf{d} \in \mathbb{R}^n$ in the order $d_1 \geq \ldots \geq d_n$. There exists a Hermitian matrix H with eigenvalues $\boldsymbol{\lambda}$ and diagonal entries $\mathbf{d}$, possibly in different order, if and only if*

$$\sum_{i=1}^{k} \lambda_{n-i+1} \leq \sum_{i=1}^{k} d_{n-i+1}, \quad k = 1, 2, \ldots, n-1, \tag{1.6}$$

and

$$\sum_{i=1}^{n} \lambda_{n-i+1} = \sum_{i=1}^{n} d_{n-i+1}. \tag{1.7}$$

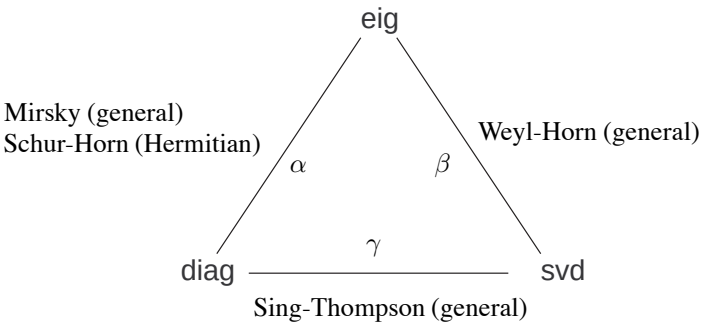

FIGURE 1.1. *Existing results concerning majorization.*

It is intriguing that merely the structure of matrices alone induces some intrinsic majorization properties. What makes the above results significant is that the conditions specified in each of the four theorems are both necessary and sufficient. For quick reference, we represent the mutual relationships by the three sides, denoted as α, β, and γ, respectively, of the triangle depicted in Figure 1.1. Given a set of data satisfying any *one side* of the triangle, a matrix satisfying the prescribed characteristics exists. Its numerical construction is an interesting but challenging task which has been extensively studied in the literature [4, 8, 9, 10, 14, 26, 44]. One fundamental feature associated with these inverse problems is that the solution is not unique. The algorithms developed thus far may serve as constructive proofs of the above theorems, but can hardly pinpoint a specific matrix. For instance, starting with a given matrix $A \in \mathbb{R}^{n\times n}$, we can calculate its eigenvalues $\boldsymbol{\lambda}$ and singular values $\boldsymbol{\sigma}$ which necessarily satisfy the inequalities (1.1) and (1.2). Applying the divide-and-conquer algorithm proposed in [10] to the set of data $\boldsymbol{\lambda}$ and $\boldsymbol{\sigma}$, we can construct a matrix B which has the very same eigenvalues $\boldsymbol{\lambda}$ and singular values $\boldsymbol{\sigma}$. However, more often than not, B is entirely different from the original A. Such discretion can easily be explained — There are more degrees of freedom in the matrix to be constructed than the prescribed data can characterize. Generally, the inverse problem has multiple solutions.

1.2. Significance of majorization. The notion of majorization has other equivalent forms and appears frequently across different fields in nature. For instance, it is closely related to the concept of "disorder" and has been exploited as a useful tool for analyzing data with inherent randomness. From a stochastic point of view, a vector $\mathbf{r}$ is said to be majorized by another vector $\mathbf{s}$ if and only if there exist permutation matrices P_j and a probability distribution $\{p_j\}$ such that

$$\mathbf{r} = \sum_j p_j P_j \mathbf{s}. \tag{1.8}$$

In other words, we regard that $\mathbf{r}$ is more disordered than $\mathbf{s}$ if it can be obtained from $\mathbf{s}$ by randomly permuting the components of $\mathbf{s}$ followed by averaging over the permutations. In this context, the uniform distribution is more disordered than *any* other probability distribution over a discrete sample space because the former is an average of the latter over the symmetric group of permutations. Majorization can also be characterized in terms of doubly stochastic matrices and unitary matrices [33, Chapters 2 and 5]. Indeed, the summation $\sum_j p_j P_j$ in (1.8) lies within the Birkhoff polytope by the well known Birkhoff-von Neumann theorem. So $\mathbf{r}$ is a double stochastic transformation of $\mathbf{s}$ and, equivalently, $\mathbf{r}$ is in the permutation polytope generated by $\mathbf{s}$. As such, majorization has found important applications in diverse areas such as statistics [2, 31], information theory [23], wireless communication [24], quantum computing [34], and quantum mechanics [33, 36].

1.3. New challenge. Referring to Figure 1.1, it becomes curious to ask whether a matrix can satisfy any *two sides* of the triangle simultaneously. Clearly, satisfying any two of the three majorization conditions should determine all three vertices of the triangle and, hence, the third condition is automatically satisfied. Thus, this problem is equivalent to the reconstruction of a matrix subject to prescribed diagonal entries, eigenvalues, and

singular values concurrently. Since such a matrix will satisfy the three sets of inequalities in Theorems 1.2, 1.1, and 1.3 all together, we shall refer to this structure as the Mirsky-Weyl-Horn-Sing-Thompson (MWHST) condition.

Note that we choose not to consider the Schur-Horn condition which is for Hermitian matrices. In the event that symmetry is part of the desirable structure, singular values are the absolute values of eigenvalues and are automatically fixed. In this case, It suffices to consider the inverse problem of satisfying the Schur-Horn condition alone, which is already solved in [4, 8, 44]. The MWHST condition constitutes a new and harder problem because the matrix under construction has no symmetric structure.

