The continuous-time Rayleigh quotient flow on the Grassmann manifold[a]

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Abstract

An extension of the Rayleigh quotient iteration (RQI) to the Grassmann manifold has been recently proposed for computing a p-dimensional eigenspace of a symmetric matrix A. Here we analyze a continuous-time flow analogous to this Grassmannian RQI. This flow achieves deflation in finite time, i.e. it converges in finite time to a subspace that includes an eigenvector of A.

1 Introduction

One of the 'classical' numerical methods used to compute a single eigenvalue, eigenvector pair for a symmetric matrix A is the *Rayleigh Quotient Iteration* [Par98]. The Rayleigh quotient iteration is also important since it is closely related to the shifted QR-algorithm, an important tool in most numerical routines used to compute eigen-decompositions of symmetric matrices (cf. Watkins [Wat82] for an excellent review of the QR algorithm).

A generalization of the RQI to the Grassmann manifold $\mathrm{Gr}(p, n)$ has been proposed in [AMSV02] for computing a p-dimensional invariant subspace of a symmetric matrix A. The generalized method involves the solution of a Sylvester equation at each iteration step for a numerical cost of $O(np^2)$. The property of cubic convergence of the RQI is retained in the generalized algorithm.

Since the early eighties there has been considerable interest in studying continuous-time flows related to algebraic iterations. The result that ignited interest in such flows was when iterates of the unshifted QR-algorithm were shown to be unit time samples of a particular Lax-pair equation [Fla74, Sym82, DNT83, Nan85]. This work sparked extensive research on

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using dynamical systems to solve linear algebraic problems [Bro89, WE88, Chu88, CD90, HM94].

A continuous-time differential equation analogous to the (classical) Rayleigh Quotient Iteration for a symmetric matrix A is studied in [MA01]. The set of all continuous solutions, termed the Rayleigh quotient flow, is shown to be a scaled version of the Newton flow for Rayleigh quotient cost functional. The scaling factor ensures that the rate of variation of the Rayleigh quotient is constant and positive along solutions. This interpretation leads to a precise phase portrait for Rayleigh quotient flow. In particular, it is shown that complete solutions of the Rayleigh quotient flow visit the eigenvectors of A in ascending order.

In the present paper, the analysis that was carried out on the sphere S^{n-1} in [MA01] is extended to the Grassmann manifold $\mathrm{Gr}(p, n)$. Namely, we consider the flow generated by the generalized Rayleigh quotient direction on the noncompact Stiefel manifold $\mathrm{ST}(p, n)$ (i.e. the set of n-by-p matrices with full column rank). This flow is shown to belong to a class of flows on $\mathrm{ST}(p, n)$ that induce a given flow on $\mathrm{Gr}(p, n)$ through the "column span" mapping from $\mathrm{ST}(p, n)$ onto $\mathrm{Gr}(p, n)$. This flow is termed the Grassmann-Rayleigh Quotient Flow (GRQF).

The connection with the Newton flow is not retained when $p > 1$, but the property of constant variation of the Rayleigh quotient is still valid for the Ritz values associated to the solutions. Moreover, for most initial conditions, if $\mathcal{Y}(t)$ is a solution of the GRQF, then there exists a finite time t^* such that $\mathcal{Y}(t^*)$ (which is an element of $\mathrm{Gr}(p, n)$, that is a p-dimensional subspace of $\mathbb{R}^n$) contains an eigenvector of A. This leads to a continuous-time flow achieving deflation.

2 The power method flow and the Rayleigh quotient flow

Because the Rayleigh quotient flow is derived from the power method, we begin this section with a brief reminder of the power method and the associated flows.

The *power method* [Par98] defines a discrete flow on the sphere S^{n-1}:

$$x_{k+1} = \frac{Ax_k}{|Ax_k|}, \quad x_0 \in S^{n-1}, \tag{2.1}$$

where $|\cdot|$ denotes the Euclidean 2-norm in $\mathbb{R}^n$. The discrete flow (almost) always converges to the maximal (in absolute value) eigenvalue, eigenvector pair of the n-by-n symmetric matrix A. The iteration (2.1) is defined on the sphere S^{n-1} but can be interpreted as a discrete-time dynamical system on the *real projective space* $\mathbb{RP}^{n-1}$, i.e. the set of one-dimensional linear subspaces of $\mathbb{R}^n$ [HM94, AMSV02].

