Stationary Iterative Methods and Krylov Subspace Methods

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Outline

1. Stationary Iterative Methods
2. Krylov Subspace Methods
3. Preconditioning
4. Summary

Stationary Iterative Methods

- Consider a linear system of equations

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \quad \mathbf{A} \in \mathbb{R}^{n \times n}, \quad \mathbf{b} \in \mathbb{R}^{n}.$$

- A *splitting* of $\mathbf{A} \in \mathbb{R}^{n \times n}$ is a decomposition

$$\mathbf{A} = \mathbf{M} - \mathbf{N},$$

  with $\mathbf{M}$ nonsingular.

- The equation

$$\mathbf{A}\mathbf{x} = (\mathbf{M} - \mathbf{N})\mathbf{x} = \mathbf{b}$$

  implies

$$\mathbf{x} = \mathbf{M}^{-1}\mathbf{N}\mathbf{x} + \mathbf{M}^{-1}\mathbf{b} := \mathbf{R}\mathbf{x} + \mathbf{c}.$$

  Given a starting vector $\mathbf{x}_0$, we obtain an iterative method

$$\mathbf{x}_{k+1} = \mathbf{R}\mathbf{x}_k + \mathbf{c}, \quad k = 0, 1, 2, \ldots$$

Stationary Iterative Methods

- Correction form

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{M}^{-1}\mathbf{r}_k,$$

where the residual

$$\mathbf{r}_k = \mathbf{b} - \mathbf{A}\mathbf{x}_k.$$

- Error recurrence

$$\mathbf{e}_k = \mathbf{x} - \mathbf{x}_k, \qquad \mathbf{e}_{k+1} = \mathbf{M}^{-1}\mathbf{N}\mathbf{e}_k$$

- Difference recurrence

$$\mathbf{d}_k = \mathbf{x}_{k+1} - \mathbf{x}_k, \qquad \mathbf{d}_{k+1} = \mathbf{M}^{-1}\mathbf{N}\mathbf{d}_k$$

- Residual recurrence

$$\mathbf{r}_{k+1} = (\mathbf{I} - \mathbf{A}\mathbf{M}^{-1})\mathbf{r}_k = \mathbf{N}\mathbf{M}^{-1}\mathbf{r}_k.$$

Stationary Iterative Methods

- Convergence criterion

  The iteration $\mathbf{x}_{k+1} = \mathbf{R}\mathbf{x}_k + \mathbf{c}$ converges to the solution of $\mathbf{A}\mathbf{x} = \mathbf{b}$ for all starting vectors $\mathbf{x}_0$ if and only if $\rho(\mathbf{R}) < 1$.

- Desirable splitting

  $\mathbf{R}\mathbf{v} = \mathbf{M}^{-1}\mathbf{N}\mathbf{v}$ and $\mathbf{c} = \mathbf{M}^{-1}\mathbf{b}$ are easy to evaluate, and $\rho(\mathbf{R})$ is small (< 1).

- Examples

  (1). Jacobi's method

  (2). Gauss–Seidel method

  (3). SOR(ω)

  (4). Domain decomposition methods

  (5). Multigrid methods

Generalized Minimal Residual Method (GMRES)

- Idea of GMRES: Consider a nonsingular linear system

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \quad \mathbf{A} \in \mathbb{R}^{n\times n}, \quad \mathbf{b} \in \mathbb{R}^n.$$

For any initial guess $\mathbf{x}_0$, at step k, GMRES finds the kth approximate solution

$$\mathbf{x}_k = \underset{\mathbf{x}\in\mathbf{x}_0+\mathcal{K}_k(\mathbf{A},\mathbf{r}_0)}{\operatorname{argmin}} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2,$$

where $\mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0$ and

$$\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0) = \operatorname{span}\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \ldots, \mathbf{A}^{k-1}\mathbf{r}_0\}.$$

For the residual $\mathbf{r}_k = \mathbf{b} - \mathbf{A}\mathbf{x}_k$, we have

$$\|\mathbf{r}_k\|_2 = \min_{\mathbf{x}\in\mathbf{x}_0+\mathcal{K}_k(\mathbf{A},\mathbf{r}_0)} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2 \quad \text{and} \quad \mathbf{r}_k \perp \mathbf{A}\mathcal{K}_k.$$

