Appendix C

Some analytical optimal results

C.1 properties of infima

- $$\inf \emptyset \triangleq \infty \tag{1479}$$
$$\sup \emptyset \triangleq -\infty \tag{1480}$$

- Given $f(x) : \mathcal{X} \to \mathbb{R}$ defined on arbitrary set $\mathcal{X}$ [148, §0.1.2]

$$\begin{aligned} \inf_{x \in \mathcal{X}} f(x) &= -\sup_{x \in \mathcal{X}} -f(x) \\ \sup_{x \in \mathcal{X}} f(x) &= -\inf_{x \in \mathcal{X}} -f(x) \end{aligned} \tag{1481}$$

$$\begin{aligned} \arg\inf_{x \in \mathcal{X}} f(x) &= \arg\sup_{x \in \mathcal{X}} -f(x) \\ \arg\sup_{x \in \mathcal{X}} f(x) &= \arg\inf_{x \in \mathcal{X}} -f(x) \end{aligned} \tag{1482}$$

- Given $f(x) : \mathcal{X} \to \mathbb{R}$ and $g(x) : \mathcal{X} \to \mathbb{R}$ defined on arbitrary set $\mathcal{X}$ [148, §0.1.2]

$$\inf_{x \in \mathcal{X}} \big(f(x) + g(x)\big) \geq \inf_{x \in \mathcal{X}} f(x) + \inf_{x \in \mathcal{X}} g(x) \tag{1483}$$

Citation: Jon Dattorro, *Convex Optimization & Euclidean Distance Geometry,* Meboo Publishing USA, 2005.

- Given $f(x) : \mathcal{X} \cup \mathcal{Y} \to \mathbb{R}$ and arbitrary sets $\mathcal{X}$ and $\mathcal{Y}$ [148, §0.1.2]

$$\mathcal{X} \subset \mathcal{Y} \Rightarrow \inf_{x\in\mathcal{X}} f(x) \geq \inf_{x\in\mathcal{Y}} f(x) \tag{1484}$$

$$\inf_{x\in\mathcal{X}\cup\mathcal{Y}} f(x) = \min\{\inf_{x\in\mathcal{X}} f(x)\,,\ \inf_{x\in\mathcal{Y}} f(x)\} \tag{1485}$$

$$\inf_{x\in\mathcal{X}\cap\mathcal{Y}} f(x) \geq \max\{\inf_{x\in\mathcal{X}} f(x)\,,\ \inf_{x\in\mathcal{Y}} f(x)\} \tag{1486}$$

- Over some convex set $\mathcal{C}$ given vector constant y or matrix constant Y

$$\arg\inf_{x\in\mathcal{C}} \|x-y\|_2 \;=\; \arg\inf_{x\in\mathcal{C}} \|x-y\|_2^2 \tag{1487}$$

$$\arg\inf_{X\in\mathcal{C}} \|X-Y\|_{\mathrm{F}} \;=\; \arg\inf_{X\in\mathcal{C}} \|X-Y\|_{\mathrm{F}}^2 \tag{1488}$$

C.2 diagonal, trace, singular and eigen values

- For $A\in\mathbb{R}^{m\times n}$ and $\sigma(A)$ denoting its singular values, [46, §A.1.6] [91, §1] (*confer* (36))

$$\begin{aligned}
\sum_i \sigma(A)_i \;=\; \operatorname{tr}\sqrt{A^TA} \;=\; \sup_{\|X\|_2\leq 1} \operatorname{tr}(X^TA) \;&=\; \begin{array}{cl}\underset{X\in\mathbb{R}^{m\times n}}{\text{maximize}} & \operatorname{tr}(X^TA)\\ \text{subject to} & \begin{bmatrix} I & X\\ X^T & I\end{bmatrix}\succeq 0\end{array}\\
&=\; \tfrac{1}{2}\begin{array}{cl}\underset{X\in\mathbb{S}^m,\ Y\in\mathbb{S}^n}{\text{minimize}} & \operatorname{tr}X + \operatorname{tr}Y\\ \text{subject to} & \begin{bmatrix} X & A\\ A^T & Y\end{bmatrix}\succeq 0\end{array}
\end{aligned} \tag{1489}$$

- For $X \in \mathbb{S}^m$, $Y \in \mathbb{S}^n$, $A \in \mathcal{C} \subseteq \mathbb{R}^{m\times n}$ for set $\mathcal{C}$ convex, and $\sigma(A)$ denoting the singular values of A [91, §3]

$$\begin{array}{ll}\underset{A}{\text{minimize}} & \sum_i \sigma(A)_i \\ \text{subject to} & A \in \mathcal{C}\end{array} \quad\equiv\quad \begin{array}{ll}\frac{1}{2}\underset{A\,,X\,,Y}{\text{minimize}} & \operatorname{tr} X + \operatorname{tr} Y \\ \text{subject to} & \left[\begin{array}{cc} X & A \\ A^T & Y\end{array}\right] \succeq 0 \\ & A \in \mathcal{C}\end{array} \tag{1490}$$

