

# Asymmetric Spectral clustering

Antoine Lejay

## ▶ To cite this version:

Antoine Lejay. Asymmetric Spectral clustering. [Technical Report] Inria Nancy - Grand Est. 2019. hal-02372570

## HAL Id: hal-02372570 https://hal.inria.fr/hal-02372570

Submitted on 20 Nov 2019

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# Asymmetric Spectral clustering

Antoine Lejay Université de Lorraine, CNRS, Inria, IECL, F-54000 Nancy, France antoine.lejay@univ-lorraine.fr

September 13, 2019 — Version 1

Abstract	This report presents the mathematical foundation of the asymmetric spectral clus-
	tering approach given in the thesis of S.E. Atev (University of Wisconsin, 2011).
	This method, implemented in a companion R package AsymmetricClustering,
	is based on a Riemannian conjugate gradient algorithm to find a minimization
	problem based on an optimization problem involving unitary matrix.
Keywords	Asymmetric Clustering — Riemannian Gradient Conjugate — Spectral Embed-
	ding

## **1** Introduction

A spectral clustering technique consists in assigning one cluster among k for a set of n data with  $k \ll n$ . More precisely, the clustering performed by combining 1) a dimension reduction based on the main eigenvalues of an affinity matrix A that encodes the similarities between any pairs of data, and 2) seeking the main direction of this reduced model. The main directions are specified as a basis of  $\mathbb{R}^k$  (or  $\mathbb{C}^k$ ), and the cluster associated to each data is given by selectionning the closest line among the k orthogonal lines specified by the basis.

Many spectral clustering techniques exists, coming from various fields. The survey [6] presents some of them with their rationale.

The affinity matrix A is usually symmetric as its coefficients are given by the distance between the pairs of data, this is not necessarily the case. In [2], S.E. Atev presents an algorithm to deal with asymmetric matrices A, with application to image analysis. He also gives a simplified Matlab code.

This report is the companion of the R package AsymmetricClustering which is a port of the above code. In particular, we present the mathematical foundation of the algorithm.

## 2 Notations

The notations given in Table 1 are used in this report.

## 3 Spectral clustering

The spectral clustering is performed through the following steps:

- We construct from *n* data  $x_1, \ldots, x_n$  a  $n \times n$  matrix *A* for which each entry  $A_{i,j}$  records a "similarity" between  $x_i$  and  $x_j$ .
- Through a spectral embedding step, we transform the matrix A into a  $k \times n$  matrix Y that keeps the main features of A, where k is the number of clusters,  $k \ll n$ . This data reduction step uses the spectral information contained in A.

$\llbracket k,n \rrbracket$	Interval for integers	$\{k,\ldots,n\}$
$\mathfrak{M}_{p \times q}(\mathbb{K})$	<i>Matrices</i> with <i>p</i> rows and <i>q</i> columns with coefficients in $\mathbb{K} = \mathbb{R}, \mathbb{C}$	
Tr M	Trace of $M \in \mathfrak{M}_{n \times n}(\mathbb{K})$	$\sum_{i=1}^{n} M_{ii}$
$M_{{\scriptscriptstyle ullet} i}$	<i>i</i> -th column	$M_{\bullet i} = \begin{bmatrix} M_{1,i} \\ \vdots \\ M_{n,i} \end{bmatrix}$
$M_{i\bullet}$	<i>i</i> -th row	$M_{i\bullet} = \begin{bmatrix} M_{1,i}^{n,i} & \cdots & M_{n,i} \end{bmatrix}$
$M^T$	<i>Transpose</i> of $M \in \mathfrak{M}_{p \times q}(\mathbb{K})$	$M^T = (M_{j,i})_{\substack{i \in [\![1,p]\!]\\j \in [\![1,q]\!]}}$
$M^H$	<i>Hermitian transpose</i> of $M \in \mathfrak{M}_{p \times n}(\mathbb{C})$	$M^{H} = \overline{M}^{T}$
$u \cdot_{\mathbb{R}} v$	Scalar product of $u, v \in \mathbb{C}^d$	$\sum_{i=1}^{d} u_i v_i = u^T v$
$u \cdot v$	<i>Hermitian scalar product</i> of $u, v \in \mathbb{C}^d$	$u \cdot v = u^T \cdot_{\mathbb{R}} \overline{v}$
$u \otimes v$	<i>Tensor product</i> $u \otimes v \in \mathfrak{M}_{k \times n}(\mathbb{C})$	$u \otimes v = uv^T$
$\mathfrak{H}_n$	Hermitian matrices of $\mathfrak{M}_{n\times n}(\mathbb{C})$ , characterized by $M = M^H$	
$\mathfrak{U}_n$	Unitary matrices of $\mathfrak{M}_{n\times n}(\mathbb{C})$ , characterized by $U^{H}U = \mathrm{Id}$	
$\mathfrak{u}_n$	Lie algebra of <i>unitary matrices</i> of $\mathfrak{M}_{n \times n}(\mathbb{C})$ , characterized by $U^H = -U$ .	

