On the Existence of Kernel Function for
Kernel-Trick of k-Means

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Abstract. This paper corrects the proof of the Theorem 2 from the Gower’s paper [3, page 5]. The correction is needed in order to establish the existence of the kernel function used commonly in the kernel trick e.g. for k-means clustering algorithm, on the grounds of distance matrix. The scope of correction is explained in section 2.

1 The background problem

Kernel based $k$-means clustering algorithm (clustering objects $1,...,m$ into $k$ clusters $1,...,k$) consists in switching to a multidimensional feature space $\mathcal{F}$ and searching therein for prototypes $\mu^\Phi_j$ minimizing the error

$$
\sum_{i=1}^{m} \min_{1 \leq j \leq k} ||\phi(i) - \mu^\Phi_j||^2
$$

where $\phi : \{1,\ldots,m\} \rightarrow \mathcal{F}$ is a (usually non-linear) mapping of the space of objects into the feature space. In analogy to the classical k-means algorithm, the prototype vectors are updated according to the equation

$$
\mu^\Phi_j = \frac{1}{n_j} \sum_{i \in C_j} \phi(i)
$$

where $n_j$ is the cardinality of the $j$-th cluster. A direct application of this equation is not possible unless the function $\phi$ is known. But it may be still feasible if we would know the so-called Kernel Matrix $K$ with elements being dot products of data points in the feature space, that is $k_{ij} = \phi(i)^T \phi(j) = K(i,j)$. Given matrix $K$, it is possible to compute the distances between the object images and prototypes in the feature space by making use of so-called called ”the kernel trick”. The ”kernel trick” relies on the fact that the following transformation is possible:

$$
||\phi(i) - \mu^\Phi_j||^2 = k_{ii} - 2 \frac{1}{n_j} \sum_{i \in C_j} k_{hi} + \frac{1}{n_j} \sum_{r \in C_j} \sum_{s \in C_j} k_{rs}
$$

1 For an overview of kernel $k$-means algorithm see e.g. [2].
where, as already stated, \( k_{ij} = \Phi(i)^T\Phi(j) = K(i,j) \).

In this way, one can update the elements of clusters without determining the prototypes explicitly.

But the question should be raised what properties the kernel matrix should have in order to

(1) be really a matrix of dot products and
(2) to enable to recover function \( \Phi() \) at the data points from the kernel matrix.

These questions may seem to be pretty easy and were partially addressed e.g. by Schölkopf \[8\]. Let \( Y \) be a matrix \( Y = (\Phi(1), \Phi(2), \ldots, \Phi(m))^T \). Then apparently \( K = YY^T \). Hence for any non-zero vector \( u \) \( u^T Ku = u^T YY^T u = (Y^T u)(Y^T u) = y^T y \geq 0 \) where \( y = Y^T u \) so \( K \) must be positive semidefinite. But a matrix is positive semidefinite iff all its eigenvalues are non-negative. Furthermore, all its eigenvectors are real numbers.

So to identify \( \Phi() \) at data points, one has to find all eigenvalues \( \lambda_l \), \( l = 1, \ldots, m \) and corresponding eigenvectors \( v_l \) of the matrix \( K \). If all eigenvalues are hereby non-negative, then construct the matrix \( Y \) that has as columns the products \( \sqrt{\lambda_l} v_l \). Rows of this matrix (up to permutations) are the values of the function \( \Phi() \) at data points \( 1, \ldots, m \). More formally, if the matrix \( V = (v_1, \ldots, v_m) \), and \( A \) is the vector of eigenvalues, then

\[
Y = V \text{diag}(\sqrt{A})
\]  

where \( \text{diag}(\cdot) \) turns a vector to diagonal matrix. It may be verified that kernel-\( k \)-means with the above \( K \) and ordinary \( k \)-means for \( Y \) would yield same results.

Closely related is the following issue: For algorithms like \( k \)-means, instead of the kernel matrix the distance matrix \( D \) between the objects may be available, being the Euclidean distance matrix in the feature space. We will call \( D \) Euclidean matrix. The question is now:

(3) can we obtain the matrix \( K \) from such data?
(4) can we obtain from the matrix \( K \) the function \( \Phi() \) such that the distances in the feature space are exactly the same as given by the \( D \) matrix?
(4) if we derived the matrix \( K \) from \( D \) and \( K \) turns out to yield \( \Phi() \), can we know then that \( D \) was really an Euclidean distance matrix?

