Is Lanczos tridiagonalization algorithm essential for solving large eigenvalue problems ?

By

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In this talk we propose an alternative approach **:**

A new type of restated Krylov method

The new method

Avoids the Lanczos algorithm

Avoids polynomial filtering

It is neither “explicit restart” nor “implicit restart”

Plan:

Part 1 : The new method

part 2 : Applications

Low-rank approximations of large sparse matrices.

Computing small eigenvalues or small singular values via **inexact inversions.**

Notations

$\mathbf{G}$ a large sparse symmetric $\mathbf{n \times n}$ matrix , $\mathbf{G^T = G}$,

with eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$

and eigenvectors $\mathbf{v_1}, \mathbf{v_2}, \ \ldots \ , \mathbf{v_n}$

$$\mathbf{G v_j} = \lambda_j \mathbf{v_j}, \quad j = 1, \ldots, n . \qquad \mathbf{G V = V D}$$

$$\mathbf{V} = [\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}] \quad , \quad \mathbf{V^T V = V V^T = I}$$

$$\mathbf{D} = \mathrm{diag}\, \{ \lambda_1, \lambda_2, \ \ldots \ , \lambda_n \}$$

$$\mathbf{G = V D V^T} = \Sigma\, \lambda_j \mathbf{v_j} \mathbf{v_j}^T$$

Aim: Computing a small number, **k**, of exterior eigenpairs.

For example, k eigenvalues with the largest moduli.

$$|\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_k| \geq \ldots \geq |\lambda_{k+\ell}| \geq \ldots \geq |\lambda_n|$$

$$\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_k, \cdots, \mathbf{v}_{k+\ell}, \cdots, \mathbf{v}_n$$

ℓ is the length of the restarted Krylov sequences

In our experiments $\ell = k + 40$

The qth iteration, $q = 1, 2, \dots,$

Starts with an $\mathbf{n} \times (\mathbf{k} + \ell)$ matrix ,

$$\mathbf{X}_{q-1} = [\, \mathbf{V}_{q-1}, \mathbf{Y}_{q-1} \,] \;,$$

that has **orthonormal columns**.

$\mathbf{V}_{q-1}$ is an $\mathbf{n} \times \mathbf{k}$ matrix that contains the current **Ritz vectors**.

$\mathbf{Y}_{q-1}$ is an $\mathbf{n} \times \ell$ matrix that contains “new” information which is obtained from a **Krylov matrix**.

The qth iteration, q = 1, 2, … ,

Step 1 : Compute the new Ritz matrix $\mathbf{V_q}$.

Step 2 : Compute a new Krylov information matrix $\mathbf{B_q}$.

Step 3 : Obtain $\mathbf{Z_q}$ by orthogonalizing $\mathbf{B_q}$ against $\mathbf{V_q}$.

Step 4 : Compute, $\mathbf{Y_q}$, an orthonormal basis of $\mathbf{Z_q}$.

Step 5 : Define $\mathbf{X_q} = [\mathbf{V_q}, \mathbf{Y_q}]$

The matrices $\mathbf{V_q}$, $\mathbf{Y_q}$ and $\mathbf{X_q}$ has orthonormal columns.

Step 1 : Compute the Rayleigh quotient matrix

$$\mathbf{S_q = X_{q-1}^T\, G\, X_{q-1}}$$

and the k largest eigenvalues of $\mathbf{S_q}$

$$|\lambda_1^{(q)}| \geq |\lambda_2^{(q)}| \geq \ldots \geq |\lambda_\kappa^{(q)}| \geq \ldots \geq |\lambda_\ell^{(q)}|$$

The related k eigenvectors are assembled into the ℓ **x k** matrix

$$\mathbf{W_q = [w_1 , w_2 , \ldots, w_k]}$$

and used to construct the **new matrix of Ritz vectors**

$$\mathbf{V_q = X_{q-1} W_q} \quad .$$

Since $\mathbf{X_{q-1}}$ and $\mathbf{W_q}$ have orthonormal columns, $\mathbf{V_q}$ inherits this property.