A natural generalization of $\mathbb{RP}^{n-1}$ is the *Grassmann manifold* $\mathrm{Gr}(p, n)$, i.e. the set of the p-dimensional subspaces of $\mathbb{R}^n$. The power method is extended to $\mathrm{Gr}(p, n)$ in the following way. Let $\mathcal{Y}$ be an element of $\mathrm{Gr}(p, n)$. Let $Y \in \mathbb{R}^{n \times p}$ be a basis of $\mathcal{Y}$. That is, the column space of Y, denoted by $\lfloor Y \rfloor$ for convenience throughout the article, is equal to $\mathcal{Y}$. Note that if Y_1 and Y_2 are two bases of $\mathcal{Y}$, then there exist a nonsingular p-by-p matrix M such that $Y_1 = Y_2 M$. The extended power method, usually termed *direct subspace iteration* [Par98], maps the subspace $\mathcal{Y}$ to the subspace $\lfloor Z \rfloor$ where

$$Z = AY. \tag{2.2}$$

It is easily verified that $\lfloor Z \rfloor$ does not depend on the basis Y chosen to represent $\mathcal{Y}$. This iteration generically converges to the largest p-dimensional eigenspace of A. In practice, in order to ensure numerical robustness, $\mathcal{Y}$ will be represented by an orthonormal basis X and the next basis will be defined by $X_+ = \mathrm{qf}(AX)$ where qf is any operator mapping general basis to orthonormal basis without altering the column space.

The continuous-time flow associated to the direct subspace iteration is

$$\dot{Y} = BY. \tag{2.3}$$

With the special choice $B = \ln(A)$, the iterates $Y_{(k)}$ of the discrete iteration (2.2) and the solution $Y(t)$ of (2.3) are related by $Y_{(k)} = Y(k)$ for all integer k provided $Y_{(0)} = Y(0)$.

The (classical) *Rayleigh Quotient Iteration* (RQI) is an inverse iteration with Rayleigh quotient shift $\rho_A(x) := (x^T Ax)/(x^T x)$, namely [Par98]

$$\begin{aligned} z &= (A - \rho_A(x_{(k)})I)^{-1} x_{(k)} \\ x_{(k+1)} &= z/|z|. \end{aligned}$$

If x is close to an eigenvector of A, then $\rho_A(x)$ is a very close (quadratic) approximation of the corresponding eigenvalue of A. This ensures cubic local convergence of the RQI to eigenvectors of A.

In [AMSV02], the RQI is extended to the Grassmann manifold in the following way. The *Grassmann Rayleigh Quotient Iteration* (GRQI) maps the subspace $\lfloor Y \rfloor$ to the subspace $\lfloor Z \rfloor$ where Z solves

$$AZ - Z(Y^T Y)^{-1} Y^T AY = Y.$$

Here again, it is possible to show that $\lfloor Z \rfloor$ does not depend on the basis Y chosen to represent $\lfloor Y \rfloor$.

By analogy to the power method flow, we define the *Grassmann-Rayleigh Quotient Flow* (GRQF) by

$$AZ_Y - Z_Y (Y^T Y)^{-1} Y^T AY = Y \tag{2.4a}$$

$$\dot{Y} = Z_Y. \tag{2.4b}$$

The solutions of (2.4) evolve on $\mathbb{R}^{n \times p}$ but, as it will be shown in Proposition 3.1, they indeed generate a unique flow on the Grassmann manifold $\mathrm{Gr}(p, n)$.

Contrary to the power method flow, the GRQF does not go through the (discrete) iterates of the GRQI. Nevertheless, this flow displays interesting convergence properties and its analysis conveys valuable ideas in terms of eigenspace computation.

The case where $p = 1$, for which the Grassmann manifold reduces to the real projective space $\mathbb{RP}^{n-1}$), has been investigated in [MA01]. It is shown in [MA01] that, when $p = 1$, $\dot{\rho}_A = 2$ along the solutions of (2.4) —i.e. the Rayleigh quotient increases at constant rate— and the solutions reach an eigenvector of A in finite time.

The present paper addresses the case $p \geq 1$. It is shown that the property $\dot{\rho}_A = 2$ extends to the eigenvalues of the matrix Rayleigh quotient $R_A(Y) = (Y^TY)^{-1}Y^TAY$. Moreover, the property that the solutions reach an eigenvector of A is still valid in the sense that, at a finite time t^*, the column span $\lfloor Y \rfloor$ of the solution Y of (2.4) contains an eigenvector of A.

3 The Grassmann-Rayleigh Quotient Flow and its representations

The following proposition proves that the equation (2.4) defines a flow on the Grassmann manifold, and that (2.4) belongs to a broader class of matrix differential equations whose solutions generate the same curve on the Grassmann manifold.

