

Since by  $(*)_1$  and  $(*)_4$  we have  $\nabla J_{u_{\ell+1}} = \nabla J_{u_\ell} + A\Delta_\ell = \nabla J_{u_\ell} - \rho_\ell Ad_\ell$ , the gradient  $\nabla J_{u_{\ell+1}}$  can be computed iteratively:

$$\begin{aligned}\nabla J_0 &= Au_0 - b \\ \nabla J_{u_{\ell+1}} &= \nabla J_{u_\ell} - \rho_\ell Ad_\ell.\end{aligned}$$

Since by Proposition 49.17 we have

$$d_k = \nabla J_{u_k} + \frac{\|\nabla J_{u_k}\|^2}{\|\nabla J_{u_{k-1}}\|^2} d_{k-1}$$

and since  $d_{k-1}$  is a linear combination of the gradients  $\nabla J_{u_i}$  for  $i = 0, \dots, k-1$ , which are all orthogonal to  $\nabla J_{u_k}$ , we have

$$\rho_k = \frac{\langle \nabla J_{u_k}, d_k \rangle}{\langle Ad_k, d_k \rangle} = \frac{\|\nabla J_{u_k}\|^2}{\langle Ad_k, d_k \rangle}.$$

It is customary to introduce the term  $r_k$  defined as

$$r_k = \nabla J_{u_k} = Au_k - b \quad (*)_7$$

and to call it the *residual*. Then the conjugate gradient method consists of the following steps. We initialize the method starting from any vector  $u_0$  and set

$$d_0 = r_0 = Au_0 - b.$$

The main iteration step is ( $k \geq 0$ ):

$$(*)_8 \quad \begin{cases} \rho_k = \frac{\|r_k\|^2}{\langle Ad_k, d_k \rangle} \\ u_{k+1} = u_k - \rho_k d_k \\ r_{k+1} = r_k - \rho_k Ad_k \\ \beta_{k+1} = \frac{\|r_{k+1}\|^2}{\|r_k\|^2} \\ d_{k+1} = r_{k+1} + \beta_{k+1} d_k. \end{cases}$$



Beware that some authors define the residual  $r_k$  as  $r_k = b - Au_k$  and the descent direction  $d_k$  as  $-d_k$ . In this case, the second equation becomes

$$u_{k+1} = u_k + \rho_k d_k.$$

Since  $d_0 = r_0$ , the equations

$$\begin{aligned}r_{k+1} &= r_k - \rho_k Ad_k \\ d_{k+1} &= r_{k+1} + \beta_{k+1} d_k\end{aligned}$$