A number of transformations yielding the kernel matrix has been proposed. The answer to the third question seems to be easily derivable from the paper by Balaji et al. \[1\]. One should use the transformation

\[
K = -\frac{1}{2}(I - \frac{11^T}{m})D_{sq}(I - \frac{11^T}{m})
\]

\[2\] Schölkopf investigates what kinds of kernel functions may lead to a distance measure in the feature space. However, he does not consider the inverse, that is Euclidean distance matrix leading to a kernel function. He does not investigate finding explicit form of the \( \Phi \) function either. He considers also \( k_{ii} \neq 0 \) which means clearly that this kernel matrix cannot be a matrix of dot products.
(where $D_{sq}$ is a matrix containing as entries squared distances from $D$) a result going back to a paper by Schoenberg [6]. The problem is that this paper of Schoenberg does not contain any such statement.

A generally accepted proof of a more general transformation can be found in the paper by Gower [3, Theorem 2, page 5], who generalizes the above result of Schoenberg [7] to

$$K = (I - 1s^T)(-\frac{1}{2} D_{sq})(I - s1^T)$$

for an appropriate choice of $s$.

But a direct inspection of the proof shows that this proof is not complete.

Hence the subsequent communication demonstrates how the transformation shall be formulated and proves the validity of such a formulation.

2 Gower formulation

Let us recall that a matrix $D \in \mathbb{R}^{m \times m}$ is an Euclidean distance matrix between points $1, \ldots, m$ if and only if there exists a matrix $X \in \mathbb{R}^{m \times n}$ rows of which $(x_1^T, \ldots, x_m^T)$ are coordinate vectors of these points in an $n$-dimensional Euclidean space and

$$d_{ij} = \sqrt{(x_i - x_j)^T(x_i - x_j)} \tag{5}$$

Gower in [3] claims that

**Theorem 1.** $D$ is Euclidean iff the matrix $F = (I - 1s^T)(-\frac{1}{2} D_{sq})(I - s1^T)$ is positive semidefinite for any vector $s$ such that $s^T1 = 1$ and $D_{sq}s \neq 0$

whereas in [5] he claims:

**Theorem 2.** $D$ is Euclidean iff the matrix $F = (I - 1s^T)(-\frac{1}{2} D_{sq})(I - s1^T)$ is positive semidefinite for any vector $s$ such that $s^T1 = 1$.

Apparently both claims do not match quite (with respect to condition $D_{sq}s \neq 0$). It must be underlined, however, that the paper [3] provides strong clues how the theorem 2 shall be proven, though incompletely, so that it what follows we use these clues to establish the result.

What we claim here is that the Gower’s theorem has the following deficiencies

- requirement $D_{sq}s \neq 0$ is not needed in Theorem 1
- the if-part of neither Theorem 1 nor of Theorem 2 was demonstrated.

It shall be noted at this point, that in a 1985 paper Gower [4] derives his theorem in the latter version from a paper by Schoenberg [7]. The problem is that first of all Gower’s result does not need this second derivation and second the paper by Schoenberg [7] does not prove what Gower [4] claims. So the issue is open and we want to address it here more thoroughly.
3 Correction of [3]

For construction purposes we need still another formulation of the theorem, which is slightly more elaborate:

**Theorem 3.** 1. if \( D \) is Euclidean then for each vector \( s \) such that \( s^T 1 = 1 \), the matrix
\[
F = (I - 1s^T)(-\frac{1}{2})D_{sq}(I - s1^T)
\] (6)
is positive semidefinite
2. if \( D \) is a symmetric matrix with zero diagonal and for a vector \( s \) such that \( s^T 1 = 1 \), the matrix \( F = (I - 1s^T)(-\frac{1}{2})D_{sq}(I - s1^T) \) is positive semidefinite then \( D \) is Euclidean
3. if \( D \) is Euclidean then for each vector \( s \) such that \( s^T 1 = 1 \) the matrix \( D \) can be derived from matrix \( F = (I - 1s^T)(-\frac{1}{2})D_{sq}(I - s1^T) \) as \( d_{ij}^2 = f_{ii} + f_{jj} - 2f_{ij} \)
4. if \( D \) is Euclidean then for each vector \( s \) such that \( s^T 1 = 1 \) then matrix \( F = (I - 1s^T)(-\frac{1}{2})D_{sq}(I - s1^T) \) can be expressed as \( F = YY^T \) where \( Y \) is a real-valued matrix, and the rows of \( Y \) can be considered as coordinates of data points the distances between which are those from the matrix \( D \).