If the MWHST condition is to be held, then any two of these three prescribed data sets $\mathbf{d}$, $\boldsymbol{\lambda}$ and $\boldsymbol{\sigma}$ must satisfy the necessary conditions required in the corresponding theorem outlined above. While a matrix satisfying two sets of prescribed data does exist and can be constructed numerically, it is not clear whether the third set of prescribed data can be met simultaneously. This question of whether a (nonsymmetric) matrix exists to meet all three prescribed data at the same time is a natural generalization with mathematical interest. As far as we know, no theory has been developed in this regard.

For the ease of conveying the idea, we limit our discussion to the real field, whereas the above four classical results remain valid over the complex field. With appropriate modifications, e.g., using unitary similarity transformations instead of orthogonal similarity transformations, our technique can be carried over to the general complex case. We shall leave the generalization to interested readers, but suggest the reference [11, Section 5] as a demonstration of such an extension.

This paper is organized as follows. The seemingly trivial problem for the case of $n = 2$ is very different from the general case. We first analyze in Section 2 that The MWHST condition itself is not enough to guarantee the existence of a 2×2 matrix. We specify what other conditions must be satisfied for the existence. For any case $n \geq 3$, we argue in Section 3 by means of optimization that generically there does exist a matrix satisfying the MWHST condition. The proof itself can be cast as a numerical algorithm, provided the inverse problem associated with the Weyl-Horn theorem is solved.

2. The case of 2×2 is special. In searching for a matrix satisfying the MWHST condition, we first consider the 2×2 case. As will be seen below, this seemingly simple problem is actually quite complicated. There are mutually exclusive situations to be considered and additional conditions must be imposed to guarantee the existence. It might be even more astounding that such a difficulty does not occur when dealing with higher dimensional cases, which will be shown in the next section.

To fix the idea, let

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

denote the 2×2 real matrix to be constructed. The Frobenius norm of A necessarily implies the equality

$$a^2 + b^2 + c^2 + d^2 = \sigma_1^2 + \sigma_2^2.$$

Assuming that the main diagonal entries are already fixed, our goal is to determine the off-diagonal entries b and c to meet the prescribed eigenvalues and singular values, which translates to the system

$$\begin{cases} bc &= ad - \lambda_1\lambda_2, \\ b^2 + c^2 &= \sigma_1^2 + \sigma_2^2 - a^2 - d^2. \end{cases} \tag{2.1}$$

The existence of a 2×2 matrix A satisfying the MWHST condition therefore boils down to finding the intersection of a hyperbola and a circle as is indicated in Figure 2.1. Obviously, the system (2.1) is solvable for the off-diagonal entries b and c only if the vertex of the hyperbola lies within the disk, that is, when

$$2|ad - \lambda_1\lambda_2| \leq \sigma_1^2 + \sigma_2^2 - a^2 - d^2. \tag{2.2}$$

In this case, there are generically four solutions per given $\mathbf{d}$, $\boldsymbol{\lambda}$, and $\boldsymbol{\sigma}$.

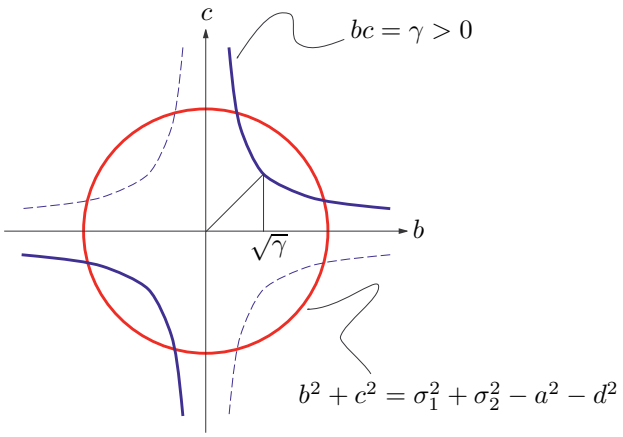

FIGURE 2.1. *Existence of $A \in \mathbb{R}^{2\times 2}$ satisfying the MWHST condition.*

On the other hand, the MWHST condition requires that the following three sets of inequalities be held simultaneously:

$$\lambda_1 + \lambda_2 = a + d; \qquad \text{(Mirsky)} \tag{2.3}$$

$$\begin{cases} |\lambda_1| \geq |\lambda_2|, \\ \sigma_1 \geq \sigma_2, \\ |\lambda_1| \leq \sigma_1, \\ |\lambda_1||\lambda_2| = \sigma_1\sigma_2; \end{cases} \qquad \text{(Weyl} - \text{Horn)} \tag{2.4}$$

$$\begin{cases} |a| \geq |d|, \\ |a| + |d| \leq \sigma_1 + \sigma_2, \\ |a| - |d| \leq \sigma_1 - \sigma_2. \end{cases} \qquad \text{(Sing} - \text{Thompson)} \tag{2.5}$$

We now examine how these inequalities play out to ensure (2.2), which guarantees a solution.

Given singular values $\boldsymbol{\sigma}$ and eigenvalues $\boldsymbol{\lambda}$, summarized in Figure 2.2 are various regions of $(a, d) \in \mathbb{R}^2$ over which the inequality (2.2) holds. Since a significant amount of information is contained in the drawing, we briefly explain its interpretation in the following theorem. The analysis is tedious but straightforward.