- For $A \in \mathbb{S}_+^N$ and $\beta \in \mathbb{R}$

$$\beta \operatorname{tr} A \;=\; \begin{array}{ll}\underset{X\in\mathbb{S}^N}{\text{maximize}} & \operatorname{tr}(XA) \\ \text{subject to} & X \preceq \beta I\end{array} \tag{1491}$$

But the following statement is numerically stable, preventing an unbounded solution in direction of a 0 eigenvalue:

$$\begin{array}{ll}\underset{X\in\mathbb{S}^N}{\text{maximize}} & \operatorname{sgn}(\beta)\operatorname{tr}(XA) \\ \text{subject to} & X \preceq \;\;\, |\beta|\, I \\ & X \succeq -|\beta|\, I\end{array} \tag{1492}$$

where $\beta \operatorname{tr} A = \operatorname{tr}(X^\star A)$. If $\beta \geq 0$, then $X \succeq -|\beta| I \leftarrow X \succeq 0$.

- For $A \in \mathbb{S}^N$ having eigenvalues $\lambda(A) \in \mathbb{R}^N$, its smallest and largest eigenvalue is respectively [9, §4.1] [31, §I.6.15] [150, §4.2] [176, §2.1]

$$\min_i\{\lambda(A)_i\} \;=\; \inf_{\|x\|=1} x^T A\, x \;=\; \begin{array}{ll}\underset{X\in\mathbb{S}_+^N}{\text{minimize}} & \operatorname{tr}(XA) \\ \text{subject to} & \operatorname{tr} X = 1\end{array} \;=\; \begin{array}{ll}\underset{t\in\mathbb{R}}{\text{maximize}} & t \\ \text{subject to} & A \succeq t\, I\end{array} \tag{1493}$$

$$\max_i\{\lambda(A)_i\} \;=\; \sup_{\|x\|=1} x^T A\, x \;=\; \begin{array}{ll}\underset{X\in\mathbb{S}_+^N}{\text{maximize}} & \operatorname{tr}(XA) \\ \text{subject to} & \operatorname{tr} X = 1\end{array} \;=\; \begin{array}{ll}\underset{t\in\mathbb{R}}{\text{minimize}} & t \\ \text{subject to} & A \preceq t\, I\end{array} \tag{1494}$$

The smallest eigenvalue of any symmetric matrix is always a concave function of its entries, while the largest eigenvalue is always convex. [46, exmp.3.10] For v_1 a normalized eigenvector of A corresponding to the largest eigenvalue, and v_N a normalized eigenvector corresponding to the smallest eigenvalue,

$$v_N = \arg \inf_{\|x\|=1} x^T A\, x \tag{1495}$$

$$v_1 = \arg \sup_{\|x\|=1} x^T A\, x \tag{1496}$$

- For $A \in \mathbb{S}^N$ having eigenvalues $\lambda(A) \in \mathbb{R}^N$, consider the unconstrained nonconvex optimization that is a projection on the rank-1 subset (§2.9.2.1) of the boundary of positive semidefinite cone $\mathbb{S}_+^N$: Defining $\lambda_1 \triangleq \max\limits_i \{\lambda(A)_i\}$ and corresponding eigenvector v_1

$$\begin{aligned}\underset{x}{\text{minimize}}\ \|xx^T - A\|_F^2 &= \underset{x}{\text{minimize}}\ \operatorname{tr}\big(xx^T(x^Tx) - 2Axx^T + A^TA\big)\\ &= \begin{cases} \|\lambda(A)\|^2\,, & \lambda_1 \leq 0 \\ \|\lambda(A)\|^2 - \lambda_1^2\,, & \lambda_1 > 0 \end{cases}\end{aligned} \tag{1497}$$

$$\arg \underset{x}{\text{minimize}}\ \|xx^T - A\|_F^2 = \begin{cases} \mathbf{0}\,, & \lambda_1 \leq 0 \\ v_1\sqrt{\lambda_1}\,, & \lambda_1 > 0 \end{cases} \tag{1498}$$

Proof. This is simply the Eckart & Young solution from §7.1.2:

$$x^\star x^{\star T} = \begin{cases} \mathbf{0}\,, & \lambda_1 \leq 0 \\ \lambda_1 v_1 v_1^T\,, & \lambda_1 > 0 \end{cases} \tag{1499}$$

Given nonincreasingly ordered diagonalization $A = Q\Lambda Q^T$ where $\Lambda = \delta\big(\lambda(A)\big)$ (§A.5), then (1497) has minimum value

$$\underset{x}{\text{minimize}}\ \|xx^T - A\|_F^2 = \begin{cases} \|Q\Lambda Q^T\|_F^2 = \|\delta(\Lambda)\|^2\,, & \lambda_1 \leq 0 \\ \left\| Q\left(\begin{bmatrix} \lambda_1 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 0 \end{bmatrix} - \Lambda\right) Q^T \right\|_F^2 = \left\| \begin{bmatrix} \lambda_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} - \delta(\Lambda) \right\|^2, & \lambda_1 > 0 \end{cases} \tag{1500}$$