Proposition 3.1 (GRQF). *Let Z_Y verify* (2.4a). *Consider the following matrix differential equation*

$$\dot{Y} = Z_Y + YR \tag{3.5}$$

where R is a (possibly time-varying) arbitrary p-by-p matrix. Note that (3.5) *reduces to* (2.4b) *for the choice $R \equiv 0$. Recall the notation $\lfloor Y \rfloor$ for the column span of Y.*
The curves $\lfloor Y(t) \rfloor$ where $Y(t)$ solves (3.5) *define a flow on the Grassmann manifold, i.e,*

1. *$\lfloor Y(t) \rfloor$ does not depend on R;*

2. *if $Y_a(t)$, $Y_b(t)$ solve* (3.5) *and $\lfloor Y_a(0) \rfloor = \lfloor Y_b(0) \rfloor$, then $\lfloor Y_a(t) \rfloor = \lfloor Y_b(t) \rfloor$ for all t.*

We call this flow the Grassmann-Rayleigh Quotient Flow (GRQF).

Proof. These properties are due to the fact that Z_Y verifies $Z_{YM} = Z_Y M$ (see [AMSV02]) and that motion of Y in the direction of YM does not alter $\lfloor Y \rfloor$. Choose an orthonormal basis $(W|W_\perp)$ of $\mathbb{R}^n$ such that $Y(0)$ is not orthogonal to W, i.e. $W^TY(0)$ is invertible. For each Y not orthogonal to W, there exists a unique $K \in \mathbb{R}^{(n-p)\times p}$ and a unique $M \in \mathbb{R}^{p\times p}$ such that

$$Y = (W + W_\perp K)M. \tag{3.6}$$

Note that $\lfloor Y \rfloor$ is uniquely defined by K. Substituting the representation (3.6) into the dynamics (3.5) yields

$$\dot{M} = W^T Z_{W+W_\perp K} M + MR \tag{3.7a}$$
$$\dot{K}M = [W_\perp^T Z_{W+W_\perp K} - KW^T Z_{W+W_\perp K}]M \tag{3.7b}$$

It is now shown that $M(t)$ is invertible for all t. Denote $B = W^T Z_{W+W_\perp K}$. The solution $M(t)$ of (3.7a) reads $M(t) = \exp[\int_0^t B(\sigma)d\sigma]\, M(0)\, \exp[\int_0^t R(\sigma)d\sigma]$. In this expression, $M(0)$ is invertible by choice of W. So, as long as the exponentials are well defined, $M(t)$ is invertible as the product of invertible matrices.
Since $M(t)$ is invertible, postmultiplying (3.7b) by M^{-1} yields

$$\dot{K} = W_\perp^T Z_{W+W_\perp K} - K W^T Z_{W+W_\perp K}$$

which only involves the coordinates K of $\lfloor Y \rfloor$. The matrices R and M are absent, which proves properties 1 and 2 respectively. □

In view of proving the deflating property of the GRQF, it is useful to represent subspaces by orthonormal bases of Ritz vectors, namely, represent $\lfloor Y \rfloor \in \mathrm{Gr}(p, n)$ by a matrix X in

$$\Gamma = \{X \in \mathbb{R}^{n\times p} : X^T X = I_p \text{ and } X^T A X \text{ is diagonal}\} \tag{3.8}$$

such that $\lfloor X \rfloor = \lfloor Y \rfloor$. This is achieved with a particular choice of R in (3.5) such that $D_t(Y^T Y) = 0$ and $D_t[(Y^T Y)^{-1} Y^T A Y]$ is diagonal:

Proposition 3.2 (structure-preserving representation of the GRQF). *The solution $Y(t)$ of (3.5) with $R = (Y^T Y)^{-1} Z_Y^T Y$,*

$$\dot{Y} = Z_Y - Y (Y^T Y)^{-1} Z_Y^T Y, \tag{3.9}$$

verifies the following properties

1. $D_t(Y^T Y) = 0$.
2. $D_t[(Y^T Y)^{-1} Y^T A Y] = 2I$.