Let \( D \in \mathbb{R}^{m \times m} \) be a matrix of Euclidean distances between objects. Let \( D_{sq} \) be a matrix of squared Euclidean distances \( d_{ij}^2 \) between objects with identifiers \( 1, \ldots, m \). This means that there must exist a matrix \( X \in \mathbb{{R}^{m \times n}} \) for some \( n \), rows of which represent coordinates of these objects in an \( n \)-dimensional space. This real-valued matrix \( X \) represents an embedding of the Euclidean distance matrix \( D \) into \( \mathbb{R}^{m \times n} \). A distance matrix can be called Euclidean if and only if an embedding exists. If \( E = XX^T \) (\( E \) with dimensions \( m \times m \)), then \( d_{ij}^2 = e_{ii} + e_{jj} - 2e_{ij} \).

As a rigid set of points in Euclidean space can be moved (shifted, rotated, flipped symmetrically\(^3\)) without changing their relative distances, there may exist many other matrices \( Y \) rows of which represent coordinates of these same objects in the same \( n \)-dimensional space after some isomorphic transformation. Let us denote the set of all such embeddings \( \mathcal{E}(D) \). And if a matrix \( Y \in \mathcal{E}(D) \), then for the product \( F = YY^T \) we have \( d_{ij}^2 = f_{ii} + f_{jj} - 2f_{ij} \). We will say that \( F \in \mathcal{E}_{dp}(D) \).

For an \( F \in \mathcal{E}_{dp}(D) \) define a matrix \( G = F + \frac{1}{2}D_{sq} \). Hence \( F = G - \frac{1}{2}D_{sq} \). Obviously then
\[
d_{ij}^2 = f_{ii} + f_{jj} - 2f_{ij}
\] (7)
\[
= (g_{ii} - \frac{1}{2}d_{ii}^2) + (g_{jj} - \frac{1}{2}d_{jj}^2) - 2(g_{ij} - \frac{1}{2}d_{ij}^2)
\] (8)
\[
= g_{ii} + g_{jj} - 2g_{ij} + d_{ij}^2
\] (9)
(as \( d_{jj} = 0 \) for all \( j \)). This implies that
\[
0 = g_{ii} + g_{jj} - 2g_{ij}
\] (10)

\(^3\) Gower does not consider flipping.
that is
\[ g_{ij} = \frac{g_{ii} + g_{jj}}{2} \]  
(11)

So \( G \) is of the form
\[ G = g1^T + 1g^T \]  
(12)

with components of \( g \in \mathbb{R}^m \) equal \( g_i = \frac{1}{2}g_{ii} \).

Therefore, to find \( F \in \mathcal{E}_{dp}(D) \) for an Euclidean matrix \( D \) we need only to consider matrices deviating from \(-\frac{1}{2}D_{sq}\) by \( g1^T + 1g^T \) for some \( g \). Let us denote with \( \mathcal{G}(D) \) the set of all matrices \( F \) such that \( F = g1^T + 1g^T - \frac{1}{2}D_{sq} \).

So for each matrix \( F \) if \( F \in \mathcal{E}_{dp}(D) \) then \( F \in \mathcal{G}(D) \), but not vice versa. We stress that we work with an Euclidean matrix \( D \) So we would like to find an \( F \) such that \( F \) is decomposable into real-valued matrices \( Y \) such that \( F = YY^T \) so that \( Y \) would represent an embedding of an Euclidean distance matrix. But first of all even if \( D \) is not Euclidean, or even not metric, such an embedding may be found. As Gower et al. [5] states, see their Theorem 1, any non-metric dissimilarity measure \( d(\mathbf{j}, \mathbf{\eta}) \) for \( \mathbf{j}, \mathbf{\eta} \in \mathcal{X} \) where \( \mathcal{X} \) is finite, can be turned into a (metric) distance function \( d'(\mathbf{j}, \mathbf{\eta}) = d(\mathbf{j}, \mathbf{\eta}) + c \) where \( c \) is a constant where \( c \geq \max_{\mathbf{j}, \mathbf{\eta} \in \mathcal{X}} \|d(\mathbf{j}, \mathbf{\eta}) + d(\mathbf{\eta}, \mathbf{\zeta}) - d(\mathbf{j}, \mathbf{\zeta})\| \).