♦

C.2.0.0.1 Exercise. *Rank-1 approximation.*
Given symmetric matrix $A\in\mathbb{S}^N$, prove:

$$v_1 = \begin{array}{cl}\arg\underset{x}{\text{minimize}} & \|xx^T - A\|_F^2 \\ \text{subject to} & \|x\| = 1\end{array} \tag{1501}$$

where v_1 is a normalized eigenvector of A corresponding to its largest eigenvalue. ▼

- (Fan) For $B\in\mathbb{S}^N$ whose eigenvalues $\lambda(B)\in\mathbb{R}^N$ are arranged in nonincreasing order, and for $1\leq k\leq N$ [9, §4.1] [158] [150, §4.3.18] [271, §2] [176, §2.1]

$$\sum_{i=N-k+1}^{N} \lambda(B)_i = \inf_{\substack{U\in\mathbb{R}^{N\times k}\\ U^TU=I}} \text{tr}(UU^TB) = \begin{array}{cl}\underset{X\in\mathbb{S}_+^N}{\text{minimize}} & \text{tr}(XB) \\ \text{subject to} & X\preceq I \\ & \text{tr}\,X = k\end{array} \tag{a}$$

$$= \begin{array}{cl}\underset{\mu\in\mathbb{R}\,,\;Z\in\mathbb{S}_+^N}{\text{maximize}} & (k-N)\mu + \text{tr}(B-Z) \\ \text{subject to} & \mu I + Z \succeq B\end{array} \tag{b}$$

$$\sum_{i=1}^{k} \lambda(B)_i = \sup_{\substack{U\in\mathbb{R}^{N\times k}\\ U^TU=I}} \text{tr}(UU^TB) = \begin{array}{cl}\underset{X\in\mathbb{S}_+^N}{\text{maximize}} & \text{tr}(XB) \\ \text{subject to} & X\preceq I \\ & \text{tr}\,X = k\end{array} \tag{c}$$

$$= \begin{array}{cl}\underset{\mu\in\mathbb{R}\,,\;Z\in\mathbb{S}_+^N}{\text{minimize}} & k\mu + \text{tr}\,Z \\ \text{subject to} & \mu I + Z \succeq B\end{array} \tag{d}$$

$$\tag{1502}$$

Given ordered diagonalization $B=Q\Lambda Q^T$, (§A.5.2) then optimal U for the infimum is $U^\star = Q(:\,,N-k+1\!:\!N)\in\mathbb{R}^{N\times k}$ whereas $U^\star = Q(:\,,1\!:\!k)\in\mathbb{R}^{N\times k}$ for the supremum. In both cases, $X^\star = U^\star U^{\star T}$. Optimization (a) searches the convex hull of the outer product UU^T of all $N\times k$ orthonormal matrices. (§2.3.2.0.1)

- For $B \in \mathbb{S}^N$ whose eigenvalues $\lambda(B) \in \mathbb{R}^N$ are arranged in nonincreasing order, and for diagonal matrix $\Upsilon \in \mathbb{S}^k$ whose diagonal entries are arranged in nonincreasing order where $1 \leq k \leq N$, we utilize the main-diagonal δ operator's self-adjointness property (1245): [10, §4.2]

$$\begin{aligned}\sum_{i=1}^{k} \Upsilon_{ii}\, \lambda(B)_{N-i+1} \;&=\; \inf_{\substack{U\in\mathbb{R}^{N\times k}\\ U^TU=I}} \operatorname{tr}(\Upsilon\, U^TBU) \;=\; \inf_{\substack{U\in\mathbb{R}^{N\times k}\\ U^TU=I}} \delta(\Upsilon)^T\delta(U^TBU) \\ &=\; \begin{array}{cll}\underset{V_i\in\mathbb{S}^N}{\text{minimize}} & \operatorname{tr}\left(B\sum_{i=1}^{k}(\Upsilon_{ii}-\Upsilon_{i+1,i+1})V_i\right) & \\ \text{subject to} & \operatorname{tr} V_i = i\;, & i=1\ldots k \\ & I \succeq V_i \succeq 0\,, & i=1\ldots k\end{array}\end{aligned} \tag{1503}$$

where $\Upsilon_{k+1,k+1} \triangleq 0$. We speculate,

$$\sum_{i=1}^{k} \Upsilon_{ii}\, \lambda(B)_i \;=\; \sup_{\substack{U\in\mathbb{R}^{N\times k}\\ U^TU=I}} \operatorname{tr}(\Upsilon\, U^TBU) \;=\; \sup_{\substack{U\in\mathbb{R}^{N\times k}\\ U^TU=I}} \delta(\Upsilon)^T\delta(U^TBU) \tag{1504}$$

