An Optimization Result With Application to Optimal Spacecraft Reaction Wheel Orientation Design

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ABSTRACT

This paper provides the globally optimal solution for both minimizing and maximizing the squared Frobenious norm of YQX (where X and Y are arbitrary compatibly dimensioned matrices) over the class of orthogonal matrices Q. The solution is in closed-form and does not require iteration. The specialization of this optimization result to 3 dimensions is found applicable to optimally orienting spacecraft reaction wheel actuators with respect to specified torque, momentum storage, and power requirements.

1 INTRODUCTION

Reaction wheels are often used as actuators for controlling spacecraft attitude. This paper takes an optimization approach to finding the best way to orient three reaction wheel actuators on an orbiting spacecraft. For this purpose, a quadratic cost function is constructed based on torque, momentum storage, and power requirements. The quadratic cost has the form of a Frobenious norm $||YQ^TX||_f^2$ where the matrix $Q \in \mathcal{R}^{3\times3}$ is orthogonal and the matrices Y and X are nonzero matrices of compatible dimensions.

In addressing this problem, the quadratic cost problem is first generalized to an arbitrary number of dimensions, i.e., for the case where $Q \in \mathcal{R}^{m\times m}$ with m arbitrary. The globally optimal solution is given in Appendix A for both minimizing and maximizing the quadratic cost over Q. The solution is provided in closed-form and does not require iteration. The optimization result is then specialized to 3 dimensions and applied to the problem of optimizing reaction wheel orientation. The full version of this work was first reported in [1].

2 BACKGROUND

Let the vector $x_w \in \mathcal{R}^3$ denote a physical quantity (e.g., torque, momentum, etc.) such that the i'th element of x_w is associated with the i'th reaction wheel, $i = 1, 2, 3$. Vectors defined in this manner will be said to be in *wheel coordinates*. The mapping from wheel coordinates to body coordinates is given by the expression,

$$x_b = A x_w \tag{2.1}$$

$$A = [a_1, a_2, a_3] \tag{2.2}$$

where $A \in \mathcal{R}^{3\times3}$ denotes a 3×3 **wheel orientation matrix** (with columns a_i, $i = 1, 2, 3$), and x_b is the corresponding vector quantity in spacecraft body coordinates. Physically, the i'th column of the A matrix denotes the orientation of the i'th reaction wheel expressed as a unit vector in body coordinates. Hence the columns of the A matrix are not arbitrary, but are each constrained to have unit norm, i.e.,

$$a_i^T a_i = 1, \quad i = 1, 2, 3 \tag{2.3}$$

Note, however, that in the present treatment, the columns of A are not required to be orthogonal. This permits the reaction wheels to attain (possibly) skewed configurations.

The approach in this paper optimizes over the complete matrix A. This parametrization is the most general possible, and avoids imposing a-priori restrictions on wheel geometry. This is in contrast to earlier results which impose special structures to simplify the problem. For example, the approach in Fleming and Ramos [6] optimizes over the single cant angle associated with a 4-wheel square pyramid configuration, while the approach in Hablani [9] optimizes over the two angles associated with a 4-wheel rectangular pyramid. In principle, the extra degrees of freedom lead to better performance, but must be traded against a potentially more complex implementation.

3 REQUIREMENTS

Reaction wheel requirements are most simply stated in terms of an *idealized* set of three reaction wheels which are assumed be oriented along each of the body axes. For example, a computer simulation can be run which assumes (artificially) that the reaction wheels are oriented along the body axes, to numerically generate the wheel torque and momentum storage requirements. For notational purposes, all quantities associated with such an idealized reaction wheel frame will be denoted with a star '$*$'.

The baseline scenario (motivated by the emerging JPL/NASA Europa orbiter mission) will involve an orbiting spacecraft which accumulates momentum in a nearly repetitive fashion due to periodic orbital dynamics and attitude histories. Because mass is a critical factor in the Europa design, the reaction wheels will be operated in a bipolar fashion, allowing for zero-rate crossings and taking advantage of their full momentum excursion.

3.1 Momentum Requirements

At some starting time $t = 0$, the spacecraft momentum is assumed to be brought (by active management) to a starting momentum "bias" level denoted as b^* (Nms) in idealized reaction wheel coordinates. The idealized reaction wheels then start accumulating momentum over the orbit with both periodic and secular components to give a total stored momentum at time t of $h^*(t)$. It will be convenient to define the momentum accumulated ***in excess of*** b^* as $\Delta h^*(t)$, so that the total stored momentum can be written as,

$$h^*(t) = b^* + \Delta h^*(t) \tag{3.1}$$

The accumulation of momentum continues until some specified time T (generally a fixed multiple or fraction of the orbital period) at which time the stored momentum is brought back again by active management to its starting bias level of b^*. The process then repeats in this fashion, defining a nominal momentum management strategy over the course of the mission.