Proof. 1. $D_t(Y^T Y) = Y^T Z - Z^T Y + (Y^T Z - Z^T Y)^T = 0$.
2. $\dot{R}_A(Y) = -(Y^T Y)^{-1} D_t(Y^T Y)(Y^T Y)^{-1} Y^T A Y$
$+(Y^T Y)^{-1}(Z^T A Y) - (Y^T Y)^{-1} Y^T Z (Y^T Y)^{-1} Y^T A Y$
$+(Y^T Y)^{-1} Y^T A Z - (Y^T Y)^{-1} Y^T A Y (Y^T Y)^{-1} Z^T Y$.
Grouping the terms appropriately and using (2.4a) yields the result $\dot{R}_A(Y) = 2I$. □

Consequently, (3.9) leaves Γ invariant:

Proposition 3.3 (Ritz representation of the GRQF). *If $X(0)$ is such that $X(0)^T X(0) = I$ and $X(0)^T A X(0) = \Sigma(0) = \mathrm{diag}(\sigma_1(0), \ldots, \sigma_p(0))$, then the solution $X(t)$ of*

$$A Z_X - Z_X X^T A X = X \tag{3.10a}$$

$$\dot{X} = Z_X - X Z_X^T X \tag{3.10b}$$

verifies $X(t)^T X(t) = I$ and

$$R_A(X(t)) = X(t)^T A X(t) = \mathrm{diag}(\sigma_1(0), \ldots, \sigma_p(0)) + 2It =: \mathrm{diag}(\sigma_1(t), \ldots, \sigma_p(t)).$$

Moreover, since (3.10) is a particular realization of (3.5), $\lfloor X(t) \rfloor$ is a solution of the GRQF.

Since $R_A(X) = \mathrm{diag}(\sigma_1(t), \ldots, \sigma_p(t))$, equation (3.10a) decouples into p equations

$$(A - \sigma_i I) Z_{:,i} = X_{:,i}, \quad i = 1, \ldots, p,$$

which shows that Z_X is well defined by (3.10a) as long as

$$\sigma_i(t) = \sigma_0 + 2t \ \notin \ \mathrm{spec}(A), \ i = 1, \ldots, p. \tag{3.11}$$

The dynamics (3.10b) of X can be interpreted in the following way. Premultiplying (3.10a) by Z^T yields

$$X^T Z_X - Z_X^T X = -[X^T A X, Z^T Z],$$

whence (3.10b) also reads

$$\dot{X} = (I - XX^T) Z_X - X[X^T A X, Z^T Z]. \tag{3.12}$$

This clarifies the structure of (3.10b). The term $(I - XX^T)Z_X$ in (3.12) is responsible for variations of the orthonormal basis X towards its orthogonal complement, producing variations of the subspace $\lfloor X \rfloor$ spanned by X. The term $X[X^T A X, Z^T Z]$, where X is multiplied by a skew-symmetric matrix, rotates X inside $\lfloor X \rfloor$ so as to preserve diagonality of $X^T A X$. This decomposition fits the decomposition of the tangent space $T_X \mathrm{St}(p, n)$ of the Stiefel manifold —i.e. the manifold of the orthonormal n-by-p matrices, which can be viewed as a principal fiber bundle over $\mathrm{Gr}(p, n)$ with group $O(p)$ [KN63]— into the vertical space $\{X\Omega : \Omega \ p\text{-by-}p \text{ skew}\}$ and the horizontal space $\{X_\perp H : H \in \mathbb{R}^{(n-p)\times p}\}$.

4 Deflation in finite time

In this section, it is proved that, under generic conditions, if $X(t)$ is a solution of (3.10), then either a column of X converges to an eigenvector of A, or X belongs to the stable manifold of an unstable set. The latter behaviour is not observed in practice.

Choose an initial condition $\lfloor Y(0) \rfloor$ such that $R_A(Y)$ and A have no eigenvalue in common (otherwise Z_Y is ill-defined). Without loss of generality, choose a coordinate system and a matrix $X(0)$ such that $\lfloor X(0) \rfloor = \lfloor Y(0) \rfloor$, $X(0)^T X(0) = I$, $X(0)^T A X(0) = \Sigma(0) = \mathrm{diag}(\sigma_1(0), \ldots, \sigma_p(0))$, $A = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$, and $\lambda_1 - \sigma_1(0) = \min\{\lambda_i - \sigma_j(0) : \lambda_i - \sigma_j(0) \geq 0\}$. Moreover, in order to simplify the forthcoming development, suppose that this minimum is unique. Then from (3.11) the first *critical time* of (3.10), i.e. time when the equation (3.10a) for Z_X is singular, is

$$t^* = (\lambda_1 - \sigma_1(0))/2$$

and at that time, $\sigma_1(t^*) = \lambda_1$.

It is claimed that (apart from a theoretically possible convergence of X to an unstable set) the first column of X converges to $\pm e_1$ as $t \to t^*$, which means that the solution $\lfloor X(t) \rfloor$ of the GRQF contains the eigenvector e_1 of A when $t = t^*$. The proof follows.

