Notes for 2015-04-20

Not all of these problems would be suitable as exam questions, but many of the ideas exercised (e.g. block Gaussian elimination, understanding convergence from a semi-logarithmic plot of residuals vs iterations, and writing an error iteration to analyze local convergence of a fixed point iteration) are things that I would expect you to be able to do on an exam.

1: A different iteration In project 3, you are asked to solve a system of equations for an equilibrium position of a electrostatically actuated cantilever subject to displacement control:

$$F(u, V^2) = \begin{bmatrix} Ku - V^2 \hat{f}_e(u) \\ e_{\mathrm{tip}}^T u - d \end{bmatrix}$$

Consider the fixed point iteration

$$x^{(k+1)} = x^{(k)} - \hat{J}_k^{-1} F(x^{(k)}), \quad x \equiv \begin{bmatrix} u \\ V^2 \end{bmatrix}$$

where

$$\hat{J}_k = \begin{bmatrix} K & -\hat{f}_e(u) \\ e_{\mathrm{tip}}^T & 0 \end{bmatrix}.$$

1. Why is this not Newton's method?
2. Describe how to compute each iterate with one solve with a pre-factored system (assuming the Cholesky factorization of K is computed at the outset)
3. Why is the constraint $e_{\mathrm{tip}} u^{(k)} = d$ always satisfied for $k > 0$?

Answer:

1. The Jacobian of F has $K - V^2 \partial \hat{f}_e / \partial u$ in the $(1, 1)$ block. Since our iteration only involves K in the $(1, 1)$ block, it is not Newton.
2. We can solve the update equation

$$\begin{bmatrix} K & -\hat{f}_e \\ e_{\mathrm{tip}}^T & 0 \end{bmatrix} \begin{bmatrix} \Delta u \\ \Delta V^2 \end{bmatrix} = \begin{bmatrix} F_1 \\ F_2 \end{bmatrix}$$

by block Gaussian elimination. This yields

$$\begin{aligned} w_{\text{tip}} &= K^{-1} e_{\text{tip}} \\ \Delta V^2 &= \frac{F_2 - w_{\text{tip}}^T F_1}{w_{\text{tip}}^T \hat{f}_e} \\ K\,\Delta u &= F_1 - \Delta V^2\, \hat{f}_e \end{aligned}$$

The solve to compute w_{tip} can be done once in a pre-computation phase, and does not need to be recomputed after. The solve for Δu is the only solve that needs to be computed at each iteration, and it can be done with two triangular solves using the Cholesky factorization $K = R^T R$.

3. The constraint $e_{\text{tip}} u^{(k)} = d$ is always satisfied for $k > 0$ because of the second update equation:

$$e_{\text{tip}}^T \Delta u^{(k)} = e_{\text{tip}}^T u^{(k)} - d.$$

Rearranging terms yiels

$$e_{\text{tip}}^T u^{(k+1)} = e_{\text{tip}}^T \left(u^{(k)} - \Delta u^{(k)} \right) = d.$$

2: Rates of convergence Typically, we plot residuals or errors on a semi-logarithmic plot in order to visually verify convergence behaviors. How can we numerically test that $\|r^{(k+1)}\| \approx C\|r^{(k)}\|^q$ by looking at successive residuals? If the residual in Newton's method decreases quadratically, must the error also decrease quadratically?

Answer: The natural thing to do is to look at logarithms. Under this model,

$$\log \frac{\|r^{(1)}\|}{\|r^{(0)}\|} \approx q \log \frac{\|r^{(2)}\|}{\|r^{(1)}\|}.$$

We can also compute the constant C from three successive residuals.

This may be worth doing when looking at a linearly convergent iteration; for quadratically convergent iterations, there are typically only one or two steps between when convergence kicks in and when the iteration is dominated by roundoff. In this case, a picture can be much more illuminating than a number.

If the Jacobian at the solution is nonsingular at the solution to a system of nonlinear equation, then the error close to convergence is well approximated by J_*^{-1} times the residual, and so quadratic convergence of the residual implies quadratic convergence of the error.

3: Pseudoinverse sensitivity Assuming $A \in \mathbb{R}^{m \times n}$ is full column rank, what is the first-order term L in the Taylor expansion

$$(A + \delta A)^\dagger = A^\dagger + \delta\left[A^\dagger\right] + O(\|\delta A\|^2)?$$

Answer: This problem involves two points: picking a useful representation for the pseudo-inverse, and understanding how to differentiate matrix-valued functions. For the representation, recall that

$$(A + \delta A)^\dagger = \left[(A + \delta A)^T (A + \delta A)\right]^{-1} (A + \delta A)^T.$$

Let's define the Gram matrix $G = A^T A$. By the product rule

$$\delta\left[A^\dagger\right] = \delta\left[G^{-1}\right] A^T + G^{-1}\, \delta A^T.$$

The derivative of a matrix inverse is

$$\delta[G^{-1}] = -G^{-1}[\delta G]G^{-1},$$

so, together with another application of the product rule, we have

$$\delta\left[G^{-1}\right] = -G^{-1}[(\delta A)^T A + A^T(\delta A)]G^{-1}$$

Putting everything together, we have

$$\delta[A^\dagger] = G^{-1}(\delta A)^T - G^{-1}\left[(\delta A)^T A + A^T(\delta A)\right] G^{-1}.$$

This is a bit of a mess, but it actually is something we can use in computation.

4: Gauss-Newton Show that Gauss-Newton iteration generally converges quadratically if the residual at the minimum is zero and the Jacobian at the origin is nonsingular, but linearly if the minimum residual is nonzero.

Answer: The Gauss-Newton iteration is

$$x_{k+1} = x_k - J_k^\dagger F_k$$

where $J_k = \partial F(x_k)/\partial x$ and $F_k = F(x_k)$. Let J_* denote the Jacobian at the solution x_*, let $x_k = x_* + e_k$, and note that

$$\begin{aligned} F_k &= F_* + J_* e_k + O(\|e_k\|^2) \\ J_k^\dagger &= J_k + E_k + O(\|e_k\|^2) \end{aligned}$$

where E_k is a complicated expression (see the previous problem). For our purposes, we mostly just care that $E_k = O(\|e_k\|)$. In this case, the error iteration for Gauss-Newton is

$$e_{k+1} = e_k - (J_*^\dagger + E_k)(F_* + J_* e_k) + O(\|e_k\|^2)$$

Note that $J_*^\dagger F_* = 0$, $E_k J_* e_k = O(\|e_k\|^2)$, and $J_*^\dagger J_* e_k = e_k$, so

$$e_{k+1} = -E_k F_* + O(\|e_k\|^2)$$

If F_* is zero, we therefore have quadratic convergence. Otherwise, convergence is linear.

One of the things that might cause us some concern is the possibility that Gauss-Newton might diverge. Indeed, this is a possibility if one starts far from the solution, but the Gauss-Newton direction *is* a descent direction. That is, looking at the Gauss-Newton direction $p_k = -J_k^\dagger F_k$ together with the gradient of the the objective function $\nabla\nabla = J_k^T F_k$ ($\phi = \|F\|^2/2$), we have

$$p^T \nabla \phi = -p^T (J_k^T J_k)^{-1} p.$$

and if the Jacobian is nonsingular at the solution point, then $J_k^T J_k$ must be positive definite for points sufficiently nearby.