It will be convenient to map the momentum bias b^* into wheel coordinates to give the vector b i.e.,

$$b = A^{-1}b^* \tag{3.2}$$

Consider a momentum storage vector $h^*(t) \in \mathcal{R}^3$ at time t in body coordinates which must be attainable using the designed wheel orientation. The momentum vector can be similarly mapped into wheel coordinates as,

$$h_w(t) = A^{-1}h^*(t) \tag{3.3}$$

It is assumed that all wheels are identical, each with a maximum momentum storage capacity of $\pm\beta$ (Nms). Then conditions which ensure that no wheel is exceeding its maximum storage capacity at time t are given by,

$$-\beta \ \mathit{1} \leq A^{-1}h^*(t) \leq \beta \ \mathit{1} \tag{3.4}$$

where,

$$\mathit{1} \triangleq \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \tag{3.5}$$

Note that using (3.1), the $t = 0$ case can be treated separately, and (3.4) can be broken into the two conditions,

$$-\beta\mathit{1} \leq b \leq \beta\mathit{1} \qquad \text{for } t = 0 \tag{3.6}$$

$$-\beta\mathit{1} \leq b + A^{-1}\Delta h^*(t) \leq \beta\mathit{1} \qquad \text{for } 0 < t \leq T \tag{3.7}$$

Constraints (3.6) and (3.7) are functions of b and A and specify the basic momentum requirements in wheel coordinates.

3.2 Torque Requirements

The torque required in body coordinates during this period of time is denoted as the time-varying torque vector $\tau^*(t) \in \mathcal{R}^3$. At each time, the torque vector $\tau^*(t)$ must be attainable using the designed wheel orientation. The torque vector can be mapped into wheel coordinates as,

$$\tau_w(t) = A^{-1}\tau^*(t) \tag{3.8}$$

where $\tau_w(t) \in \mathcal{R}^3$ denotes the torque vector in wheel coordinates. It is assumed that all wheels are identical, each with maximum torque capability of $\pm\gamma$ (Nm). Then the condition which ensures that no wheel is exceeding its maximum torque capacity at time t is given by,

$$-\gamma \mathit{1} \leq A^{-1}\tau^*(t) \leq \gamma \mathit{1} \tag{3.9}$$

Constraint (3.9) is a function of A and specifies the basic torque requirements in wheel coordinates.

3.3 Power Requirements

Let the total power expended due to reaction wheels at time t associated with a specific wheel configuration be denoted by $P(t)$. The power dissipated $P(t)$ will be assumed to be approximated by the model $P_1(t)$ defined as,

$$P_1(t) = p_0 + \alpha||w(t)||_1 \tag{3.10}$$

where the wheel speed vector $w(t) = [w_1(t), w_2(t), w_3(t)]^T$ has components $w_i(t)$ which correspond to the speed of the i'th wheel, and $||\cdot||_1$ denotes the standard L_1 vector norm,

$$||w(t)||_1 = \sum_{i=1}^{3} |w_i(t)| \tag{3.11}$$

The constant p_0 in (3.10) accounts for power loss in the electronics and other fixed dissipative effects. The wheel rate term $w(t)$ captures long term dissipation effects associated with countering frictional torques. The value for α is best obtained by fitting empirical data. The angular acceleration $\dot{w}$ is intentionally omitted from this model since it is not a major contributor to long-term power dissipation issues. However, it is important for calculating peak-power requirements (e.g., during maneuvers) and should be checked against the final design.

For optimization purposes, the P_1 power model (3.10) will be replaced by the P_2 model given below,

$$P_2(t) = p_0 + \alpha||w(t)||_2 \tag{3.12}$$

where $||\cdot||_2$ denotes the standard L_2 (Euclidean) vector norm,

$$||w(t)||_2 = \left(\sum_{i=1}^{3} |w_i(t)|^2\right)^{\frac{1}{2}} \tag{3.13}$$

The P_2 model (3.12) only approximates the P_1 model, but has the advantage of leading to a more tractable optimization problem. The L_1 norm can be bounded on either side by the L_2 norm as [8],

$$||w(t)||_2 \leq ||w(t)||_1 \leq \sqrt{2} \cdot ||w(t)||_2 \tag{3.14}$$

Hence, the minimization of P_2 power indirectly acts to minimize P_1 power to within a factor of $\sqrt{2}$. Numerical results indicate that this approximate approach can be very effective.