Table 1: Notations

We look for an orthogonal (if A is symmetric) or unitary matrix U whose axes encoding an orthonormal basis {u<sub>1</sub>,..., u<sub>k</sub>} on ℝ<sup>k</sup> or ℂ<sup>k</sup>. This matrix is selected to minimaize the overall distance between the columns vectors of Y, seen as elements of ℝ<sup>k</sup>, and the rays emanating from 0 in one of the direction u<sub>i</sub>. If the *j*-th column vector of Y is closest to the line in the direction u<sub>i</sub> than in any other direction u<sub>ℓ</sub>, ℓ ∋, then we assign the data x<sub>i</sub> to the *i*-th cluster.

#### 3.1 Dealing with asymmetric matrices

We consider a  $n \times n$  matrix A which is not necessarily symmetric.

**Lemma 1.** The transform  $H : \mathfrak{M}_{n \times n}(\mathbb{R}) \to \mathfrak{H}_n$  defined by

$$H(A) = \frac{1}{2}(A + A^{T}) + \frac{1}{2}i(A - A^{T})$$

is one-to-one with inverse  $H^{-1}(M) = \Re M + \Im M$  for  $M \in \mathfrak{H}_n$ .

As the matrix H(A) is Hermitian, we may consider the eigenvalue problem

$$H(A)x = \lambda x, \ x \in \mathbb{C}^d, \ \lambda \in \mathbb{R}$$

The eigenvectors are orthogonal for the Hermitian scalar product. Therefore, we summarize the eigenvalue problem as

$$V\Lambda V^H = H(A) \tag{1}$$

where V is a unitary matrix and

$$\Lambda = \begin{bmatrix} \lambda_1 & 0 & 0\\ 0 & \ddots & 0\\ 0 & 0 & \lambda_d \end{bmatrix}$$

with  $\lambda_1 \geq \ldots \geq \lambda_n$  is a diagonal matrix containing the eigenvalues. The eigenvector of norm 1 corresponding to  $\lambda_i$  is encoded into  $V_{i}$ .

#### 3.2 Spectral embedding

The spectral embedding step consists in transforming the coordinates of the  $n \times n$  matrix A to a matrix Y of size  $k \times n$ , where k is the number of clusters. This is a dimension reduction.

Following [2], the package AsymmetricClustering considers by default the following spectral embedding princple. Other choices are possible [2, Table 3.2, p. 23].

**Principle 1** (Spectral embedding step). Using  $\Lambda$  and V as in (1), we define

$$Y = \begin{bmatrix} \lambda_1^{-1/2} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_k^{-1/2} \end{bmatrix} \begin{bmatrix} V_{\bullet 1} & \dots & V_{\bullet k} \end{bmatrix}^H \in \mathfrak{M}_{n \times k}(\mathbb{C}).$$

As explained in [4], the spectral embedding step stems from the following principle: "Truncation of the eigenbasis amplifies any unevenness in the distribution of points on the *d*-dimensional hypersphere by causing points of high affinity to move toward each other and other to move apart."

*Remark* 1. With this matrix *Y*, we have

$$YV_{\cdot i} = \begin{cases} \lambda_i^{-1/2} & \text{if } 1 \le i \le k, \\ 0 & \text{otherwise.} \end{cases}$$

The matrix *Y* satisfies  $YAY^* = Id$ .

#### **3.3** Transformation into an optimization problem

The problem is now rewritten as an optimization problem.

**Lemma 2.** Given a point  $y \in \mathbb{C}^k$ ,  $n \ge 1$  and a direction  $u \in \mathbb{C}^k$ , the distance d(y, u) between y and its orthogonal projection on u is given by

$$d(y,u) = \sqrt{\overline{y}^T (\operatorname{Id} - u \otimes \overline{u}) y}.$$
(2)

**Principle 2** (General principle of spectral clustering). Given a matrix  $Y \in \mathfrak{M}_{k \times n}(\mathbb{C})$ , we consider finding a unitary matrix  $U \in \mathfrak{U}_{k \times k}$  such that  $d(Y_{\cdot i}, U_{\sigma(i)})$  is minimal for each  $i \in [\![1, n]\!]$ , where  $\sigma : [\![1, n]\!] \to [\![1, k]\!]$ . The cluster of the column *i* is given by  $\sigma(i)$ .

