Block CG Solvers Documentation
github.com/lkeegan/blockCG

Liam Keegan
liam@keegan.ch

May 25, 2018

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 $L \times n_{\mathrm{RHS}}$ block–vectors, and greek letters represent scalars or $n_{\mathrm{RHS}} \times n_{\mathrm{RHS}}$ matrices.

2 Solvers

2.1 CG

Algorithm 1 CG: Solve $Ax = b$

$x, p, r, t \in \mathcal{C}^L$; $\alpha, \beta \in \mathcal{R}$
$x_0 = t_0 = p_0 = 0$, $r_0 = b$, $\alpha_0 = b^\dagger b$
for $k = 1, 2, \dots$ until $|Ax_k - b| \, / \, |b| < \epsilon$ **do**
    $p_k \leftarrow r_{k-1} + p_{k-1}\alpha_{k-1}$
    $t_k \leftarrow Ap_k$
    $\beta_k \leftarrow (p_k^\dagger t_k)^{-1}(r_{k-1}^\dagger r_{k-1})$
    $r_k \leftarrow r_{k-1} - t_k\beta_k$
    $x_k \leftarrow x_{k-1} + p_k\beta_k$
    $\alpha_k \leftarrow (r_{k-1}^\dagger r_{k-1})^{-1}(r_k^\dagger r_k)$
end for

2.2 SCG

3 Block Solvers

3.1 BCG

Algorithm 2 BCG: Solve $AX = B$

$X, P, R, T \in \mathcal{C}^{L \times n_{\mathrm{RHS}}}$; $\alpha, \beta \in \mathcal{C}^{n_{\mathrm{RHS}} \times n_{\mathrm{RHS}}}$
$X_0 = T_0 = P_0 = 0,\ R_0 = B,\ \alpha_0 = B^\dagger B$
for $k = 1, 2, \ldots$ until $|AX_k - B| \,/\, |B| < \epsilon$ **do**
    $P_k \leftarrow R_{k-1} + P_{k-1}\alpha_{k-1}$
    $T_k \leftarrow AP_k$
    $\beta_k \leftarrow (P_k^\dagger T_k)^{-1}(R_{k-1}^\dagger R_{k-1})$
    $R_k \leftarrow R_{k-1} - T_k\beta_k$
    $X_k \leftarrow X_{k-1} + P_k\beta_k$
    $\alpha_k \leftarrow (R_{k-1}^\dagger R_{k-1})^{-1}(R_k^\dagger R_k)$
end for

3.2 BCGrQ

Algorithm 3 BCGrQ: Solve $AX = B$

$X, P, R, T \in \mathcal{C}^{L \times n_{\mathrm{RHS}}}$; $\alpha, \beta, \delta \in \mathcal{C}^{n_{\mathrm{RHS}} \times n_{\mathrm{RHS}}}$
$X_0 = T_0 = P_0 = 0,\ \{R_0, \delta_0\} = \mathrm{qr}(B), \alpha_0 = 1$
for $k = 1, 2, \ldots$ until $\max\limits_i \sqrt{\delta_k(i,i)/\delta_0(i,i)} < \epsilon$ **do**
    $P_k \leftarrow R_{k-1} + P_{k-1}\alpha_{k-1}^\dagger$
    $T_k \leftarrow AP_k$
    $\beta_k \leftarrow (P_k^\dagger T_k)^{-1}$
    $\{R_k, \alpha_k\} \leftarrow \mathrm{qr}(R_{k-1} - T_k\beta_k)$
    $X_k \leftarrow X_{k-1} + P_k\beta_k\delta_{k-1}$
    $\delta_k \leftarrow \alpha_k\delta_{k-1}$
end for