THEOREM 2.1. *Given three sets of data $\mathbf{d}$, $\boldsymbol{\lambda}$, and $\boldsymbol{\sigma}$ satisfying the MWHST condition, then a 2×2 matrix A exists with prescribed diagonal entries $\mathbf{d}$, eigenvalues $\boldsymbol{\lambda}$, and singular values $\boldsymbol{\sigma}$ if and only if the following (additional) conditions on $\mathbf{d}$ hold.*

1. *Given $\boldsymbol{\sigma}$, the shape of "kissing fish" in Figure 2.2 represents the feasible region of the diagonal (a, d) in order to satisfy the Sing-Thompson condition (2.5) alone. (See [9] for details.)*
2. *The Weyl-Horn condition (2.4) defines two mutually exclusive cases — either $\lambda_1\lambda_2 = \sigma_1\sigma_2$ or $\lambda_1\lambda_2 = -\sigma_1\sigma_2$.*
3. *When eigenvalues λ_1 and λ_2 are either complex conjugate or real valued with the same sign, then*
   (a) *The only feasible diagonal entries must be further restricted to the union of the red, cyan, and green regions in Figure 2.2.*
   (b) *When $ad \geq \sigma_1\sigma_2$, the (a, d) must come from the red region.*
4. *When eigenvalues λ_1 and λ_2 are of opposite sign,*
   (a) *The only feasible diagonal entries must be further restricted to the union of the blue, purple, and green regions in Figure 2.2.*
   (b) *When $ad \leq -\sigma_1\sigma_2$, the (a, d) must come from the blue region.*
5. *The green region is when both $|a + d| \leq \sigma_1 - \sigma_2$ and $|a - d| \leq \sigma_1 - \sigma_2$.*

The above elaboration on the 2×2 case is illuminating. It manifests that satisfying the MWHST condition alone by the prescribed diagonal entries, eigenvalues, and singular values is not sufficient to guarantee the exis-

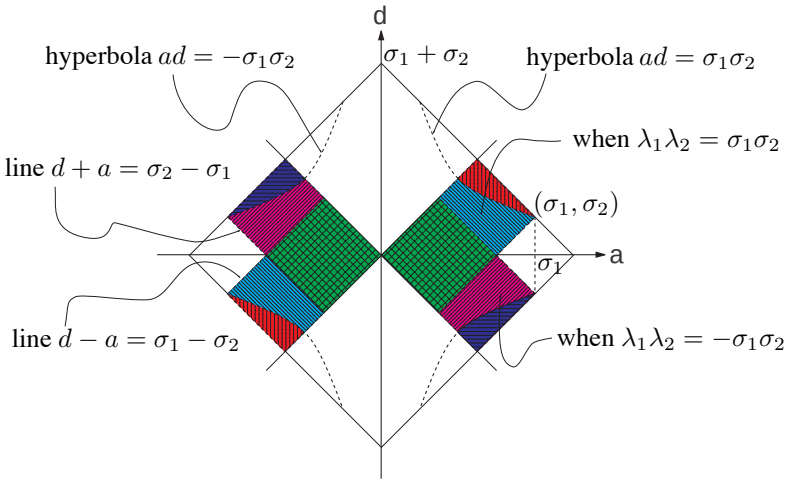

FIGURE 2.2. *Domain of feasible diagonal entries* (a, d)*, given* $\{\sigma_1, \sigma_2\}$ *and* $\{\lambda_1, \lambda_2\}$.

tence of a 2×2 matrix. Indeed, depending on other factors such as the sign of $\lambda_1\lambda_2 = \pm\sigma_1\sigma_2$, the location of the diagonal entries (a, d) also comes to play in the solvability of the inverse problem for the 2×2 case. Such a simple fact is of interest in its own right. For instance, the following corollary is a special case of Theorem 2.1.

COROLLARY 2.2. *Suppose that the MWHST condition holds for three given sets of data* $\mathbf{d}$*,* $\boldsymbol{\lambda}$*, and* $\boldsymbol{\sigma}$*. If, in addition,* $|a + d| \leq \sigma_1 - \sigma_2$ *and* $|a - d| \leq \sigma_1 - \sigma_2$*, then there exists a* 2×2 *real matrix with diagonal entries* $\mathbf{d}$*, eigenvalues* $\boldsymbol{\lambda}$*, and singular values* $\boldsymbol{\sigma}$*.*

The understanding of the 2×2 case seems to suggest that the pursuit for a matrix satisfying all inequalities simultaneously in the MWHST condition should have been ended. However, the 2×2 matrices discussed above is only an exception. In the next section, we argue that the inverse problem of constructing a real-valued matrix satisfying the MWHST condition is generically solvable when $n \geq 3$.

3. Existence in general case. A rough count of the dimensionality might give clue to the solvability, though in reality the MWHST condition consists of inequalities which make the dimensionality analysis not so straightforward. In the case $n = 2$, the task was to determine the two off-diagonal entries b and c so as to result in having two prescribed eigenvalues and two prescribed singular values. At first glance, this might seem to be an over-determined system. However, the Mirsky condition (2.3) and the last equality in the Weyl-Horn condition (2.4) imply that actually there are only one eigenvalue condition and one singular value condition to be satisfied. Thus, the reconstruction problem amounts to solving two equations in two unknowns, such as that of (2.1). In order to ensure that this nonlinear problem has a solution (indeed, four solutions generically, if it is ever solvable), we have concluded in the preceding section that some additional constraints are required. For the case $n \geq 3$, it is difficult to use a geometric argument directly. Instead, we prove the existence by an entirely different strategy.

