congrad

The nonlinear conjugate gradient method is an iterative method using the conjugacy property of the matrix to solve a nonlinear system of equations. Details of the method can be found in *Numerical Optimization*(Nocedal, J., & Wright, S. (2006). Numerical optimization. Springer Science & Business Media.).

[called by: solvers.] [calls: packdof.]

Basic algorithm

The basic nonlinear conjugate gradient algorithm used in FOCUS is a hybrid of **Algorithm 5.4** and **Equation (5.49)** from *Numerical Optimization* and Dai & Yuan. This version of conjugate gradient method converges globally, provided the line search satisfies the standard Wolfe conditions.

Our target function is $\chi^2(\mathbf{X})$, while $\mathbf{X}$ is the variables vector. As we mentioned before, we can calculate the gradient $G(\mathbf{X}) = \frac{\partial \chi^2}{\partial \mathbf{X}}$ accurately with analytical expressions. The structure of the algorithm is as below.

$k = 0$: for initial $\mathbf{X}_0$, evaluate $\chi^2(\mathbf{X}_0)$ and $G(\mathbf{X}_0)$; $p_0 = -G_0$;
while $G_k > \epsilon$:
$\mathbf{X}_{k+1} = \mathbf{X}_k + \alpha_k p_k$ (α_k satisfies strong Wolfe condition);
$\beta_{k+1} = \frac{|G_{k+1}|^2}{(G_{k+1} - G_k)^T p_k}$;
$p_{k+1} = -G_{k+1} + \beta_{k+1} p_k$;
$k = k + 1$;
end(while)

The line search algorithm is applying the **Algorithm 3.5 & 3.6** in the book to satisfy the strong Wolfe conditions.

congrad.f90 last modified on 020-01-06 09:52:50.; Focus subroutines;