Computing The Best Positive Semi-Definite Approximation of a Symmetric Matrix Using a Flow

by

Kenneth R. Driessel

5 March 2007

INTRODUCTION

We work in the space Sym(n) of real symmetric matrices with the "Frobenius" (or "euclidean") inner product. We consider the following problem:

Problem: **Positive semi-definite approximation.** Given a matrix A in Sym(n), find the semi-definite matrix which is closest to A.

If $A = QDQ^T$ where Q is an orthogonal matrix and $D =$ Diag$(a_1 \geq a_2 \geq \cdots \geq a_n)$ is a diagonal matrix, then the product QDQ^T is called the **spectral decomposition of** A. The diagonal entries of D are the **eigenvalues of** A.

Proposition 1. *Assume that A has distinct nonzero eigenvalues. Let $A = QDQ^T$ be the spectral decomposition of A. Let $D^* :=$ Diag$(a_1 > a_2 > \cdots > a_k > 0, \ldots, 0)$ where k is the number of positive eigenvalues of A and let $A^* := QD^*Q^T$. Then A^* is the positive semi-definite matrix which most closely approximates A in the Frobenius norm.*

I describe a differential equation which proves this result and which computes the solution of the semi-definite approximation problem.

Let W be a real vector space with an inner product $\langle \cdot, \cdot \rangle$. Let S be a subset of W and let $f : S \to \mathbb{R}$ be a real-valued function on S. Then $m \in S$ is a **local minumum** of f on S, if there is a neighborhood N of m such that $f(m)$ is a minimum of f on N. I say that $f : S \to \mathbb{R}$ has the **unique local minimum property** if f is bounded below and has a unique local minimum. In this case the local minimum is also the global minimum. Usually an optimization problem has numerous (mostly undesirable) local minimums. An optimization problem with the unique local minimum property is an especially nice optimization problem.

Let WeakPos(n) denote the set of n-by-n positive semi-definite matrices. I show that if A has distinct non-zero eigenvalues then the function f : WeakPos$(n) \to \|X - A\|$ has the unique local minimum property.

SETTING UP THE DIFFERENTIAL EQUATION

Let $Gl(n)$ denote the general linear group of n by n, invertible, real matrices. Recall that two matrices X and Y in Sym(n) are **congruent** if there exists a matrix $G \in Gl(n)$ such that $Y = GXG^T$. Also recall that every matrix M in Sym(n) is congruent to a diagonal matrix with ones, minus ones and zeros on its main diagonal. The triple (r_+, r_-, r_0) where r_+, r_- and r_0 are the number of ones, minus ones and zeros respectively is the **inertia** of M.

We can use the group $Gl(n)$ to "parameterize" the matrices with fixed inertia as follows. We have the following group action:

$$Gl(n) \times \text{Sym}(n) \to \text{Sym}(n) : (G, X) \mapsto GXG^T.$$

For $M \in$ Sym(n), let Orbit(M) denote the orbit of M under this group action; in symbols, Orbit$(M) := \{GMG^T : G \in Gl(n)\}$.

Proposition 2. *Let (r_+, r_-, r_0) be a triple of natural numbers satifying $r_+ + r_- + r_0 = n$ and let M be any matrix with this inertia. Then the set of matrices with inertia (r_+, r_-, r_0) is the same as the orbit of M under the given group action; in symbols, Inert$(r_+, r_-, r_0) =$ Orbit(M) where Inert$(r_+, r_-, r_0) := \{X \in$ Sym(n) : Inertia$(X) = (r_+, r_-, r_0)\}$.*

Let Tan.Orbit$(M).B$ denote the space tangent to Orbit(M) at B.

Proposition 3. *Let M and B be matrices in Sym(n) with B on the orbit of M. Then the space tangent to the the orbit of M at B is given by*

$$\text{Tan.Orbit}(M).B = \{XB + BX^T : X \in \mathbb{R}^{n \times n}\}.$$

Proof. We simply compute the derivative of the parameterizing map. We have

$$D(G \mapsto GBG^T).I.X = XB + BX^T.$$

□

For symmetric matrix B, consider the following linear map:

$$L_B := \mathbb{R}^{n \times n} \to \text{Sym}(n) : X \mapsto XB + BX^T.$$

The range of this map equals the space tangent to the orbit of B at B.

