ON THE APPROXIMATION OF LOW-RANK RIGHTMOST EIGENPAIRS OF A CLASS OF MATRIX-VALUED LINEAR OPERATORS

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Linear Operators

Let $\mathcal{A}$ be a real matrix-valued linear operator,

$$\mathcal{A} : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$$

that is $X \in \mathbb{R}^{n\times n} \implies \mathcal{A}(X) \in \mathbb{R}^{n\times n}$.
Examples of such operators are the following:

(i) $\mathcal{A}(X) = AX + XB$ (Sylvester equation);

(ii) $\mathcal{A}(X) = \sum_i B_i X C_i$;

(iii) $\mathcal{A}(X) = A \bullet X$ (componentwise multiplication);

(iv) A combination of previous cases.

The problem

Let us consider

$$\mathcal{A}(X) = \lambda X, \quad X \neq \mathrm{O} \qquad (1)$$

where X and λ are allowed to be complex-valued.

- We call a solution X of (1) eigenmatrix of the operator $\mathcal{A}$.
- As usual, the eigenvalues of $\mathcal{A}$ coincide with the eigenvalues of its matrix representation, $A \in \mathbb{R}^{n^2 \times n^2}$.
- We focus on computing either the rightmost eigenvalue λ_1 when this is real (and simple) or the righmost complex-conjugate pair (which is generically unique).

We make, a priori, the following hypothesis :

(H) X has quickly decaying singular values.

This motivates to constrain the search of approximate eigensolutions to a low-rank manifold.

A suited system of ODEs

We consider the following system of ODEs

$$\begin{cases} \dot{X}(t) & = & \mathcal{A}(X(t)) - \alpha(X(t))\,X(t) \\ X(0) & = & X_0, \qquad \|X_0\| = 1 \end{cases} \tag{2}$$

for general real initial data, where $\alpha(X) = \langle \mathcal{A}(X(t)), X(t) \rangle$.
In the sequel we omit – when not necessary – the dependence on t.

For a pair of matrices $A, B \in \mathbb{R}^{n\times n}$ we let

$$\langle A, B \rangle = \mathrm{trace}(A^{\mathrm{T}} B) = \sum_{i,j=1}^{n} A_{ij} B_{ij}$$

denote the Frobenius inner product and $\|A\| = \langle A, A \rangle^{1/2}$ the associated Frobenius norm.

Properties of the system

a. Norm conservation :

$$X(t) \in \mathbb{B}, \qquad \mathbb{B} = \{Z \in \mathbb{R}^{n\times n} : \|Z\| = 1\}.$$

b. Equilibria: A matrix $X \in \mathbb{B}$ is an equilibrium of (2) if and only if it is an eigenmatrix of $\mathcal{A}$.

c. Assume that $\mathcal{A}$ has a unique rightmost eigenvalue λ_1, which is assumed to be real. Let $V \in \mathbb{B}$ be an eigenmatrix associated with a simple eigenvalue $\lambda \in \mathbb{R}$ of $\mathcal{A}$. Then V is a stable equilibrium of (2) if and only if $\lambda = \lambda_1$.

d. If $\mathcal{A}$ has all real and simple eigenvalues, the solution of (2) cannot be periodic.

e. If that $X_0 \in \mathrm{span}\left(V, \overline{V}\right) \cap \mathbb{R}^{n\times n}$, where V is a complex eigenvector of $\mathcal{A}$. Then $X(t)$ tends to a periodic solution.

f. If $\mathcal{A}$ has a unique simple real rightmost eigenvalue λ_1, with associated eigenmatrix V_1, and generically that $\langle X_0, V_1 \rangle \neq 0$; then the solution of (2) is such that

$$\lim_{t\to\infty} X(t) = \pm V_1.$$

Low rank approximation

Idea: find an approximate solution to the differential equation, working only with its low-rank approximation[1].
A natural criterion is the following:

$$\|\dot{X}(t) - F(X(t))\| \longrightarrow \min$$

with

$$F(X(t)) = \mathcal{A}(X(t)) - \langle \mathcal{A}(X(t)), X(t) \rangle X(t)$$

where the minimization is over all matrices that are tangent to $X(t)$ on the manifold $\mathcal{M}_r$ of matrices of rank r, and the norm is the Frobenius norm.