Furthermore, Gower et al. [5] recall that any dissimilarity matrix \( D \) may be turned to an Euclidean distance matrix, see their Theorem 7, by adding an appropriate constant, e.g. \( d'(\mathbf{j}, \mathbf{\eta}) = \sqrt{d(\mathbf{j}, \mathbf{\eta})^2 + h} \) where \( h \) is a constant such that \( h \geq -\lambda_m \), \( \lambda_m \) being the smallest eigenvalue of \((I - 11^T/m)(-1/2D_{sq})(I - 11^T/m)\), \( D_{sq} \) is the matrix of squared values of elements of \( D \), \( m \) is the number of rows/columns in \( D \). Obviously also, even if \( D \) is actually an Euclidean distance matrix, and \( F = -\frac{1}{2}D_{sq} \) by \( g1^T + 1g^T \), there is no warranty, that the distance matrix induced by corresponding \( Y \) is identical with \( D \).

For an \( F \in \mathcal{G}(D) \) consider the matrix \( F^* = (I - 1s^T)F(I - 1s^T)^T \). We obtain
\[
F^* = (I - 1s^T)F(I - 1s^T)^T 
= (I - 1s^T)(1g^T + g1^T - \frac{1}{2}D_{sq})(I - 1s^T)^T 
= (I - 1s^T)1g^T(I - 1s^T)^T + (I - 1s^T)g1^T(I - 1s^T)^T - \frac{1}{2}(I - 1s^T)D_{sq}(I - 1s^T)^T 
\]
(15)

Let us investigate \((I - 1s^T)1g^T(I - 1s^T)^T\):
\[
(I - 1s^T)1g^T(I - 1s^T)^T = 1g^T - 1g^Ts1^T - 1s^T1g^T + 1s^T1g^Ts1^T 
\]
(16)

Let us make the following choice (always possible) of \( s \) with respect to \( g \):
\[ s^T1 = 1, s^Tg = 0. \]

Then we obtain from the above equation
\[
(I - 1s^T)1g^T(I - 1s^T) = 1g^T - 1g^T1s1^T - 1s^T1g^T + 1s^T1g^Ts1^T = 00^T 
\]
(17)

By analogy...
exist a positive semidefinite matrix $F$, then there exists an $s$ from $M$ such that

$$ \mathbf{v}$$

is shifted to a new location in the Euclidean space. So the distances between objects computed is the same as those from $Y$, hence if $F \in \mathcal{E}_{dp}(D)$, then $Y^* \in \mathcal{E}(D)$.

Therefore, to find a matrix $F \in \mathcal{E}_{dp}(D)$, yielding an embedding of $D$ in the Euclidean $n$ dimensional space we need only to consider matrices of the form $-\frac{1}{2} (I - 1s^T) D_sq(I - 1s^T)^T$, subject to the already stated constraint $s^T 1 = 1$, that is ones from $\mathcal{M}(D)$.

So we can conclude: If $D$ is a matrix of Euclidean distances, then there must exist a positive semidefinite matrix $F = -\frac{1}{2} (I - 1s^T) D_sq(I - 1s^T)^T$ for some vector $s$ such that $s^T 1 = 1$, $\text{det}((I - 1s^T)) = 0$ and $D_sq s \neq 0$. So if $D$ is an Euclidean distance matrix, then there exists an $F \in \mathcal{M}(D) \cap \mathcal{E}_{dp}(D)$.

Let us investigate other vectors $t$ such that $t^T 1 = 1$, Noted that

$$ (I - 1t^T)(I - 1s^T) = I - 1t^T - 1s^T + 1t^T 1s^T$$

$$ = I - 1t^T - 1s^T + 1s^T$$

$$ = I - 1t^T$$

Therefore, for a matrix $F \in \mathcal{M}(D)$

$$ (I - 1t^T)F(I - 1t^T)^T = -\frac{1}{2} (I - 1t^T)(I - 1s^T) D_sq(I - 1s^T)^T(I - 1t^T)^T$$

