Numerical and Scientific Computing (CSL361) Take-home for Minor II
October 14, 2009

Note: You may submit by the end of the mid-semester break. Please include a declaration of originality. Please submit jointly if you collaborate on the entire problem with somebody else and please give credits if you obtain any part of your solutions from somebody else or some other source.

Consider the problem of drawing a map of n cities given the pair-wise distances between them.

More formally, we have n cities, an array D of the n^2 distances, $D_{ij} = dist(city_i, city_j)$ ($D_{ij} = D_{ji}$ with ordinary luck!), and we want to know if there are points P_i in the plane such that $dist(P_i, P_j) = D_{ij}$. We may also wish to find an appropriate "approximate solution" if such P_i's do not exist (perhaps by fudging a little).

Please do not despair. The situation is not that bad! Just read on...

Let us first see if there are such points in $\mathbb{R}^n$. If there are, we may shift the lot so that the center of mass is at origin. Then the distances can be related to the inner products in the following way. Assuming that $\sum_i P_i = 0$, you can show that the inner products are $P_i^t P_j = A_{ij}$, where

$$S_i = \frac{1}{n}\sum_{j=1}^{n} D_{ij}^2, \qquad T = \frac{1}{n^2}\sum_{i,j=1}^{n} D_{ij}^2, \qquad A_{ij} = -\frac{1}{2}\left(D_{ij}^2 - S_i - S_j + T\right)$$

Thus, if such $P_i \in \mathbb{R}^n$ can be found whose inner products are A_{ij}, we can readily compute that $dist(P_i, P_j) = D_{ij}$. Also if X is the matrix with the P_i's as columns, the problem reduces to one of finding if there is a X such that $A = X^t X$. Clearly, in such a case, A must be symmetric and positive definite, since if v is any vector in $\mathbb{R}^n$ then $v^t A v = (Xv)^t (Xv) \geq 0$. Is this related to triangular inequality?

So, now our (actually your) problem is as follows:
Given a symmetric matrix A, **(a)** how do we decide if there are n-dimensional vectors whose inner products are the entries of A? **(b)** How do we know if they lie in a plane? **(c)** How do we find them if they exist? and **(d)** fudge if they do not?

Here are a few **hints**: **(a)** positive definite symmetric matrices have an orthonormal basis of real eigenvectors and corresponding positive eigenvalues; (you may show this for A by considering the *SVD* of X) **(b)** if you want the points to lie on a plane, you want X to be a $2 \times n$ matrix; **(c)** same as **(a)**; **(d)** think of a galaxy of stars in $\mathbb{R}^3$. Some galaxies (like ours!), while contained in $\mathbb{R}^3$, are pretty close to being planar. Least-squares appears to be a good choice for projection on to a plane which will overall be close to preserving inter-point distances. Of-course you will have to find the "residual error" in such a case.

So now you can write out the formal solutions to **(a)**, **(b)**, **(c)** and **(d)** (not so hard after all!).

You can also throw some more light on the problem

1. Verify the relationship between $[D_{ij}]$ and $[A_{ij}]$. Can you think of a geometric interpretation?

2. Can you relate the necessary condition that A is positive definite to triangular inequality?

3. If the solution exists then it is normalized for translation. We have achieved this by putting the center of mass at origin. Can we normalize for rotation and reflection?

Will it help to show that X exists *iff* an upper-triangular X exists (with +ve diagonal entries) such that $X^t X = A$? Can we then say that if the solution exists then it is essentially unique (modulo rotation and translation which we can normalize). You may wish to read up about *Given's rotations*.

4. What does it mean if some eigenvalues of A are negative?

5. What if the matrix D is not symmetric (may be different measurements have made some $D_{ij} \neq D_{ji}$). Can we still approximate? Think in terms of SVD.