To set up Principle 2 in practive, we need to rewrite it by defining a cost function. For that,  $\sigma$  is replaced by  $W \in \mathfrak{M}_{k \times n}$  containing exactly one and only one 1 on each row. The *cost function*<sup>1</sup> is

$$J(Y, U, W) = \sum_{i=1}^{n} \sum_{j=1}^{k} W_{j,i} D_{j,i} \text{ with } D_{j,i} = d(Y_{\bullet i}, U_{\bullet j})^2$$
(3)

for  $Y \in \mathfrak{M}_{k \times n}(\mathbb{C})$ ,  $U \in \mathfrak{U}_{k \times k}$  and  $W \in \mathfrak{M}_{k \times n}(\mathbb{R})$  with the constraint

$$W_{j,i} \in \{0,1\}$$
 and  $\sum_{j=1}^{k} W_{j,i} = 1$  for  $i = 1, ..., n$ . (4)

**Principle 3.** Fix  $1 \le k \le n$ . Given  $Y \in \mathfrak{M}_{k,n}(\mathbb{R})$ , find  $U \in \mathfrak{M}_{k \times k}(\mathbb{C})$  and  $W \in \mathfrak{M}_{k \times n}(\mathbb{R})$  satisfying (4) such that

$$J(Y, U, W) \text{ is minimal}$$
  
with  $U \in \mathfrak{U}_k$  and  $W$  satisfies (4). (5)

The constraint (4) is relaxed into

$$0 \le W_{i,j} \le 1 \text{ and } \sum_{j=1}^{k} W_{j,i} = 1 \text{ for } i = 1, \dots, n.$$
 (6)

We coefficients  $W_{i,j}$  are then seen as *weights* that quantify the probability to belong to a class k.

**Principle 4** (Minimization of the cost function, relaxed version of Principle 3). Fix  $1 \le k \le n$ . Given  $Y \in \mathfrak{M}_{k,n}(\mathbb{R})$ , find  $U \in \mathfrak{M}_{k \le k}(\mathbb{C})$  and  $W \in \mathfrak{M}_{k \le n}(\mathbb{R})$  satisfying (4) such that

$$J(Y, U, W) \text{ is minimal}$$
  
with  $U \in \mathfrak{U}_k$  and  $W$  satisfies (6). (7)

The cluster for the column *i* of *Y* is given by  $\arg \max_{1 \le i \le k} W_{j,i}$ 

The minimization problem 7 is solved using an iterative approach in which we alternatively optimize over the weights and over unitary matrices, up to reaching a state in which the update are small. A "temperature" parameter is updated at each global step.

<sup>&</sup>lt;sup>1</sup>In [2], the matrix W is defined as the transpose of ours.

## **4** Numerical algorithms

#### 4.1 Algorithm 1: updating the weights

When U is fixed, the weight matrix W is updated through

$$W_{j,i}(\sigma, Y, U) = \frac{\exp(-D_{j,i}/\sigma)}{\sum_{\ell=1}^{k} \exp(-D_{\ell,i}/\sigma)} \text{ for } j \in [\![1,k]\!], \ i \in [\![1,n]\!],$$

with  $D_{j,i} = d(Y_{\bullet i}, U_{\bullet j})^2$  (see (3)) for a scale parameter  $\sigma$ . Thus, the column  $W_{\bullet,i}$  is the output the softmax function

$$S\left(\begin{bmatrix}x_1\\\vdots\\x_k\end{bmatrix},\sigma\right) = \frac{1}{\sum_{i=1}^k \exp(x_i/\sigma)} \left(\begin{bmatrix}\exp(x_1/\sigma)\\\vdots\\\exp(x_k/\sigma)\end{bmatrix}\right)$$

applied to the vector  $D_{\bullet,i}$ . The function  $\sigma \mapsto J(Y, U, W(\sigma, Y, U))$  is non-decreasing. Reducing  $\sigma$  reduces the cost function. At the end of the *m*-th step, we update the scale parameter  $\sigma$  as