It is known that the wheel speed is proportional to the wheel momentum, i.e.,

$$I_w w(t) = h_w(t) = A^{-1} h^*(t) \tag{3.15}$$

where I_w ($Kg\ m^2$) is a scalar value for the individual wheel inertia (assumed to be the same for all wheels). Using (3.15), the P_2 power model (3.12) can be rewritten as,

$$P_2(t) = p_0 + \frac{\alpha}{I_w} ||A^{-1} h^*(t)||_2 \tag{3.16}$$

The condition for power $P_2(t)$ to be less than some desired specified value P_d is then given by,

$$||A^{-1} h^*(t)||_2 \leq \frac{\overline{p}\ I_w}{\alpha} \tag{3.17}$$

where $\overline{p} = P_d - p_0$. As done for the momentum, the $t = 0$ case can be broken out separately to give the two constraints,

$$||b||_2 \leq \frac{\overline{p}\ I_w}{\alpha}, \quad \text{for } t = 0 \tag{3.18}$$

$$||b + A^{-1} \Delta h^*(t)||_2 \leq \frac{\overline{p}\ I_w}{\alpha}, \quad \text{for } 0 < t \leq T \tag{3.19}$$

Constraints (3.18) and (3.19) are functions of b and A and specify the basic power requirements.

3.4 Discussion

A *feasible design* of b and A is defined as one which meets the momentum storage requirements (3.6)(3.7), torque requirements (3.9), and power requirements (3.18)(3.19). The present approach will be to optimize a certain cost function which tends to drive b and A towards a feasible design. The cost function is discussed in the next section.

4 COST FUNCTION

The optimization problem will focus on a specific discrete set of times t_k, $k = 1, ..., n$. At each time t_k, let the desired torque be given as $\tau^*(k)$ and the excess accumulated momentum be given as $\Delta h^*(k)$. Here, the t dependence has been replaced by k for notational simplicity, since the set of constraint times is now finite.

The goal is to optimize a cost function $C(b, A)$ over the choice of both the initial bias momentum b and the reaction wheel orientation A, i.e.,

$$\min_{b,A} C(b, A) \tag{4.1}$$

The cost function is taken to be the sum of three components:

$$C(b, A) = C_M + C_T + C_P \tag{4.2}$$

where each component is defined below.

Momentum Cost Function

$$C_M(b, A) = \frac{1}{\beta^2}\left(||b||_2^2 + \sum_{k=1}^{n} ||b + A^{-1}\Delta h^*(k)||_2^2\right) \tag{4.3}$$

Torque Cost Function

$$C_T(b, A) = \frac{1}{\gamma^2}\sum_{k=1}^{n} ||A^{-1}\tau^*(k)||_2^2 \tag{4.4}$$

Power Cost Function

$$C_P(b, A) = \frac{\alpha^2}{\overline{p}^2\, I_w^2}\left(||b||_2^2 + \sum_{k=1}^{n} ||b + A^{-1}\Delta h^*(k)||_2^2\right) \tag{4.5}$$

The cost function (4.2) is a weighted sum of L_2 norms (i.e,. weighted least squares criteria) where the weightings are chosen to normalize the importance of each term according to their specified requirements. For example, the $\frac{1}{\beta^2}$ weighting associated with C_M cost in (4.3) is motivated by the need to satisfy the momentum storage requirements given in (3.6)(3.7). Similarly the scalings for C_T and C_P above are motivated by the need to satisfy the torque requirements (3.9), and power requirements (3.18)(3.19), respectively. These scalings transform the cost into dimensionless units, and drive each of the quantities to satisfy their desired constraints. This overcomes the usual difficulty of scaling costs in problems with multiple objectives.

Numerical values for $\beta, \gamma, \alpha, \overline{p}, I_\omega$ are needed to properly scale the optimization problem. In practice, these parameters can be chosen based on a nominal reaction wheel design. The choice of times t_k at which to enforce the constraints is left up to the designer. For the present paper, t_k will not be interpreted as time, but rather, k will be used as an index to define a set of linear constraints forming a simplex which overbounds the region containing all simulated momentum and torque values. Specifically, the eight corners of a box aligned with the body axes will be used to specify the constraints associated with the idealized star frame. Similar formulations making use of torque boxes and momentum cylinders have appeared elsewhere in the literature [5][9].

5 OPTIMIZATION PROCEDURE

5.1 Parametrization of Orientation Matrix

It will be convenient for optimization purposes to represent the matrix A in terms of its QR factors (cf., [8]), i.e.,

$$A = QR \tag{5.1}$$

where $Q \in \mathcal{R}^{3\times3}$ is an orthogonal matrix (i.e., $QQ^T = Q^TQ = I$) and R is an upper triangular matrix. Intuitively, the R matrix represents the skewness of the wheel coordinate frame, and the Q matrix represents any rotations and/or reflections.

