Dummy's note: (2) Convergence of iteration scheme

S. Yoshida

April 6, 2005

Root finding of general non-linear (set of) equation(s),

$$\boldsymbol{x} - \boldsymbol{f}[\boldsymbol{x}] = \boldsymbol{0}\ ; \qquad \text{x and f could be vectors}, \tag{1}$$

can be regarded as finding fixed points of map,

$$\boldsymbol{x} \xrightarrow{\boldsymbol{f}} \boldsymbol{f}[\boldsymbol{x}]. \tag{2}$$

1 Direct iteration

We name an iterative procedure with the following scheme as *direct iteration*:

1. Choose initial guess of solution x_0 (0-th step solution).
2. Map the already given k-th step solution x_k with Eq.(2) to obtain $(k+1)$-th step solution x_{k+1},
$$x_{k+1} = f[x_k]. \tag{3}$$
3. Ideally, $k \to \infty$ gives us a root. For numerical computation, we monitor a residual and if it becomes smaller than some criterion, we stop computation.

From a point of view of fixed point finding, the situation when the direct iteration breaks down is picturized (Fig.1). Suppose we start from an initial guess x_0, slightly right of X_S. The mapping is done in two steps: 1) computing $y = f[x_0]$. 2) Set $y \to x_1$. After this mapping, x_1 is closer to X_S than x_0, that is, $|x_1 - X_S| < |x_0 - X_S|$. This ensures that the procedure converges. On the other hand, the procedure diverges for another root X_U. Thus the direct iteration is not used to compute X_U. The criterion of convergence for this simplest case is

$$|f'[X_S]| < 1 \qquad \text{(contractive map)} \tag{4}$$

For more general multi-dimensional case, the condition is expressed by Jacobian of the map.

2 Newton-Raphson

To see how Newton-Raphson (N-R) works, we here stick to one-dimensional case.

Suppose we want to compute a zero $x = x_0$, of $x - f[x] = 0$. Naturally we assume the regularity of $f[x]$ around $x = x_0$,

$$f[x_0 + \epsilon] = x_0 + a\epsilon + b\epsilon^2 + ... \tag{5}$$

N-R scheme for $x - f[x] := g[x] = 0$ is written as,

$$x_{n+1} = x_n - \frac{g[x_n]}{g'[x_n]} \tag{6}$$

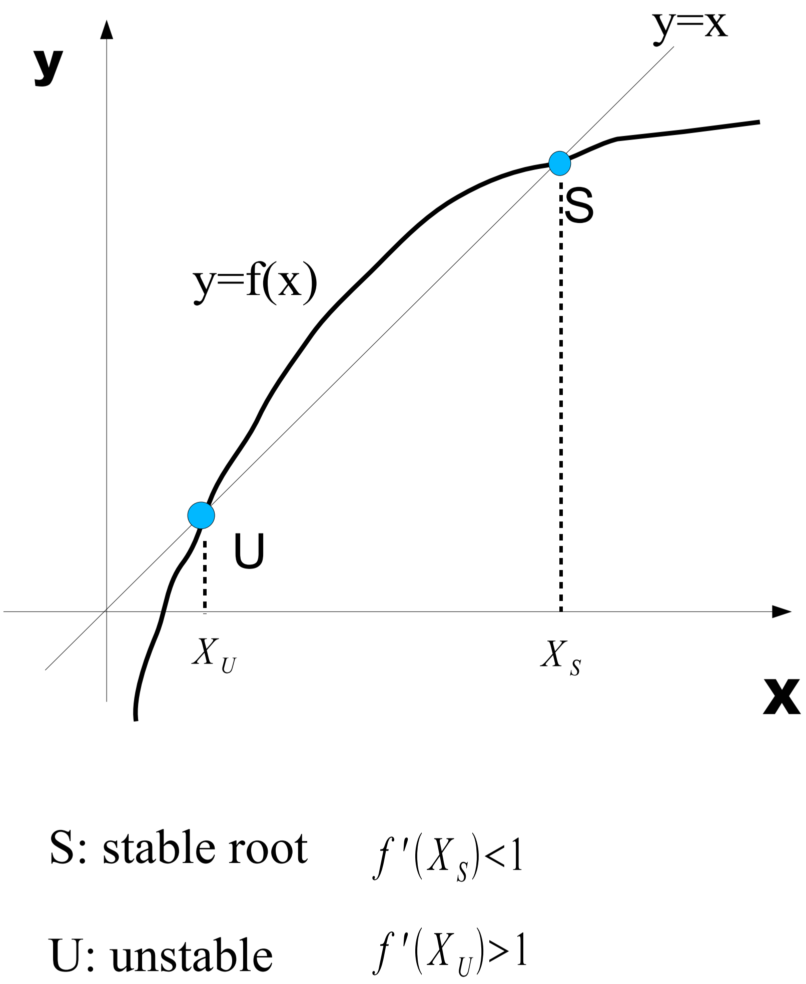

Figure 1: Schematic figure of stable and unstable roots of non-linear equation $x = f(x)$.

This scheme is equivalent to Eq.(3) with substitution of $f \to F = x - \frac{g[x]}{g'[x]}$. Therefore, the condition of stable iteration for F is,

$$
\begin{aligned}
& F'[x_0 + \epsilon] < 1 \\
\Rightarrow \quad & 1 > 1 - \left. \frac{(g'[x])^2 - g[x]g''[x]}{(g'[x])^2} \right|_{x=x_0+\epsilon} \\
& = \frac{g[x]g''[x]}{(g'[x])^2} = \frac{(x - f[x])(-f''[x])}{(1 - f'[x])^2} \\
& = \left. \frac{(-a\epsilon)(-2b)}{(1-a)^2} \right|_{x_0+\epsilon} \\
& = \frac{2ab}{(1-a)^2}\epsilon
\end{aligned}
\tag{7}
$$

It is clear that unless $a = 1$, we have stability of N-R scheme for the choice of sufficiently small ϵ. This is even true for unstable root in direct iteration. If we chose initial guess appropriately (sufficiently small ϵ), N-R is absolutely stable. If accidentally $f'(x_0) = 1$ at zero, we should go to higher (2nd order) N-R scheme.