The monotonicity property

The eigenvalues of the matrix $V_q^T G V_q$

$$|\lambda_1^{(q)}| \geq |\lambda_2^{(q)}| \geq \ldots \geq |\lambda_\kappa^{(q)}|$$

interlace those of the matrix $[V_q, Y_q]^T G [V_q, Y_q]$

$$|\lambda_1^{(q+1)}| \geq |\lambda_2^{(q+1)}| \geq \ldots \geq |\lambda_\kappa^{(q+1)}|$$

and therefore

$$|\lambda_j| \geq |\lambda_j^{(q+1)}| \geq |\lambda_\kappa^{(q)}|$$

for $j = 1, \ldots, k$ and $q = 1, 2, \ldots$.

This holds for any choice of B_q !

The basic Krylov matrix

$$\mathbf{B_q} = [\mathbf{b_1}, \mathbf{b_2}, \ldots, \mathbf{b}_\ell]$$

The columns span a Krylov subspace of G that is generated by the following **three term recurrence relation**

For $\mathbf{j = 2, \ldots, k}$

$$\mathbf{b_j = G\, b_{j-1}}$$

Orthogonalize $\mathbf{b_j}$ against $\mathbf{b_{j-1}}$

Orthogonalize $\mathbf{b_j}$ against $\mathbf{b_{j-2}}$

Normalize $\mathbf{b_j}$.

The starting vector $\mathbf{b_0}$

is a unit vector in the direction

$$\mathbf{V_q e} = [\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_k}]\mathbf{e} = \mathbf{v_1} + \mathbf{v_2} + \ldots + \mathbf{v_k}$$

where $\mathbf{v_1} + \mathbf{v_2} + \ldots + \mathbf{v_k}$ are the current Ritz vectors .

Computing $\mathbf{b_0}$: Set $\mathbf{b_0} = \mathbf{V_q e}$,
normalize $\mathbf{b_0}$.

Computing $\mathbf{b_1}$: Set $\mathbf{b_1} = \mathbf{G b_0}$
orthogonalize $\mathbf{b_1}$ against $\mathbf{b_0}$,
normalize $\mathbf{b_1}$.

Comparison with "Explicit Restart"

Step 1 : Compute the new Ritz matrix $\mathbf{V_q}$.

Step 2 : Compute a new Krylov information matrix $\mathbf{B_q}$.

Step 3 : Obtain $\mathbf{Z_q}$ by orthogonalizing $\mathbf{B_q}$ against $\mathbf{V_q}$.

Step 4 : Compute, $\mathbf{Y_q}$, an orthonormal basis of $\mathbf{Z_q}$.

Step 5 : Define $\mathbf{X_q} = [\, \mathbf{V_q} , \mathbf{Y_q} \,]$

Step 1 : Compute a Ritz matrix $\mathbf{V_q}$ from $\mathbf{T_{q-1}}$.

Step 2 : Compute a new tridiagonal matrix $\mathbf{T_q}$.

(Starting from the direction of $\mathbf{V_q e}$.)

Comparison with "Implicit Restart"

Step 1 : Compute the new Ritz matrix $\mathbf{V_q}$.

Step 2 : Compute a new Krylov information matrix $\mathbf{B_q}$.

Step 3 : Obtain $\mathbf{Z_q}$ by orthogonalizing $\mathbf{B_q}$ against $\mathbf{V_q}$.

Step 4 : Compute, $\mathbf{Y_q}$, an orthonormal basis of $\mathbf{Z_q}$.

Step 5 : Define $\mathbf{X_q} = [\ \mathbf{V_q}, \mathbf{Y_q}\ ]$

Step 1 : Compute the new Ritz matrix $\mathbf{V_q}$ from $\mathbf{T_{q-1}}$.

Step 2 : Compute a new tridiagonal matrix $\mathbf{T_q}$,
(Using "polynomial filtering" .)

Applications

* **Low-rank approximations of large sparse matrices.**

* **Exact/Inexact inversions:**

Inner-outer iterative methods for calculating **small eigenvalues** and **small singular values.**

Low-rank approximation

of a large sparse m x n matrix **A**

is carried out by replacing **G** with $\mathbf{A}^T \mathbf{A}$

In practice **G** is never computed . Instead, matrix-vector products of the form

$\mathbf{z} = \mathbf{G}\mathbf{x}$ are computed in two steps: First compute $\mathbf{y} = \mathbf{A}\mathbf{x}$ then $\mathbf{z} = \mathbf{A}^T\mathbf{y}$.

Advantage: The left singular vectors (and left Ritz vectors) are not needed. **This leads to significant saving of computer storage** with respect to Lanczos bidiagonalization. (The final approximation can be expressed as $\mathbf{A}\mathbf{V}\mathbf{V}^T = \mathbf{U}\mathbf{V}^T$.)

