

# Global Iterative Methods for Sparse Approximate Inverses of Symmetric Positive-Definite Matrices

GAMM Workshop on  
Applied and Numerical Linear Algebra  
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October 23, 2025  
(revised in December 2025)



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# Introduction

## The "What?", the "Why?" and the "How?"

- ▶ Given a sparse matrix  $A \in \mathbb{R}^{n \times n}$ , we seek a sparse matrix  $M \in \mathbb{R}^{n \times n}$  such that  $I_n - AM$  is small in some sense:

We say that  $M$  is a right sparse approximate inverse (SPAI) of  $A$ .

- ▶ In this talk, we aim at minimizing the Frobenius residual norm:

Find a sparse  $M \in \mathbb{R}^{n \times n}$  s.t.  $f(M) := \|I_n - AM\|_F^2$  is minimized

- ▶ SPAIs are good candidates to precondition the iterative solve of linear systems.
- ▶ Existing methods to find SPAIs include:
  - Method of Hotelling and Bodewig,
  - Steepest descent (SD) method,
  - Minimal residual (MR) method.

To which non-zero dropping strategies are added.

- ▶ Our experiments show that, even without dropping strategy deployed, some of these methods struggle to achieve symmetric positive definite (SPD) spectra for  $M$  when  $A$  is SPD.

# One-dimensional descent methods

## One-dimensional descent methods

- ▶ For this problem, it is standard to consider the Frobenius inner product  $(X, Y)_F := \text{tr}(X^T Y)$  with induced norm  $\|X\|_F := (X, X)_F^{1/2}$ .
- ▶ In this work:
  - We look into descent methods as projections with carefully defined orthogonality constraints.
  - Orthogonality:  $\mathbb{R}^{m \times n} \ni X \perp \mathcal{S} \subset \mathbb{R}^{m \times n} \iff (X, Y)_F = 0 \forall Y \in \mathcal{S}$ .

### Definition (One dimensional descent methods)

- Given  $A \in \mathbb{R}^{n \times n}$  and  $M_0 \in \mathbb{R}^{n \times n}$  a sequence of one-dimensional descent iterates with search directions  $P_i \in \mathbb{R}^{n \times n}$  is defined by:

$$M_{i+1} \in M_i + \text{span}\{P_i\} \quad \text{s.t.} \quad R_{i+1} := I_n - AM_{i+1} \perp A \text{span}\{P_i\}$$

for  $i = 0, 1, \dots$

- This leads to the update formula:

$$M_{i+1} = M_i + \alpha_i P_i \quad \text{where} \quad \alpha_i = \frac{(R_i, AP_i)_F}{\|AP_i\|_F^2} \quad \text{for} \quad i = 0, 1, \dots$$

## Steepest descent method

- ▶ Of particular interest for the definition of a search direction in a descent method is the gradient given by:

$$\nabla_M f(M) = -2AR = -2(I_n - AM)$$

- ▶ The steepest descent (SD) method is obtained by setting the search direction opposed to the gradient direction:

$$P_i := AR_i \text{ for } i = 0, 1, \dots$$

The resulting algorithm is given by:

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### Algorithm 1 SD( $A, M_0$ )

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- 1:  $R_0 := I_n - AM_0$
  - 2:  $P_0 := AR_0$
  - 3: **for**  $i = 0, 1, \dots$  **do**
  - 4:    $\alpha_i := (R_i, AP_i)_F / \|AP_i\|_F^2$
  - 5:    $M_{i+1} := M_i + \alpha_i P_i$
  - 6:    $R_{i+1} := R_i - \alpha_i AP_i$
  - 7:    $P_{i+1} := AR_{i+1}$
-

## Minimal residual method

- ▶ Alternatively, the minimal residual (MR) method (Chow and Saad, 1998) is formed by setting the search direction to the residual:

$$P_i := R_i \text{ for } i = 0, 1, \dots$$

The resulting algorithm is given by:

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### Algorithm 2 MR( $A, M_0$ )