Alizadeh shows: [9, §4.2]

$$\begin{aligned}\sum_{i=1}^{k} \Upsilon_{ii}\, \lambda(B)_i \;&=\; \begin{array}{cll}\underset{\mu\in\mathbb{R}^k,\, Z_i\in\mathbb{S}^N}{\text{minimize}} & \sum_{i=1}^{k} i\mu_i + \operatorname{tr} Z_i & \\ \text{subject to} & \mu_i I + Z_i - (\Upsilon_{ii}-\Upsilon_{i+1,i+1})B \succeq 0\,, & i=1\ldots k \\ & Z_i \succeq 0\,, & i=1\ldots k\end{array} \\ &=\; \begin{array}{cll}\underset{V_i\in\mathbb{S}^N}{\text{maximize}} & \operatorname{tr}\left(B\sum_{i=1}^{k}(\Upsilon_{ii}-\Upsilon_{i+1,i+1})V_i\right) & \\ \text{subject to} & \operatorname{tr} V_i = i\;, & i=1\ldots k \\ & I \succeq V_i \succeq 0\,, & i=1\ldots k\end{array}\end{aligned} \tag{1505}$$

where $\Upsilon_{k+1,k+1} \triangleq 0$.

- The largest eigenvalue magnitude μ of $A \in \mathbb{S}^N$

$$\max_i \{\, |\lambda(A)_i|\, \} \;=\; \begin{array}{cl}\underset{\mu\in\mathbb{R}}{\text{minimize}} & \mu \\ \text{subject to} & -\mu I \preceq A \preceq \mu I\end{array} \tag{1506}$$

is minimized over convex set $\mathcal{C}$ by semidefinite program: (*confer* §7.1.5)

$$\begin{array}{ll}\underset{A}{\text{minimize}} & \|A\|_2\\ \text{subject to} & A\in\mathcal{C}\end{array} \quad\equiv\quad \begin{array}{ll}\underset{\mu\,,\,A}{\text{minimize}} & \mu\\ \text{subject to} & -\mu I \preceq A \preceq \mu I\\ & A\in\mathcal{C}\end{array} \tag{1507}$$

id est,

$$\mu^\star \triangleq \max_i \{\, |\lambda(A^\star)_i| \;,\; i=1\ldots N \,\} \in \mathbb{R}_+ \tag{1508}$$

- For $B\in\mathbb{S}^N$ whose eigenvalues $\lambda(B)\in\mathbb{R}^N$ are arranged in nonincreasing order, let $\Pi\,\lambda(B)$ be a permutation of eigenvalues $\lambda(B)$ such that their absolute value becomes arranged in nonincreasing order: $|\Pi\,\lambda(B)|_1 \geq |\Pi\,\lambda(B)|_2 \geq \cdots \geq |\Pi\,\lambda(B)|_N$. Then, for $1\leq k\leq N$ [9, §4.3][C.1]

$$\sum_{i=1}^k |\Pi\,\lambda(B)|_i \;=\; \begin{array}{ll}\underset{\mu\in\mathbb{R}\;,\;Z\in\mathbb{S}_+^N}{\text{minimize}} & k\mu+\operatorname{tr} Z\\ \text{subject to} & \mu I + Z + B\succeq 0\\ & \mu I + Z - B \succeq 0\end{array} \;=\; \begin{array}{ll}\underset{V\,,W\in\mathbb{S}_+^N}{\text{maximize}} & \langle B\,,\,V-W\rangle\\ \text{subject to} & I\succeq V\,,W\\ & \operatorname{tr}(V+W)=k\end{array} \tag{1509}$$

For diagonal matrix $\Upsilon\in\mathbb{S}^k$ whose diagonal entries are arranged in nonincreasing order where $1\leq k\leq N$

$$\begin{aligned}\sum_{i=1}^k \Upsilon_{ii}|\Pi\,\lambda(B)|_i \;&=\; \begin{array}{lll}\underset{\mu\in\mathbb{R}^k\,,\;Z_i\in\mathbb{S}^N}{\text{minimize}} & \sum\limits_{i=1}^k i\mu_i + \operatorname{tr} Z_i & \\ \text{subject to} & \mu_i I + Z_i + (\Upsilon_{ii}-\Upsilon_{i+1,i+1})B\succeq 0\,, & i=1\ldots k\\ & \mu_i I + Z_i - (\Upsilon_{ii}-\Upsilon_{i+1,i+1})B\succeq 0\,, & i=1\ldots k\\ & Z_i\succeq 0\,, & i=1\ldots k\end{array}\\ &=\; \begin{array}{lll}\underset{V_i\,,W_i\in\mathbb{S}^N}{\text{maximize}} & \operatorname{tr}\left(B\sum\limits_{i=1}^k(\Upsilon_{ii}-\Upsilon_{i+1,i+1})(V_i-W_i)\right) & \\ \text{subject to} & \operatorname{tr}(V_i+W_i)=i\;, & i=1\ldots k\\ & I\succeq V_i\succeq 0\,, & i=1\ldots k\\ & I\succeq W_i\succeq 0\,, & i=1\ldots k\end{array}\end{aligned} \tag{1510}$$

where $\Upsilon_{k+1,k+1}\triangleq 0$.

[C.1] We eliminate a redundant positive semidefinite variable from Alizadeh's minimization. There exist typographical errors in [218, (6.49) (6.55)] for this minimization.