$$ = -\frac{1}{2} (I - 1t^T) D_sq(I - 1t^T)^T$$

But if $F = YY^T \in \mathcal{E}_{dp}(D)$, then

$$ F' = (I - 1t^T)F(I - 1t^T)^T$$

$$ = (I - 1t^T) YY^T (I - 1t^T)^T$$

$$ = (Y - 1(t^T Y)) (Y - 1(t^T Y))^T$$
and hence each \(-\frac{1}{2}(I - 1s^T)D_{sq}(I - 1s^T)^T\) is also in \(E_{dp}(D)\), though with a different placement (by a shift) in the coordinate systems of the embedded data points. So if one element of \(M(D)\) is in \(E_{dp}(D)\), then all of them are.

So we have established that: if \(D\) is an Euclidean distance matrix then there exists a decomposable matrix \(F = YY^T \in E_{dp}(D)\) which is in \(G(D)\), hence \(E_{dp}(D) \subset G(D)\). For each matrix in \(G(D) \cap E_{dp}(D)\) there exists a multiplicative form matrix in \(M(D) \cap E_{dp}(D)\). But if it exists, all multiplicative forms are there: \(M(D) \subset E_{dp}(D)\).

In this way we have proven points 1, 3 and 4 of the Theorem and also the only-if-part of Theorem of Gower.

However, two things remain to be clarified and are not addressed in Gower: the if-part of (given a matrix \(D\) such that \(-0.5(I - 1s^T)D_{sq}(I - 1s^T)^T\) is positive semidefinite, is \(D\) an Euclidean distance matrix? – see point 2 of the Theorem) and the status of the additional condition \(D_{sq}s \neq 0\) in Theorem 1.

Gower makes the following remark: \(F = (I - 1s^T)\left(-\frac{1}{2}D_{sq}\right)(I - s1^T)\) is to be positive semidefinite for Euclidean \(D\). However, for non-zero vectors \(u\)

\[
\begin{align*}
    u^TFu &= \frac{1}{2}u^T(I - 1s^T)D_{sq}(I - 1s^T)^Tu = \frac{1}{2}(I - 1s^T)^TuD_{sq}((I - 1s^T)^Tu) \\
    (29)
\end{align*}
\]

But \(D_{sq}\) is known to be not negative semidefinite, so that \(F\) would not be positive semidefinite in at least the following cases: \(\det((I - 1s^T)) \neq 0\) and \(D_{sq}s = 0\). Let us have a brief look at these conditions and why they are neither welcome nor actually existent:

1. Situation \(\det((I - 1s^T)) \neq 0\) is not welcome, because there exists a vector \(u'\) such that \(u'^TD_{sq}u' > 0\) and under \(\det((I - 1s^T)) \neq 0\) we could solve the equation \((I - 1s^T)^Tu = u'\) and thus demonstrate that for some \(u\) \(u^TFu < 0\):

   However this situation is impossible, because for \(F \in M(D)\) \((I - 1s^T)1 = 1 - 1 = 0\) which means that the rows are linearly dependent, hence \(\det((I - 1s^T)) = 0\) is guaranteed by earlier assumption about \(s\); so this concern by Gower needs to be dismissed as pointless.

2. Situation \(D_{sq}s = 0\) is not welcome, because then \(u^T(I - 1s^T)D_{sq}(I - 1s^T)^Tu = u^TD_{sq}(I - 1s^T)^Tu = u^Tu > 0\) and thus \(u^TFu < 0\), denying positive semidefiniteness of \(F\). Gower does not consider this further, but such a situation is impossible. Recall that because \(D\) is Euclidean, there must exist a vector \(v\) such that \(v^T1 = 1\) and \(F(v) = Yv^T = -frac{12}{1s^T}D_{sq}(I - 1v^T)\) is in \(E_{dp}(D)\). Hence for any \(s\) such that \(s^Tv = 1\) \((I - 1s^T)\left(-\frac{1}{2}D_{sq}\right)(I - s1^T)\) is positive semidefinite. This allows us to conclude that for such \(s\) \(Ds \neq 0\). Therefore if \(Ds = 0\) then \(s^Tv = 0\). What is more, if \(det(D) \neq 0\) then \(D_{sq}s = 0\) implies \(s = 0\), for which of course \(s^Tv = 0\).

\[\text{This means that there exists a matrix } X \text{ such that rows are coordinates of objects in an Euclidean space with distances as in } D\]
Hence the last assumption of if-part of Theorem 1 needs to be dropped as unnecessary which simplifies it to Theorem 2.