By the orthogonality of Q the unit norm constraints (2.3) on the columns of A become unit norm constraints on the columns of R. Hence, R is upper triangular with unit norm columns. Accordingly, it will be parametrized as follows,

$$R = \begin{bmatrix} 1 & \overline{a} & \overline{c} \\ 0 & (1-\overline{a}^2)^{\frac{1}{2}} & \overline{b}(1-\overline{c}^2)^{\frac{1}{2}} \\ 0 & 0 & (1-\overline{b}^2)^{\frac{1}{2}}(1-\overline{c}^2)^{\frac{1}{2}} \end{bmatrix} \tag{5.2}$$

It can be verified that the columns of R are unit norm by construction. In order to prevent the square-root terms in R from becoming imaginary, it will be convenient to impose the following linear constraints,

$$\begin{aligned} -1 &\leq \overline{a} \leq 1 \\ -1 &\leq \overline{b} \leq 1 \\ -1 &\leq \overline{c} \leq 1 \end{aligned} \tag{5.3}$$

It is proved in [1] that without loss of generality, the square roots in the definition of R (5.2) can always be taken as positive.

5.2 Three Wheel Optimization Algorithm

Using the QR factorization of A, the cost function (4.2)-(4.5) can be rewritten as,

$$C(b, R, Q) = \frac{1}{c^2}||b||_2^2 + \frac{1}{c^2}\sum_{k=1}^{n}||b + R^{-1}Q^T\Delta h^*(k)||_2^2 + \frac{1}{\gamma^2}\sum_{k=1}^{n}||R^{-1}Q^T\tau^*(k)||_2^2 \tag{5.4}$$

where,

$$\frac{1}{c^2} = \frac{1}{\beta^2} + \frac{\alpha^2}{\overline{p}^2\, I_w^2} \tag{5.5}$$

subject to Q orthogonal, and R upper triangular with unit norm columns.

The basic approach to minimizing $C(b, R, Q)$ is outlined in the following sequence of steps.

Step 0: Initialize

$$\widehat{Q} = I \tag{5.6}$$

Step 1: Optimize over b, R

$$\widehat{b}, \widehat{R} = \arg\min_{b,R}\ C(b, R, \widehat{Q}) \tag{5.7}$$

subject to R upper triangular with unit norm columns.

Step 2:

Calculate the bias in body frame $\widehat{b}^*$

$$\widehat{b}^* = \widehat{Q}\widehat{R}\widehat{b} \tag{5.8}$$

Step 3: Optimize over Q

$$\widehat{Q} = \arg\min_{Q}\ C(\widehat{R}^{-1}Q^T\widehat{b}^*, \widehat{R}, Q) \tag{5.9}$$

subject to Q being an orthogonal matrix i.e., $Q^TQ = I$.

Step 4: Repeat

Repeat Steps 1 to 3 until convergence is obtained.

5.3 Discussion

In Step 1, the matrix R is parametrized as (5.2), subject to linear constraints (5.3), thus ensuring that it will be upper triangular with unit norm columns as desired. The nonlinear cost function is optimized subject to linear constraints using Sequential Quadratic Programming (SQP). Details can be found in Appendix A of [1]. It is worth noting that Step 1 is equivalent to,

$$\widehat{b}^*, \widehat{R} = \arg\min_{b^*,R}\ C(R^{-1}\widehat{Q}^T b^*, R, \widehat{Q}) \tag{5.10}$$

where it is emphasized that this optimization is equivalently taken over the optimal bias momentum in *body frame coordinates* b^*. This fact is important for conceptual reasons discussed below. However, for the actual numerical optimization, it is more convenient to use the bias momentum b in *reaction wheel coordinates* since it is b and not b^* that appears linearly inside the various norm terms of C.

In Step 2, the calculation of the momentum bias in body frame $\widehat{b}^*$ is made for explicit use in the expression (5.9) which keeps it invariant during optimization of Q in Step 3.

In Step 3, the optimization over Q is performed using a globally optimal analytical solution derived in Theorem A.1 of Appendix A.

Together, the optimization in (5.10) and (5.9) (equivalently, Steps 1 and 3) constitute alternating minimizations between the two *independent* parameter sets $\{b^*, R\}$ and $\{Q\}$. This *relaxation* type approach ensures that the algorithm gives a sequence of solutions with a monotonically decreasing cost. Since the cost is bounded below (by zero), the cost converges. Hence the algorithm is convergent in the sense of the cost. However, it cannot be claimed that the converged solution is the globally optimal solution to the original problem. Rather, the main motivation for this approach is to take advantage of a new result in Appendix A which provides a closed-form analytical solution to the subproblem of optimizing over Q.