- For $A, B \in \mathbb{S}^N$ whose eigenvalues $\lambda(A), \lambda(B) \in \mathbb{R}^N$ are respectively arranged in nonincreasing order, and for nonincreasingly ordered diagonalizations $A = W_A \Upsilon W_A^T$ and $B = W_B \Lambda W_B^T$ [149] [176, §2.1]

$$\lambda(A)^T \lambda(B) \;=\; \sup_{\substack{U\in\mathbb{R}^{N\times N}\\ U^TU=I}} \operatorname{tr}(A^T U^T B U) \;\geq\; \operatorname{tr}(A^T B) \qquad (1528)$$

(*confer* (1533)) where optimal U is

$$U^\star = W_B W_A^T \in \mathbb{R}^{N\times N} \qquad (1525)$$

We can push that upper bound higher using a result in §C.4.2.1:

$$|\lambda(A)|^T |\lambda(B)| \;=\; \sup_{\substack{U\in\mathbb{C}^{N\times N}\\ U^HU=I}} \operatorname{Re}\operatorname{tr}(A^T U^H B U) \qquad (1511)$$

For step function ψ as defined in (1387), optimal U becomes

$$U^\star = W_B \sqrt{\delta(\psi(\delta(\Lambda)))}^H \sqrt{\delta(\psi(\delta(\Upsilon)))}\, W_A^T \in \mathbb{C}^{N\times N} \qquad (1512)$$

C.3 Orthogonal Procrustes problem

Given matrices $A, B \in \mathbb{R}^{n\times N}$, their product having full singular value decomposition (§A.6.3)

$$AB^T \triangleq U\Sigma Q^T \in \mathbb{R}^{n\times n} \qquad (1513)$$

then an optimal solution $R^\star$ to the orthogonal Procrustes problem

$$\begin{array}{cl}\underset{R}{\text{minimize}} & \|A - R^T B\|_{\mathrm F}\\ \text{subject to} & R^T = R^{-1}\end{array} \qquad (1514)$$

maximizes $\operatorname{tr}(A^T R^T B)$ over the nonconvex manifold of orthogonal matrices: [150, §7.4.8]

$$R^\star = QU^T \in \mathbb{R}^{n\times n} \qquad (1515)$$

A necessary and sufficient condition for optimality

$$AB^T R^\star \succeq 0 \qquad (1516)$$

holds whenever $R^\star$ is an orthogonal matrix. [114, §4]

Solution to problem (1514) can reveal rotation/reflection (§5.5.2, §B.5) of one list in the columns of A with respect to another list B. Solution is unique if $\operatorname{rank} BV_{\mathcal{N}} = n$. [77, §2.4.1] The optimal value for objective of minimization is

$$\begin{aligned} \operatorname{tr}\big(A^TA + B^TB - 2AB^TR^\star\big) &= \operatorname{tr}(A^TA) + \operatorname{tr}(B^TB) - 2\operatorname{tr}(U\Sigma U^T) \\ &= \|A\|_F^2 + \|B\|_F^2 - 2\delta(\Sigma)^T\mathbf{1} \end{aligned} \tag{1517}$$

while the optimal value for corresponding trace maximization is

$$\sup_{R^T=R^{-1}} \operatorname{tr}(A^TR^TB) \;=\; \operatorname{tr}(A^TR^{\star T}B) \;=\; \delta(\Sigma)^T\mathbf{1} \;\geq\; \operatorname{tr}(A^TB) \tag{1518}$$

The same optimal solution $R^\star$ solves

$$\begin{array}{cl} \underset{R}{\text{maximize}} & \|A + R^TB\|_F \\ \text{subject to} & R^T = R^{-1} \end{array} \tag{1519}$$

C.3.1 Effect of translation

Consider the impact of dc offset in known lists $A, B \in \mathbb{R}^{n\times N}$ on problem (1514). Rotation of B there is with respect to the origin, so better results may be obtained if offset is first accounted. Because the geometric centers of the lists AV and BV are the origin, instead we solve

$$\begin{array}{cl} \underset{R}{\text{minimize}} & \|AV - R^TBV\|_F \\ \text{subject to} & R^T = R^{-1} \end{array} \tag{1520}$$

where $V \in \mathbb{S}^N$ is the geometric centering matrix (§B.4.1). Now we define the full singular value decomposition

$$AVB^T \triangleq U\Sigma Q^T \in \mathbb{R}^{n\times n} \tag{1521}$$

and an optimal rotation matrix

$$R^\star = QU^T \in \mathbb{R}^{n\times n} \qquad (1515)$$

The desired result is an optimally rotated offset list

$$R^{\star T}BV + A(I - V) \approx A \tag{1522}$$

which most closely matches the list in A. Equality is attained when the lists are precisely related by a rotation/reflection and an offset. When $R^{\star T}B = A$ or $B\mathbf{1} = A\mathbf{1} = \mathbf{0}$, this result (1522) reduces to $R^{\star T}B \approx A$.