As we can see from the first point above, $F$, given by $F = -0.5(I - 1s^T)D_{sq}(I - 1s^T)^T$ does not need to identify uniquely a matrix $D$, as $(I - 1s^T)$ is not invertible. Though of course it identifies an Euclidean distance matrix.

Let us now demonstrate the missing part of Gower’s proof that $D$ is uniquely defined given a decomposable $F$.

So assume that for some $D$ (of which we do not know if it is Euclidean, but is symmetric and with zero diagonal), $F = -0.5(I - 1s^T)D_{sq}(I - 1s^T)^T$ and $F$ is decomposable that is $F = YY^T$. Let $D(Y)$ be the distance matrix derived from $Y$ (that is the distance matrix for which $Y$ is an embedding). That means $F$ is decomposable into properly distanced points with respect to $D(Y)$. And $F$ is in additive form with respect to it, that is $F \in G(D(Y))$. Therefore there must exist some $s'$ such that the $F' = -0.5(I - 1s'^T)D(Y)_{sq}(I - s'1^T)$ as valid multiplicative form with respect to $D(Y)$, and it holds that $F' = (I - 1s'^T)F(I - s'1^T)$. But recall that $(I - 1s^T)F(I - s'1^T) = (I - 1s'^T)((-0.5(I - 1s^T)D_{sq}(I - s1^T)(I - s'1^T) = -0.5((I - 1s'^T)(I - 1s^T))D_{sq}((I - 1s'^T)(I - 1s^T))^T = -0.5(I - 1s'^T)^TD_{sq}(I - s'1^T)$.

Hence $-0.5(I - 1s^T)D_{sq}(I - s1^T) = -0.5 (I - 1s'^T)D(Y)_{sq}(I - s'1^T)$.

So we need to demonstrate that for two symmetric matrices with zero diagonals $D, D'$ such that

$$-rac{1}{2}(I - 1s^T)D_{sq}(I - s1^T) = -rac{1}{2}(I - 1s^T)D'_{sq}(I - s1^T)$$

the equation $D = D''$ holds.

It is easy to see that

$$-rac{1}{2}(I - 1s^T)(D_{sq} - D'_{sq})(I - s1^T) = 00^T$$

Denote $\Delta = D_{sq} - D'_{sq}$.

$$(I - 1s^T)\Delta(I - s1^T) = 00^T$$

$$\Delta - 1s^T\Delta - \Delta s1^T + 1s^T\Delta s1^T = 00^T$$

With $\Delta$ denote the vector $\Delta s$ and with $c$ the scaler $s^T\Delta s$. So we have

$$\Delta - 1\Delta^T - \Delta 1^T + c11^T = 00^T$$

So in the row $i$, column $j$ of the above equation we have: $\delta_{ij} + c - \overline{\delta}_i - \overline{\delta}_j = 0$. Let us add cells $ii$ and $jj$ and subtract from them cells $ij$ and $ji$. $\delta_{ii} + c - \overline{\delta}_i - \overline{\delta}_i + \delta_{jj} + c - \overline{\delta}_j - \overline{\delta}_j - \delta_{ij} - c + \overline{\delta}_i + \overline{\delta}_j - \delta_{ji} - \delta_{ij} - \delta_{ji} = \delta_{ii} + \delta_{jj} - \delta_{ij} - \delta_{ji} = 0$. But as the diagonals of $D$ and $D'$ are zeros, hence $\delta_{ii} = \delta_{jj} = 0$. So $-\delta_{ij} - \delta_{ji} = 0$. But $\delta_{ij} = \delta_{ji}$ because $D, D'$ are symmetric. Hence $-2\delta_{ji} = 0$ so $\delta_{ji} = 0$. This means that $D = D'$. 
This means that $D$ and $D(Y)$ are identical. Hence decomposition of $F = -0.5(I - 1s^T)D_{sq}(I - 1s^T)^T$ is sufficient to prove Euclidean space embedding of $D$ and yields this embedding. This proves the if-part of Gower’s Theorem 1 and 2 and point 2 of Theorem 3.

4 A numerical example

Let us illustrate the process of generating a kernel matrix from a distance table and show that the distances between the objects in the feature space really match the distances of the original distance matrix.

