Notes on Nonlinear Newton Iterations at a Typical Singularity

Given a nonlinear n-vector-valued function $f(x)$ of an n-vector x, a solution z of the equation $f(z) = o$ is often sought by means of *Newton's Iteration* $x_{k+1} := Nf(x_k)$ wherein *Newton's Iterating Function* $Nf(x) := x - f'(x)^{-1}\cdot f(x)$. Here $f'(x) := \partial f(x)/\partial x$ is the n-by-n *Jacobian Matrix* of first partial derivatives; it is usually presumed adequately differentiable and invertible at all x in some open neighborhood of the desired solution z, and then

$$Nf(x) - z = f'(x)^{-1}\cdot\big(f''(x)\cdot(x-z) + \dots\big)\cdot(x-x) \approx O(x-z)^2 \text{ as } x \to z .$$

Those presumptions imply at least *Quadratic Convergence*. This happens almost always.

The iteration's behavior is not so easy to characterize in some singular situations. Among these the most common has $\det(f'(x)) = 0$ but $\partial \det(f'(x))/\partial x \ne o\grave{}$ at $x = z$. Thus $\det(f'(x)) = 0$ along some curve $(n = 2)$ or (hyper)surface $(n \ge 3)$ that passes through z but does not intersect itself there, not even tangentially. Call this locus " \$ ". It divides some open neighborhood of z into two open regions in which $\det(f'(x))$ takes opposite signs. $Nf(x)$ is either ambiguous or infinite on \$ because $f'(x)$ is not invertible there. These notes explore the behavior of Newton's iteration when it converges to z but no iterate falls into \$. Convergence turns out to be *Linear* rather than quadratic, and iterates approaching z usually tend to avoid \$, as we shall see. Our conclusions are summarized on p. 3 and illustrated by examples on p. 4.

The Derivative row $h\grave{}(x) := \partial\det(f'(x))/\partial x$.

Jacobi's Formula for the derivative of a determinant says $d\det(B) = \mathrm{Trace}(\mathrm{Adj}(B)\cdot dB)$ wherein the Trace is the sum of all diagonal elements, and $\mathrm{Adj}(B)$ is the *Classical Adjoint* or *Adjugate*: $\mathrm{Adj}(B) := \det(B)\cdot B^{-1}$ when $\det(B) \ne 0$ and is otherwise defined by the continuity of what turns out to be a polynomial function of the elements of B defined by $B\cdot\mathrm{Adj}(B) \equiv \mathrm{Adj}(B)\cdot B \equiv \det(B)\cdot I$ in general. There are other equivalent definitions of $\mathrm{Adj}(B)$ in terms of determinants or the *Characteristic Polynomial* of B, but all we need from them is this fact: $\mathrm{Adj}(B) \ne O$ just when the n-by-n matrix B has $\mathrm{Rank}(B) \ge n-1$, and then $\mathrm{Rank}(\mathrm{Adj}(B)) = n - (n-1)\cdot(n - \mathrm{Rank}(B))$. Jacobi's formula is derived at `<www.cs.berkeley.edu/~wkahan/MathH110/jacobi.pdf>`.

Jacobi's formula says $d\det(f'(x)) = \mathrm{Trace}(\mathrm{Adj}(f'(x))\cdot f''(x)\cdot dx)$ wherein the second derivative f'' is a bilinear operator that maps n-vectors y and z each linearly to an n-vector $f''(x)\cdot y\cdot z$ that, in general, varies nonlinearly with x and, if continuously, $f''(x)\cdot y\cdot z = f''(x)\cdot z\cdot y$. In particular $f''(x)\cdot dx$ is a matrix whose every element depends linearly upon column dx, so there must be some row n-vector $h\grave{}(x) = \partial\det(f'(x))/\partial x$ satisfying $d\det(f'(x)) = h\grave{}(x)\cdot dx$ for all dx; and if $h\grave{}(z) \ne o\grave{}$ then the equation of the plane tangent to \$ at z is $h\grave{}(z)\cdot(x-z) = 0$.