3.1. Variational formulation. We begin with the assumption that an $n \times n$ real-valued matrix A satisfying the Weyl-Horn condition is already in hand. The existence of such a matrix with prescribed singular values $\boldsymbol{\sigma}$ and eigenvalues $\boldsymbol{\lambda}$ is guaranteed in theory and is obtainable numerically. Referring to the diagram in Figure 1.1, we assume that the β side (Weyl-Horn condition) of the triangular relationship is already satisfied by A. If we can establish the α side (Mirsky condition) in the diagram, then the γ side follows automatically. In other words, given the desired main diagonal elements $\mathbf{d}$ satisfying both the Mirsky condition and the Sing-Thompson condition, our goal now is to somehow transform the matrix A so that the resulting diagonal elements agree with elements of the prescribed $\mathbf{d}$. A critical question is what kinds of transformations are allowed.

Foremost, we want to preserve the spectrum of the given A so as not to upset the Weyl-Horn condition. So we have to employ similarity transformations. Likewise, to preserve the singular values we must perform orthogonal equivalence transformations. To keep both the eigenvalues and the singular values invariant, therefore, the only

option is to apply orthogonal similarity transformations to the matrix A.

Let $\mathcal{O}(n) \subset \mathbb{R}^{n\times n}$ denote the group of $n \times n$ real orthogonal matrices. Also, let $\mathsf{diag}(M)$ denote the diagonal matrix whose main diagonal is the same as that of the matrix M and $\mathsf{diag}(\mathbf{v})$ the diagonal matrix whose main diagonal entries are formed from the vector $\mathbf{v}$. Using the same notation diag for both M and $\mathbf{v}$ will prove convenient in the discussion. Any ambiguity can be clarified from the context. Our idea of driving the diagonal of $Q^\top AQ$ to that of the specified vector $\mathbf{d}$ is to formulate the minimization problem

$$\min_{Q\in\mathcal{O}(n)} F(Q) := \frac{1}{2}\|\mathsf{diag}(Q^\top AQ) - \mathsf{diag}(\mathbf{d})\|_F^2, \tag{3.1}$$

where $\|\cdot\|_F$ stands for the Frobenius matrix norm. Since the matrix A is real, $\mathsf{diag}(Q^\top AQ) = \mathsf{diag}(Q^\top A^\top Q)$. Therefore,

$$\mathsf{diag}(Q^\top AQ)) = \mathsf{diag}(Q^\top \frac{A+A^\top}{2}Q). \tag{3.2}$$

Define the matrix

$$S := \frac{A+A^\top}{2}. \tag{3.3}$$

It is more convenient to work on the (symmetrized) optimization problem[1]

$$\min_{Q\in\mathcal{O}(n)} F(Q) := \frac{1}{2}\|\mathsf{diag}(Q^\top SQ) - \mathsf{diag}(\mathbf{d})\|_F^2. \tag{3.4}$$

The optimizer of problem (3.1) is the same as that of problem (3.4), and vice versa.

Denote

$$\eta(Q) := \mathsf{diag}(Q^\top SQ) - \mathsf{diag}(\mathbf{d}). \tag{3.5}$$

If we can find an orthogonal matrix $Q \in \mathcal{O}(n)$ such that $\eta(Q) = 0$, then the very same Q will make the main diagonal entries, the eigenvalues, and the singular values of the matrix $Q^\top AQ$ satisfy the MWHST condition simultaneously. In the remainder of this paper, we focus on proving that such an optimizer $Q \in \mathcal{O}(n)$ ensuring $\eta(Q) = 0$ does exist.

3.2. Projected gradient flow. We shall deal with the optimization problem (3.4) by directly applying the conventional optimization techniques to the matrices. Theoretical basis for the manipulations of matrix calculus needed below can be found in our earlier work [11]. The techniques permit easy calculation of the projected gradient and the projected Hessian without resorting to Lagrange multiplier theory.

Let the Frobenius inner product between two matrices M, N of the same size be denoted by

$$\langle M, N\rangle := \sum_{i,j} m_{ij}n_{ij}.$$

The Fréchet derivative of F at Q acting on an arbitrary matrix $H \in \mathbb{R}^{n\times n}$ is given by

$$\begin{aligned} F'(Q).H &= \langle \eta(Q), \eta'(Q).H\rangle = 2\left\langle \eta(Q), \mathsf{diag}(Q^\top SH)\right\rangle \\ &= 2\left\langle \eta(Q), Q^\top SH\right\rangle = 2\left\langle SQ\eta(Q), H\right\rangle. \end{aligned} \tag{3.6}$$

[1]Obviously, if A happens to be a skew-symmetric matrix, then $S = 0$ and $F(Q)$ is a constant. In this case, we cannot do anything with (3.4). Instead, if A is skew-symmetric, then the discussion in this paper can be equally applied to (3.1) with appropriate changes of sign due to the fact that $A^\top = -A$. To save space, we shall not analyze this case in this article by assuming that generically the matrix A constructed to satisfy the Weyl-Horn condition is not skew-symmetric.

In (3.6), the second equality follows from the linearity of the operator diag; the third equality results from the fact $\eta(Q)$ is a diagonal matrix; and the fourth equality is due to the adjoint property. By the Riesz representation theorem, the gradient ∇F at Q can be represented as

$$\nabla F(Q) = 2SQ\eta(Q). \tag{3.7}$$

Because of the constraint that Q must be in $\mathcal{O}(n)$, we next calculate the projected gradient $g(Q)$ of $\nabla F(Q)$ onto the tangent space $\mathcal{T}_Q\mathcal{O}(n)$ of $\mathcal{O}(n)$.