6 NUMERICAL RESULTS

A case study is given in this section to demonstrate the use of the algorithm in Section 5.2 for optimizing reaction wheel orientations. This example is consistent with requirements for the Europa orbiter mission based on preliminary modeling results. The requirements are more stringent in the Y axis because it corresponds to the orbit normal direction.

6.1 Nominal Wheel Characteristics

```
Individual wheel inertia
Iw=.0509305 (Kg-m^2)
Max individual wheel momentum storage capacity
beta=8 (Nms)
Max single wheel torque capability
gamma=.02 (Nm)
Power dissipation scale factor
alpha=.025 watt/(rad/sec)
```

6.2 Initial Conditions

The initial design is taken as the identity $A = I$, and the initial momentum bias is taken to be zero $b^* = 0$.

6.3 Requirements (Europa Example)

```
Momentum Box x,y,z (Nms)
              X             Y             Z
Max     3.4300e+000   3.8000e-003   6.9700e+000
Min    -2.2200e-001  -4.9800e+000   2.9400e+000

Torque Box x,y,z (Nm)
              X             Y             Z
```

```
Max     1.7700e-003  1.7500e-003  1.4000e-003
Min    -1.7200e-003 -9.8600e-003 -4.8500e-004

Total power allocation-pbar (watts)
  3.1500e+001
*************************************************************
```

Itrn	Cost	Max Momentum	Max Torque	Max Power
Allocation:		8.0000e+000	2.0000e-002	3.1500e+001
0	7.0418e+000	6.9700e+000	9.8600e-003	7.5495e+000
1	3.1403e+000	1.0241e+001	8.2358e-003	9.2542e+000
2	3.0414e+000	4.0107e+000	7.5552e-003	3.9294e+000
.	.	.	.	.
.	.	.	.	.
29	3.0374e+000	4.8707e+000	7.5861e-003	3.1461e+000
30	3.0374e+000	4.8750e+000	7.5826e-003	3.1506e+000

The final optimized wheel configuration is summarized below and is depicted graphically in Figure 6.1.

$$A = \begin{bmatrix} 5.8700e-001 & 2.8918e-001 & -5.3041e-001 \\ 8.0345e-001 & -2.3296e-001 & 8.0643e-001 \\ -9.9452e-002 & 9.2850e-001 & 2.6143e-001 \end{bmatrix}; \quad b^* = \begin{bmatrix} -1.4257 \\ 2.2116 \\ -4.4042 \end{bmatrix} \tag{6.1}$$

As expected, the strong projections [-8.0345e-001,2.3296e-001,-8.0643e-001] in the second row of $\widehat{A}$ indicate that the y axis is favored by the optimized wheel configuration. As an intuition check, the optimized momentum bias is seen to be close to the values [-1.6040,2.4881,-4.9550] which center the momentum box about zero.

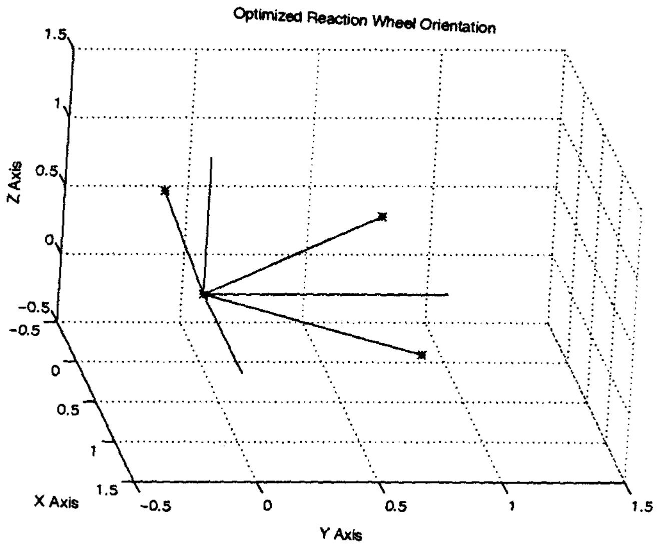

Figure 6.1: Optimized Reaction Wheel Orientation

7 CONCLUSIONS

This paper has developed an optimization-based approach to orienting three reaction wheels on an orbiting spacecraft. The main consideration has been to find an orientation matrix which minimizes mass and power of the required reaction wheels, while meeting torque and momentum storage requirements and allowing a specified maximum amount of time between momentum dumps.

