Block CG Solvers Documentation github.com/lkeegan/blockCG

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1 Introduction

Formulations of block CG solvers. Notation conventions used: A is the hermitian positive definite $L \times L$ matrix to be inverted, lowercase Roman letters respresent L-component vectors, uppercase Roman letters represent $L \times n_{\rm RHS}$ block-vectors, and greek letters represent scalars or $n_{\rm RHS} \times n_{\rm RHS}$ matrices.

2 Solvers

2.1 CG

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Algorithm 1 CG: Solve Ax = b

1: x, p, r, t \in C^L; \alpha, \beta \in \mathbb{R}

2: x_0 = t_0 = p_0 = 0, r_0 = b, \alpha_0 = b^{\dagger}b

3: for k = 1, 2, ... until |Ax_k - b| / |b| < \epsilon do

4: p_k \leftarrow r_{k-1} + p_k \alpha_k

5: t_k \leftarrow Ap_k

6: \beta_k \leftarrow (p_k^{\dagger}t_k)^{-1}(r_{k-1}^{\dagger}r_{k-1})

7: r_k \leftarrow r_{k-1} - t_k \beta_k

8: x_k \leftarrow x_{k-1} + p_k \beta_k

9: \alpha_k \leftarrow (r_{k-1}^{\dagger}r_{k-1})^{-1}(r_k^{\dagger}r_k)

10: end for
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2.2 SCG

3 Block Solvers

3.1 BCG

Algorithm 2 BCG: Solve AX = B

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1: X, P, R, T \in \mathcal{C}^{L \times n_{\text{RHS}}}; \alpha, \beta \in \mathcal{C}^{n_{\text{RHS}} \times n_{\text{RHS}}}

2: X_0 = T_0 = P_0 = 0, R_0 = B, \alpha_0 = B^{\dagger}B

3: \mathbf{for} \ k = 1, 2, \dots until |AX_k - B| / |B| < \epsilon do

4: P_k \leftarrow R_{k-1} + P_k \alpha_k

5: T_k \leftarrow AP_k

6: \beta_k \leftarrow (P_k^{\dagger}T_k)^{-1}(R_{k-1}^{\dagger}R_{k-1})

7: R_k \leftarrow R_{k-1} - T_k \beta_k

8: X_k \leftarrow X_{k-1} + P_k \beta_k

9: \alpha_k \leftarrow (R_{k-1}^{\dagger}R_{k-1})^{-1}(R_k^{\dagger}R_k)

10: \mathbf{end} for
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3.2 SBCGrQ