Proposition 4. Adjoint of the tangent space map. *The adjoint L_B^* of the linear map L_B is the map Sym$(n) \to \mathbb{R}^{n \times n} : Y \mapsto 2YB$.*

Proof. We have

$$\langle L_B(X), Y \rangle = \langle XB + BX^T, Y \rangle = \langle X, YB^T \rangle + \langle X^T, B^T Y \rangle = \langle X, YB + (BY)^T \rangle.$$

□

I call the composition $L_B \circ L_B^*$ a "quasi-projection" map.

For A in Sym(n), we define the **objective function** f_A **determined by** A as the following function: Sym$(n) \to \mathbb{R} : X \mapsto (1/2)\langle X - A, X - A \rangle$.

Proposition 5. Gradient of the objective function. *Let A and B be matrices in $\mathbb{R}^{m \times n}$. The gradient of the objective function f_A at B is $B - A$; in symbols,*

$$\nabla f_A(B) = B - A.$$

We have a gradient vector field on Sym(n) defined by $X \mapsto \nabla f_A(X) = X - A$. But this vector field is generally not tangent to the constant inertia surfaces. In other words, the corresponding differential equation does not preserve inertia. We want to adjust the gradient vector field so that the corresponding vector field does preserve inertia. We can use the quasi-projection map to do so.

We now compute the quasi-projection of the negative gradient onto the tangent space. For B on the orbit of K, we have

$$(L_B \circ L_B^*)(-\nabla f_A(B)) = L_B(2(A - B)B) = (A - B)B^2 + B^2(A - B).$$

In the next section we use this formula to define a vector field on the space Sym(n). We then see that the corresponding differential equation provides a solution of the constrained optimization problem of interest.

PROPERTIES OF THE DIFFERENTIAL EQUATION

Let the vector field F on Sym(n) be defined by

$$F(X) := (1/2)(L_X \circ L_X^*)(A - X) = (A - X)X^2 + X^2(A - X).$$

We consider the differential equation associated with this vector field:

$$X' = F(X). \qquad (*)$$

Note that this differential equation is clearly inertia preserving since the vector $F(X)$ is tangent to the space Inertia$(X) =$ Orbit(X) at X.

The following proposition says that for any solution $X(t)$ of the differential equation (*), the distance between $X(t)$ and A decreases.

Proposition 6. Lyapunov function. *The objective function f_A is a Lyapunov function for the differential equation (*).*

Proof. Let $X(t)$ be any solution of (*). To simplify the notation, let $f := f_A$ and $L := L_X$. We have

$$\begin{aligned}(d/dt)(f(X(t)) &= (1/2)(d/dt)\langle X - A, X - A \rangle = \langle X - A, X' \rangle \\ &= \langle X - A, -(L \circ L^*)(X - A) \rangle = -\langle L^*(A - X), L^*(A - X) \rangle \leq 0.\end{aligned}$$

□

Proposition 7. Equilibrium conditions. *Let E be an element of Sym(n). Then the following conditions are equivalent:*

(i) E is an equilibrium point of the differential equation (*).
(ii) E satisfies the equations $AE = E^2$ and $EA = E^2$.
(iii) $A - E$ is orthogonal to the space tangent the orbit of E at E.
(iv) E is a critical point of the objective function.

Proposition 8. Commuting relations. *Let E be an equilibrium point of the differential equation (*). Then $AE = EA$.*

Proposition 9. *If the matrix A has distinct nonzero eigenvalues, then the differential equation (*) has isolated equilibrium points and solutions converge.*

Proof. Choose ann ortho-normal basis so that A is a diagonal matrix of ordered eigenvalues:

$$A = \text{Diag}(a_1 > a_2 > \cdots > a_n).$$

Claim: If a matrix E is an equilibrium point of the differential equation then E is a diagonal matrix.

Recall that E must satisfy $AE = EA$.

Claim: Let $E :=$ Diag$(e_1, \ldots, e_n)$ be an equilibrium point of the differential equation. Then, for $i = 1, 2, \ldots, n$, either $e_i = a_i$ or $e_i = 0$.

Since the vector field vanishes at E, we have

$$0 = (a_i - e_i)e_i^2 + e_i^2(a_i - e_i) = 2(a_i - e_i)e_i^2.$$

Claim: The solutions of the differential equation (*) converge.

