Vectorization

Goal represent linear functions $\mathbb{R}^{m\times n} \to \mathbb{R}^{p\times q}$.

For instance, to deal with problems like the following one.

Sylvester equation

$$AX - XB = C$$

$A \in \mathbb{C}^{m\times m}$, $C, X \in \mathbb{C}^{m\times n}$, $B \in \mathbb{C}^{n\times n}$.

This must be a $mn \times mn$ linear system, right?

Vectorization gives us an explicit way to construct it.

Vectorization: definition

$$\operatorname{vec} X = \operatorname{vec} \left[\begin{array}{c|c|c|c} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & \cdots & x_{mn} \end{array}\right] := \left[\begin{array}{c} x_{11} \\ x_{21} \\ \vdots \\ x_{m1} \\ \hline x_{12} \\ x_{22} \\ \vdots \\ x_{m2} \\ \hline \vdots \\ \hline \\ x_{1n} \\ x_{2n} \\ \vdots \\ x_{mn} \end{array}\right].$$

Vectorization: comments

Column-major order: leftmost index 'changes more often'. Matches Fortran, Matlab standard (C/C++ prefer row-major instead).

Converting indices in the matrix into indices in the vector:

$$(X)_{ij} = (\operatorname{vec} X)_{i+mj} \qquad \text{0-based,}$$

$$(X)_{ij} = (\operatorname{vec} X)_{i+m(j-1)} \qquad \text{1-based.}$$

vec(AXB)

First, we will work out the representation of a simple linear map, $X \mapsto AXB$ (for fixed matrices A, B of compatible dimensions).

If $X \in \mathbb{R}^{m \times n}$, $AXB \in \mathbb{R}^{p \times q}$, we need the $pq \times mn$ matrix that maps $\operatorname{vec} X$ to $\operatorname{vec}(AXB)$.

$$(AXB)_{hl} = \sum_j (AX)_{hj}(B)_{jl} = \sum_j \sum_i A_{hi} X_{ij} B_{jl}$$

$$= \left[\begin{array}{cccc|cccc|c} A_{h1}B_{1l} & A_{h2}B_{1l} & \ldots & A_{hm}B_{1l} & A_{h1}B_{2l} & A_{h2}B_{2l} & \ldots & A_{hm}B_{2l} & \ldots \end{array} \right.$$

$$\left. \begin{array}{|ccc} A_{h1}B_{nl} & A_{h2}B_{nl} & A_{hm}B_{nl} \end{array} \right] \operatorname{vec} X$$

Kronecker product: definition

$$\operatorname{vec}(AXB) = \begin{bmatrix} b_{11}A & b_{21}A & \dots & b_{n1}A \\ b_{12}A & b_{22}A & \dots & b_{n2}A \\ \vdots & \vdots & \ddots & \vdots \\ b_{1q}A & b_{2q}A & \dots & b_{nq}A \end{bmatrix} \operatorname{vec} X$$

Each block is a multiple of A, with coefficient given by the corresponding entry of $B^\top$.

Definition

$$X \otimes Y := \begin{bmatrix} x_{11}Y & x_{12}Y & \dots & x_{1n}Y \\ x_{21}Y & x_{22}Y & \dots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ x_{m1}Y & x_{m2}Y & \dots & x_{mn}Y \end{bmatrix}.$$

so the matrix above is $B^\top \otimes A$.

Properties of Kronecker products

$$X \otimes Y = \begin{bmatrix} x_{11}Y & x_{12}Y & \dots & x_{1n}Y \\ x_{21}Y & x_{22}Y & \dots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ x_{m1}Y & x_{m2}Y & \dots & x_{mn}Y \end{bmatrix}.$$

- $\operatorname{vec} AXB = (B^\top \otimes A) \operatorname{vec} X$. (Warning: not B^*, if complex).
- $(A \otimes B)(C \otimes D) = (AC \otimes BD)$, when dimensions are compatible. Proof: $B(DXC^\top)A^\top = (BD)X(AC)^\top$.
- $(A \otimes B)^\top = A^\top \otimes B^\top$.
- orthogonal $\otimes$ orthogonal $=$ orthogonal.
- upper triangular $\otimes$ upper triangular $=$ upper triangular.
- One can "factor out" several decompositions, e.g.,

  $$A \otimes B = (U_1 S_1 V_1^*) \otimes (U_2 S_2 V_2^*) = (U_1 \otimes U_2)(S_1 \otimes S_2)(V_1 \otimes V_2)^*.$$

- In particular, $\|A \otimes B\| = \|A\| \|B\|$.