The optimization is nonlinear in both the cost and constraints. A QR factorization of the wheel-to-body transformation allows separate optimization over the rotation Q and skewness R of the reaction wheel frame. The initial momentum bias b is also optimized for momentum management purposes. The optimization over the Q matrix has been performed analytically based on a specialization of a new result proved in Appendix A, which gives a general expression for the globally optimal Q of arbitrary dimensions. The R, b parameters are optimized using Sequential Quadratic Programming (SQP).

A numerical example based on NASA's emerging Europa orbiter, was given to show that the algorithm converged as expected, leading to a final (intuitively reasonable) orientation which tended to favor the body axis having the most stringent requirements.

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A APPENDIX A: Frobenious Norm Optimization

This appendix discusses Step 3 of the algorithm in Section 5.2 where the cost $C(\hat{R}^{-1}Q^T b^*, \hat{R}, Q)$ in (5.4) is optimized with respect to the orthogonal matrix Q. The cost in Step 3 in conveniently put into the following form,

$$C(\hat{R}^{-1}Q^T\hat{b}^*, \hat{R}, Q) = ||YQ^TX||_f^2 \tag{A.1}$$

where,

$$X = [\frac{\hat{b}^*}{c}, \frac{\hat{b}^* + \Delta h^*(1)}{c}, \ldots, \frac{\hat{b}^* + \Delta h^*(n)}{c}, \frac{\tau^*(1)}{\gamma}, \ldots, \frac{\tau^*(n)}{\gamma}] \tag{A.2}$$

$$Y = \hat{R}^{-1} \tag{A.3}$$

Here, $||M||_f$ denotes the Frobenious norm of a given matrix M [8],

$$||M||_f = Tr\{M^TM\}^{\frac{1}{2}} \tag{A.4}$$

and corresponds simply to the sum of squares of the elements of M. The optimization of (A.1) over choice of $Q \in \mathcal{R}^{3\times 3}$ is a special case of the general problem treated in the following result which is applicable to the case where $Q \in \mathcal{R}^{m\times m}$ with m arbitrary.

THEOREM A.1 *Let $X \in \mathcal{R}^{m\times n}$, $Y \in \mathcal{R}^{\ell\times m}$ be arbitrary but non-zero matrices. Consider the following cost function involving the Frobenious norm,*

$$C(Q) = ||YQ^TX||_f^2 = Tr\{X^TQY^TYQ^TX\} \tag{A.5}$$

where the matrix $Q \in \mathcal{R}^{m \times m}$ is constrained to be orthogonal, i.e.,

$$Q^T = Q^{-1} \tag{A.6}$$

Let P_x and P_y be orthogonal matrices obtained from the following eigenvector decompositions,

$$Y^T Y = P_y \Lambda_y P_y^T \tag{A.7}$$

$$X X^T = P_x \Lambda_x P_x^T \tag{A.8}$$

$$\Lambda_x = diag\{\lambda_{x1}, ..., \lambda_{xm}\} \tag{A.9}$$

$$\Lambda_y = diag\{\lambda_{y1}, ..., \lambda_{ym}\} \tag{A.10}$$

where the eigenvalues in Λ_x and Λ_y are each assumed to be ordered in a monotonically non-increasing sequence, i.e.,

$$\lambda_{x1} \geq \lambda_{x2} \geq ... \geq \lambda_{xm} \geq 0 \tag{A.11}$$

$$\lambda_{y1} \geq \lambda_{y2} \geq ... \geq \lambda_{ym} \geq 0 \tag{A.12}$$

Then a choice of Q which globally maximizes $C(Q)$ is given by,

$$\overline{Q} = P_x P_y^T \tag{A.13}$$

and a choice of Q which globally minimizes $C(Q)$ is given by,

$$\underline{Q} = P_x J P_y^T \tag{A.14}$$

where J is the reverse identity,

$$J \triangleq \begin{bmatrix} 0 & \cdots & 0 & 1 \\ \vdots & & 1 & 0 \\ 0 & & & \vdots \\ 1 & 0 & \cdots & 0 \end{bmatrix} \tag{A.15}$$

■

The proof of Theorem A.1 will require some preliminary definitions and results.