$$\sigma_{m+1} = \frac{J(Y, U_m, W(\sigma_m, Y, U_m))}{n \cdot m}$$

To avoid numerical problems with the softmax function S, we actually use the formula

$$S\left(\begin{bmatrix} x_1\\ \vdots\\ x_k \end{bmatrix}, \sigma\right) = \frac{1}{\sum_{i=1}^k \exp\left(\frac{x_i - m}{\sigma}\right)} \left(\begin{bmatrix} \exp\left(\frac{x_1 - m}{\sigma}\right)\\ \vdots\\ \exp\left(\frac{x_k - m}{\sigma}\right) \end{bmatrix}\right) \text{ with } m = \max_{j=1,\dots,k} x_j.$$

See [3] for numerical considerations on the computation of the softmax function.

#### 4.2 Algorithm 2: minimization over the unitary matrices

During this optimisation step, the matrix W is fixed. The problem is then to optimize over unitary matrices. For this, a conjugate gradient method is used in the framework of a Riemannian algorithm [5] that takes profits from the geometry of the Lie group of unitary matrices. The algorithm implements the method of [1].

At each point U of  $\mathfrak{U}_n$ , the tangent space  $T_U \mathfrak{U}_n$  is the set

$$T_U \mathfrak{U}_n = \{SU \mid S \in \mathfrak{u}_n\}$$
 with  $\mathfrak{u}_n = \{S \in \mathfrak{M}_{n \times n}(\mathbb{C}) \mid S^H = -S\}$ .

The tangent space is also identified with the set

$$T_U \mathfrak{U}_n = \{ S \in \mathfrak{M}_{n \times n}(\mathbb{C}) \mid U^H S + S^H U = 0 \}.$$

On  $\mathfrak{M}_{n \times n}(\mathbb{C})$ , we define a scalar product as

$$\langle\!\langle M, N \rangle\!\rangle = \frac{1}{2} \Re \operatorname{Tr}(M N^H).$$

**Lemma 3.** For  $M \in \mathfrak{M}_{n \times n}(\mathbb{C})$ , write  $M_a = \frac{1}{2}(M - M^H)$ . The map  $p^{\perp} : M \mapsto M_a$  is the orthogonal projection from  $\mathfrak{M}_{n \times n}(\mathbb{C})$  to  $\mathfrak{u}_n$  for  $\langle\!\langle \cdot, \cdot \rangle\!\rangle$ .

*Proof.* For this scalar product, Hermitian and anti-Hermitian matrices are orthogonal. Any matrix M is decomposed as  $M = M_s + M_a$  with  $M_s = \frac{1}{2}(M + M^H)$  which is Hermitian and  $M_a$  which is anti-Hermitian.

As any element of  $T_U \mathfrak{U}_n$  is writen SU for some  $S \in \mathfrak{u}_n$  and  $U^{-1} = U^*$ , a scalar product is naturally on  $T_U \mathfrak{U}_n$  for any  $U \in \mathfrak{U}_n$  as

$$\langle V, W \rangle_U = \langle \langle VU^{-1}, WU^{-1} \rangle = \frac{1}{2} \Re \operatorname{Tr}(VU^H UW^H) = \langle \langle V, W \rangle.$$

This way,  $\langle \cdot, \cdot \rangle$  gives rise to a Riemannian metric.

**Lemma 4.** The orthogonal projection of  $M \in \mathfrak{M}_{n \times n}(\mathbb{C})$  onto  $T_U \mathfrak{U}$  for  $U \in \mathfrak{U}_n$  is

$$p_U^{\perp}(M) = M - U M^H U.$$
(8)

*Proof.* We set  $p_U^{\perp}$ :  $M \mapsto p^{\perp}(MU^{-1})U$ . It is easily checked that  $\langle p_U^{\perp}(M), W \rangle_U = 0$  for any  $W \in W \in T_U \mathfrak{U}_n$ . Using Lemma 3, this leads to (8).

The geodesics emanating from U in the direction  $SU \in T_U \mathfrak{U}_n$ , that is for  $S \in \mathfrak{u}_n$ , are then

$$\gamma(t) = \exp(tS)U$$

where  $S \mapsto \exp(S)$  is the matrix exponential.