[1] O. Koch and C. Lubich. Dynamical low-rank approximation. *SIMAX*, 2007

A constrained integration

Every real rank-r matrix X of dimension $n \times n$ can be written in the form

$$X = USV^{\mathrm{T}}$$

where $U \in \mathbb{R}^{n \times r}$ and $V \in \mathbb{R}^{n \times r}$ have orthonormal columns, i.e.,

$$U^{\mathrm{T}} U = I_r, \quad V^{\mathrm{T}} V = I_r,$$

(with the identity matrix I_r of dimension r), and $S \in \mathbb{R}^{r \times r}$ is nonsingular.

Orthogonal projection

Lemma (Koch&Lubich)

The orthogonal projection onto the tangent space $T_X\mathcal{M}_r$ *at* $X = USV^{\mathrm{T}} \in \mathcal{M}_r$ *is given by*

$$\begin{aligned} P_X(Z) &= Z - (I - UU^{\mathrm{T}})Z(I - VV^{\mathrm{T}}) \\ &= ZVV^{\mathrm{T}} - UU^{\mathrm{T}}ZVV^{\mathrm{T}} + UU^{\mathrm{T}}Z \end{aligned}$$

for $Z \in \mathbb{R}^{n\times n}$.

Projected equation

In the differential equation (2), we replace the right-hand side by its orthogonal projection to $T_X\mathcal{M}_r$, so that solutions starting with rank r will retain rank r for all times:

$$\dot{X} = P_X\Big(\mathcal{A}(X) - \langle X, \mathcal{A}(X)\rangle X\Big). \qquad (3)$$

Since $X \in T_X\mathcal{M}_r$, we have $P_X(X) = X$ and $\langle X, Z\rangle = \langle X, P_X(Z)\rangle$, and hence the differential equation can be rewritten as

$$\dot{X} = P_X(\mathcal{A}(X)) - \langle X, P_X(\mathcal{A}(X))\rangle X, \qquad (4)$$

which differs from (2), only in that $\mathcal{A}(X)$ is replaced by its orthogonal projection to $T_X\mathcal{M}_r$.

Lemma (Koch & Lubich, 2007)

For $X = USV^{\mathrm{T}} \in \mathcal{M}_r$ with nonsingular $S \in \mathbb{R}^{r\times r}$ and with $U \in \mathbb{R}^{n\times r}$ and $V \in \mathbb{R}^{r\times r}$ having orthonormal columns, the equation $\dot{X} = P_X(Z)$ is equivalent to $\dot{X} = \dot{U}SV^{\mathrm{T}} + U\dot{S}V^{\mathrm{T}} + US\dot{V}^{\mathrm{T}}$, where

$$
\begin{aligned}
\dot{S} &= U^{\mathrm{T}}ZV \\
\dot{U} &= (I - UU^{\mathrm{T}})ZVS^{-1} \\
\dot{V} &= (I - VV^{\mathrm{T}})Z^{\mathrm{T}}US^{-\mathrm{T}}.
\end{aligned}
\tag{5}
$$

Remarks:

- Replacing Z by $F(X)$ in (6), we obtain the projected system of ODEs (5), written in terms of the factors U, S and V of X.
- Norm conservation: If $\|X(0)\| = 1$, then, the solution of (4) has the property $\|X(t)\| = 1 \quad \forall t \geq 0$.

Equilibria

The following result characterizes possible equilibria of (5).

Theorem

Let $X = USV^{\mathrm{T}}$ *(with* $U \in \mathbb{R}^{n\times r}$ *and* $V \in \mathbb{R}^{n\times r}$ *have orthonormal columns and* $S \in \mathbb{R}^{r\times r}$ *is nonsingular).* X *is an equilibrium of* (5) *if and only if*

$$\begin{cases} F\left(USV^{\mathrm{T}}\right)V &= O \\ U^{\mathrm{T}}F\left(USV^{\mathrm{T}}\right) &= O \end{cases}$$

under the constraints $U^{\mathrm{T}}U = I_r$, $V^{\mathrm{T}}V = I_r$, $\|S\| = 1$.