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- 1:  $R_0 := I_n - AM_0$
  - 2: **for**  $i = 0, 1, \dots$  **do**
  - 3:    $\alpha_i := (R_i, AR_i)_F / \|AR_i\|_F^2$
  - 4:    $M_{i+1} := M_i + \alpha_i R_i$
  - 5:    $R_{i+1} := R_i - \alpha_i AR_i$
- 

- ▶ Both the SD and MR methods are optimal in the sense that:

$$\|I_n - AM_{i+1}\|_F = \min_{M \in M_i + \text{span}\{P_i\}} \|I_n - AM\|_F \text{ for } i = 0, 1, \dots$$

Chow, E., & Saad, Y. (1998). Approximate inverse preconditioners via sparse-sparse iterations. *SIAM Journal on Scientific Computing*, 19(3), 995-1023.

# Locally optimal variants

## Local optimality

- ▶ The term "locally optimal" was coined by Andrew Knyazev (2001) to refer to the enrichment with previous search directions of the search space used for the subspace optimization of Rayleigh quotients of symmetric matrices.
- ▶ To apply local optimality to the subspace minimization of  $f(M)$ , we stress that the MR search directions constitute a trivial case of:

$$P_i \in \text{span}\{P_{i-1}, R_i\}. \quad (1)$$

### Theorem (Local optimality)

Given  $A \in \mathbb{R}^{n \times n}$  and  $M_0 \in \mathbb{R}^{n \times n}$  with search directions satisfying Eq. (1) and  $P_{-1} := 0_{n \times n}$ , we have:

$$\min_{M \in M_i + \text{span}\{P_{i-1}, R_i\}} f(M) \leq \min_{M \in M_i + \text{span}\{R_i\}} f(M)$$

- ▶ Similarly, local optimality can be stated with respect to SD-like iterates.

Andrew Knyazev (2001). Toward the optimal preconditioned eigensolver: Locally optimal block preconditioned conjugate gradient method. SIAM journal on scientific computing, 23(2):517–541.

## Local optimal minimal residual method

- ▶ Upon deploying a locally optimal iteration in the context of the MR approach, we obtain the following locally optimal minimal residual (LOMR) method:

### Definition (LOMR)

- Given  $A \in \mathbb{R}^{n \times n}$  and  $M_0 \in \mathbb{R}^{n \times n}$ , a sequence of LOMR iterates is defined by:

$$M_{i+1} := \arg \min_{M \in M_i + \text{span}\{P_{i-1}, R_i\}} \|I_n - AM\|_F \quad \text{for } i = 0, 1, \dots$$

- The main iterates are given by:

$$M_{i+1} := M_i + \delta_i R_i + \gamma_i P_{i-1} \quad \text{for } i = 0, 1, \dots$$

where the optimal step sizes  $\delta_i$  and  $\gamma_i$  depend on:

$$(R_i, AR_i)_F, \|AR_i\|_F^2, \|AP_{i-1}\|_F^2, (AR_i, AP_i)_F, (R_i, AP_i)_F.$$

# Conjugate gradient methods

## Nonlinear conjugate gradient method

- ▶ We introduce the nonlinear conjugate gradient (NCG) method as follows:

### Definition (NCG)

- Given  $A \in \mathbb{R}^{n \times n}$  and  $M_0 \in \mathbb{R}^{n \times n}$ , a sequence of NCG iterates is defined by:

$$M_{i+1} \in M_i + \text{span}\{P_i\} \quad \text{s.t.} \quad R_{i+1} := I_n - AM_{i+1} \perp \text{span}\{P_i\}$$

for  $i = 0, 1, \dots$ , with search direction  $P_i \in \mathbb{R}^{n \times n}$  defined as

$$P_i \in -G_i + \text{span}\{P_{i-1}\} \quad \text{s.t.} \quad P_i \perp A \text{span}\{P_{i-1}\} \quad \text{for } i = 1, 2, \dots$$

with  $P_0 := -G_0$  and  $G_i := -AR_i$ , where  $G_i$  denotes the gradient direction of  $f(M)$  at  $M_i$ .