Gradients are computed with respect to the complex conjugate derivative operator

$$\frac{\partial}{\partial U^H} = \frac{1}{2} \left( \frac{\partial}{\partial \Re U} + \mathrm{i} \frac{\partial}{\partial \Im U} \right).$$

The Riemannian gradient of  $f : \mathfrak{U}_n \to \mathbb{R}$  at U is the orthogonal projection of  $\frac{\partial f}{\partial U^H}$  onto  $T_U \mathfrak{U}_n$ , so that with (8),

$$\nabla_{\mathfrak{U}} f(U) = \frac{\partial f}{\partial U^H} - U \left(\frac{\partial f}{\partial U^H}\right)^H U.$$
(9)

#### 4.2.1 The conjugate gradient

**Notation 1.** The gradient of the cost function J(Y, U, W) at point  $U \in \mathfrak{U}_n$  is denoted by  $\Gamma(U) = \frac{\partial J(Y, U, W)}{\partial U^H}$ .

The conjugate gradient algorithm consists in finding successive points  $U_k$  in  $\mathfrak{U}_n$  by

• At  $U_k$ , the next point  $U_{k+1}$  is computed by following the geodesic through a search direction  $-H_k \in T_{U_k} \mathfrak{U}_n$ , as

$$U_{k+1} = \exp(-\mu H_k)U_k \text{ with } \mu = \arg\min J(Y, \exp(-\mu H_k)U_k, W).$$

The scalar  $\mu$  is choosen according to a line search algorithm presented in § 4.2.3.

• At  $U_{k+1}$ , the search direction is updated by combining the direction given by steepest descent gradient

$$G_{k+1} = \Gamma(U_{k+1})U_{k+1}^{H} - U_{k+1}\Gamma(U_{k})^{H}$$

and  $H_k$ . As  $G_{k+1} \in T_{U_{k+1}} \mathfrak{U}_n$  and  $H_k \in U_{T_k} \mathfrak{U}_n$ ,  $H_k$  a parallel transport is used, so that  $H_k$  is transformed into

$$H_k = H_k \exp(-\mu H_k) U_k = H_k U_{k+1}.$$

The new search direction is defined so that

$$-H_{k+1} = -G_{k+1} - \theta H_k$$
(10)

where  $\theta$  is selected so that  $H_{k+1}$  and  $\widetilde{H}_k$  are Hessian conjugate, that is

$$H_{k+1}^T$$
 Hess  $J(Y, U_{k+1}, W)\widetilde{H}_k = 0.$ 

The value of  $\theta$  is actually computed using the Polak-Ribière approximation [1, Eq. (10), § 2.4],

$$\theta = \frac{\Re \operatorname{Tr}((G_{k+1} - G_k)^H G_{k+1})}{\Re \operatorname{Tr} G_k^H G_k}.$$
(11)

#### 4.2.2 The gradient

Let us compute first the gradient of the distance  $d(y, u)^2$  given by (2) for two vectors y and u in  $\mathbb{C}^k$ . We note first that

$$\frac{\partial u_i}{\partial u_i^H} = 0 \text{ for } i \neq j, \ \frac{\partial \overline{u}_j}{\partial u_i^H} = 1 \text{ for } i \neq j \text{ and } \frac{\partial u_i \overline{u}_i}{\partial u_i^H} = u_i.$$

Therefore,

$$\frac{\partial d(y,u)^2}{\partial u_i^H} = -\sum_{p=1}^k \overline{y}_p u_p y_i = -(y^H \cdot u) y_i.$$

Applied to the cost function,

$$\frac{\partial J(Y, U, W)}{\partial U_{r,c}^{H}} = -\sum_{i=1}^{n} W_{c,i} ((Y_{\bullet i})^{H} \cdot U_{\bullet c}) Y_{r,i} = -\sum_{i=1}^{n} \sum_{j=1}^{k} W_{c,i} (Y^{H}U)_{i,c} Y_{r,i}.$$

#### 4.2.3 The line search

The line search algorithm consists in finding the minimal point of the cost function along a geodesic curve. More precisely, of

$$G(\mu) = J(Y, \exp(-\mu H)U, W)$$

for a direction  $H \in \mathfrak{u}_n$ , as  $\mu \mapsto \exp(-\mu H)U$  is a geodesic passing through U in the direction HU.

Here, *H* is the *search direction*: it is either the steepest descent (computed from the Riemannian Gradient  $\nabla_{\mathfrak{U}} J(Y, U, W)$ ) given by (9)) or the conjugate gradient (see (10) and (11)).

We rewrite

$$G(\mu) = J(Y, (1+Z)U, W)$$
 with  $Z = \exp(-\mu H) - 1$ .