Remark

The existence and the number of equilibria for (5) *(equivalently of* (6)*) is non trivial, given the nonlinearity of the problem. The asymptotic behaviour of the solution of* (5) *is also more complicated to determine.*

Numerical integration

Goal: integrate the $n \times n$ matrix differential equation

$$\begin{cases} \dot{X}(t) & = & F(X(t)) = P_X(\mathcal{A}(X(t))) - \langle \mathcal{A}(X(t)), X(t) \rangle X(t), \\ X(t) & \in & \mathcal{M}_r, \; X(0) = X_0 \in \mathcal{M}_r, \qquad \|X_0\| = 1. \end{cases}$$

which is equivalent to the system (6) of differential equations for the factors U, S, V of $X \in \mathcal{M}_r$.

Projector splitting integrator

We consider a slight variant of the projector-splitting integrator of Lubich&Oseledets [2], such that, the unit Frobenius norm is preserved.

- It is a first-order method with an error bound that is independent of possibly small singular values of X_0 or X_1.
- The algorithm starts from the factorized rank-r matrix of unit norm

$$X_0 = U_0 S_0 V_0^{\mathrm{T}}, \qquad \|S_0\| = 1$$

  at time $t_0 = 0$.
- After one step, it computes the factors of the approximation $X_1 = U_1 S_1 V_1^{\mathrm{T}}$, again of unit Frobenius norm, at the next time $t_1 = t_0 + h$.

[2] C. Lubich and I. V. Oseledets. A projector-splitting integrator for dynamical low-rank approximation. *BIT*, 2014.

1. With $F_0 = F(X_0)$, set
$$K_1 = U_0 S_0 + hF_0 V_0$$
and, via a QR decomposition, compute the factorization
$$U_1 \widehat{S}_1 \widehat{\sigma}_1 = K_1$$
with U_1 having orthonormal columns, with an $r \times r$ matrix $\widehat{S}_1$ of unit Frobenius norm, and a positive scalar $\widehat{\sigma}_1$.

2. Set
$$\widetilde{\sigma}_0 \widetilde{S}_0 = \widehat{S}_1 - h\, U_1^{\mathrm{T}} F_0 V_0,$$
where $\widetilde{S}_0$ is of unit Frobenius norm and $\widetilde{\sigma}_0 > 0$.

3. Set
$$L_1 = V_0 \widetilde{S}_0^{\mathrm{T}} + hF_0^{\mathrm{T}} U_1$$
and, via a QR decomposition, compute the factorization
$$V_1 S_1^{\mathrm{T}} \sigma_1 = L_1,$$
with V_1 having orthonormal columns, with an $r \times r$ matrix S_1 of unit Frobenius norm, and a positive scalar σ_1.

Example

Let us consider the operator:

$$\mathcal{A}(X) = AX + XA^{\mathrm{T}} + BXC^{\mathrm{T}}$$

for given matrices $A, B, C, X \in \mathbb{R}^{n \times n}$.
We consider:

- A diagonal
- B, C of moderate norm
- this suggests that the eigenvectors of $\mathcal{A}$ are reasonably close to those of $AX + XA^{\mathrm{T}}$ which have rank-1.
- We choose $n = 50$

$$A = \begin{pmatrix} -1 & 0 & \dots & 0 \\ 0 & -2 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & -n \end{pmatrix},$$

B and C full random matrices of Frobenius norm σn with $\sigma \in [0.1, 1]$.

Example

σ	r	$\frac{\lvert\hat{\lambda}_1-\lambda_1\rvert}{\lvert\lambda_1\rvert}$	$\lVert X_1 - USV^{\mathrm{T}}\rVert$
0.1	1	1.6681 $e-4$	0.0160
0.1	2	3.7769 $e-5$	0.0061
0.2	1	0.0025	0.0609
0.2	2	1.2001 $e-4$	0.0154
0.2	3	3.2617 $e-5$	0.0068
0.5	2	0.0625	0.2459
0.5	3	0.0102	0.1809
0.5	4	0.0052	0.1087
0.5	8	0.0019	0.0350
1.0	2	0.0792	0.3265
1.0	4	0.0335	0.3158
1.0	8	0.0298	0.1419
1.0	15	9.5427 $e-4$	0.0463

Table: Computed values for Example 1.

