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Asymmetric Spectral clustering

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Abstract This report presents the mathematical foundation of the asymmetric spectral clustering 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 Embedding

1 Introduction

A spectral clustering technique consists in assigning one cluster among k for a set of n data with $k \lll n$. 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, \dots, 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, $k \lll n$. This data reduction step uses the spectral information contained in A .

$\llbracket k, n \rrbracket$	Interval for integers	$\{k, \dots, n\}$
$\mathfrak{M}_{p \times q}(\mathbb{K})$	<i>Matrices</i> with p rows and q columns with coefficients in $\mathbb{K} = \mathbb{R}, \mathbb{C}$	
$\text{Tr } M$	Trace of $M \in \mathfrak{M}_{n \times n}(\mathbb{K})$	$\sum_{i=1}^n M_{ii}$
$M_{\bullet i}$	i -th column	$M_{\bullet i} = \begin{bmatrix} M_{1,i} \\ \vdots \\ M_{n,i} \end{bmatrix}$
$M_{i\bullet}$	i -th row	$M_{i\bullet} = [M_{1,i} \ \dots \ M_{n,i}]$
M^T	Transpose of $M \in \mathfrak{M}_{p \times q}(\mathbb{K})$	$M^T = (M_{j,i})_{\substack{i \in \llbracket 1, p \rrbracket \\ j \in \llbracket 1, q \rrbracket}}$
M^H	Hermitian transpose of $M \in \mathfrak{M}_{p \times n}(\mathbb{C})$	$M^H = \overline{M}^T$
$u \cdot_{\mathbb{R}} v$	Scalar product of $u, v \in \mathbb{C}^d$	$\sum_{i=1}^d u_i v_i = u^T v$
$u \cdot v$	Hermitian scalar product of $u, v \in \mathbb{C}^d$	$u \cdot v = u^T \cdot_{\mathbb{R}} \bar{v}$
$u \otimes v$	Tensor product $u \otimes v \in \mathfrak{M}_{k \times n}(\mathbb{C})$	$u \otimes v = uv^T$
\mathfrak{S}_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 $U^H U = \text{Id}$	
\mathfrak{u}_n	Lie algebra of unitary matrices 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 $\{u_1, \dots, u_k\}$ on \mathbb{R}^k or \mathbb{C}^k . This matrix is selected to minimize the overall distance between the columns vectors of Y , seen as elements of \mathbb{R}^k , and the rays emanating from 0 in one of the direction u_i . If the j -th column vector of Y is closest to the line in the direction u_i than in any other direction u_ℓ , $\ell \neq i$, then we assign the data x_j 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 $H : \mathfrak{M}_{n \times n}(\mathbb{R}) \rightarrow \mathfrak{H}_n$ 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

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

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

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 principle. Other choices are possible [2, Table 3.2, p. 23].

Principle 1 (Spectral embedding step). Using Λ and V as in (1), we define

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

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

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

The matrix Y satisfies $Y A Y^* = \text{Id}$.

3.3 Transformation into an optimization problem

The problem is now rewritten as an optimization problem.

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

$$d(y, u) = \sqrt{y^T (\text{Id} - u \otimes \bar{u}) y}. \quad (2)$$

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 $i \in \llbracket 1, n \rrbracket$, where $\sigma : \llbracket 1, n \rrbracket \rightarrow \llbracket 1, k \rrbracket$. The cluster of the column i is given by $\sigma(i)$.

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

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

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

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

Principle 3. Fix $1 \leq k \leq n$. 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

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

The constraint (4) is relaxed into

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

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 $1 \leq k \leq n$. 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 (6) such that

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

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

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.

¹In [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

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

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

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

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

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

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

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

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

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

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. \square

As any element of $T_U \mathfrak{U}_n$ is written 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

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

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*

$$p_U^\perp(M) = M - UM^H U. \quad (8)$$

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 $W \in T_U \mathfrak{U}_n$. Using Lemma 3, this leads to (8). \square

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

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

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

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

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 μ is chosen 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 $H_k \in T_{U_k} \mathfrak{U}_n$, H_k a parallel transport is used, so that H_k is transformed into

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

The new search direction is defined so that

$$-H_{k+1} = -G_{k+1} - \theta \tilde{H}_k \quad (10)$$

where θ is selected so that H_{k+1} and \tilde{H}_k are Hessian conjugate, that is

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

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

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

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

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

Therefore,

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

Applied to the cost function,

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

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 $\nabla_U J(Y, U, W)$) given by (9)) or the conjugate gradient (see (10) and (11)).

We rewrite

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

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

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

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 $\exp(-\mu H) = Q \text{Diag}(e^{-\mu i \omega_1}, \dots, e^{-\mu i \omega_k}) Q^H$ 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 $\mu \mapsto \exp(-\mu i \omega_j)$ and $\mu \mapsto \exp(-2\nu i \omega_j)$.

With $\omega = \max_{i=1, \dots, k} |\omega_i|$, 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,

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

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 $\mu_k = \frac{k\pi}{P\omega}$, $k = 1, \dots, P$. Hence,

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

With the approximation

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

we obtain

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

The a_i are then found by solving the linear system

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

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.

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