Permutation Matrices [2] A permutation matrix P of order m is an $m \times m$ matrix possessing exactly a single element of value "1" in each row and column, with all other elements zero. There are known to be exactly $m!$ permutation matrices of any given order m. ■

Doubly Stochastic Matrices [2] A square matrix $A \in \mathcal{R}^{m \times m}$ is *doubly stochastic* if its elements $A = \{a_{ij}\}$ satisfy the following conditions,

$$a_{ij} \geq 0 \tag{A.16}$$

$$\sum_{i=1}^{m} a_{ij} = 1; \quad \sum_{j=1}^{m} a_{ij} = 1 \tag{A.17}$$

■

Birkhoff's Theorem [2][4] Any doubly stochastic matrix $A \in \mathcal{R}^{m \times m}$ can be written as a convex combination of permutation matrices, i.e.,

$$A = \sum_{k=1}^{m!} w_k P_k \tag{A.18}$$

$$w_k \geq 0; \quad \sum_{k=1}^{m!} w_k = 1 \tag{A.19}$$

where $\{P_k\}$, $k = 1, ..., m!$ denotes the set of permutation matrices of order m. ■

Hardy's Theorem [3] Let $\{b_1, ..., b_m\}$ and $\{c_1, ..., c_m\}$ be monotonically nonincreasing sequences of numbers. Associate with each $i = 1, ..., m$ a distinct index j to define the mapping between indices $j(i)$. Then the sum-of-products cost $\sum_{i=1}^{m} b_i c_{j(i)}$ is maximized when $j(i) = i$ for all i, and minimized when $j(i) = m - i + 1$ for all i. ■

It is necessary to first prove the following result.

LEMMA A.1 (Bounds on an inner product) *Consider vectors $b = [b_1, ..., b_m]^T$ and $[c_1, ..., c_m]^T$ where $\{b_1, ..., b_m\}$ and $\{c_1, ..., c_m\}$ are monotonically nonincreasing sequences of numbers. Let $A \in \mathcal{R}^{m \times m}$ be a doubly stochastic matrix. Then the inner product $b^T Ac$ can be bounded above and below as follows,*

$$b^T Jc \leq b^T Ac \leq b^T c \tag{A.20}$$

where J is the reverse identity given by (A.15). Furthermore, the lower bound is achieved with equality by choosing $A = J$, and the upper bound is achieved with equality by choosing $A = I$. ■

Proof: Using Birkhoff's Theorem (A.18)(A.19), the matrix A in the expression $b^T Ac$ can be replaced by the convex combination of permutation matrices (A.18) to give,

$$b^T Ac = \sum_{k=1}^{m!} w_k b^T P_k c \tag{A.21}$$

Without loss of generality, we can define the first two permutation matrices as,

$$P_1 = I; \quad P_2 = J \tag{A.22}$$

It is noted that each inner-product term $b^T P_k c$ appearing in the summation of (A.21) can be interpreted as a sum-of-products of elements of b with elements of c, as reordered by multiplication with the permutation matrix P_k. Accordingly, by Hardy's theorem, the largest of the terms $\{b^T P_k c\}_{k=1}^{m!}$ is given by using the identity permutation $P_k = P_1 = I$. Hence, an upper bound on the convex combination (A.21) is found by putting all of the weight into the first term (i.e. $w_1 = 1, w_i = 0 \; for \; i \neq 1$) to give,

$$b^T Ac = \sum_{k=1}^{m!} w_k b^T P_k c \leq b^T P_1 c = b^T c \tag{A.23}$$

This establishes the upper bound in (A.20). Note that this upper bound is achieved with equality when $A = I$.

Similarly, by Hardy's theorem, the smallest of the inner-product terms $\{b^T P_k c\}_{k=1}^{m!}$ is given by using the reverse-ordering permutation $P_k = P_2 = J$. Hence, a lower bound on the convex combination (A.21) is found by putting all of the weight into the second term (i.e. $w_2 = 1,\ w_i = 0\ for\ i \neq 2$) to give,

$$b^T A c = \sum_{k=1}^{m!} w_k b^T P_k c \geq b^T P_2 c = b^T J c \qquad \text{(A.24)}$$

This establishes the lower bound in (A.20). Note that this lower bound is achieved with equality when $A = J$. ∎

At this point Theorem A.1 can be proved. The basic idea is to first show that the cost $C(Q)$ has the special inner product form $b^T Ac$, as treated in Lemma A.1. Second, it is shown that the upper and lower bounds on the cost ensured by result (A.20) of Lemma A.1, are achieved with equality for the optimal choices of Q given by (A.13) and (A.14) of Theorem A.1. As desired, this implies that they are in fact global extrema.