C.3.1.1 Translation of extended list

Suppose an optimal rotation matrix $R^\star \in \mathbb{R}^{n\times n}$ were derived as before from matrix $B\in\mathbb{R}^{n\times N}$, but B is part of a larger list in the columns of $[\,C \;\; B\,]\in\mathbb{R}^{n\times M+N}$ where $C\in\mathbb{R}^{n\times M}$. In that event, we wish to apply the rotation/reflection and translation to the larger list. The expression supplanting the approximation in (1522) makes $\mathbf{1}^T$ of compatible dimension;

$$R^{\star T}[\,C - B\mathbf{1}\mathbf{1}^T\tfrac{1}{N} \quad BV\,] \;+\; A\mathbf{1}\mathbf{1}^T\tfrac{1}{N} \tag{1523}$$

id est, $C - B\mathbf{1}\mathbf{1}^T\frac{1}{N}\in\mathbb{R}^{n\times M}$ and $A\mathbf{1}\mathbf{1}^T\frac{1}{N}\in\mathbb{R}^{n\times M+N}$.

C.4 Two-sided orthogonal Procrustes

C.4.0.1 Minimization

Given symmetric $A\,,B\in\mathbb{S}^N$, each having diagonalization (§A.5.2)

$$A \triangleq Q_A\Lambda_A Q_A^T\;, \qquad B \triangleq Q_B\Lambda_B Q_B^T \tag{1524}$$

where eigenvalues are arranged in their respective diagonal matrix Λ in nonincreasing order, then an optimal solution [86]

$$R^\star = Q_B Q_A^T \in\mathbb{R}^{N\times N} \tag{1525}$$

to the two-sided orthogonal Procrustes problem

$$\begin{array}{cl}\underset{R}{\text{minimize}} & \|A - R^TBR\|_{\mathrm F}\\ \text{subject to} & R^T = R^{-1}\end{array} \;=\; \begin{array}{cl}\underset{R}{\text{minimize}} & \operatorname{tr}\big(A^TA - 2A^TR^TBR + B^TB\big)\\ \text{subject to} & R^T = R^{-1}\end{array} \tag{1526}$$

maximizes $\operatorname{tr}(A^TR^TBR)$ over the nonconvex manifold of orthogonal matrices. Optimal product $R^{\star T}BR^\star$ has the eigenvectors of A but the eigenvalues of B. [114, §7.5.1] The optimal value for the objective of minimization is, by (40)

$$\|Q_A\Lambda_A Q_A^T - R^{\star T}Q_B\Lambda_B Q_B^T R^\star\|_{\mathrm F} \;=\; \|Q_A(\Lambda_A-\Lambda_B)Q_A^T\|_{\mathrm F} \;=\; \|\Lambda_A-\Lambda_B\|_{\mathrm F} \tag{1527}$$

while the corresponding trace maximization has optimal value

$$\sup_{R^T=R^{-1}} \operatorname{tr}(A^TR^TBR) \;=\; \operatorname{tr}(A^TR^{\star T}BR^\star) \;=\; \operatorname{tr}(\Lambda_A\Lambda_B) \;\geq\; \operatorname{tr}(A^TB) \tag{1528}$$

C.4.0.2 Maximization

Any permutation matrix is an orthogonal matrix. Defining a row- and column-swapping permutation matrix (a reflection matrix, B.5.2)

$$\Xi \;=\; \Xi^T \;=\; \begin{bmatrix} \mathbf{0} & & & 1 \\ & & \cdot & \\ & \cdot & & \\ & 1 & & \\ 1 & & & \mathbf{0} \end{bmatrix} \tag{1529}$$

then an optimal solution $R^\star$ to the maximization problem [*sic*]

$$\begin{array}{ll} \underset{R}{\text{maximize}} & \|A - R^TBR\|_{\rm F} \\ \text{subject to} & R^T = R^{-1} \end{array} \tag{1530}$$

minimizes $\operatorname{tr}(A^TR^TBR)$: [149] [176, §2.1]

$$R^\star = Q_B \Xi Q_A^T \in \mathbb{R}^{N\times N} \tag{1531}$$

The optimal value for the objective of maximization is

$$\begin{aligned} \|Q_A\Lambda_A Q_A^T - R^{\star T}Q_B\Lambda_B Q_B^T R^\star\|_{\rm F} \;&=\; \|Q_A\Lambda_A Q_A^T - Q_A\Xi^T\Lambda_B\Xi Q_A^T\|_{\rm F} \\ &=\; \|\Lambda_A - \Xi\Lambda_B\Xi\|_{\rm F} \end{aligned} \tag{1532}$$

while the corresponding trace minimization has optimal value

$$\inf_{R^T=R^{-1}} \operatorname{tr}(A^TR^TBR) \;=\; \operatorname{tr}(A^TR^{\star T}BR^\star) \;=\; \operatorname{tr}(\Lambda_A\Xi\Lambda_B\Xi) \tag{1533}$$