We assume henceforth that $h\grave{}(z) \ne o\grave{}$ and $\det(f'(z)) = 0$, whence $\mathrm{Rank}(f'(z)) = n-1$ and hence $\mathrm{Rank}(\mathrm{Adj}(f'(z))) = 1$, so $\mathrm{Adj}(f'(z)) = w\cdot v\grave{}$ for two nonzero vectors satisfying $f'(z)\cdot w = o$ and $v\grave{}\cdot f'(z) = o\grave{}$. Consequently

$$h\grave{}(z)\cdot dx = \mathrm{Trace}(\mathrm{Adj}(f'(z))\cdot f''(z)\cdot dx) = \mathrm{Trace}(w\cdot v\grave{}\cdot f''(z)\cdot dx) = \mathrm{Trace}(v\grave{}\cdot f''(z)\cdot w\cdot dx)$$

and therefore $h\grave{}(z) = v\grave{}\cdot f''(z)\cdot w = \partial\det(f'(x))/\partial x$ at $x = z$. We shall need this formula later.

A *Taylor Series* expansion of f will be presumed valid for x in some open neighborhood of z :

$$f(x) = o + f'(z)\cdot(x-z) + \tfrac{1}{2} f''(z)\cdot(x-z)\cdot(x-z) + \tfrac{1}{6} f'''(z)\cdot(x-z)\cdot(x-z)\cdot(x-z) + \dots .$$

$$f'(x) = f'(z) + f''(z)\cdot(x-z) + \tfrac{1}{2} f'''(z)\cdot(x-z)\cdot(x-z) + \dots ; \quad \det(f'(z)) = 0 ; \quad \mathrm{Adj}(f'(z)) = w\cdot v` .$$

$$\det(f'(x)) = h`\cdot(x-z) + \dots \ \text{wherein} \ h` := v`\cdot f''(z)\cdot w \ne o` .$$

Needed next is a Taylor series expansion for Newton's iterating function:

$$Nf(x) = x - f'(x)^{-1}\cdot f(x)$$

$$= z + \tfrac{1}{2}\left(f' + f''\cdot(x-z) + \tfrac{1}{2} f'''\cdot(x-z)\cdot(x-z) + \dots\right)^{-1}\cdot\left(f''\cdot(x-z) + \tfrac{2}{3} f'''\cdot(x-z)\cdot(x-z) + \dots\right)\cdot(x-z)$$

in which all derivatives of $f(x)$ are evaluated at x = z . This is too messy. It must be simplified.

A Change of Coordinates.

By a process akin to *Gaussian Elimination* with *Pivotal Exchanges* of both rows and columns, we can obtain a diagonal matrix $L^{-1}\cdot f'(z)\cdot U^{-1} = M := \begin{bmatrix} I & o \\ o' & 0 \end{bmatrix}$ using suitably permuted lower- and upper-triangular matrices L and U . These figure in a simplifying change of variables from x to $u := U\cdot(x-z)$. Let $g(u) := L^{-1}\cdot f(z + U^{-1}\cdot u)$ so that Newton's iterating function for g is $Ng(u) := u - g'(u)^{-1}\cdot g(u) = U\cdot(Nf(z + U^{-1}\cdot u) - z)$. In other words, the iteration $x_{k+1} := Nf(x_k)$ starting from x_0 is mimicked by the iteration $u_{k+1} := Ng(u_k)$ starting from $u_0 := U\cdot(x_0 - z)$ in so far as every $u_k = U\cdot(x_k - z)$. Iterates $x_k \to z$ just as fast (if at all) as $u_k \to o$.

Thus no generality is lost by assuming $z = o = f(o)$, $f'(o) = M := \begin{bmatrix} I & o \\ o' & 0 \end{bmatrix}$, $\mathrm{Adj}(f'(o)) = \begin{bmatrix} O & o \\ o' & 1 \end{bmatrix} = v\cdot v`$ in which $w` = v` = [o` \ \ 1]$, and the foregoing Taylor series for $Nf(x)$ is simplified to …

$$Nf(x) = \tfrac{1}{2}\left(M + f''\cdot x + \tfrac{1}{2} f'''\cdot x\cdot x + \dots\right)^{-1}\cdot\left(f''\cdot x + \tfrac{2}{3} f'''\cdot x\cdot x + \dots\right)\cdot x$$

$$= \tfrac{1}{2} x - \tfrac{1}{2}\left(M + f''\cdot x + \tfrac{1}{2} f'''\cdot x\cdot x + \dots\right)^{-1}\cdot\left(M - \tfrac{1}{6} f'''\cdot x\cdot x + \dots\right)\cdot x$$