Proof of Theorem A.1: Define the cost function as,

$$C(Q) = ||YQ^T X||_f^2 = Tr\{X^T Q Y^T Y Q^T X\} \qquad \text{(A.25)}$$

Rearranging using the eigenvalue decompositions (A.7)(A.8) and standard trace identities gives,

$$\begin{aligned}
C(Q) &= Tr\{QY^T Y Q^T X X^T\} && \text{(A.26)}\\
&= Tr\{QP_y \Lambda_y P_y^T Q^T P_x \Lambda_x P_x^T\} && \text{(A.27)}\\
&= Tr\{\Lambda_y P_y^T Q^T P_x \Lambda_x P_x^T Q P_y\} && \text{(A.28)}\\
&= Tr\{\Lambda_y L^T \Lambda_x L\} && \text{(A.29)}\\
&= Tr\{\Lambda_y^{\frac{1}{2}} \Lambda_y^{\frac{1}{2}} L^T \Lambda_x^{\frac{1}{2}} \Lambda_x^{\frac{1}{2}} L\} && \text{(A.30)}\\
&= Tr\{\Lambda_y^{\frac{1}{2}} L^T \Lambda_x^{\frac{1}{2}} \Lambda_x^{\frac{1}{2}} L \Lambda_y^{\frac{1}{2}}\} && \text{(A.31)}\\
&= ||\Lambda_x^{\frac{1}{2}} L \Lambda_y^{\frac{1}{2}}||_f^2 && \text{(A.32)}\\
&= \sum_{i=1}^{m}\sum_{j=1}^{m}\left(\lambda_{xi}^{\frac{1}{2}}\lambda_{yj}^{\frac{1}{2}}\ell_{ij}\right)^2 = \sum_{i=1}^{m}\sum_{j=1}^{m}\lambda_{xi}\lambda_{yj}\ell_{ij}^2 && \text{(A.33)}\\
&= \lambda_x^T A \lambda_y && \text{(A.34)}
\end{aligned}$$

where the following quantities have been defined,

$$L \triangleq P_x^T Q P_y = \{\ell_{ij}\} \qquad \text{(A.35)}$$

$$\lambda_x = [\lambda_{x1}, ..., \lambda_{xm}]^T \in \mathcal{R}^m \tag{A.36}$$

$$\lambda_y = [\lambda_{y1}, ..., \lambda_{ym}]^T \in \mathcal{R}^m \tag{A.37}$$

$$A = L \otimes L = \{a_{ij} = \ell_{ij}^2\} \tag{A.38}$$

Equation (A.29) follows from (A.28) by the definition of the orthogonal matrix L in (A.35); equation (A.33) follows from the fact that a squared Frobenious norm of a matrix is the sum-of-squares its elements; and equation (A.34) follows by vectorizing equation (A.33), where the symbol $\otimes$ denotes the Hadamard product (i.e., the element-by-element multiplication of two matrices).

Since L is an orthogonal matrix (i.e., $L^T L = LL^T = I$) each of its rows and columns have unit norm so that the matrix A in (A.38) is doubly stochastic. In addition, the elements of vectors λ_x, λ_y are ordered from highest to lowest, so that the result (A.20) of Lemma A.1 can be applied to the inner product (A.34) to give,

$$\lambda_x^T J \lambda_y \leq C(Q) \leq \lambda_x^T \lambda_y \tag{A.39}$$

The lower bound in (A.39) is achieved with equality by the choice $A = J$, which using (A.38) gives

$$L = J^{\frac{1}{2}} \tag{A.40}$$

where $J^{\frac{1}{2}}$ denotes any Hadamard square root of the matrix J (i.e., any $J^{\frac{1}{2}}$ such that $J = J^{\frac{1}{2}} \otimes J^{\frac{1}{2}}$). Substituting (A.40) into (A.35), and solving for Q gives the global minimum as,

Global Minimum

$$\underline{Q} = P_x J^{\frac{1}{2}} P_y^T \tag{A.41}$$

For simplicity one can choose (non-uniquely) $J^{\frac{1}{2}} = J$ which gives (A.14) as desired. However, $J^{\frac{1}{2}}$ can alternatively be chosen as one of 2^m possible Hadamard roots of J formed by changing the sign on any combination of 1's in J. Any one of these choices gives a alternative global maximum.

The upper bound in (A.39) is achieved with equality with the choice $A = I$ which using (A.38) gives,

$$L = I^{\frac{1}{2}} \tag{A.42}$$

where $I^{\frac{1}{2}}$ denotes any Hadamard square root of the identity matrix I. Substituting (A.42) into (A.35) and solving for Q gives the global maximum as,

Global Maximum

$$\overline{Q} = P_x I^{\frac{1}{2}} P_y^T \tag{A.43}$$

For simplicity one can choose (non-uniquely) $I^{\frac{1}{2}} = I$ which gives (A.13) as desired. However, $I^{\frac{1}{2}}$ can alternatively be chosen as one of 2^m possible Hadamard roots of I formed by changing the sign on any combination of 1's in the identity I. Any one of these choices gives an alternative global maximum. ∎