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# Asymmetric Spectral clustering

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## **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 ℝ<sup>*k*</sup> (or ℂ<sup>*k*</sup>), 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  $\vec{A}$  into a  $\vec{k} \times \vec{n}$  matrix  $\vec{Y}$  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 $p$ rows and $q$ columns with coefficients in $K = \mathbb{R}, \mathbb{C}$	
Tr M	Trace of $M \in \mathfrak{M}_{n \times n}(\mathbb{K})$	$\sum_{i=1}^n M_{ii}$
$M_{\bullet i}$	$i$ -th column	$\label{eq:matrixM} \begin{aligned} M_{\bullet i} &= \begin{bmatrix} M_{1,i} \\ \vdots \\ M_{n,i} \end{bmatrix} \\ M_{i\bullet} &= \begin{bmatrix} M_{1,i} & \cdots & M_{n,i} \end{bmatrix} \end{aligned}$
$M_{i_{\bullet}}$	$i$ -th row	
$M^T$	<i>Transpose</i> of $M \in \mathfrak{M}_{p \times q}(\mathbb{K})$	$M^T = (M_{i,i})_{i \in [1,p]}$
$M^H$	<i>Hermitian transpose</i> of $M \in \mathfrak{M}_{n \times n}(\mathbb{C})$	$M^H = \overline{M}^T \overset{j \in [\![1,q]\!]}{\leq}$
$u \cdot_{\mathbb{R}} v$	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 $u, v \in \mathbb{C}^d$	$u \cdot v = u^T \cdot_{\mathbb{R}} \overline{v}$
$u \otimes v$	Tensor product $u \otimes v \in \mathfrak{M}_{k \times n}(\mathbb{C})$	$u \otimes v = uv^T$
$\mathfrak{H}_n$	<i>Hermitian matrices</i> 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 $U^HU = Id$	
$\mathfrak{u}_n$	Lie algebra of <i>unitary matrices</i> of $\mathfrak{M}_{n \times n}(\mathbb{C})$ , charac- terized 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  $\{u_1, \ldots, u_k\}$  on  $\mathbb{R}^k$  or  $\mathbb{C}^k$ . This matrix is selected to minimaize 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  $u_e$ ,  $e \ni$ , 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*  $H : \mathfrak{M}_{n \times n}(\mathbb{R}) \to \mathfrak{H}_n$  *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  $V_{\boldsymbol{i}i}$ .

#### **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 dimensension 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

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

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

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

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

$$
d(y, u) = \sqrt{\overline{y}^T (\text{Id} - u \otimes \overline{u}) y}.
$$
 (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  $d(Y_{i}, U_{\sigma(i)})$  is minimal for each  $i \in [\![1, n]\!]$ , where  $\sigma : [\![1, n]\!] \to [\![1, k]\!]$ .<br>The cluster of the column *i* is given by  $\sigma(i)$ . 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

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

**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

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

The constraint (4) is relaxed into

$$
0 \le W_{i,j} \le 1
$$
 and  $\sum_{j=1}^{k} W_{j,i} = 1$  for  $i = 1, ..., n$ . (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  $1 \leq k \leq n$ . Given *Y* ∈  $\mathfrak{M}_{k,n}(\mathbb{R})$ , 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 (6). (7)

The cluster for the column *i* of *Y* is given by arg max<sub> $1 \le i \le k$ </sub>  $W_{i,i}$ 

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

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

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

**Lemma 3.** *For*  $M \in \mathfrak{M}_{n \times n}(\mathbb{C})$ *, write*  $M_a = \frac{1}{2}$  $\frac{1}{2}(M - M^H)$ . 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  $M_s = \frac{1}{2}$  $\frac{1}{2}(M + M^H)$  which is Hermitian and  $M_a$  which is anti-Hermitian.

As any element of  $T_U \mathcal{U}_n$  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

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

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* 

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

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

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

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

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),

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

 $\bullet$  At  $U_k$ , the next point  $U_{k+1}$  is computed by following the geodesic through a *search direction* −*H*<sub>k</sub> ∈  $T_{U_k}$ ,  $\mathfrak{U}_n$ , 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

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

The new search direction is defined so that

$$
-H_{k+1} = -G_{k+1} - \theta \widetilde{H}_k
$$
\n<sup>(10)</sup>

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

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

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

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

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

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*  $\omega_1 \leq \cdots \leq \omega_k$  *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  $\omega = \max_{i=1,...,k} |\omega_i|$ , 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,

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

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  $\mu_k = \frac{k\pi}{R}$  $\frac{k\pi}{P\omega}$ ,  $k = 1, \ldots, P$ . 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  $a_0 + a_1 \mu + \cdots + a_p \mu^p = 0$  if it exist. Otherwise, it returns 0, and a new direction is computed.

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