We took a $n = 4$-dimensional data matrix with $m = 7$ objects.

$$X = \begin{pmatrix} 76 & 98 & 2 & 6 \\ 32 & 5 & 41 & 43 \\ 1 & 21 & 57 & 54 \\ 46 & 19 & 85 & 25 \\ 62 & 35 & 96 & 40 \\ 5 & 28 & 66 & 78 \\ 36 & 75 & 51 & 86 \\ 76 & 98 & 2 & 6 \end{pmatrix}$$

and derived from it an original Euclidean distance matrix

$$D = \begin{pmatrix} 116.1 & 129.9 & 120 & 119 & 138.6 & 104.5 & 0 \\ 0 & 39.9 & 51.5 & 69.5 & 55.7 & 82.9 & 116.1 \\ 39.9 & 0 & 60.4 & 75.1 & 26.9 & 72.1 & 129.9 \\ 51.5 & 60.4 & 0 & 29.3 & 70.2 & 90.1 & 120 \\ 69.5 & 75.1 & 29.3 & 0 & 75.1 & 80.1 & 119 \\ 55.7 & 26.9 & 70.2 & 75.1 & 0 & 58.8 & 138.6 \\ 82.9 & 72.1 & 90.1 & 80.1 & 58.8 & 0 & 104.5 \\ 116.1 & 129.9 & 120 & 119 & 138.6 & 104.5 & 0 \end{pmatrix}$$

We applied to it the transformation from equation [1] using the vector $s = [0.16, 0.28, 0.1, 0.07, 0.07, 0.2, 0.12, 0.16]^T$ and obtained the matrix

$$F = \begin{pmatrix} -1364.6 & -2934.7 & -1254.2 & -779.7 & -3802.8 & 728.3 & 9587.3 \\ 1158.6 & 495.5 & 400.9 & -332.6 & 39.3 & -1453.6 & -1364.6 \\ 495.5 & 1426.4 & 33.8 & -598.7 & 1366.2 & -487.7 & -2934.7 \\ 400.9 & 33.8 & 2295.3 & 2223.8 & -304.3 & -1509.2 & -1254.2 \\ -332.6 & -598.7 & 2223.8 & 3010.3 & -301.8 & -303.7 & -779.7 \\ 39.3 & 1366.2 & -304.3 & -301.8 & 2028.1 & 684.2 & -3802.8 \\ -1453.6 & -487.7 & -1509.2 & -303.7 & 684.2 & 2799.3 & 728.3 \\ -1364.6 & -2934.7 & -1254.2 & -779.7 & -3802.8 & 728.3 & 9587.3 \end{pmatrix}$$
After eigen-decomposition of $F$, we get via equation (4) the embedding matrix (after ignoring columns with next to zero eigenvalues)

$$Y = \begin{pmatrix}
97.5 & 4 & 4.6 & -6.2 \\
-14.9 & 9.3 & 26.5 & 12.1 \\
-31.1 & -10.3 & 11.6 & -14.7 \\
-14.9 & 44.7 & -5.9 & -6.6 \\
-8.1 & 43 & -33 & 1.9 \\
-38 & -21.5 & -9.8 & -5.2 \\
10.9 & -34.6 & -38.3 & 3.9 \\
97.5 & 4 & 4.6 & -6.2
\end{pmatrix}$$

which produces the distance matrix

$$D' = \begin{pmatrix}
116.1 & 129.9 & 120 & 119 & 138.6 & 104.5 & 0 \\
0 & 39.9 & 51.5 & 69.5 & 55.7 & 82.9 & 116.1 \\
39.9 & 0 & 60.4 & 75.1 & 26.9 & 72.1 & 129.9 \\
51.5 & 60.4 & 0 & 29.3 & 70.2 & 90.1 & 120 \\
69.5 & 75.1 & 29.3 & 0 & 75.1 & 80.1 & 119 \\
55.7 & 26.9 & 70.2 & 75.1 & 0 & 58.8 & 138.6 \\
82.9 & 72.1 & 90.1 & 80.1 & 58.8 & 0 & 104.5 \\
116.1 & 129.9 & 120 & 119 & 138.6 & 104.5 & 0
\end{pmatrix}$$

It can be easily seen that $D'$ is (nearly) identical with $D$, though the embeddings $X$ and $Y$ differ.

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