It is easy to see that the tangent space of $\mathcal{O}(n)$ at Q can be identified as either the left translation or the right translation of the subspace of skew-symmetric matrices, that is,

$$\mathcal{T}_Q\mathcal{O}(n) = \{QK \,|\, K \text{ is skew-symmetric}\} = \{KQ \,|\, K \text{ is skew-symmetric}\}. \tag{3.8}$$

The following lemma serves as a recipe to compute the projected gradient onto the tangent space of $\mathcal{O}(n)$. For a proof, readers are referred to [11].

LEMMA 3.1. *Let $Q \in \mathcal{O}(n)$ be a fixed orthogonal matrix. The projection of any given matrix $X \in \mathbb{R}^{n\times n}$ onto the tangent space $\mathcal{T}_Q\mathcal{O}(n)$ is given by*

$$\mathbb{P}_{\mathcal{T}_Q\mathcal{O}(n)}(X) = \frac{1}{2}Q\left\{Q^\top X - X^\top Q\right\} = \frac{1}{2}\left\{XQ^\top - QX^\top\right\}Q. \tag{3.9}$$

For our application, it suffices to take the left translation. The projected gradient $g(Q) := \mathbb{P}_{\mathcal{T}_Q\mathcal{O}(n)}(\nabla F(Q))$ of $\nabla F(Q)$ onto $\mathcal{O}(n)$ can be calculated explicitly as

$$\begin{aligned} g(Q) &= \frac{1}{2}Q\left(Q^\top\nabla F(Q) - \nabla F(Q)^\top Q\right) \\ &= Q\left[Q^\top SQ, \eta(Q)\right], \end{aligned} \tag{3.10}$$

where, for convenience, we adopt the Lie bracket notation

$$[M, N] = MN - NM.$$

By now, if we define the dynamical system

$$\dot{Q} = -g(Q), \quad Q(0) = I, \tag{3.11}$$

then the solution flow $Q(t)$ to (3.11) stays on the manifold $\mathcal{O}(n)$ and moves in the steepest descent direction for the objective function $F(Q)$. In the following two subsections, we argue for two points. First, the asymptotically stable equilibria of this projected gradient flow are necessarily a geometrically isolated. Second, any such an equilibrium point provides the orthogonal matrix Q at which $\eta(Q) = 0$. In this way, we establish the existence of a matrix satisfying the MWHST condition.

3.3. Geometric isolation of equilibrium points. Consider the gradient flow[2]

$$\dot{\mathbf{x}} = -\nabla F(\mathbf{x}) \tag{3.12}$$

for minimizing an objective function $F(\mathbf{x})$. It is known that if $\mathbf{x}(t)$ is a bounded semi-orbit of (3.12) and if F is differentiable, then the set of accumulation points, that is,

$$\omega(\mathbf{x}(0)) := \{\mathbf{x}^* \in \mathbb{R}^n \,|\, \mathbf{x}(t_\nu) \to \mathbf{x}^* \text{ for some sequence } t_\nu \to \infty\} \tag{3.13}$$

[2]Without causing ambiguity, we use the same notation F for a general objective function which eventually goes back to our F defined in (3.4) or, more correctly, the potential function whose gradient is our projected gradient $g(Q)$ in (3.11). An analytic expression of the potential function is obtainable, but not needed in our subsequent analysis.

is a non-empty, compact, and connected subset of stationary points

$$\mathcal{C} := \{\mathbf{x} \in \mathbb{R}^n \,|\, \nabla F(\mathbf{x}) = 0\}\,. \tag{3.14}$$

There are examples showing that $\omega(\mathbf{x}(0))$ can form a periodic orbit [1] . For analytic gradient flow, however, more can be said about the limiting behavior in (3.13). The main reason hinges upon the fact that the ratio of an analytic function to its gradient is bounded in a specific way known as the Łojasiewicz gradient inequality. This classical result has found rather striking applications in the theory of ordinary and partial differential equations, in particular, to gradient flows.

THEOREM 3.2. *(Łojasiewicz Inequality [6, 27, 28]) Suppose that $F : U \to \mathbb{R}$ is real analytic in an open set $U \subset \mathbb{R}^n$. Then for any point $\mathbf{p} \in U$, there exists a neighborhood W of $\mathbf{p}$, constants $\theta \in [\frac{1}{2}, 1)$ and $c > 0$ such that*

$$\|F(\mathbf{x}) - F(\mathbf{p})\|^\theta \leq c\|\nabla F(\mathbf{x})\| \quad \textit{for all } \mathbf{x} \in W\,. \tag{3.15}$$

An important consequence of the Łojasiewicz inequality is that the semi-orbit of any analytic gradient flow is necessarily of finite arc length. Equivalently, the set $\omega(\mathbf{x}(0))$ of any analytic gradient flow $\mathbf{x}(t)$ is necessarily a singleton. This fundamental fact is well known in the field of dynamical systems for gradient flow applications. We recommend [1, Theorem 2.2] and [35] for its proof.

THEOREM 3.3. *([1, 35]) Suppose that $F : U \to \mathbb{R}$ is real analytic in an open set $U \subset \mathbb{R}^n$. Then for any bounded semi-orbit of (3.12), there exists a point $\mathbf{x}^* \in \omega(\mathbf{x}(0))$ such that $\mathbf{x}(t) \to \mathbf{x}^*$ as $t \to \infty$.*

In our gradient flow (3.11), it is obvious from (3.10) that the vector field is a multi-variate polynomial in the entries of Q. So definitely the vector field is analytic in Q. By Theorem 3.3, the flow $Q(t)$ defined by (3.11) converges to a single point.