in which all derivatives of $f(x)$ are evaluated at x = o . Further progress requires a partition of $f''\cdot x = \begin{bmatrix} Xx & C\cdot x \\ x'\cdot R' & h'\cdot x \end{bmatrix}$ in which Xx is an (n–1)-by-(n–1) matrix whose every element is a linear function of x . Similarly for the column $C\cdot x$, the row $x`\cdot R`$ and the scalar $h`\cdot x$ . In fact $h`\cdot x = v`\cdot f''\cdot x\cdot v = v`\cdot f''\cdot v\cdot x = [v`\cdot R` \ \ h`\cdot v]\cdot x$ so $h` = [v`\cdot R` \ \ h`\cdot v] = \partial \det(f'(x))/\partial x$ at x = o as expected, and $h` \ne o`$ has been assumed. Later much of our analysis will be affected by whether the last element of $h`$, namely $h`\cdot v$, is zero.

Let $\begin{bmatrix} W & \mu\cdot c \\ \mu\cdot r' & \mu \end{bmatrix} := f'(x)^{-1} = \left(M + f''\cdot x + \tfrac{1}{2} f'''\cdot x\cdot x + \dots\right)^{-1} = \left(\begin{bmatrix} I + Xx & C\cdot x \\ x'\cdot R' & h'\cdot x \end{bmatrix} + \tfrac{1}{2} f'''\cdot x\cdot x + \dots\right)^{-1}$.

Here a process akin to Gaussian elimination provides estimates

$\mu(x) = \det(I + Xx + O(x)^2)/\det(f'(x)) = 1/(\ h`\cdot x + O(x)^2\ )$,

column $c(x) = -(I-Xx)\cdot C\cdot x + O(x)^2$,

row $r`(x) = -x`\cdot R`\cdot(I-Xx) + O(x)^2$, and

matrix $W(x) = I-Xx + \mu(x)\cdot c(x)\cdot r`(x) + O(x)^2$ as $x \to o$.

These estimates produce an estimate of $\mathrm{N}f(\mathrm{x}) = \frac{1}{2}\begin{bmatrix} \mathrm{I}-\mathrm{W} & \mathrm{o} \\ -\mu\cdot\mathrm{r}' & 1 \end{bmatrix}\cdot\mathrm{x} + \mu(\mathrm{x})\cdot O(\mathrm{x})^3$.

What happens next depends upon whether x approaches z (= o) too nearly tangentially to the surface \$ on which $\det(f'(\mathrm{x})) = 0$. If so, $\mathrm{h}`\cdot\mathrm{x} = O(\mathrm{x})^2$, and then $\mu(\mathrm{x}) = 1/O(\mathrm{x})^2$ can be arbitrarily big, so big that the computation of $f'(\mathrm{x})^{-1}\cdot f(\mathrm{x})$ and thus $\mathrm{N}f(\mathrm{x})$ malfunctions because of roundoff if not division by zero.

To avoid that malfunction we must keep $|\mathrm{h}`\cdot\mathrm{x}| >> O(\mathrm{x})^2$ , though $\mathrm{h}`\cdot\mathrm{x} = O(\mathrm{x})$, so that terms like $\mu(\mathrm{x})\cdot O(\mathrm{x})^2$ stay no bigger than $O(\mathrm{x})$ as $\mathrm{x} \to \mathrm{o}$. Under these circumstances $\mathrm{W}(\mathrm{x}) = \mathrm{I} + O(\mathrm{x})$ and then $\mathrm{N}f(\mathrm{x}) = \frac{1}{2}([-\mu\cdot\mathrm{r}` \;\; 1]\cdot\mathrm{x})\cdot\mathrm{v} + O(\mathrm{x})^2 = O(\mathrm{x})\cdot\mathrm{v} + O(\mathrm{x})^2$. Thus, if $\mathrm{N}f(\mathrm{x})$ is not $O(\mathrm{x})^2$ it is likely to take the form $\mathrm{N}f(\mathrm{x}) = ß\cdot\mathrm{v} + O(ß)^2$ for some tiny scalar $ß = O(\mathrm{x})$. Whether these circumstances persist and avoid malfunctions depends upon whether the last element $\mathrm{h}`\cdot\mathrm{v}$ of h\` is zero.

If, as is most likely, $\mathrm{h}`\cdot\mathrm{v} \neq 0$ then iterates of the form $\mathrm{x} = ß\cdot\mathrm{v} + O(ß)^2$ for sufficiently tiny nonzero scalars ß turn into $\mathrm{N}f(\mathrm{x}) = \frac{1}{2}ß\cdot\mathrm{v} + O(ß)^2 \approx \frac{1}{2}\mathrm{x}$ because $\mu(\mathrm{x}) = 1/\big(ß\cdot\mathrm{h}`\cdot\mathrm{v} + O(ß)^2\big)$ is not too tiny, and then convergence is linear with rate log(2) and iterates approach z along a direction v that is *Transverse* (not tangential) to the surface \$.

