

libcKrylov algorithm collection

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

```
1:  $x_0 := 0$ 
2:  $r_0 := b - Ax_0 = b$ 
3:  $p_0 := r_0$ 
4: for  $k = 0, \dots, N_{CG} - 1$  do
5:    $\alpha_k = \frac{r_k^H r_k}{p_k^H A p_k}$ 
6:    $x_{k+1} = x_k + \alpha_k p_k$ 
7:    $r_{k+1} = r_k - \alpha_k A p_k$ 
8:    $\beta_k = \frac{r_{k+1}^H r_{k+1}}{r_k^H r_k}$ 
9:    $p_{k+1} = r_{k+1} + \beta_k p_k$ 
10: end for
```

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

```
1:  $x_0 := 0$ 
2:  $r_0 := b - Ax_0 = b$ 
3:  $z_0 := M^{-1} r_0$ 
4:  $p_0 := z_0$ 
5: for  $k = 0, \dots, N_{CG} - 1$  do
6:    $\alpha_k = \frac{r_k^H p_k}{p_k^H A p_k}$ 
7:    $x_{k+1} = x_k + \alpha_k p_k$ 
8:    $r_{k+1} = r_k - \alpha_k A p_k$ 
9:    $z_{k+1} := M^{-1} r_{k+1}$ 
10:   $\beta_k = \frac{r_{k+1}^H z_{k+1}}{r_k^H z_k}$ 
11:   $p_{k+1} = z_{k+1} + \beta_k p_k$ 
12: end for
```

Algorithm 3 GMRES (Saad, 2003, algorithm 6.9)

```
1:  $r_0 := b - Ax_0 = b$ 
2:  $\beta = \|r_0\|_2$ 
3:  $v_1 := r_0/\beta$ 
4: for  $j = 1, \dots, m$  do
5:   compute  $w_j = Av_j$ 
6:   for  $i = 1, \dots, j$  do
7:      $h_{ij} = (w_j, v_i)$ 
8:      $w_j = W_j - h_{ij}v_i$ 
9:   end for
10:   $h_{j+1,j} = \|w_j\|_2$ . If  $h_{j+1,j} = 0$ , set  $m = j$  and go to
11:   $v_{j+1} = w_j/h_{j+1,j}$ 
12:  solve least-squares problem  $\min_y \left\| \begin{bmatrix} \beta \\ 0 \\ \dots \\ 0 \end{bmatrix} - \tilde{H}_m y \right\|_2$  by Givens rotation
13:   $x_m = x_0 + V_m y_m$ 
14: end for
```

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

```
1:  $r_0 := b - Ax_0 = b$ 
2:  $\beta = \|r_0\|_2$ 
3:  $v_1 := r_0/\beta$ 
4: for  $j = 1, \dots, m$  do
5:   compute  $w_j = AM^{-1}v_j$ 
6:   for  $i = 1, \dots, j$  do
7:      $h_{ij} = (w_j, v_i)$ 
8:      $w_j = W_j - h_{ij}v_i$ 
9:   end for
10:   $h_{j+1,j} = \|w_j\|_2$ . If  $h_{j+1,j} = 0$ , set  $m = j$  and go to
11:   $v_{j+1} = w_j/h_{j+1,j}$ 
12:  solve least-squares problem  $\min_y \left\| \begin{bmatrix} \beta \\ 0 \\ \dots \\ 0 \end{bmatrix} - \tilde{H}_m y \right\|_2$  by Givens rotation
13:   $x_m = x_0 + M^{-1}V_m y_m$ 
14: end for
```