3.4. Projected Hessian. The optimization problem (3.4) may have many stationary points. A stationary point as is defined by (3.14) may be a local minimizer, maximizer, or saddle point. To fully analyze the local behavior of its stationary points, we need to know the definiteness of the projected Hessian of $F(Q)$ over the tangent space at the stationary point [16, 17]. For a general constrained optimization problem, computing the projected Hessian is a theoretically desirable but practically difficult task. For problem (3.4), nonetheless, we can compute the projected Hessian explicitly by the technique developed in [11].

First, we formally extend the projected gradient $g(Q)$ for $Q \in \mathcal{O}(n)$ to the function $G : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$ via the definition

$$G(Z) := Z\left[Z^\top SZ, \eta(Z)\right]. \tag{3.16}$$

Note that $G(Z)$ is only a mechanical generalization of $g(Q)$. Second, we calculate action of the Fréchet derivative of G at $Z \in \mathbf{R}^{n\times n}$ on an arbitrary $H \in \mathbb{R}^{n\times n}$ as

$$G'(Z).H = H\left[Z^\top SZ, \eta(Z)\right] + Z\left[H^\top SZ + Z^\top SH, \eta(Z)\right] + Z\left[Z^\top SZ, \mathsf{diag}(H^\top SZ + Z^\top SH)\right]. \tag{3.17}$$

Then, the information of the projected Hessian can be obtained by restricting the action of (3.17) to the case where $Q \in \mathcal{O}(n)$ is a stationary point and $H \in \mathcal{T}_Q\mathcal{O}(n)$.

More specifically, we know that Q is a stationary point of (3.4) if and only if $\left[Q^\top SQ, \eta(Q)\right] = 0$ by (3.10). We know also that $H \in \mathcal{T}_Q\mathcal{O}(n)$ if and only if H is of the form $H = QK$ for some skew-symmetric matrix $K \in \mathbb{R}^{n\times n}$. So, upon substitution, the projected Hessian $G'(Q)$ acting on QK is given by

$$\begin{aligned}
\langle QK, G'(Q).QK\rangle &= \left\langle QK, Q\left[\left[Q^\top SQ, K\right], \eta(Q)\right] + Q\left[Q^\top SQ, \operatorname{diag}\left[Q^\top SQ, K\right]\right]\right\rangle \\
&= \left\langle K, \left[\left[Q^\top SQ, K\right], \eta(Q)\right] + \left[Q^\top SQ, \operatorname{diag}\left[Q^\top SQ, K\right]\right]\right\rangle \\
&= \left\langle \left[Q^\top SQ, K\right], [K, \eta(Q)] + \operatorname{diag}\left[Q^\top SQ, K\right]\right\rangle.
\end{aligned} \tag{3.18}$$

With (3.18) in hand, the second-order optimality condition can be stated as follows [16, 17].

LEMMA 3.4. *Suppose that $Q \in \mathcal{O}(n)$ is a stationary point for (3.4). Then a necessary condition for Q to be a local minimizer is that*

$$\langle QK, G'(Q).QK\rangle \geq 0 \quad \textit{for all skew-symmetric matrices } K. \tag{3.19}$$

Conversely, if the strict inequality in (3.19) holds at Q, then Q is guaranteed to be a local minimizer.

3.5. Asymptotically stable equilibrium. We now apply the above theory to establish the existence of a matrix satisfying the MWHST condition. As explained earlier, we need to find an orthogonal matrix Q such that $\eta(Q) = 0$. Our approach is to argue that if $\eta(Q) \neq 0$ for a stationary point Q, then there is a direction along which the value of the objective function F can be further reduced. As such, our gradient flow $Q(t)$ will bypass[3] this stationary point and continue to descend until a local minimizer at which $\eta(Q) = 0$ is found.

We first make the following simple claim.

LEMMA 3.5. *Suppose that the three given sets of data $\mathbf{d}$, $\boldsymbol{\lambda}$, and $\boldsymbol{\sigma}$ satisfy the MWHST condition. Suppose also that a matrix A satisfying the Weyl-Horn condition is already found and is now skew-symmetric. Let S be the symmetric matrix defined in (3.3). Then for any $Q \in \mathcal{O}(n)$, $\eta(Q)$ cannot be a constant diagonal unless it is identically zero.*

Proof. Suppose that $\eta(Q) = \mathsf{diag}(Q^\top SQ) - \mathsf{diag}(\mathbf{d}) = cI$ for some constant c. Summing over the diagonal entries, by the Mirsky condition, we have $\mathrm{trace}(\eta(Q)) = \mathrm{trace}(\mathsf{diag}(Q^\top AQ) - \sum_{i=1}^n d_i) = \sum_{i=1}^n \lambda_i - \sum_{i=1}^n d_i = 0 = nc$. It follows that $c = 0$. ∎

For simplicity, we assume the generic situation that all eigenvalues of S are distinct. The analysis for the case of equal eigenvalues is more involved[4], but the asymptotic behavior should be similar. By using the gradient flow, here is our major result for proving the solvability.