In tbe unlikely case that $\mathrm{h}`\cdot\mathrm{v} = 0$ the iteration's behavior is difficult to predict because, although iterates x tend often to come close to the form $\mathrm{x} = ß\cdot\mathrm{v} + O(ß)^2$, it is too nearly tangential to \$.

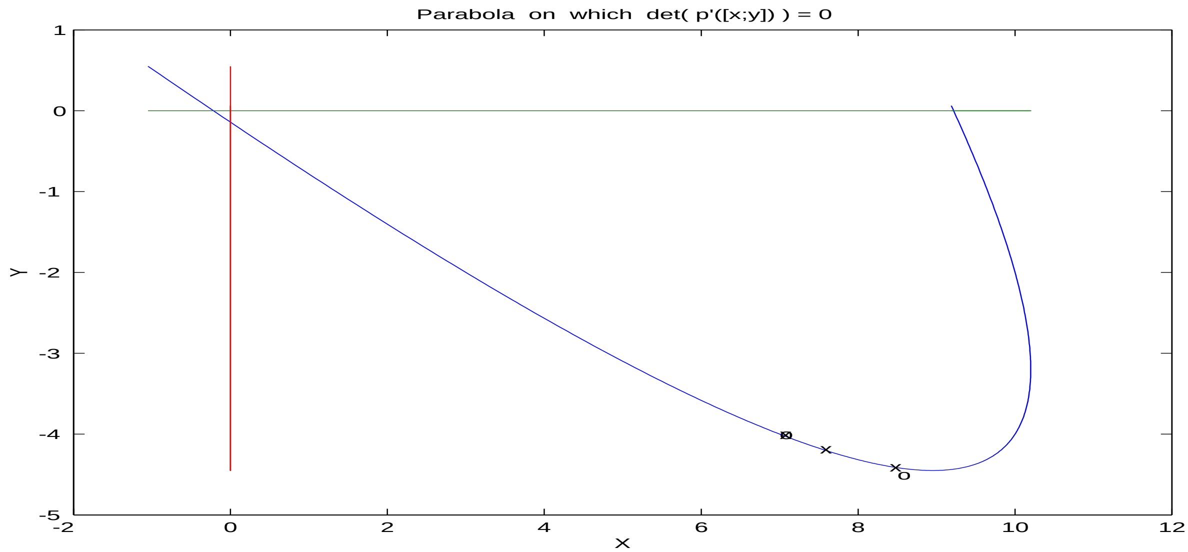
Summary.
If $f(\mathrm{z}) = \mathrm{o}$ and $\det(f'(\mathrm{z})) = 0$ and Newton's iteration is started close enough to z but not too much closer to the locus \$ on which $\det(f'(\mathrm{x})) = 0$, the iteration's convergence to z is linear with rate log(2) provided a technical condition $\big(\partial \det(f'(\mathrm{x}))/\partial\mathrm{x}$ at $\mathrm{x} = \mathrm{z}\big)\cdot\mathrm{Adj}(f'(\mathrm{z})) \neq \mathrm{o}`$ is satisfied by the second derivative $f''(\mathrm{z})$ , as is usually the case. This technical condition can be described in terms of nonzero null-vectors $\mathrm{v}` \neq \mathrm{o}` = \mathrm{v}`\cdot f'(\mathrm{z})$ and $\mathrm{w} \neq \mathrm{o} = f'(\mathrm{z})\cdot\mathrm{w}$ of singular matrix $f'(\mathrm{z})$: it is that $\mathrm{v}`\cdot f''(\mathrm{z})\cdot\mathrm{w}\cdot\mathrm{w} \neq 0$. And then iterates $\mathrm{x}_{k+1} := \mathrm{x}_k - f'(\mathrm{x}_k)^{-1}\cdot f(\mathrm{x}_k)$ approach the desired zero z very nearly like $\mathrm{z} + (ß/2^k)\cdot\mathrm{w}$ for some small nonzero scalar constant ß.