## Nonlinear conjugate gradient method, con'd

- ▶ We introduce the nonlinear conjugate gradient (NCG) method as follows:

### Definition (NCG, cont'd)

- The iterates of the NCG method are given by:

$$M_{i+1} := M_i + \alpha_i P_i \quad \text{where} \quad \alpha_i := -\frac{(R_i, G_i)_F}{(P_i, AP_i)_F} \quad \text{and} \quad G_i := -AR_i$$

for  $i = 0, 1, \dots$ , in which the search direction is updated as follows:

$$P_i := -G_i + \beta_i P_{i-1} \quad \text{where} \quad \beta_i := \frac{(R_i, G_i)_F}{(R_{i-1}, G_{i-1})_F} \quad \text{for} \quad i = 1, 2, \dots$$

## Nonlinear conjugate gradient method, con'd

- ▶ The NCG method can be seen as a Krylov method:

### Theorem (Global optimality of NCG iterates)

*The NCG iterates are equivalently given by*

$$M_i \in M_0 + \mathcal{K}_i(A^2, G_0) \quad \text{s.t.} \quad R_i := I_n - AM_i \perp \mathcal{K}(A^2, G_0) \quad \text{for } i = 1, 2, \dots$$

*and the right-approximate inverse  $M_i$  is optimal in the sense that*

$$\|A^{-1} - M_i\|_{F,A} = \min_{M \in M_0 + \mathcal{K}_i(A^2, G_0)} \|A^{-1} - M\|_{F,A} \quad \text{for } i = 1, 2, \dots$$

*That is, the NCG iterate minimizes the Frobenius  $A$ -norm of the error  $E := A^{-1} - M$  over the affine Krylov subspace of  $A^2$  generated by the initial gradient  $G_0 := -AR_0$ .*

## Conjugate gradient method

- ▶ Lastly, we implement a conjugate gradient (CG) method which corresponds to the standard conjugate gradient algorithm with matrix iterates and Frobenius inner products:

### Definition (CG)

- Given  $A \in \mathbb{R}^{n \times n}$  and  $M_0 \in \mathbb{R}^{n \times n}$ , a sequence of CG iterates is defined by:

$$M_{i+1} \in M_i + \text{span}\{P_i\} \quad \text{s.t.} \quad R_{i+1} := I_n - AM_{i+1} \perp \text{span}\{P_i\}$$

for  $i = 0, 1, \dots$ , with search direction  $P_i \in \mathbb{R}^{n \times n}$  defined as

$$P_i \in R_i + \text{span}\{P_{i-1}\} \quad \text{s.t.} \quad P_i \perp A \text{span}\{P_{i-1}\} \quad \text{for } i = 1, 2, \dots$$

with  $P_0 := R_0$ .

# Non-zero dropping strategies

## Non-zero dropping strategy — main iterate

► Non-zero values are dropped in the main iterate,  $M \mapsto \widehat{M}$ , to try and decrease the residual norm achieved after dropping, i.e.,  $\|\widehat{R}\|_F < \|R\|_F$ :

① Symmetrize  $M$ :  $\widehat{M} := (M + M^T) / 2$ .

② Drop insignificant non-diagonal components:

$\widehat{m}_{k\ell} := 0 \forall |\widehat{m}_{k\ell}| < u$  with  $k \neq \ell$ , where  $u$  denotes the unit round-off.

③ If  $|\mathcal{NNZ}(\widehat{M})| > nnz$ :

$$\text{For } (k, \ell) \in \mathcal{D} = \underset{\substack{\mathcal{S} \subset \mathcal{NNZ}(\widehat{M}) \setminus \{(k, k), k=1, \dots, n\} \\ |\mathcal{NNZ}(\widehat{M})| - |\mathcal{S}| = nnz}}{\text{arg}} \min \left\{ \sum_{(k, \ell) \in \mathcal{S}} \widehat{m}_{k\ell}^2 \|Ae_k\|_2^2 + 2 \sum_{(k, \ell) \in \mathcal{S}} \widehat{m}_{k\ell} \cdot (AR)_{k\ell} \right\},$$

set  $\widehat{m}_{k\ell} := 0$ .

