On extensions of the Newton-Raphson iterative scheme to arbitrary orders

Gilbert Labelle, LaCIM-UQAM, Montréal (Québec) Canada

FPSAC’10, San Francisco, August 2010
Definition
Let \( t_n \to a \). The convergence is said to be of order \( p \) if

\[
t_{n+1} - a = O \left( \left( t_n - a \right)^p \right), \text{ as } n \to \infty.
\]

Theorem (Classical Newton-Raphson)
Let \( U \subseteq \mathbb{R} \) be open and \( f : U \to \mathbb{R} \) be twice differentiable. If \( a \in U \) is a simple root of \( f \left( t \right) = 0 \), then the iterative scheme,

\[
t_{n+1} = N \left( t_n \right), \quad n = 0, 1, 2, ..., \quad \text{with} \quad N \left( t \right) = t - \frac{f \left( t \right)}{f' \left( t \right)}
\]

produces a quadratically convergent \(( p = 2 \) sequence of approximations \( t_n \to a \), as \( n \to \infty \), whenever the first approximation, \( t_0 \), is sufficiently near to \( a \).
Higher order convergence can also be achieved:

**Theorem (Householder, \( p = 3 \))**

\[
\mathcal{N}(t) = t - \frac{f(t)}{f'(t)} \left(1 + \frac{f(t)f''(t)}{2f'(t)^2}\right).
\]

**Theorem (Halley, \( p = 3 \))**

\[
\mathcal{N}(t) = t - \frac{2f(t)f'(t)}{2f'(t)^2 - f(t)f''(t)}.
\]

**Theorem (Householder, \( p = k + 1 \))**

\[
\mathcal{N}(t) = t + k \frac{(1/f)^{(k-1)}(t)}{(1/f)^{(k)}(t)}.
\]
Theorem (Extension of Newton-Raphson to order $p = k + 1$)

Let $f$ be of class $C^{k+1}$ around the simple root $a$ and let

$$
\mathcal{N}(t) = \sum_{\nu=0}^{k} (-1)^\nu \frac{f(t)^\nu}{\nu!} \left( \frac{1}{f'(t)D} \right)^\nu t.
$$

Then for every $t_0$ sufficiently near to $a$, the sequence $(t_n)_{n \geq 0}$, defined by $t_{n+1} = \mathcal{N}(t_n)$, converges to $a$ to the order $k + 1$:

$$
t_{n+1} - a \sim C \cdot (t_n - a)^{k+1}, \quad n \to \infty,
$$

where

$$
C = (-1)^{k+1} \left[ \frac{f'(t)^{k+1}}{(k+1)!} \left( \frac{1}{f'(t)D} \right)^{k+1} t \right]_{t=a}.
$$

Proof (Sketch).

$a = f^{-1}(0) = f^{-1}(f(t) - f(t)) = f^{-1}(f(t) + u)|_{u=-f(t)}$.  \hfill \Box
The last iteration step can also be rewritten as,

\[ \mathcal{N}(t) = \sum_{\nu=0}^{k} (-1)^\nu \left( \frac{f(t)}{f'(t)} D^\nu \right) t, \]

where \( \binom{z}{\nu} = \frac{z(z-1)(z-2)\cdots(z-\nu+1)}{\nu!}. \)

**Corollary**

Let \( f \) be analytic around the simple root \( a \). Then, for every \( g \), analytic around \( a \) and \( t \) sufficiently near to \( a \):

\[ g(a) = \sum_{\nu=0}^{\infty} (-1)^\nu \frac{f(t)^\nu}{\nu!} \left( \frac{1}{f'(t)} D^\nu \right) g(t). \]

\[ = \sum_{\nu=0}^{\infty} (-1)^\nu \left( \frac{f(t)}{f'(t)} D^\nu \right) g(t). \]
Typical illustrations (order = $k + 1$):

- **Root extraction**, $f(t) = t^n - c = 0$, $a = c^{1/n}$, $g(t) = t^{m/n}$:

  $$
  \mathcal{N}(t) = \sum_{\nu=0}^{k} (-1)^{\nu} \left( \frac{1}{n} \right)^{\nu} t \left( 1 - \frac{c}{t^n} \right)^{\nu},
  $$

  $$
  c^{m/n} = \sum_{\nu=0}^{\infty} (-1)^{\nu} \left( \frac{m}{n} \right)^{\nu} t^{m} \left( 1 - \frac{c}{t^n} \right)^{\nu}.
  $$