Denoting $X_{ij} = e_i^T X e_j$ and $X_j = Xe_j$, the element-by-element expression of (3.10) is

$$\dot{X}_{ij} = (\lambda_i - \sigma_j)^{-1} X_{ij} - \sum_{km} X_{ik} (\lambda_m - \sigma_k)^{-1} X_{mk} X_{mj} \tag{4.13}$$

where $\sigma_l = X_l^T A X_l$. Separating the terms that will blow up first (at $t = t^*$) yields

$$\dot{X}_{11} = \frac{1}{\lambda_1 - \sigma_1} X_{11}(1 - X_{11}^2) \qquad - \sum_{(k,m)\neq(1,1)} X_{ik}(\lambda_m - \sigma_k)^{-1} X_{mk} X_{mj} \tag{4.14a}$$

$$\dot{X}_{ij} = -\frac{1}{\lambda_1 - \sigma_1} X_{i1} X_{1j} X_{11} \quad + \frac{1}{\lambda_i - \sigma_j} X_{ij} - \sum_{(k,m)\neq(1,1)} X_{ik}(\lambda_m - \sigma_k)^{-1} X_{mk} X_{mj}. \tag{4.14b}$$

Define the new time variable

$$\tau = -\ln(\lambda_1 - \sigma_1(t)) = -\ln(2(t^* - t)),\ t \leq t^*,$$

and denote D_τ by $'$. Then, denoting $\xi = \lambda_1 - \sigma_1$, (4.14) becomes

$$X'_{11} = X_{11}(1 - X_{11}^2) + \xi K_{11}(X) \tag{4.15a}$$
$$X'_{ij} = -X_{i1} X_{1j} X_{11} + \xi K_{ij}(X) \tag{4.15b}$$
$$\xi' = -\xi \tag{4.15c}$$

where $K(X)$ is bounded on $t \in [0, t^*]$ because X is orthonormal and $\lambda_m - \sigma_k$ for $(k, m) \neq (1, 1)$ evolves linearly with t (see (3.11)) and does not vanish for $t \in [0, t^*]$ by hypothesis. Restrict the analysis to the invariant manifold Γ (see (3.8)) which is stable (non asymptotically) for the GRQF by Proposition 3.2. The equilibrium points of (4.15) are

$$\{\xi = 0,\ X_{11} = \pm 1\}\ \cup\ \{\xi = 0,\ X_{11} = 0\}.$$

Linearization of (4.15) at $\bar{\xi} = 0$, $\bar{X}_{11} = \pm 1$ yields

$$X'_{11} = -2X_{11} + \xi \bar{K}_{11} \tag{4.16a}$$
$$X'_{ij} = \dots \tag{4.16b}$$
$$\xi' = -\xi \tag{4.16c}$$

and the set $\{\xi = 0,\ X_{11} = \pm 1\}$ is stable. Linearization of (4.15) at $\bar{\xi} = 0$, $\bar{X}_{11} = 0$ yields

$$X'_{11} = X_{11} + \xi \bar{K}_{11} \tag{4.17a}$$
$$X'_{ij} = -\bar{X}_{i1} \bar{X}_{1j} X_{11} + \xi \bar{K}_{ij} \tag{4.17b}$$
$$\xi' = -\xi \tag{4.17c}$$

and the set $\{\xi = 0,\ X_{11} = 0\}$ is unstable. Moreover, since K_{11} is bounded and $\xi = e^{-\tau}$, equation (4.15a) implies that either

- $X_{11} \to 0$. This happens only if $X(0)$ belongs to the stable manifold of the unstable set $\{\xi = 0,\ X_{11} = 0\}$. Or
- $X_{11} \to \pm 1$. This means that the first column of X converges to the eigenvector $\pm e_1$ of A.

When $X_{11} = 1$, then one has $\sigma_1 = \lambda_1$ and Z_X is not defined. A possible continuation of the flow is to deflate the problem by freezing X_1 and continuing the flow inside the orthogonal complement of X_1 with initial point $X_{:,2:p}$.

5 Conclusion

We have studied a continuous flow associated to a Rayleigh quotient iteration on the Grassmann manifold $\mathrm{Gr}(p,n)$ [AMSV02]. The analysis of this Grassmannian flow is carried out using its Ritz representation on the Stiefel manifold. The property of constant variation of the Rayleigh quotient along the solutions in the particular case $p = 1$ [MA01], extends when $p \geq 1$ to the Ritz values associated to the solutions. Moreover, for most initial conditions, one of the Ritz vectors of the solution converges to an eigenvector of A in finite time. This property leads to a continuous-time flow achieving deflation.

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