- The matrix  $AR$  is already formed at each iteration.
- The dot products  $\|Ae_1\|_2^2, \dots, \|Ae_n\|_2^2$  need be computed only once, at the start of the algorithm.

## Non-zero dropping strategy — search direction

► Similarly, we drop non-zero values in the search direction iterate,  $P \mapsto \hat{P}$ , simply by:

① If  $|\mathcal{NNZ}(P)| > nnz$ :

$$\text{For } (k, \ell) \in \mathcal{D}_P = \underset{\substack{\mathcal{S} \subset \mathcal{NNZ}(P) \\ |\mathcal{NNZ}(P)| - |\mathcal{S}| = m}}{\text{arg min}} \left\{ \sum_{(k, \ell) \in \mathcal{S}} |p_{k\ell}| \right\},$$

set  $\hat{p}_{k\ell} := 0$ , otherwise  $\hat{p}_{k\ell} := p_{k\ell}$ .

② Otherwise,  $\hat{P} := P$ .

# Summary of methods

## Summary of computing cost per iteration

Method	Operation count per iteration (without dropping)
MR	1 SpGEMM <sup>†</sup> + 1 SpFIP <sup>◦</sup> + 1 SpFN <sup>•</sup> + 2 SpGEAMs*
SD	2 SpGEMMs + 1 SpFIP + 1 SpFN + 2 SpGEAMs
NCG	2 SpGEMMs + 2 SpFIPs + 3 SpGEAMs
CG	1 SpGEMM + 1 SpFIP + 1 SpFN + 3 SpGEAMs
LOMR	2 SpGEMMs + 3 SpFIPs + 2 SpFNs + 5 SpGEAMs

†: General product of sparse matrices    ◦: Frobenius inner product of sparse matrices  
•: Frobenius norm of sparse matrix    \*: General addition of sparse matrices

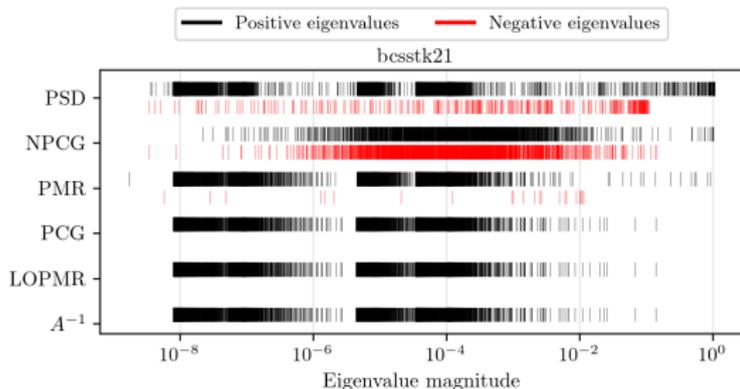
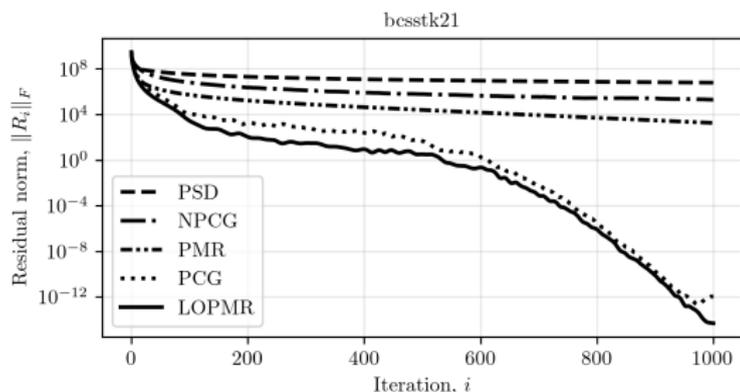
Method	Operation count per iteration (with dropping)
MR	2 SpGEMM + 1 SpFIP + 1 SpFN + 2 SpGEAMs
SD	3 SpGEMMs + 1 SpFIP + 1 SpFN + 2 SpGEAMs
NCG	3 SpGEMMs + 2 SpFIPs + 3 SpGEAMs
CG	2 SpGEMMs + 1 SpFIP + 1 SpFN + 3 SpGEAMs
LOMR	3 SpGEMMs + 3 SpFIPs + 2 SpFNs + 4 SpGEAMs

A substantial added cost is induced by dropping zeros and changing the data structures of the sparse iterates.

