libcKrylov algorithm collection

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Algorithm 1 Conjugate gradient algorithm for solving $Ax = b$ ($A^H = A$) (Shewchuk, 1994)

$x_0 := 0$
$r_0 := b - Ax_0 = b$
$p_0 := r_0$
for $k = 0, \cdots, N_{CG} - 1$ **do**
    $\alpha_k = \frac{r_k^H r_k}{p_k^H A p_k}$
    $x_{k+1} = x_k + \alpha_k p_k$
    $r_{k+1} = r_k - \alpha_k A p_k$
    $\beta_k = \frac{r_{k+1}^H r_{k+1}}{r_k^H r_k}$
    $p_{k+1} = r_{k+1} + \beta_k p_k$
end for

Algorithm 2 Preconditioned Conjugate gradient algorithm for solving $Ax = b$ (Saad, 2003, algorithm 9.1)

$x_0 := 0$
$r_0 := b - Ax_0 = b$
$z_0 := M^{-1} r_0$
$p_0 := z_0$
for $k = 0, \cdots, N_{CG} - 1$ **do**
    $\alpha_k = \frac{r_k^H p_k}{p_k^H A p_k}$
    $x_{k+1} = x_k + \alpha_k p_k$
    $r_{k+1} = r_k - \alpha_k A p_k$
    $z_{k+1} := M^{-1} r_{k+1}$
    $\beta_k = \frac{r_{k+1}^H z_{k+1}}{r_k^H z_k}$
    $p_{k+1} = z_{k+1} + \beta_k p_k$
end for

Algorithm 3 GMRES (Saad, 2003, algorithm 6.9)

$r_0 := b - Ax_0 = b$
$\beta = \|r_0\|_2$
$v_1 := r_0/\beta$
for $j = 1, \cdots, m$ **do**
  compute $w_j = Av_j$
  for $i = 1, \cdots, j$ **do**
    $h_{ij} = (w_j, v_i)$
    $w_j = W_j - h_{ij}v_i$
  end for
  $h_{j+1,j} = \|w_j\|_2$. If $h_{j+1,j} = 0$, set $m = j$ and go to
  $v_{j+1} = w_j/h_{j+1,j}$
  solve least-squares problem $\min_y \| \begin{bmatrix} \beta \\ 0 \\ \cdots \\ 0 \end{bmatrix} - \tilde{H}_m y\|_2$ by Givens rotation
  $x_m = x_0 + V_m y_m$
end for

Algorithm 4 GMRES with right preconditioning (Saad, 2003, algorithm 9.5)

$r_0 := b - Ax_0 = b$
$\beta = \|r_0\|_2$
$v_1 := r_0/\beta$
for $j = 1, \cdots, m$ **do**
  compute $w_j = AM^{-1}v_j$
  for $i = 1, \cdots, j$ **do**
    $h_{ij} = (w_j, v_i)$
    $w_j = W_j - h_{ij}v_i$
  end for
  $h_{j+1,j} = \|w_j\|_2$. If $h_{j+1,j} = 0$, set $m = j$ and go to
  $v_{j+1} = w_j/h_{j+1,j}$
  solve least-squares problem $\min_y \| \begin{bmatrix} \beta \\ 0 \\ \cdots \\ 0 \end{bmatrix} - \tilde{H}_m y\|_2$ by Givens rotation
  $x_m = x_0 + M^{-1}V_m y_m$
end for

Algorithm 5 BiCGStab (Chen et al., 2016), improved version from (Van der Vorst, 1992)

$r_0 = b - Ax_0$, $\tilde{r}_0$ arbitrary but $(\tilde{r}_0, r_0) \neq 0$
$p_0 = r_0$
for $j = 0, 1, \cdots$, until convergence **do**
  $\alpha_j = (r_j, \tilde{r}_0)/(Ap_j, \tilde{r}_0)$
  $s_j = r_j - \alpha_j Ap_j$
  $\omega_j = (As_j, s_j)/(As_j, As_j)$
  $x_{j+1} = x_j + \alpha_j p_j + \omega_j s_j$
  $r_{j+1} = s_j - \omega_j As_j$
  $\beta_j = (r_{j+1}, \tilde{r}_0)/(r_j, \tilde{r}_0) \cdot \alpha_j/\omega_j$
  $p_{j+1} = r_{j+1} + \beta_j(p_j - \omega_j Ap_j)$
end for

Algorithm 6 BiCGStab with right preconditioning (Flexible BiCGStab) (Chen et al., 2016)

$r_0 = b - Ax_0$, $\tilde{r}_0$ arbitrary but $(\tilde{r}_0, r_0) \neq 0$
$p_0 = r_0$
for $j = 0, 1, \cdots$ until convergence **do**
  $\tilde{p}_j = M^{-1} p_j$
  $\alpha_j = (r_j, \tilde{r}_0)/(A\tilde{p}_j, \tilde{r}_0)$
  $s_j = r_j - \alpha_j A\tilde{p}_j$
  $\tilde{s}_j = M^{-1} s_j$
  $\omega_j = (A\tilde{s}_j, s_j)/(A\tilde{s}_j, A\tilde{s}_j)$
  $x_{j+1} = x_j + \alpha_j p_j + \omega_j s_j$
  $r_{j+1} = s_j - \omega_j A\tilde{s}_j$
  $\beta_j = (r_{j+1}, \tilde{r}_0)/(r_j, \tilde{r}_0) \cdot \alpha_j/\omega_j$
  $p_{j+1} = r_{j+1} + \beta_j (p_j - \omega_j A\tilde{p}_j)$
end for

Algorithm 7 CGNR (Saad, 2003, algorithm 8.4)

$r_0 = b - Ax_0$
$z_0 = A^H r_0$
$p_0 = z_0$
for $j = 0, 1, \cdots$ until convergence **do**
  $w_i = Ap_i$
  $\alpha_j = (z_j, z_j)/(w_j, w_j)$
  $x_{j+1} = x_j + \alpha_j p_j$
  $r_{j+1} = r_j - \alpha_j w_j$
  $z_{j+1} = A^H r_{j+1}$
  $\beta_j = (z_{j+1}, z_{j+1})/(z_j, z_j)$
  $p_{j+1} = z_{j+1} + \beta_j p_j$
end for

Algorithm 8 CGNE (Craig's method) (Saad, 2003, algorithm 8.5)

$r_0 = b - Ax_0$
$p_0 = A^H r_0$
for $j = 0, 1, \cdots$ until convergence **do**
  $\alpha_j = (r_j, r_j)/(p_j, p_j)$
  $x_{j+1} = x_j + \alpha_j p_j$
  $r_{j+1} = r_j - \alpha_j A p_j$
  $\beta_j = (r_{j+1}, r_{j+1})/(r_j, r_j)$
  $p_{j+1} = A^H r_{j+1} + \beta_j p_j$
end for

References

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