The cost function J is quadratic in U, so that there exists  $J_1$  linear and  $J_2$  bilinear on  $\mathfrak{M}_{k\times k}(\mathbb{C})$  such that

$$G(\mu) = G(0) + J_1 \cdot (\exp(-\mu H) - 1) + J_2 \cdot (\exp(-\mu H) - 1) \otimes (\exp(-\mu H) - 1).$$
(12)

Let us recall a standard result on the spectral decomposition of anti-Hermitian matrices.

**Lemma 5.** The spectrum of *H* is purely imaginary, so that  $\exp(-\mu H) = Q \operatorname{Diag}(e^{-\mu i\omega_1}, \dots, e^{-\mu i\omega_k})Q^H$  for  $\omega_1 \leq \dots \leq \omega_k$  and *Q* a unitary matrix.

It follows from the above property and (12) that  $G(\mu)$  is the linear superposition of function of type  $\mu \mapsto \exp(-\mu i \omega_i)$  and  $\mu \mapsto \exp(-2\nu i \omega_i)$ .

With  $\omega = \max_{i=1,...,k} |\omega_i|$ , we then restrict the search of the minimum of  $G(\mu)$  to the interval  $[0, 2\pi/q\omega]$  with q = 2, as  $G(\mu + 2\pi\omega)$  is close to  $G(\mu)$ .

With the chain rule and the definition of the Riemannian gradient,

$$G'(\mu) = -2\Re \operatorname{Tr} \left( \nabla_{\mathfrak{U}} J(Y, \exp(-\mu H)U, W) U^H \exp(-\mu H)^H H^H \right)$$

since the derivative of  $\mu \mapsto \exp(-\mu H)U$  is  $H \exp(-\mu H)U \in T_{\exp(-\mu H)U} \mathfrak{U}_n$ .

As the search direction imposes that G'(0) < 0, to find the minimum of  $G(\mu)$ , we look for the smallest zero-crossing of the derivative.

To avoid the high cost of computing the exponential  $\exp(-\mu H)$  too frequently, we use a polynomial approximation of  $G'(\mu)$ . Thus,  $G'(\mu)$  is evaluated at the *P* spaced point  $\mu_k = \frac{k\pi}{P_{\omega}}$ , k = 1, ..., P. Hence,

$$\exp(-\mu_k G) = \exp(-\mu_1 G)^k$$
 for  $k = 1, ..., P$ .

With the approximation

$$G'(\mu) \approx G'(0) + \sum_{k=1}^{P} a_k \mu^k,$$

we obtain

$$G'(\mu_i) \approx G'(0) + \sum_{k=1}^{P} a_k \mu_i^k$$
 for  $i = 1, ..., P$ 

The  $a_i$  are then found by solving the linear system

$$\begin{bmatrix} G'(\mu_1) - G'(0) \\ \vdots \\ G'(\mu_P) - G'(0) \end{bmatrix} = \begin{bmatrix} \mu_1 & \cdots & \mu_1^P \\ \vdots & \vdots & \vdots \\ \mu_k & \cdots & \mu_k^P \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_P \end{bmatrix}.$$

The line search algorithm returns the smallest positive root of  $a_0 + a_1\mu + \dots + a_p\mu^P = 0$  if it exist. Otherwise, it returns 0, and a new direction is computed.

## References

- T. Abrudan, J. Eriksson, and V. Koivunen. "Conjugate gradient algorithm for optimization under unitary matrix constraint". In: *Signal Processing* 89.9 (Sept. 2009), pp. 1704–1714. DOI: 10.1016/ j.sigpro.2009.03.015.
- [2] S. E. Atev. "Using Asymmetry in the Spectral Clustering of Trajectories". University of Minnesota, 2011.
- [3] P. Blanchard, D. J. Higham, and N. J. Higham. *Accurate Computation of the Log-Sum-Exp and Softmax Functions*. 2019. arXiv: 1909.03469.
- [4] M. Brand and K. Huang. "A unifying theorem for spectral embedding and clustering". In: AISTATS. 2003.
- [5] A. Edelman, T. A. Arias, and S. T. Smith. "The Geometry of Algorithms with Orthogonality Constraints". In: SIAM Journal on Matrix Analysis and Applications 20.2 (Jan. 1998), pp. 303–353. DOI: 10.1137/s0895479895290954.
- [6] U. von Luxburg. "A tutorial on spectral clustering". In: *Statistics and Computing* 17.4 (Dec. 2007), pp. 395–416. DOI: 10.1007/s11222-007-9033-z.