Note that every solution stays in a compact set since the distance to A decreases. Hence the solutions cannot blow up. Also recall that a gradient flow with isolated equilibrium points converges. □

Proposition 10. Best semi-definite approximation. *Let $X(t)$ be the solution of the differential equation (*) with initial value $X(0) = M$ where M is a positive definite matrix. If A has distinct non-zero eigenvalues then the $X(t)$ converges to a limit $X(+\infty)$ which is the unique best semi-definite approximation of A.*

Proof. We want to classify the equilibrium points. We compute the linearization of the differential equation at E:

$$\begin{aligned}D.F.E.X &= -XE^2 + (A - E)(XE + EX) + (XE + EX)(A - E) - E^2X \\ &= (A - E)XE + EX(A - E) - XE^2 - E^2X.\end{aligned}$$

We regard $D.F.E$ as a linear map on the space tangent to the orbit of E at E. The nature of the equilibrium is determined by this linear map. In particular, the equilibrium point E is stable if the eigenvalues of this map are all negative. We want to see that exactly one of the equilibrium points has all eigenvalues negative (a stable situation) and that all of the other equilibrium points are unstable.

We have

$$(D.F.E.X)_{ij} = (a_i - e_i)x_{ij}e_j + e_i x_{ij}(a_j - e_j) - e_i^2 x_{ij} - x_{ij}e_j^2 = \alpha_{ij}x_{ij}$$

where $\alpha_{ij} := (a_i - e_i)e_j + e_i(a_j - e_j) - e_i^2 - e_j^2$. Note that $\alpha_{ij} = \alpha_{ji}$. These are the eigenvalues of $D.F.E$ and $E^{ij} + E^{ji}$ are corresponding eigenvectors.

Since the initial point M is positive definite, the solution $X(t)$ is positive definite for all positive t (by the invariance of inertia). Hence the limit $X(+\infty)$ must be positive semi-definite. It follows that we only need to consider positive semi-definite equilibrium points. These have the form Diag$(e_1, \ldots, e_k, 0, \ldots, 0)$ where k is the number of positive eigenvalues of A.

Claim: The diagonal matrix $E^* :=$ Diag$(a_1, \ldots, a_k, 0, \ldots, 0)$, where k is the number of positive eigenvalues of A, is a stable equilibrium point.

Simply compute the eigenvalues of $D.F.E^*$.

Claim: Let E be an equilibrium point that is different than E^*. Then E is unstable. In particular, every neighborhood of E contains a semi-definite diagonal matrix which is closer to A than E.

For $i = 1, \ldots, k$, let ϵ_i denote a small positive number if $e_i = 0$ and let $\epsilon_i = 0$ if $e_i = a_i$. Let $D :=$ Diag$(\epsilon_1, \ldots, \epsilon_k, 0, \ldots, 0)$. Consider the matrix $E + D$. Note that this matrix is positive semi-definite. Also note that

$$A - E = \text{Diag}(a_1 - e_1, \ldots, a_k - e_k, a_{k+1}, \ldots, a_n)$$

and

$$A - (E + D) = \text{Diag}(a_1 - (e_1 + \epsilon_1), \ldots, a_k - (e_k + \epsilon_k), a_{k+1}, \ldots, a_n).$$

If we choose the positive ϵ_i small enough to satisfy $\epsilon_i < a_i$ then $E + D$ is closer to A than E, since, for all $i = 1, \ldots, k$, either $a_i - e_i = 0$ (in case $e_i = a_i$) or $a_i - e_i > a_i - e_i - \epsilon_i = a_i - \epsilon_i > 0$ (in case $e_i = 0$). □

Examples

Example: We begin with the case $n = 1$. In this case we want to approximate a given number a by means of a weakly positive (that is, nonnegative) number. The differential equation reduces to the following scalar equation on the real line:

$$x' = 2(a - x)x^2.$$

A point e on is an equilibrium point if and only if $e = 0$ or $e = a$. The linearization of the differential equation at e is the following differential equation:

$$x' = -2e^2.$$

We assume that the initial condition is $x(0) = m$ where m is a positive number. We consider two cases. (We ignore the case $a = 0$.) If a is a positive number then the flow is to the limit point a. The eigenvalue is $-2a^2$ which is a stable situation. If a is a negative number then the flow is to the limit point 0.

Phase Portraits

Example: We consider the case $n = 2$. Let

$$A := \begin{pmatrix} a_1 & 0 \\ 0 & a_2 \end{pmatrix} \text{ and } X := \begin{pmatrix} x_1 & x_3 \\ x_3 & x_2 \end{pmatrix}.$$

Recall the differential equation (*):

$$X' = F(X) := (A - X)X^2 + X^2(A - X).$$

Note that

$$F\begin{pmatrix} x_1 & 0 \\ 0 & x_2 \end{pmatrix} = 2\begin{pmatrix} (a_1 - x_1)x_1^2 & 0 \\ 0 & (a_2 - x_2)x_2^2 \end{pmatrix}.$$