Example p :
For column 2-vector arguments x let column 2-vector $\mathrm{p}(\mathrm{x}) := \mathrm{a} + \mathrm{B}\cdot\mathrm{x} + \begin{bmatrix} \mathrm{x}'\cdot\mathrm{C}_1\cdot\mathrm{x} \\ \mathrm{x}'\cdot\mathrm{C}_2\cdot\mathrm{x} \end{bmatrix}/2$ in which

$\mathrm{a} = \begin{bmatrix} -15/2 \\ 11 \end{bmatrix}$, $\mathrm{B} = \begin{bmatrix} 1 & -2 \\ 0 & 2 \end{bmatrix}$, $\mathrm{C}_1 = \begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix}$, $\mathrm{C}_2 = \begin{bmatrix} 2 & 3 \\ 3 & 4 \end{bmatrix}$. Now $\mathrm{p}\left(\begin{bmatrix} 17/2 \\ -9/2 \end{bmatrix}\right) = \mathrm{o}$ and $\mathrm{p}'\left(\begin{bmatrix} 17/2 \\ -9/2 \end{bmatrix}\right) = \begin{bmatrix} 1 & 3 \\ 7 & 19 \end{bmatrix}/2$ is nonsingular, so Newton's iteration converges quadratically to this zero of p as expected. But

$p(\begin{bmatrix}7\\-4\end{bmatrix}) = o$ has a singular $p'(\begin{bmatrix}7\\-4\end{bmatrix}) = \begin{bmatrix}0 & 0\\2 & 7\end{bmatrix}$; now $v` = [1 \;\; 0]$, $w = \begin{bmatrix}7\\-2\end{bmatrix}$ and $v`\cdot f''(z)\cdot w\cdot w = 5 \neq 0$, so Newton's iterates x_k tend to this "double" zero z of p linearly like $z + (ß/2^k)\cdot w$. Try it!

Newton's iterating function $Np(x) := x - p'(x)^{-1}\cdot p(x)$ may tend to infinity as x tends to the parabola on which $\det(p'(x)) = 0$. The equation $-\det(p'(\begin{bmatrix}\xi\\\eta\end{bmatrix})) = (\xi+\eta-7)^2 + 5\xi - 51 = 0$ of the parabola is solved by its parametrization: $\xi = \xi(\tau) := 7 + 8\tau - 5\tau^2$ and $\eta = \eta(\tau) := 5\tau^2 - 3\tau - 4$. $Np(x)$ becomes indeterminate at two points on this parabola: One is the "double" zero $z = \begin{bmatrix}7\\-4\end{bmatrix}$ and the second is the point $x = \begin{bmatrix}8.4\\-4.4\end{bmatrix}$. As x approaches a third point $\begin{bmatrix}338/45\\-188/45\end{bmatrix}$ on the parabola, the direction of $Np(x)-x = -p'(x)^{-1}\cdot p(x)$ approaches tangency with the parabola; elsewhere than near these three points, the direction of $Np(x)-x$ throws Newton's iterate $Np(x)$ violently across the parabola as x approaches it.



Example q :

For column 2-vector arguments x let column 2-vector $q(x) := a + B\cdot x + \begin{bmatrix}x'\cdot C_1\cdot x\\x'\cdot C_2\cdot x\end{bmatrix}/2$ in which

$a = \begin{bmatrix}-6\\-4\end{bmatrix}$, $B = \begin{bmatrix}-2 & 0\\0 & 2\end{bmatrix}$, $C_1 = \begin{bmatrix}1 & 2\\2 & 3\end{bmatrix}$, $C_2 = \begin{bmatrix}2 & 3\\3 & 4\end{bmatrix}$. Now $q(\begin{bmatrix}-6\\4\end{bmatrix}) = o$ and $q'(\begin{bmatrix}-6\\4\end{bmatrix}) = O$ has rank 0 so the analysis displayed above cannot explain the linear convergence of Newton's iteration to this zero z . Worse, $q(x) = o$ all along the line whose equation is $[1 \;\; 1]\cdot x = -2$ and thereon, except at this zero z , $q'(x)$ is a nonzero scalar multiple of $[1 \;\; 1]\cdot[1 \;\; 1]`$ , so $v`$ and $w`$ are nonzero scalar multiples of $[1 \;\; -1]$ whence $v`\cdot f''(z)\cdot w\cdot w = 0$. Consequently the analysis displayed above does not explain why Newton's iterates x_k converge to no zero of q on that line other than the zero $z = \begin{bmatrix}-6\\4\end{bmatrix}$, and converges to it like $z + (ß/2^k)\cdot w$. Try it!