A particular example

Consider the problem (with separable coefficients)

$$u_t = \varepsilon \Delta u + \phi_1(x)\psi_1(y)u_x + \phi_2(x)\psi_2(y)u_y$$

with zero Dirichlet boundary conditions on the domain $[0,1] \times [0,1]$. Using standard finite differences and defining $U_{ij} = u(x_i, y_j)$ for $i, j = 1, \dots n$, yields

$$\dot{U} = \mathcal{A}(U) = TU + UT + \Phi_1 B U \Psi_1^{\mathrm{T}} + \Psi_2 U \left(\Phi_2 B\right)^{\mathrm{T}} \tag{6}$$

with $U \in \mathbb{R}^{n \times n}$. Denoting the stepsize k, the matrices are given by

$$T = \frac{\varepsilon}{k^2}\mathrm{trid}(1, -2, 1), \qquad B = \frac{1}{2k}\mathrm{trid}(-1, 0, 1)$$

and - for $\ell = 1, 2$ -

$$\Phi_\ell = \mathrm{diag}\left(\phi_\ell(x_1), \dots, \phi_\ell(x_n)\right), \qquad \Psi_\ell = \mathrm{diag}\left(\psi_\ell(y_1), \dots, \psi_\ell(y_n)\right).$$

Setting

- $\varepsilon = 1/10$ and $n = 50$,
- $\phi_1(x) = \phi_2(x) = \sin(\pi x)$
- $\psi_1(y) = \psi_2(y) = \cos(\pi y)$

we obtain a largest eigenvalue $\lambda_1 = -2.79071\ldots$ to which corresponds the eigenmatrix U_1 , whose five leading singular values are given by:

$$\sigma_1 \approx 0.8808, \quad \sigma_2 \approx 0.4561, \quad \sigma_3 \approx 0.1243, \quad \sigma_4 \approx 0.0255, \quad \sigma_5 \approx 0.0041.$$

This suggests that the eigenvalue problem may be well approximated restricting the search of eigenmatrices to $\mathcal{M}_3$ or $\mathcal{M}_4$, the manifolds of rank-3 and rank-4 $n \times n$-matrices.
Applying the method we have presented,

(i) looking for a rank-3 approximation of U_1, we obtain an approximated eigenvalue $\widetilde{\lambda}_1 \approx -2.7814\ldots$ and an approximated eigenmatrix $\widetilde{U}_1 \in \mathcal{M}_3$ with

$$\frac{\|U_1 - \widetilde{U}_1\|_F}{\|U_1\|_F} \approx 0.0950.$$

(2) looking for a rank-4 approximation of U_1, we obtain an approximated eigenvalue $\widehat{\lambda}_1 \approx -2.7945\ldots$ and an approximated eigenmatrix $\widehat{U}_1 \in \mathcal{M}_4$ with

$$\frac{\|U_1 - \widehat{U}_1\|_F}{\|U_1\|_F} \approx 0.0910.$$

Comparison to the ALS method

We compare our approach based on the modified projector splitting integrator (MPS) with the ALS method on a symmetric operator of the type

$$\mathcal{A}(X) = AX + XA + BXB$$

with A diagonal and B symmetric, of dimensions 50×50.

Details:

- The exact value for the maximum eigenvalue is $\lambda = -1.7391$.
- The initial data are randomly chosen for both codes.
- We set $r = 1, 3, 5, 7$, as values of the rank.

Comparison to the ALS method

	ALS				MPS			
r	$\lambda_{\max}$	d_X	d_{X_r}	Time	$\lambda_{\max}$	d_X	d_{X_r}	Time
1	-1.7988	0.0443	0.5768	0.0155	-1.8010	0.0619	0.0460	0.0942
3	-1.7583	0.0482	0.0471	1.4616	-1.7404	0.0296	0.0047	0.0915
5	-1.7395	0.0151	0.0151	2.7483	-1.7392	0.0046	0.0045	0.0966
7	-1.7392	0.0044	$2.55e-4$	7.5043	-1.7391	$3.50e-4$	$2.45e-4$	0.3932

Details:

- d_X is distances between the rank r eigenmatrix computed by a method and the exact eigenvector X
- d_{X_r} is the distance between the computed eigenmatrix and X_r, the best rank r approximation of X.
- Time is in seconds.

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