Conjugate Gradients (CG)

- Idea of CG: Consider an SPD linear system

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \quad \mathbf{A} \in \mathbb{R}^{n\times n}, \quad \mathbf{b} \in \mathbb{R}^n.$$

For initial guess $\mathbf{x}_0$, at step k, the conjugate gradient method finds an approximate solution

$$\mathbf{x}_k \in \mathbf{x}_0 + \mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)$$

satisfying

$$\mathbf{r}_k := \mathbf{b} - \mathbf{A}\mathbf{x}_k \perp \mathcal{K}_k(\mathbf{A}, \mathbf{r}_0),$$

where

$$\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0) := \operatorname{span}\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \ldots, \mathbf{A}^{k-1}\mathbf{r}_0\}.$$

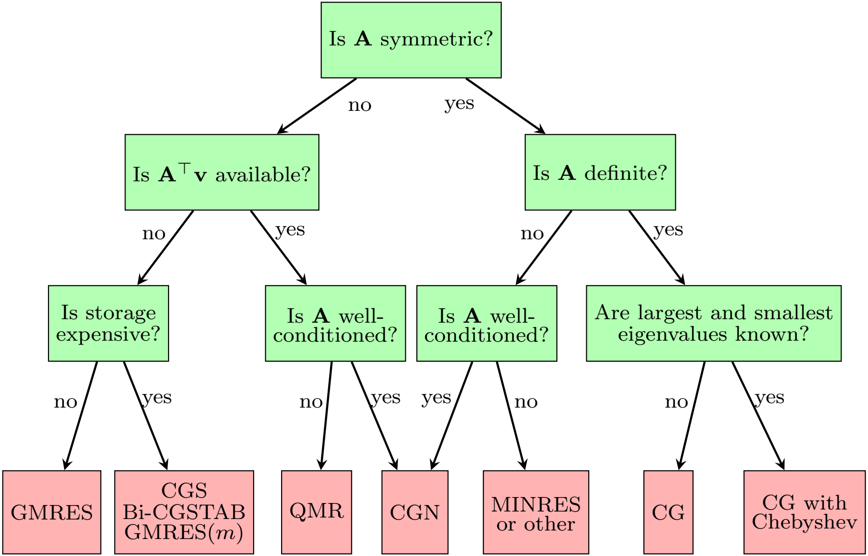
We have

$$\|\mathbf{x} - \mathbf{x}_k\|_{\mathbf{A}} = \min_{\mathbf{z}\in\mathbf{x}_0+\mathcal{K}_k(\mathbf{A},\mathbf{r}_0)} \|\mathbf{x} - \mathbf{z}\|_{\mathbf{A}}.$$

Krylov Subspace Methods

- Matrix-free implementation: $\mathbf{A}\mathbf{v}$ and $\mathbf{A}^\top\mathbf{v}$ are enough.
- GMRES = generalized minimal residual; MINRES
- CG = conjugate gradient; CGN; CGLS; LSQR
- Bi-CG = bi-conjugate gradient
  COCG = Bi-CG for complex symmetric systems
- CGS = conjugate gradients squares
  transpose free, but is twice as erratic
- Bi-CGSTAB = stabilized Bi-CG (via stabilizing CGS)
  Significantly smooths the convergence of Bi-CG, transpose free
- QMR = quasi-minimal residuals
  Pronounced effect on the smoothness of convergence
- TFQMR = tanspose-free QMR
  transpose free and smooth convergence of QMR
- ...