THEOREM 3.6. *Suppose that the symmetric matrix S has distinct eigenvalues. Let $Q \in \mathcal{O}(n)$ denote a stationary point for the problem (3.4). If $\eta(Q) \neq 0$, then there exists a skew-symmetric matrix K such that $\langle QK, G'(Q)QK\rangle < 0$. In other words, if $\eta(Q) \neq 0$, then Q is not a local minimizer for the objective function F in (3.4).*

Proof. Because Q is a stationary point, by (3.10) we have $\left[Q^\top SQ, \eta(Q)\right] = 0$. Since S is symmetric, let $S = U^\top \Pi U$ denote its spectral decomposition where columns of $U^\top$ are the orthonormal eigenvectors and $\Pi = \mathrm{diag}\{\pi_1, \ldots, \pi_n\}$ is the diagonal matrix of eigenvalues. Define the matrix

$$V := (UQ)\eta(Q)(UQ)^\top. \tag{3.20}$$

Then $[\Pi, V] = 0$. Since the diagonal matrix Π has distinct diagonal entries, V must also be a diagonal matrix. Write $V = \mathrm{diag}\{v_1, \cdots, v_n\}$. Because $\eta(Q)$ is itself a diagonal matrix, the relationship (3.20) implies that $\{v_1, \cdots, v_n\}$ is a permutation of $\{\pi_1, \ldots, \pi_n\}$.

Suppose that $\eta(Q) \neq 0$. We may assume, after a similarity transformation by permutation matrices if necessary, that $\eta(Q)$ is of the form

$$\eta(Q) = \mathrm{diag}\{\eta_1 I_{n_1}, \cdots, \eta_k I_{n_k}\},$$

where I_{n_i} is the $n_i \times n_i$ identity matrix for $i = 1, \cdots, k$, and $\eta_1 > \cdots > \eta_k$. By Lemma 3.5, we know that $\eta(Q)$ has more than one diagonal block, i.e., $k > 1$. Write $Y := Q^\top SQ$ for abbreviation. The commutativity $[Y, \eta(Q)] = 0$ implies that Y must be of block diagonal form

$$Y = \mathrm{diag}\{Y_{11}, \cdots, Y_{kk}\}, \tag{3.21}$$

where Y_{ii}, $i = 1, \cdots, k$, is an $n_i \times n_i$ symmetric matrix. Note that columns of $(UQ)^\top$ are orthonormal eigenvectors of Y with corresponding eigenvalues $\{\pi_1, \ldots, \pi_n\}$ which are distinct, so the matrix UQ must have the same block structure as that of Y.

[3] Unless $Q(t)$ happens to stay on a heteroclinic orbit, which is numerically unlikely due to the ubiquitous floating-point arithmetic errors.

[4] In this case, we still have $[\Pi, V] = 0$ as in the proof of Theorem 3.6. If Π has repeated entries, then V is block diagonal, but still orthogonally similar to the diagonal matrix $\eta(Q)$. From this point on, the same idea in the proof carries through with a little bit manipulation of block forms.

Let $K \in \mathbb{R}^{n\times n}$ denote an arbitrary skew-symmetric matrix partitioned in block form $K = [K_{ij}]$ where the block sizes of $K_{ij}, i, j = 1, \ldots, k$, are conformal to those of Y as in (3.21) and $K_{ii} = 0$ for $i = 1, \cdots, k$. Note that $k > 1$, so we may assume that $K \neq 0$. Clearly, $\operatorname{diag}\left[Q^\top SQ, K\right] = 0$. With respect to this matrix K and at the stationary point Q, the projected Hessian (3.18) becomes

$$\begin{aligned}\langle QK, G'(Q).QK\rangle &= \left\langle \left[Q^\top SQ, K\right], [K, \eta(Q)]\right\rangle = -\left\langle V\tilde{K} - \tilde{K}V, \Pi\tilde{K} - \tilde{K}\Pi\right\rangle \\ &= -2\sum_{i<j}(\pi_i - \pi_j)(v_i - v_j)\tilde{k}_{ij}^2, \end{aligned} \tag{3.22}$$

where $\tilde{K} = \left[\tilde{k}_{ij}\right] := (UQ)K(UQ)^\top$ remains to be skew-symmetric since UQ is orthogonal.

Finally, given any fixed ordering in both sets $\{\pi_1, \ldots, \pi_n\}$ and $\{v_1, \ldots, v_n\}$, it is obvious from (3.22) that we may choose appropriate values of $\tilde{k}_{ij}$ such that $\langle QK, G'(Q).QK\rangle < 0$. ∎

The implication of Theorem 3.6 is as follows. If Q is a stationary point with $\eta(Q) \neq 0$, then at this point there exists at least one tangent direction, i.e., QK for a certain skew-symmetric matrix K, along which $F(Q)$ can be further decreased. This point is an unstable equilibrium for the gradient dynamics. Therefore, the flow must continue until an isolated limit point at which $\eta(Q) = 0$ is found.

Based on this understanding, we conclude that the convergence of $Q(t)$ to an asymptotically stable equilibrium point Q at which $\eta(Q) = 0$ is guaranteed. When this limit point is achieved, even though it is only a local minimum for the objective function F, the corresponding matrix $Q^\top AQ$ will maintain the prescribed diagonal entries, eigenvalues, and singular values. The existence of a matrix satisfying the MWHST condition is hereby established.

4. Numerical example. The proof used to derive the theoretical existence can actually be implemented as a numerical scheme, albeit we have not considered its efficiency. To maintain the orthogonality of $Q(t)$, for example, structure preserving techniques from the field of geometric integration should have been used for speed and precision [19, 22] . For the time being, we only want to demonstrate workability of the differential system (3.11), which is the basis of our existence proof.