# Numerical experiments

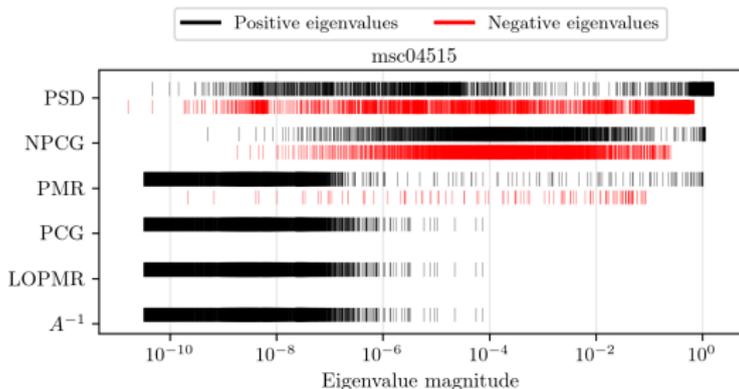
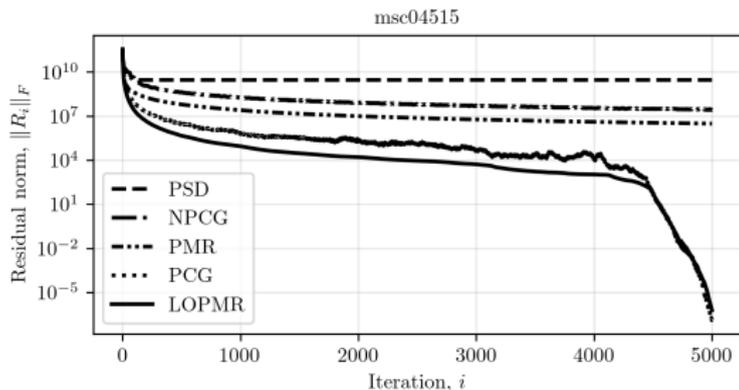
# Dropping-free experiments

► bcsstk21 matrix (from SuiteSparse Collection), with Jacobi preconditioner:



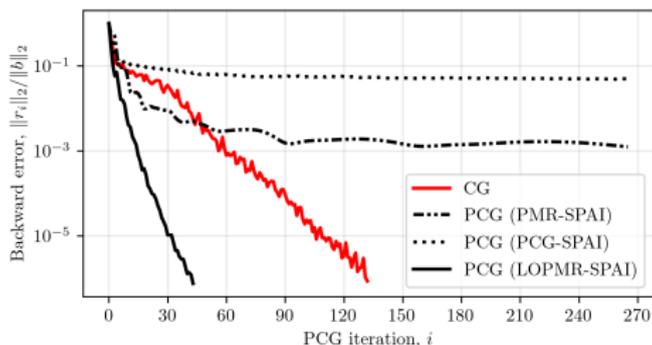
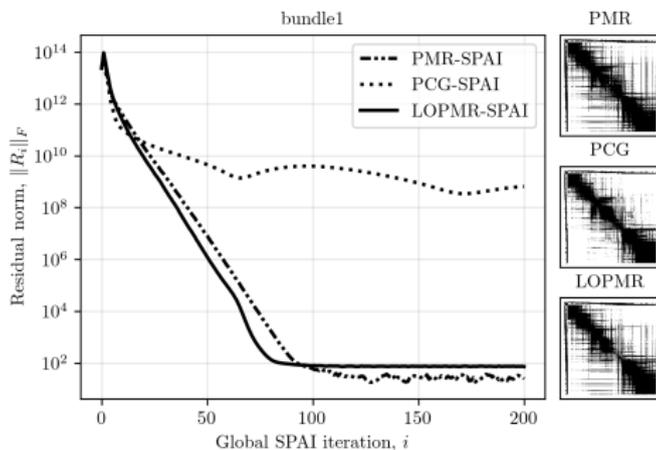
# Dropping-free experiments, cont'd

