Supplements 6 to Chapter V — E. Gekeler

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Supplements to Section 5.8.

(c) Step Length Control Let $m = 3, 4, \ldots$ be the step number of the continuation method, $\| \circ \| = \| \circ \|_2$ and $e_i \in \mathbb{R}_{n+1}$ the i-th *rowwise* unit vector. Further, let

h_m step length, $x^m \in \mathbb{R}$ approximation, $t^m \in \mathbb{R}^{n+1}$ numerical tangent.

For the start of the method `pitcon.m` we need the values

$$x^1\,,\ x^2\,,\ x^3\quad t^1\,,\ t^2$$

in MATLAB-compatible notation. For the computation of a new step length in the *predictor step* the solution path $x^*(\sigma)$ is approximated at the point x^m by a vector-valued *quadratic polynomial*:

$$\begin{aligned} q(\sigma) &= x^m + \sigma\, t^m + \frac{1}{2}\sigma^2 w^m \\ w^m &= \frac{1}{\Delta s_m}(t^m - t^{m-1})\,,\quad \Delta s_m = \|x^m - x^{m-1}\|\,. \end{aligned}$$

Then

$$q(x^m) = x^m\,,\ q'(0) = t^m\,,\ q(-\Delta s_m) = t^{m-1}\,. \tag{1}$$

For the *curvature* at the point x^m we choose the approximation

$$\kappa_m := \mathrm{Max}\left\{\kappa_{\min}\,,\ \|w^m\| + \frac{\Delta s_m}{\Delta s_m + \Delta s_{m-1}}\big(\|w^m\| - \|w^{m-1}\|\big)\right\}$$

where $\kappa_{\min} > 0$ is a certain *threshold value*. For the distance between tangent and solution path the *estimation*

$$\frac{1}{2}\sigma^2\|w^m\| = \|q(\sigma) - x^*(\sigma)\| + \mathcal{O}(\mathrm{Max}\{|\sigma|, \Delta s_m\})$$

is chosen (F sufficiently smooth). The maximum distance shall be smaller than a certain *tolerance* $\varepsilon > 0$ for which by geometrical reasons is chosen

$$\varepsilon_m = \begin{cases} \varepsilon_{\min}\Delta s_m & \text{for} \quad \sigma^* \le \varepsilon_{\min}\Delta s_m \\ \Delta s_m & \text{for} \quad \sigma^* \ge \Delta s_m \\ \sigma^* & \text{else} \end{cases}$$

where $\varepsilon_{\min} > 0$, is a suitable *threshold value*, e.g. $\varepsilon_{\min} = 0.01$. The threshold value σ^* can be calculated by the start values or can be specified in advance. Now we choose a first estimation for the new step length

$$\widetilde{h}_m = \left(\frac{2\varepsilon_m}{\kappa_m}\right)^{1/2}\,,$$

and compute the final step length h_m by the requirement

$$e^{i(m)}(x^m + h_m t^m) = e^{i(m)} q(\widetilde{h}_m)$$

with the chosen unit vector $e^{i(m)}$. Then

$$h_m = \widetilde{h}_m\left[1 + \frac{\widetilde{h}_m}{2\Delta s_m}\left(1 - \frac{e^{i(m)}t(x^{m-1})}{e^{i(m)}t(x^m)}\right)\right]\,.$$

Some savety bounds must also be applied:

$$\frac{1}{\chi}\Delta s_m \leq h_m \leq \chi \Delta s_m\,, \quad h_{\min} \leq h_m \leq h_{\max}$$

with a factor χ, e.g. $\chi = 3$, and bounds $h_{\min}$, $h_{\max}$ which depend on the one side of the machine exactness and one the other side of the basic problem.

(d) PITCON Computation of index $i(m)$ for correcture, m step number:

$$j = \mathrm{Max}_i\{|e^i t^m|\}\,, \quad k = \mathrm{Max}_{i\neq j}\{|e^i t^m|\}$$

Then $[t^m]_j$ is the maximum absolute value and $[t^m]_k$ the second-largest value of t^m.
Preventer for limit points:

$$|e^j t^m| < |e^j t^{m-1}|\,, \quad |e^k t^m| > |e^k t^{m-1}|\,, \quad |e^k t^m| \geq \mu |e^j t^m|\,, \tag{2}$$