For convenience, we choose to use the standard routine ode15s from MATLAB as our integrator. The local error tolerance is set at $\mathsf{AbsTol} = \mathsf{RelTol} = 10^{-10}$. To demonstrate the robustness of the approach, we challenge ourselves with the 8×8 Rosser matrix R with integer elements

$$R = \begin{bmatrix} 611 & 196 & -192 & 407 & -8 & -52 & -49 & 29 \\ 196 & 899 & 113 & -192 & -71 & -43 & -8 & -44 \\ -192 & 113 & 899 & 196 & 61 & 49 & 8 & 52 \\ 407 & -192 & 196 & 611 & 8 & 44 & 59 & -23 \\ -8 & -71 & 61 & 8 & 411 & -599 & 208 & 208 \\ -52 & -43 & 49 & 44 & -599 & 411 & 208 & 208 \\ -49 & -8 & 8 & 59 & 208 & 208 & 99 & -911 \\ 29 & -44 & 52 & -23 & 208 & 208 & -911 & 99 \end{bmatrix}.$$

The matrix R is known for its difficulty in that it has a double eigenvalue, three nearly equal eigenvalues, a zero eigenvalue, two dominant eigenvalues of opposite sign and a small nonzero eigenvalue. We use its diagonal entries $\mathbf{d}$ and the *computed* eigenvalues and singular values

$$\boldsymbol{\lambda} = \begin{bmatrix} -1.020049018429997e{+}03 \\ 1.020049018429997e{+}03 \\ 1.020000000000000e{+}03 \\ 1.019901951359278e{+}03 \\ 1.000000000000001e{+}03 \\ 9.999999999999998e{+}02 \\ 9.804864072152601e{-}02 \\ 4.851119506099622e{-}13 \end{bmatrix}, \boldsymbol{\sigma} = \begin{bmatrix} 1.020049018429997e{+}03 \\ 1.020049018429996e{+}03 \\ 1.020000000000000e{+}03 \\ 1.019901951359279e{+}03 \\ 1.000000000000000e{+}03 \\ 9.999999999999998e{+}02 \\ 9.804864072162672e{-}02 \\ 1.054603342667098e{-}14 \end{bmatrix}$$

as the test data. So the MWHST condition is automatically satisfied[5]. This example also serves to demonstrate the case that even though the matrix S in Theorem 3.6 does have multiple eigenvalues, the gradient flow still

[5]Strictly speaking, the MWHST condition is satisfied only up to the machine precision. See, for example, the smallest computed eigenvalue is not exactly zero.

works. Using the recursive algorithm proposed in [10] for the above λ and σ, we obtain first the following matrix A needed in Section 3.1:

$$A = \begin{bmatrix} 1.0200e{+}03 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1.0200e{+}03 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.0200e{+}03 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.0199e{+}03 & 0 & 0 & 1.4668e{-}09 & 0 \\ 0 & 0 & 0 & 0 & 1.0000e{+}03 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.0000e{+}03 & 0 & 0 \\ 0 & 0 & 0 & -1.5257e{-}05 & 0 & 0 & 9.8049e{-}02 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1.4045e{-}07 & 0 \end{bmatrix},$$

where for the convenience of running text we display all numbers in only 5 digits. Defining S according to (3.3) and integrating our differential equation (3.11) numerically, we are able to find this matrix

$$B = \begin{bmatrix} 611.0000 & -184.6972 & 93.4026 & -177.9840 & 50.0103 & -66.4451 & -364.8367 & -230.1007 \\ -184.6972 & 899.0000 & 84.6701 & -18.4713 & 86.7552 & -70.4723 & -143.9197 & -161.0699 \\ 93.4026 & 84.6701 & 899.0000 & -136.2380 & -152.2550 & 106.6705 & -2.4645 & 191.7090 \\ -177.9840 & -18.4713 & -136.2380 & 611.0000 & -282.3676 & 196.8994 & -260.5891 & 85.8062 \\ 50.0103 & 86.7552 & -152.2550 & -282.3676 & 411.0000 & 592.8768 & 367.9171 & -228.2314 \\ -66.4451 & -70.4723 & 106.6705 & 196.8994 & 592.8768 & 411.0000 & -481.0590 & 348.2056 \\ -364.8367 & -143.9197 & -2.4645 & -260.5891 & 367.9171 & -481.0590 & 99.0000 & 459.5032 \\ -230.1007 & -161.0699 & 191.7090 & 85.8062 & -228.2314 & 348.2056 & 459.5032 & 99.0000 \end{bmatrix}.$$

It can been seen that the diagonal entries of B are almost identical to those of R. Indeed, the total difference is within a 2-norm of 2×10^{-9} in absolute error. Likewise, we can check that the eigenvalues and singular values of B agree with $\boldsymbol{\lambda}$ and $\boldsymbol{\sigma}$ within the tolerance 10^{-9}. However, note that the off-diagonal entries of B are very different from those of the original R, indicating that the inverse problem has multiple solutions.

5. Conclusion. We studied the theoretical problem of whether a matrix with prescribed main diagonal entries, eigenvalues, and singular values exists when these data satisfy the equalities and inequalities entailed by the Mirsky, Weyl-Horn, and Sing-Thompson theorems simultaneously. We employ an argument involving an array of tools to establish the existence of such a matrix when $n \geq 3$. Extra conditions are needed for the case $n = 2$. The existence theory is new in the field. The dynamical system approach might be useful for other types of existence problems.

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