Computing small eigenvalues

Assume for simplicity that the eigenvalues of G satisfy

$$\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n > 0$$

and we want to compute the k smallest eigenvalues.

In this case there is a minor change in Step 1.

Step 1* : Compute the Rayleigh quotient matrix

$$\mathbf{S_q = X_{q-1}^{T}\, G\, X_{q-1}}$$

and the k smallest eigenvalues of $\mathbf{S_q}$

$$\lambda_1^{(q)} \geq \lambda_2^{(q)} \geq \ldots \geq \lambda_{n+1-k}^{(q)} \geq \ldots \geq \lambda_n^{(q)}$$

The related k eigenvectors are assembled into the ℓ **x k** matrix

$$\mathbf{W_q = [w_1 , w_2 , \ldots, w_k]}$$

and used to construct the **new matrix of Ritz vectors**

$$\mathbf{V_q = X_{q-1} W_q}$$

Since $\mathbf{X_{q-1}}$ and $\mathbf{W_q}$ have orthonormal columns, $\mathbf{V_q}$ inherits this property.

Exact inversions

This improvement is carried out by replacing $\mathbf{G}$ with $\mathbf{G}^{-1}$ in the construction of the Krylov matrix $\mathbf{B_q} = [\mathbf{b_1}, \mathbf{b_2}, \ldots, \mathbf{b_\ell}]$.

Here the columns of $\mathbf{B_q}$ span a **Krylov subspace of $\mathbf{G}^{-1}$** that is generated by the following **three term recurrence relation**

For $\mathbf{j = 2, \ldots, k}$

Set $\mathbf{b_j = G^{-1} b_{j-1}}$

Orthogonalize $\mathbf{b_j}$ against $\mathbf{b_{j-1}}$

Orthogonalize $\mathbf{b_j}$ against $\mathbf{b_{j-2}}$

Normalize $\mathbf{b_j}$.

Exact inversions

In practice, the columns of $\mathbf{B_q}$ span a **Krylov subspace of G^{-1}** that is obtained by using a **direct method** to solve the related linear systems.

For $j = 2, \ldots, k$

Compute $\mathbf{b_j}$ by solving the linear system $\mathbf{Gx = b_{j-1}}$

Orthogonalize $\mathbf{b_j}$ against $\mathbf{b_{j-1}}$

Orthogonalize $\mathbf{b_j}$ against $\mathbf{b_{j-2}}$

Normalize $\mathbf{b_j}$.

Comparison with "Implicit Restart"

Step 1 : Compute the smallest Ritz eigenpairs $\mathbf{V_q}$ of $\mathbf{G}$.

Step 2 : Compute a new Krylov information matrix $\mathbf{B_q}$ of $\mathbf{G^{-1}}$.

Step 3 : Obtain $\mathbf{Z_q}$ by orthogonalizing $\mathbf{B_q}$ against $\mathbf{V_q}$.

Step 4 : Compute, $\mathbf{Y_q}$, an orthonormal basis of $\mathbf{Z_q}$.

Step 5 : Define $\mathbf{X_q} = [\ \mathbf{V_q}, \mathbf{Y_q}\ ]$

Step 1 : Use $\mathbf{T_{q-1}}$ to compute the largest Ritz eigenpairs of $\mathbf{G^{-1}}$.

Step 2 : Compute a new Lanczos matrix $\mathbf{T_q}$ of $\mathbf{G^{-1}}$.

Inexact inversions

The columns of $\mathbf{B_q}$ approximate a **Krylov subspace of $\mathbf{G^{-1}}$** that is is obtained by using an **iterative method** to solve the related linear systems. (Such as CG, MINRES or GMRES, equiped with a suitable preconditioner.)

For $j = 2, \dots, k$

Set $\mathbf{b_j}$ to be an **approximate solution** of the linear system $\mathbf{Gx = b_{j-1}}$.

Orthogonalize $\mathbf{b_j}$ against $\mathbf{b_{j-1}}$.

Orthogonalize $\mathbf{b_j}$ against $\mathbf{b_{j-2}}$.

Normalize $\mathbf{b_j}$.

Comparison with "Implicit Restart"

Step 1 : Compute the smallest Ritz eigenpairs $\mathbf{V_q}$ of $\mathbf{G}$.