Solvability criterion

Theorem

The Sylvester equation is solvable for all C iff $\Lambda(A) \cap \Lambda(B) = \emptyset$.

$AX - XB = C \iff$

$$(I_n \otimes A - B^\top \otimes I_m)\,\mathrm{vec}(X) = \mathrm{vec}(C).$$

Schur decompositions of $A, B^\top$: $A = Q_A T_A Q_A^*$, $B^\top = Q_B T_B Q_B^*$.
Then,

$$I_n \otimes A - B^\top \otimes I_m = (Q_B \otimes Q_A)(I_n \otimes T_A - T_B \otimes I_m)(Q_B \otimes Q_A)^*.$$

is a Schur decomposition.
What is on the diagonal of $I_n \otimes T_A - T_B \otimes I_m$?
If $\Lambda(A) = \{\lambda_1, \ldots, \lambda_m\}$, $\Lambda(B) = \{\mu_1, \ldots, \mu_n\}$, then it's
$\Lambda(I_n \otimes A - B^\top \otimes I_m) = \{\lambda_i - \mu_j : i, j\}$.

Solution algorithms

The naive algorithm costs $O((mn)^3)$. One can get down to $O(m^3 n^2)$ (full steps of GMRES, for instance.)

Bartels–Stewart algorithm (1972): $O(m^3 + n^3)$.

Idea: invert factor by factor the decomposition

$$(Q_B \otimes Q_A)(I_n \otimes T_A - T_B \otimes I_m)(Q_B \otimes Q_A)^*.$$

- Solving orthogonal systems $\iff$ multiplying by their transpose, $O(m^3 + n^3)$ using the $\otimes$ structure.
- Solving upper triangular system $\iff$ back-substitution; costs $O(\text{nnz}) = O(m^3 + n^3)$.

Bartels–Stewart algorithm

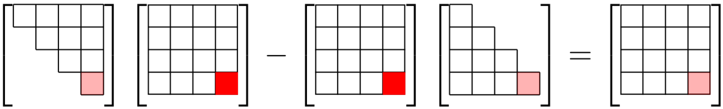
A more operational description...

Step 1: reduce to a triangular equation.

$$Q_A T_A Q_A^* X - X \overline{Q_B} T_B^\top Q_B^\top = C$$

$$T_A Y - Y T_B^* = D, \quad Y = Q_A^* X \overline{Q_B}, D = Q_A^* C \overline{Q_B}.$$

Step 2: We can compute each entry Y_{ij}, by using the (i, j)th equation, as long as we have computed all the entries below and to the right of Y_{ij}.



Step 3: $X = Q_a Y Q_B^\top$.

Comments

- Works also with the real Schur form: back-sub yields block equations which are tiny 2×2 or 4×4 Sylvesters.
- It works also for $X + AXB = C$ and $AXB + CXD = E$ (with some complications).
- It does not work for three-term equations, $AXB + CXD + EXF = G$.

Backward stability

This method is backward stable (as a system of mn linear equations), i.e., the computed $\mathrm{vec}(\tilde{X})$ solves a linear system close to $(I \otimes A - B^\top \otimes I)\,\mathrm{vec}(X) = \mathrm{vec}(C)$.
(Follows from the interpretation as orthogonal transformations + back-sub.)

However, it is not always backward stable in the sense that $\widetilde{X}$ solves a nearby matrix equation $\widetilde{A}\widetilde{X} - \widetilde{X}\widetilde{B} = \widetilde{C}$ [Higham '93].