C.4.1 Procrustes' relation to linear programming

Although these two-sided Procrustes problems are nonconvex, a connection with linear programming [64] was discovered by Anstreicher & Wolkowicz [10, §3] [176, §2.1]: Given $A\,,B\in\mathbb{S}^N$, this semidefinite program in S and T

$$\begin{array}{ll} \underset{R}{\text{minimize}} & \operatorname{tr}(A^TR^TBR) \\ \text{subject to} & R^T = R^{-1} \end{array} \;=\; \begin{array}{ll} \underset{S\,,\,T\in\mathbb{S}^N}{\text{maximize}} & \operatorname{tr}(S+T) \\ \text{subject to} & A^T\otimes B - I\otimes S - T\otimes I \succeq 0 \end{array} \tag{1534}$$

(where $\otimes$ signifies Kronecker product (§D.1.2.1)) has optimal objective value (1533). These two problems are strong duals (§2.13.1.0.3). Given ordered diagonalizations (1524), make the observation:

$$\inf_{R} \operatorname{tr}(A^T R^T B R) = \inf_{\hat{R}} \operatorname{tr}(\Lambda_A \hat{R}^T \Lambda_B \hat{R}) \tag{1535}$$

because $\hat{R} \triangleq Q_B^T R Q_A$ on the set of orthogonal matrices (which includes the permutation matrices) is a bijection. This means, basically, diagonal matrices of eigenvalues Λ_A and Λ_B may be substituted for A and B, so only the main diagonals of S and T come into play;

$$\begin{array}{ll} \underset{S,T\in\mathbb{S}^N}{\text{maximize}} & \mathbf{1}^T\delta(S+T) \\ \text{subject to} & \delta(\Lambda_A \otimes (\Xi\Lambda_B\Xi) - I\otimes S - T\otimes I) \succeq 0 \end{array} \tag{1536}$$

a linear program in $\delta(S)$ and $\delta(T)$ having the same optimal objective value as the semidefinite program (1534).

We relate their results to Procrustes problem (1526) by manipulating signs (1481) and permuting eigenvalues:

$$\begin{array}{lll} \underset{R}{\text{maximize}} & \operatorname{tr}(A^T R^T B R) & = \ \underset{S\,,\,T\in\mathbb{S}^N}{\text{minimize}} \quad \mathbf{1}^T\delta(S+T) \\ \text{subject to} & R^T = R^{-1} & \quad\ \ \text{subject to} \quad \delta(I\otimes S + T\otimes I - \Lambda_A\otimes\Lambda_B) \succeq 0 \\ & & = \ \underset{S\,,\,T\in\mathbb{S}^N}{\text{minimize}} \quad \operatorname{tr}(S+T) \\ & & \quad\ \ \text{subject to} \quad I\otimes S + T\otimes I - A^T\otimes B \succeq 0 \end{array} \tag{1537}$$

This formulation has optimal objective value identical to that in (1528).

C.4.2 Two-sided orthogonal Procrustes via SVD

By making left- and right-side orthogonal matrices independent, we can push the upper bound on trace (1528) a little further: Given real matrices $A\,,B$ each having full singular value decomposition (§A.6.3)

$$A \triangleq U_A\Sigma_A Q_A^T \in \mathbb{R}^{m\times n}\,, \qquad B \triangleq U_B\Sigma_B Q_B^T \in \mathbb{R}^{m\times n} \tag{1538}$$

then a well-known optimal solution $R^\star$, $S^\star$ to the problem

$$\begin{array}{ll} \underset{R\,,\,S}{\text{minimize}} & \|A - SBR\|_F \\ \text{subject to} & R^H = R^{-1} \\ & S^H = S^{-1} \end{array} \tag{1539}$$

maximizes $\operatorname{Re}\operatorname{tr}(A^TSBR)$: [238] [215] [38] [144] optimal orthogonal matrices

$$S^\star = U_A U_B^H \in \mathbb{R}^{m\times m}\,, \qquad R^\star = Q_B Q_A^H \in \mathbb{R}^{n\times n} \tag{1540}$$

[*sic*] are not necessarily unique [150, §7.4.13] because the feasible set is not convex. The optimal value for the objective of minimization is, by (40)

$$\|U_A\Sigma_A Q_A^H - S^\star U_B\Sigma_B Q_B^H R^\star\|_{\rm F} \;=\; \|U_A(\Sigma_A-\Sigma_B)Q_A^H\|_{\rm F} \;=\; \|\Sigma_A-\Sigma_B\|_{\rm F} \tag{1541}$$

while the corresponding trace maximization has optimal value [31, §III.6.12]

$$\sup_{\substack{R^H=R^{-1}\\ S^H=S^{-1}}} |\operatorname{tr}(A^TSBR)| \;=\; \sup_{\substack{R^H=R^{-1}\\ S^H=S^{-1}}} \operatorname{Re}\operatorname{tr}(A^TSBR) \;=\; \operatorname{Re}\operatorname{tr}(A^TS^\star BR^\star) \;=\; \operatorname{tr}(\Sigma_A^T\Sigma_B) \;\geq\; \operatorname{tr}(A^TB) \tag{1542}$$

for which it is necessary

$$A^TS^\star BR^\star \succeq 0\,, \qquad BR^\star A^TS^\star \succeq 0 \tag{1543}$$

The lower bound on inner product of singular values in (1542) is due to von Neumann. Equality is attained if $U_A^HU_B = I$ and $Q_B^HQ_A = I$.