Step 2 : Compute an **approximate** Krylov matrix $\mathbf{B_q}$ of $\mathbf{G^{-1}}$.

Step 3 : Obtain $\mathbf{Z_q}$ by orthogonalizing $\mathbf{B_q}$ against $\mathbf{V_q}$.

Step 4 : Compute, $\mathbf{Y_q}$, an orthonormal basis of $\mathbf{Z_q}$.

Step 5 : Define $\mathbf{X_q} = [\ \mathbf{V_q}, \mathbf{Y_q}\ ]$

Step 1 : Use $\mathbf{T_{q-1}}$ to compute the largest Ritz eigenpairs of $\mathbf{G^{-1}}$.

Step 2 : Compute an **approximate** Lanczos matrix $\mathbf{T_q}$ of $\mathbf{G^{-1}}$.

Computing small singular values

A is a large sparse m x n matrix with singular values

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n \geq 0 \quad ,$$

and we want to compute the k smallest singular triplets.

This task is carried out by introducing the following modifications in Steps 1 and 2 of the basic iteration.

Computing small singular values:

The qth iteration , $q = 1, 2, \ldots$.

Step 1 :** Compute the **k** smallest singular values of $\mathbf{A X_{q-1}}$ and the related matrix of right Ritz vectors $\mathbf{V_k}$.

Step 2 :** Compute an **approximate** Krylov matrix $\mathbf{B_q}$ of $\mathbf{(A^T A)^{-1}}$.

Step 3 : Obtain $\mathbf{Z_q}$ by orthogonalizing $\mathbf{B_q}$ against $\mathbf{V_q}$.

Step 4 : Compute, $\mathbf{Y_q}$, an orthonormal basis of $\mathbf{Z_q}$.

Step 5 : Define $\mathbf{X_q} = [\, \mathbf{V_q}, \mathbf{Y_q} \,]$

Step 1 :** Compute the Rayleigh matrix

$$\mathbf{H_q = A X_{q-1}}$$

and the **k smallest singular values** of $\mathbf{H_q}$

$$\sigma_1^{(q)} \geq \sigma_2^{(q)} \geq \ldots \geq \sigma_{n+1-k}^{(q)} \geq \ldots \geq \sigma_n^{(q)}$$

The related **k right singular vectors** are assembled into the ℓ **x k** matrix

$$\mathbf{W_q = [w_1 , w_2 , \ldots , w_k]}$$

and used to construct the **new matrix of Ritz vectors**

$$\mathbf{V_q = X_{q-1} W_q}$$

Since $\mathbf{X_{q-1}}$ and $\mathbf{W_q}$ have orthonormal columns, $\mathbf{V_q}$ inherits this property.

Step 2** : Inexact inversion of A^TA

The columns of B_q approximate a **Krylov subspace of** $(A^TA)^{-1}$ using an **iterative method** to solve the related linear systems.

For j = 2, … , k

Set b_j to be an **approximate solution** of the linear system $A^TAx = b_{j-1}$.

Orthogonalize b_j against b_{j-1} .

Orthogonalize b_j against b_{j-2} .

Normalize b_j .

Computing small singular triplets

The new method

Step 1: Compute $\mathbf{V_q}$ the smallest right Ritz vectors of $\mathbf{A}$.

Step 2: Compute an **approximate** Krylov matrix $\mathbf{B_q}$ of $\mathbf{(A^TA)^{-1}}$.

Step 3: Obtain $\mathbf{Z_q}$ by orthogonalizing $\mathbf{B_q}$ against $\mathbf{V_q}$.

Step 4: Compute, $\mathbf{Y_q}$, an orthonormal basis of $\mathbf{Z_q}$.

Step 5: Define $\mathbf{X_q = [\ V_q , Y_q\ ]}$.

Lanczos bidiagonalization

Step 1: Use $\mathbf{B_{q-1}}$ to compute the largest Ritz eigenpairs of $\mathbf{A^{-1}}$.

Step 2: Compute a lower bidiagonal matrix $\mathbf{B_q}$ from $\mathbf{A^{-1}}$.

Concluding remarks

The new method is useful for the following purposes:

* A reduced storage approach for calculating low-rank approximations of large matrices.

* The use of exact/inexact inversions for calculating small eigenvalues and small singular triplets.
  (In this case most of the computation time is spent on the linear solver.)

* The method is easily adapted to use "shift and invert" techniques.

The END

Thank You