Sketch of proof: backward error given by the minimum-norm solution of the underdetermined system

$$\underbrace{\begin{bmatrix} \widetilde{X}^\top \otimes I & -I \otimes \widetilde{X} & -I \end{bmatrix}}_{=:M} \begin{bmatrix} \mathrm{vec}\,\delta_A \\ \mathrm{vec}\,\delta_B \\ \mathrm{vec}\,\delta_C \end{bmatrix} = -\,\mathrm{vec}(A\widetilde{X} - \widetilde{X}B - C).$$

Assume WLOG $\widetilde{X}$ diagonal and compute it via the pseudoinverse $M^+ = M^\top (MM^\top)^{-1}$.

Comments

Condition number: ratio between

$$\sigma_{\max}(I\otimes A - B^\top \otimes I) = \|I\otimes A - B^\top \otimes I\| \leq \|I\otimes A\| + \|B^\top \otimes I\| \leq \|A\| + \|B\|$$

and

$$\operatorname{sep}(A, B) := \sigma_{\min}(I \otimes A - B^\top \otimes I) = \min_Z \frac{\|AZ - ZB\|_F}{\|Z\|_F}.$$

(Note that $\|\operatorname{vec}(X)\| = \|X\|_F$.)

We have seen $\lambda_{\min}(I \otimes A - B^\top \otimes I) = \min_{\lambda \in \Lambda(A), \mu \in \Lambda(B)} |\lambda - \mu|$ (minimum difference between their eigenvalues).

If A, B are both normal, this difference is also $\operatorname{sep}(A, B) = \sigma_{\min}(I \otimes A - B^\top \otimes I)$. Otherwise, $\sigma_{\min}$ is smaller; no simple expression for it.

Decoupling eigenvalues

Solving a Sylvester equation means finding

$$\begin{bmatrix} I & -X \\ 0 & I \end{bmatrix} \begin{bmatrix} A & C \\ 0 & B \end{bmatrix} \begin{bmatrix} I & X \\ 0 & I \end{bmatrix} = \begin{bmatrix} A & 0 \\ 0 & B \end{bmatrix}.$$

Idea Indicates how 'difficult' (ill-conditioned) it is to go from block-triangular to block-diagonal.

Compare also with the scalar case:

$$\begin{bmatrix} \lambda & 1 \\ 0 & \mu \end{bmatrix} \text{ is similar to } \begin{bmatrix} \lambda & 0 \\ 0 & \mu \end{bmatrix},$$

if $\lambda \neq \mu$, but

$$\begin{bmatrix} \lambda & 1 \\ 0 & \lambda \end{bmatrix} \text{ is not similar to } \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix}.$$

Application: reordering Schur forms

In a (complex) Schur form $A = QTQ^*$, the T_{ii} are the eigenvalues of A.

Problem

Given a Schur form $A = QTQ^*$, compute another Schur form $A = \hat{Q}\hat{T}\hat{Q}^*$ that has the eigenvalues in another (different) order.

This can be solved with the help of Sylvester equations.

It is enough to have a method to 'swap' two blocks of eigenvalues.

Reordering Schur forms

Let X solve the Sylvester equation $AX - XB = C$.
Since

$$\begin{bmatrix} 0 & I \\ I & -X \end{bmatrix} \begin{bmatrix} A & C \\ 0 & B \end{bmatrix} \begin{bmatrix} X & I \\ I & 0 \end{bmatrix} = \begin{bmatrix} B & 0 \\ 0 & A \end{bmatrix},$$

the matrix $\left[\begin{smallmatrix} X & I \\ I & 0 \end{smallmatrix}\right]$ does the job, but it is not orthogonal. We replace it with its QR factor:

$Q = \mathrm{qr}(\left[\begin{smallmatrix} X & I \\ I & 0 \end{smallmatrix}\right])$ is such that $Q^* \begin{bmatrix} A & C \\ 0 & B \end{bmatrix} Q = \begin{bmatrix} T_{11} & T_{12} \\ 0 & T_{22} \end{bmatrix}$ with $\Lambda(T_{11}) = \Lambda(B)$, $\Lambda(T_{22}) = \Lambda(A)$.

Matlab example: computing the stable invariant subspace with `ordschur`.

Invariant subspaces

Invariant subspace of a matrix M: any subspace $\mathcal{U}$ such that $M\mathcal{U} \subseteq \mathcal{U}$.