Decision Tree for Choosing Krylov Solvers



Preconditioning

- To improve the convergence of Krylov subspace methods, it is important to have a preconditioner (suitable approximation for the original coefficient matrix $\mathbf{A}$), denoted by $\mathbf{M}$.
- Left preconditioning, i.e.,

$$\mathbf{M}^{-1}\mathbf{A}\mathbf{x} = \mathbf{M}^{-1}\mathbf{b}.$$

- Right preconditioning is often used, i.e.,

$$\mathbf{A}\mathbf{M}^{-1}\mathbf{z} = \mathbf{b}, \quad \mathbf{x} = \mathbf{M}^{-1}\mathbf{z},$$

  because it produces the unpreconditioned residual.
- If $\mathbf{M}$ is SPD, two-sided preconditioning:

$$\mathbf{M} = \mathbf{L}\mathbf{L}^{\top}, \quad (\mathbf{L}^{-1}\mathbf{A}\mathbf{L}^{-\top})\mathbf{L}^{\top}\mathbf{x} = \mathbf{L}^{-1}\mathbf{b}.$$

Preconditioning

- How to find a good preconditioner? It's problem dependent.

  Example. Let

  $$\mathcal{A} = \begin{bmatrix} \mathbf{A} & \mathbf{B}^\top \\ \mathbf{C} & \mathbf{0} \end{bmatrix}$$

  and

  $$\mathcal{M} = \begin{bmatrix} \mathbf{A} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}\mathbf{A}^{-1}\mathbf{B}^\top \end{bmatrix},$$

  where $\mathbf{A} \in \mathbb{R}^{m\times m}$ is invertible, and $\mathbf{B}, \mathbf{C} \in \mathbb{R}^{n\times m}$ with $m \geq n$. Assume that $-\mathbf{C}\mathbf{A}^{-1}\mathbf{B}^\top$ is invertible.

  The preconditioned matrix $\mathcal{M}^{-1}\mathcal{A}$ is diagonalizable and has at most three distinct eigenvalues

  $$1, \quad (1+\sqrt{5})/2, \quad (1-\sqrt{5})/2.$$

  GMRES converges within three steps.

Preconditioning

- Stationary iterative methods

  Any iterative technique can be used as a preconditioner.
- Algebraic preconditioning

  Incomplete Cholesky or LU factorization.
- Physical approximation problem preconditioning

  Constant-coefficient or symmetric approximation.

  Splitting of a multi-term operator.

  Dimensional splitting or ADI.

  Periodic or convolution approximation.
- Polynomial preconditioning

  PROXY-GMRES (SIMAX 2021).
- Multipreconditioning: Flexible GMRES
- ...

Preconditioning in Practice

- In many cases (e.g., multigrid methods and domain decomposition methods) the structure of $\mathbf{M}$ is unknown or $\mathbf{M}$ is expensive to compute.
- We never explicitly form $\mathbf{M}^{-1}$. Only the action of applying the preconditioner solve operation $\mathbf{M}^{-1}$ to a given vector is computed in iterative methods. So $\mathbf{M}^{-1}\mathbf{z}$ must be cheap.
- Example: we would like to use a stationary method

$$\mathbf{x}_k = \mathbf{M}^{-1}\mathbf{N}\mathbf{x}_{k-1} + \mathbf{M}^{-1}\mathbf{b}$$

as a preconditioner, but we do not know explicitly $\mathbf{M}$. If

$$\texttt{function} \quad \texttt{xk} = \texttt{stationary}(\texttt{A}, \texttt{b}, \texttt{x0}, \texttt{k}),$$

then

$$\mathbf{M}^{-1}\mathbf{z} = \texttt{stationary}(\texttt{A}, \texttt{z}, 0, 1),$$

$$\mathbf{M}^{-1}\mathbf{A}\mathbf{z} = \mathbf{z} - \texttt{stationary}(\texttt{A}, 0, \texttt{z}, 1).$$

Summary

- Krylov subspace methods (with preconditioning) can be used in a matrix-free way.
- All the iterative methods like Jacobi, Gauss–Seidel, and SOR, should be used as preconditioners for a Krylov method. The Krylov method serves as an accelerator of convergence.
- We never explicitly form $\mathbf{M}^{-1}$. Only the action of applying the preconditioner solve operation $\mathbf{M}^{-1}$ to a given vector is computed in iterative methods.
- PETSc: the Portable, Extensible Toolkit for Scientific Computation
- Automatic selection of solvers and preconditioners???

A Reference Book

- Iterative Methods and Preconditioners for Systems of Linear Equations

  Authors: Gabriele Ciaramella and Martin J. Gander

  SIAM, 2022