In terms of coordinates, if $x_3 = 0$ then the differential equation becomes

$$x_1' = 2(a_1 - x_1)x_1^2,$$
$$x_2' = 2(a_2 - x_2)x_2^2,$$
$$x_3' = 0.$$

In other words, the x_1x_2-plane $\{(x_1, x_2, 0) : x_1, x_2 \in \mathbb{R}\}$ is an invariant set. This set contains all the equilibrium points. Furthermore, if $x_2 = 0$ and $x_3 = 0$ then the differential equation becomes

$$x_1' = 2(a_1 - x_1)x_1^2,$$
$$x_2' = 0,$$
$$x_3' = 0.$$

In other words, the lines $\{(x_1, 0, 0) : x_1 \in \mathbb{R}\}$ and $\{(x_1, a_2, 0) : x_1 \in \mathbb{R}\}$ are invariant sets. Similarly, if $x_1 = 0$ and $x_3 = 0$ then the differential equation becomes

$$x_1' = 0,$$
$$x_2' = 2(a_2 - x_2)x_x^2,$$
$$x_3' = 0.$$

In other words, the lines $\{(0, x_2, 0) : x_2 \in \mathbb{R}\}$ and $\{(a_1, x_2, 0) : x_2 \in \mathbb{R}\}$ are invariant.

Phase Portraits

1 APPENDIX: FROBENIUS INNER PRODUCT

We use the "Frobenius" (or "euclidean") inner product in the space $\mathbb{R}^{m \times n}$ of m by n real matrices. For X and Y in this space, the **Frobenius inner product** is defined by

$$\langle X, Y \rangle := \text{Trace}(XY^T).$$

In terms of coordinates, $\langle X, Y \rangle = \sum\{X_{ij}Y_{ij} : i = 1, \ldots, m, j = 1, \ldots, n\}$. Here we review a few of the properties of this inner product.

Proposition 11. Adjoints of multiplication maps. *Let B and Z be elements of $\mathbb{R}^{m \times n}$.*

- *For $X \in \mathbb{R}^{m \times m}$, $\langle XB, Z \rangle = \langle X, ZB^T \rangle$.*
- *For $Y \in \mathbb{R}^{n \times n}$, $\langle BY, Z \rangle = \langle Y, B^T Z \rangle$.*

Proof. We have

$$\text{Trace}(XBZ^T) = \text{Trace}(X(ZB^T)^T)$$

and

$$\text{Trace}(BYZ^T) = \text{Trace}(YZ^T B) = \text{Trace}(Y(B^T Z)^T).$$

□

Proposition 12. Orthogonal invariance. *Let U be an m by m real orthogonal matrix and let V be an n by n real orthogonal matrix. Then, for all X and Y in $\mathbb{R}^{m \times n}$,*

- *$\langle UX, UY \rangle = \langle X, Y \rangle$ and*
- *$\langle XV, YV \rangle = \langle X, Y \rangle$.*

Proof. Use the result concerning the adjoints of multiplication maps.

□

REFERENCES

- Chu, M. (1984) *The generalized Toda flow, the QR algorithm, and the centre manifold theory*, SIAM J. Alg. Discr. Math. 5, 187-201.
- Chu, M. (1986) *A differential equation approach to the singular value decomposition of bidiagonal matrices*, Lin. Alg. Appl. 80, 71-80.
- Chu, M. and Driessel, K.R. (1990) *The projected gradient method for least squares approximation with spectral constraints*, SIAM J. Numerical Analysis 27, 1050-1060.
- Deift, P., Nanda, T. and Tomei, C. (1983) *Differential equations for the symmetric eigenvalue problem*, SIAM J. Numer. Analysis 20, 1-22.
- Demmel, J.W. (1997) *Applied Numerical Linear Algebra*, SIAM.
- Driessel, K.R. (2003) *On computing cannonical forms using flows*, Lin. Alg. Appl. 379, 353-379.
- Driessel, K.R. (2007) *A globally convergent flow for computing the best low rank approximation of a matrix*, http://www.arxiv.org, math.OC/07022621.
- Nanda, T. (1982) *Isospectral flows on band matrices*, Doctoral Dissertation, Courant Institute, New York.
- Nanda, T. (1985) *Differential equations and the QR algorithm*, SIAM J. Numer. Analysis 22, 310-321.
- Symes, W.W. (1982) *The QR algorithm and scattering for the finite nonperiodic Toda lattice*, Physica 4D, 275-280.
- Watkins, D.S. (1984) *Isospectral flows*, SIAM Review 26, 379-391.