There is a matrix A associated to the linear operator M on the space $\mathcal{U}$ (with basis U_1), i.e., $MU_1 = U_1 A$.

If $Av = \lambda v$, then $M(U_1 v) = \lambda U_1 v$, i.e., $\Lambda(A) \subseteq \Lambda(M)$.

Completing a basis U_1 to one $U = \begin{bmatrix} U_1 & U_2 \end{bmatrix}$ of $\mathbb{C}^m$, we get

$$U^{-1} M U = \begin{bmatrix} A & C \\ 0 & B \end{bmatrix}.$$

Invariant subspaces $\iff$ block triangular decomposition $\iff$ part of the spectrum/eigenvectors of a matrix.

Examples (stable invariant subspaces)

Idea: invariant subspaces are 'the span of some eigenvectors' (usually) or Jordan chains (more generally).

Example 1 $\operatorname{span}(v_1, v_2, \dots, v_k)$ (eigenvectors).

Example 2 Invariant subspaces of $\begin{bmatrix} \lambda & 1 \\ 0 & \lambda \end{bmatrix}$: $\operatorname{span}(e_1)$ and $\operatorname{span}(e_1, e_2)$.

Example 3 Invariant subspaces of a larger Jordan block: $\operatorname{span}(e_1, \dots, e_k)$ for all k ("beginnings" of Jordan chains).

Example 4: stable invariant subspace: vectors x_0 s.t. $\lim_{k\to\infty} A^k x_0 = 0$

(These give the general case — idea: a Jordan chain of A can always be extended to one of M.)

Sensitivity of invariant subspaces

If we perturb M to $M + \delta_M$, how much does an invariant subspace U_1 change?

We can assume $U = I$ for simplicity (orthogonal change of basis): $\begin{bmatrix} I \\ 0 \end{bmatrix}$ spans an invariant subspace of $M = \begin{bmatrix} A & C \\ 0 & B \end{bmatrix}$.

Theorem [Stewart Sun book V.2.2]

Let $M = \begin{bmatrix} A & C \\ 0 & B \end{bmatrix}$, $\delta_M = \begin{bmatrix} \delta_A & \delta_C \\ \delta_D & \delta_B, \end{bmatrix}$, $a = \|\delta_A\|_F$ and so on.

If $4(\operatorname{sep}(A, B) - a - b)^2 - d(\|C\|_F + c) \geq 0$, then there is a (unique) X with $\|X\|_F \leq 2\frac{d}{\operatorname{sep}(A,B)-a-b}$ such that $\begin{bmatrix} I \\ X \end{bmatrix}$ spans an invariant subspace of $M + \delta_M$.

Proof (sketch)

- $M + \delta M = \begin{bmatrix} A+\delta_A & C+\delta_C \\ \delta_D & B+\delta_B \end{bmatrix}$
- Look for a transformation $V^{-1}(M + \delta M)V$ of the form $V = \begin{bmatrix} I & 0 \\ X & I \end{bmatrix}$ that zeroes out the $(2, 1)$ block.
- Formulate a Riccati equation $X(A + \delta_A) - (B + \delta_B)X = \delta_D - X(C + \delta C)X.$
- See it as a fixed-point problem

$$X_{k+1} = \hat{T}^{-1}(\delta_D - X_k(C + \delta C)X_k)$$

- Take norms, show that the iteration map sends a ball $B(0, \rho)$ (for sufficiently small ρ) to itself:

$$\|X_{k+1}\|_F \leq \|\hat{T}^{-1}\|(d + \|X_k\|_F^2(\|C\|_F + c)).$$

- $\|\hat{T}^{-1}\|^{-1} = \sigma_{\min}(\hat{T}) \geq \sigma_{\min}(T) - a - b$ (from SVD perturbation results.)

Applications of Sylvester equations

Apart from the ones we have already seen:

- As a step to compute matrix functions.
- Stability of linear dynamical systems.
  Lyapunov equations $AX + XA^\top = B$, B symmetric.
- As a step to solve more complicated matrix equations (Newton's method $\to$ linearization).

We will re-encounter them later in the course.