C.4.2.1 Symmetric matrices

Now optimizing over the complex manifold of unitary matrices (§B.5.1), the upper bound on trace (1528) is thereby raised: Suppose we are given diagonalizations for (real) symmetric $A\,,B$ (§A.5)

$$A = W_A\Upsilon W_A^T \in \mathbb{S}^n\,, \qquad \delta(\Upsilon)\in\mathcal{K}_{\mathcal{M}} \tag{1544}$$

$$B = W_B\Lambda W_B^T \in \mathbb{S}^n\,, \qquad \delta(\Lambda)\in\mathcal{K}_{\mathcal{M}} \tag{1545}$$

having their respective eigenvalues in diagonal matrices $\Upsilon\,,\Lambda\in\mathbb{S}^n$ arranged in nonincreasing order (membership to the monotone cone $\mathcal{K}_{\mathcal{M}}$ (377)). Then by splitting eigenvalue signs, we invent a symmetric SVD-like decomposition

$$A \triangleq U_A\Sigma_A Q_A^H \in \mathbb{S}^n\,, \qquad B \triangleq U_B\Sigma_B Q_B^H \in \mathbb{S}^n \tag{1546}$$

where $U_A\,, U_B\,, Q_A\,, Q_B \in \mathbb{C}^{n\times n}$ are unitary matrices defined by (*confer* §A.6.5)

$$U_A \triangleq W_A\sqrt{\delta(\psi(\delta(\Upsilon)))}\,, \quad Q_A \triangleq W_A\sqrt{\delta(\psi(\delta(\Upsilon)))}^H, \quad \Sigma_A = |\Upsilon| \tag{1547}$$

$$U_B \triangleq W_B\sqrt{\delta(\psi(\delta(\Lambda)))}\,, \quad Q_B \triangleq W_B\sqrt{\delta(\psi(\delta(\Lambda)))}^H, \quad \Sigma_B = |\Lambda| \tag{1548}$$

where step function ψ is defined in (1387). In this circumstance,

$$S^\star = U_A U_B^H = R^{\star T} \in \mathbb{C}^{n\times n} \tag{1549}$$

optimal matrices (1540) now unitary are related by transposition. The optimal value of objective (1541) is

$$\|U_A\Sigma_A Q_A^H - S^\star U_B\Sigma_B Q_B^H R^\star\|_F = \|\,|\Upsilon| - |\Lambda|\,\|_F \tag{1550}$$

while the corresponding optimal value of trace maximization (1542) is

$$\sup_{\substack{R^H=R^{-1}\\ S^H=S^{-1}}} \operatorname{Re}\operatorname{tr}(A^T SBR) = \operatorname{tr}(|\Upsilon|\,|\Lambda|) \tag{1551}$$

C.4.2.2 Diagonal matrices

Now suppose A and B are diagonal matrices

$$A = \Upsilon = \delta^2(\Upsilon) \in \mathbb{S}^n\,, \quad \delta(\Upsilon) \in \mathcal{K}_{\mathcal{M}} \tag{1552}$$

$$B = \Lambda = \delta^2(\Lambda) \in \mathbb{S}^n\,, \quad \delta(\Lambda) \in \mathcal{K}_{\mathcal{M}} \tag{1553}$$

both having their respective main diagonal entries arranged in nonincreasing order:

$$\begin{array}{ll} \underset{R\,,\,S}{\text{minimize}} & \|\Upsilon - S\Lambda R\|_F \\ \text{subject to} & R^H = R^{-1} \\ & S^H = S^{-1} \end{array} \tag{1554}$$

Then we have a symmetric decomposition from unitary matrices as in (1546) where

$$U_A \triangleq \sqrt{\delta(\psi(\delta(\Upsilon)))}\,, \quad Q_A \triangleq \sqrt{\delta(\psi(\delta(\Upsilon)))}^H, \quad \Sigma_A = |\Upsilon| \tag{1555}$$

$$U_B \triangleq \sqrt{\delta(\psi(\delta(\Lambda)))}\,, \quad Q_B \triangleq \sqrt{\delta(\psi(\delta(\Lambda)))}^H, \quad \Sigma_B = |\Lambda| \tag{1556}$$

Procrustes solution (1540) again sees the transposition relationship

$$S^\star = U_A U_B^H = R^{\star T} \in \mathbb{C}^{n\times n} \qquad (1549)$$

but both optimal unitary matrices are now themselves diagonal. So,

$$S^\star\Lambda R^\star = \delta(\psi(\delta(\Upsilon)))\Lambda\delta(\psi(\delta(\Lambda))) = \delta(\psi(\delta(\Upsilon)))|\Lambda| \tag{1557}$$