- msc04515 matrix (from SuiteSparse Collection), with Jacobi preconditioner:



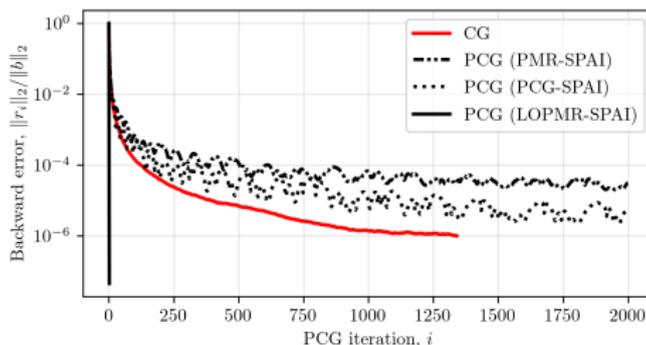
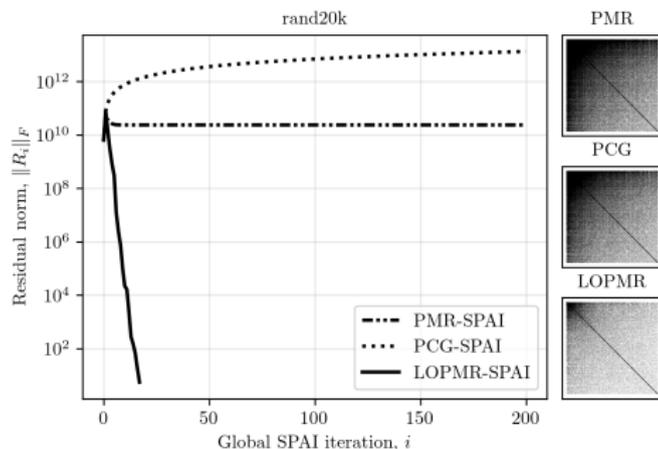
# With dropping experiments

- ▶ bundle1 matrix (from SuiteSparse Collection) with Jacobi preconditioner, and 3% density:



# With dropping experiments, cont'd

- ▶ rand20k matrix ([github.com/venkovic/matrix-market](https://github.com/venkovic/matrix-market)) with Jacobi preconditioner, and 3% density:



# Closing remarks

# Conclusion

## ► Findings:

Global iterative methods were introduced for the approximation of SPAIs of SPD matrices:

- SD, MR and NCG all fail to consistently yield SPAIs with SPD spectra for SPD matrices, even without dropping.
- LOMR and CG both consistently yield SPAIs with SPD spectra for SPD matrices, without dropping.
- LOMR achieves better SPAIs, with dropping, than CG.

## ► Dissemination:

### - Preprint:

N. Venkovic and H. Anzt (2025) Global iterative methods for sparse approximate inverses of symmetric positive-definite matrices. arXiv preprint, arXiv:2511.09753.

### - Repository allowing reproducible experiments:

[github.com/venkovic/julia-global-spd-spai](https://github.com/venkovic/julia-global-spd-spai)

### - Find this presentation at:

[venkovic.github.io/research](https://venkovic.github.io/research)

## Related ongoing and future work

- ▶ Randomized short-recurrence iterative methods for approximate low-rank matrix factorizations:

Venkovic & Anzt (in progress). Randomized first-order short-recurrence subspace iterative methods for approximate low-rank matrix factorizations.

[github.com/venkovic/julia-iterative-low-rank](https://github.com/venkovic/julia-iterative-low-rank)

- ▶ Related future works:

- SPAs:
  - Parallelization.
- Low-rank approximation:
  - Application to matrix recovery (completion and sensing problems).
  - Non-negative matrix factorizations.
  - Tensor factorizations.