Set $i(m) = j$, but if (2) is fulfilled with a certain $\mu > 0$ then set $i(m) = k$.
NEWTON method: New predictor point:

$$v^m = x^m + h_m t^m$$

Solve

$$\widetilde{F}(x) = \begin{bmatrix} F(x) \\ e^{i(m)}(x - v^m) \end{bmatrix} = 0 \tag{3}$$

iteratively with one of the following both iterations for $j = 1, 2, \ldots j_{\max}$

$$\begin{aligned} y^{[j+1]} &= y^{[j]} - [\nabla \widetilde{F}(y^{[j]})]^{-1}\widetilde{F}(y^{[j]})\,, \quad y^{[0]} = v^m\,, \quad j_{\max} = 10\,; \\ y^{[j+1]} &= y^{[j]} - [\nabla \widetilde{F}(v^m)]^{-1}\widetilde{F}(y^{[j]})\,, \quad y^{[0]} = v^m\,, \quad j_{\max} = 20\,. \end{aligned}$$

Stopping criterium for NEWTON's method: Let $\vartheta = 2$ for $j = 1$ and $\vartheta = 1.05$ for $j \geq 2$. Stopping if one of the following three conditions is fulfilled:

$$\begin{aligned} \|\widetilde{F}(y^{[j]})\|_\infty &\geq \vartheta\, \|\widetilde{F}(y^{[j-1]})\|_\infty && \text{f"ur ein } j \geq 1 \\ \|y^{[j]} - y^{[j-1]}\|_\infty &\geq \vartheta\, \|y^{[j-1]} - y^{[j-2]}\|_\infty && \text{f"ur ein } j \geq 2 \\ j &\geq j_{\max}\,. \end{aligned}$$

If NEWTON's method fails to converge, set $h_m := h/2$ until convergence happens or $h_m < h_{\min}$. In the latter case the entire methods fails.

The correcture in this method runs by (3) not perpendicular to the tangent but perpendicular to the unit vector $e^{i(m)}$, which can be used advantageously in solving the linear system of equation in the NEWTON step: One may solve at first $\nabla F(x)dy = -F(x)$ for $[dy]^{i(m)} = 0$ – a system with n unknowns and n equations – and can ensuing set $[dy]^{i(m)} = [v^m]^{i(m)}$. Nevertheless the tangent must be computed but here without QR-decomposition. To this end one chooses a vector $0 \neq d^m \in \mathbb{R}_{n+1}$ with $d^m\, t^m > 0$ where t^m is the tangent *still being unknown*. Then on computes

$$\begin{bmatrix} \nabla F(x^m) \\ d^m \end{bmatrix} u = e_{n+1}\,, \quad t^m = u/\|u\|_2\,.$$

This choice of d^m for unknown t^m is only a small, optical drawback which does not play a role numerically. In starting the method, d^1 is chosen arbitrarily and possibly adapted, during the iteration $d^m = e^{i(m-1)}$ or $d^m = t^{m-1}$ is chosen in the hope that no trouble arises.

(e) Nonlinear Method of Conjugate Gradients [Allgower90].

START: Choose tolerance *tol*, step length h and step number $N \in \mathbb{N}$.
(1°) Find starting value x such that $F(x) \simeq 0$.
(2°) Find tangent t with $|t| = 1$ and $\nabla F(x)t \simeq 0$.
$n = 0$
WHILE NOT $n \geq N$
  $u := x + ht$ *predictor step*
  Compute lower triangular matrix L such that

$$LL^T \simeq \nabla F(u) \nabla F(u)^T \qquad \textit{preconditioner} \tag{4}$$

  $g_u := \nabla F(u)(LL^T)^{-1} F(u)\,;\ d := g_u$ *gradient*
  done $= 0$
  WHILE NOT done *corrector loop*

$$\varrho^* \simeq \operatorname{Arg\,Min}_{\varrho \geq 0} \frac{1}{2} \|L^{-1} F(u - \varrho d)\|^2 \qquad \textit{Linesearch}$$

$$v := u - \varrho^* d \qquad \textit{corrector step}$$

$$g_v := [\nabla F(v)]^T (LL^T)^{-1} F(v) \qquad \textit{new gradient}$$

$$\gamma := (g_v - g_u)^T g_u / \|g_u\|^2$$

$$d := g_v + \gamma d \qquad \textit{new conjugate gradient}$$

$$u := v\,;\ g_u := g_v$$

    done $= \|F(v)\| < \text{tol}$
  END
  Adapt step length h
  $t := (v - x)/\|v - x\|$ *approximation of* $t(\nabla F(v))$
  $x := v$ *new value for* $F(x) = 0$
END