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

```
1:  $r_0 = b - Ax_0$ ,  $\tilde{r}_0$  arbitrary but  $(\tilde{r}_0, r_0) \neq 0$ 
2:  $p_0 = r_0$ 
3: for  $j = 0, 1, \dots$ , until convergence do
4:    $\alpha_j = (r_j, \tilde{r}_0)/(Ap_j, \tilde{r}_0)$ 
5:    $s_j = r_j - \alpha_j Ap_j$ 
6:    $\omega_j = (As_j, s_j)/(As_j, As_j)$ 
7:    $x_{j+1} = x_j + \alpha_j p_j + \omega_j s_j$ 
8:    $r_{j+1} = s_j - \omega_j As_j$ 
9:    $\beta_j = (r_{j+1}, \tilde{r}_0)/(r_j, \tilde{r}_0) \cdot \alpha_j/\omega_j$ 
10:   $p_{j+1} = r_{j+1} + \beta_j(p_j - \omega_j Ap_j)$ 
11: end for
```

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

```
1:  $r_0 = b - Ax_0$ ,  $\tilde{r}_0$  arbitrary but  $(\tilde{r}_0, r_0) \neq 0$ 
2:  $p_0 = r_0$ 
3: for  $j = 0, 1, \dots$  until convergence do
4:    $\tilde{p}_j = M^{-1}p_j$ 
5:    $\alpha_j = (r_j, \tilde{r}_0)/(A\tilde{p}_j, \tilde{r}_0)$ 
6:    $s_j = r_j - \alpha_j A\tilde{p}_j$ 
7:    $\tilde{s}_j = M^{-1}s_j$ 
8:    $\omega_j = (A\tilde{s}_j, s_j)/(A\tilde{s}_j, A\tilde{s}_j)$ 
9:    $x_{j+1} = x_j + \alpha_j p_j + \omega_j s_j$ 
10:   $r_{j+1} = s_j - \omega_j A\tilde{s}_j$ 
11:   $\beta_j = (r_{j+1}, \tilde{r}_0)/(r_j, \tilde{r}_0) \cdot \alpha_j/\omega_j$ 
12:   $p_{j+1} = r_{j+1} + \beta_j(p_j - \omega_j A\tilde{p}_j)$ 
13: end for
```

Algorithm 7 CGNR (Saad, 2003, algorithm 8.4)

```
1:  $r_0 = b - Ax_0$ 
2:  $z_0 = A^H r_0$ 
3:  $p_0 = z_0$ 
4: for  $j = 0, 1, \dots$  until convergence do
5:    $w_j = Ap_j$ 
6:    $\alpha_j = (z_j, z_j)/(w_j, w_j)$ 
7:    $x_{j+1} = x_j + \alpha_j p_j$ 
8:    $r_{j+1} = s_j - \alpha_j w_j$ 
9:    $z_{j+1} = A^H r_{j+1}$ 
10:   $\beta_j = (z_{j+1}, z_{j+1})/(z_j, z_j)$ 
11:   $p_{j+1} = z_{j+1} + \beta_j p_j$ 
12: end for
```

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

```
1:  $r_0 = b - Ax_0$ 
2:  $p_0 = A^H r_0$ 
3: for  $j = 0, 1, \dots$  until convergence do
4:    $\alpha_j = (r_j, r_j)/(p_j, p_j)$ 
5:    $x_{j+1} = x_j + \alpha_j p_j$ 
6:    $r_{j+1} = s_j - \alpha_j Ap_j$ 
7:    $\beta_j = (r_{j+1}, r_{j+1})/(r_j, r_j)$ 
8:    $p_{j+1} = A^H r_{j+1} + \beta_j p_j$ 
9: end for
```

References

- Chen, J., McInnes, L. C., and Zhang, H. (2016). Analysis and practical use of flexible bicgstab. *Journal of Scientific Computing*, 68(2):803–825.
- Saad, Y. (2003). *Iterative Methods for Sparse Linear Systems*. SIAM, Philadelphia.
- Shewchuk, J. R. (1994). An introduction to the conjugate gradient method without the agonizing pain. Technical Report Computer Science Technical Report CMU-CS-94-125, School of computer science, Carnegie Mellon University.
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