- **Computing logarithms**, $f(t) = e^t - c$, $a = \ln(c)$, $g$ analytic:

  $$
  \mathcal{N}(t) = t - \sum_{\nu=1}^{k} \frac{(1 - ce^{-t})^{\nu}}{\nu},
  $$

  $$
  g(\ln(c)) = \sum_{\nu=0}^{\infty} (ce^{-t} - 1)^{\nu} \left( \frac{D}{\nu} \right) g(t).
  $$
Another illustration (order = $2p + 1$):

- Approximating $\pi$, $f(t) = \sin(t) = 0$, $a = \pi$, $g$ analytic:

\[
\frac{3}{4}\pi < t_0 < \frac{5}{4}\pi, \quad t_{n+1} = N(t_n) \rightarrow \pi \quad \text{where}
\]

\[
N(t) = t - \tan(t) + \frac{\tan(t)^3}{3} - \frac{\tan(t)^5}{5} + \cdots + (-1)^{2p-1}\frac{\tan(t)^{2p-1}}{2p-1}.
\]

Moreover,

\[
g(\pi) = \sum_{\nu=0}^{\infty} (-1)^\nu \binom{\tan(t)D}{\nu} g(t), \quad \text{for } t \text{ near } \pi.
\]
Given a combinatorial species, \( R \), the species, \( A = A(X) \), of \( R \)-enriched rooted trees is recursively defined by

\[
A = XR(A).
\]

**Figure:** An \( R \)-enriched rooted tree \((X = \bullet)\)

Hence, \( A \) is the solution of \( F(T) = 0 \) where \( F(T) = T - XR(T) \).
Let $D = d/dT$ denote the combinatorial differentiation operator with respect to singletons of sort $T$. Note that

$$-F(T) = XR(T) - T \quad \text{and} \quad DF(T) = F'(T) = 1 - XR'(T).$$

This suggests that for some actions of the symmetric groups $\mathfrak{S}_\nu$:

**Theorem**

Let $m \geq 0$. If $\alpha$ coincides with the species $A$ of $R$-enriched rooted trees on sets up to cardinality $m$, then

$$N(\alpha) = \sum_{\nu=0}^{k} \frac{1}{\mathfrak{S}_\nu} (XR(\alpha) - \alpha)^\nu \left[ \left( \frac{1}{1 - XR'(T)} D \right)^\nu T \right]_{T := \alpha},$$

coincides with $A$ on sets up to cardinality $(k + 1)(m + 1)$. 

In other words,

\[ \alpha = A|_{\leq m} \Rightarrow \mathcal{N}(\alpha)|_{\leq (k+1)(m+1)} = A|_{\leq (k+1)(m+1)}. \]

Proof ($m = 6$ fixed).

- $\alpha$-structures are called \textit{light R-enriched rooted trees}.
- ($XR(\alpha) - \alpha$)-structures are called \textit{m-broccolis}:

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{broccoli}
\caption{A $m$-broccoli for $m = 6$}
\end{figure}
\[ \mathcal{D} = \frac{1}{1 - X R'(T)} D \] is called an \textit{eclosion operator} \( (T = \blacktriangle) \):

![Diagram of eclosion operator applied to a species \( K(X, T) \)]

\textbf{Figure:} The eclosion operator \( \mathcal{D} \) applied to a species \( K(X, T) \)
Now let $\tau$ be an $A$-structure on a set of size $\leq (k + 1)(m + 1)$. Let $\nu$ be the number of broccolis contained in $\tau$. Then $0 \leq \nu \leq k$. Number arbitrarily these broccolis from 1 to $\nu$ as in Figure (a), then detach these broccolis as in Figure (b), (here $m = 6$, $\nu = 3$):

(a) Numbering broccolis

(b) Detached broccolis

**Figure:** Visualizing $(XR(\alpha) - \alpha)^\nu \left[ \left( \frac{1}{1-XR'(T)D} \right)^\nu T \right]_{T:=\alpha}$

We conclude using the fact that $\mathcal{G}_\nu$ acts on these structures.
Corollary

Let $A = XR(A)$ and $G$ be an arbitrary species. Then, according to the number $\nu$ of leaves, the following expansions hold:

\[
A = \sum_{\nu=0}^{\infty} \frac{1}{\mathcal{S}_\nu} X^\nu \left[ \left( \frac{R(0)}{1 - XR'(T)D} \right)^\nu T \right]_{T:=0},
\]

\[
G(A) = \sum_{\nu=0}^{\infty} \frac{1}{\mathcal{S}_\nu} X^\nu \left[ \left( \frac{R(0)}{1 - XR'(T)D} \right)^\nu G(T) \right]_{T:=0}.
\]

Proof.

Take $m = 0$ and $\alpha = 0$. The 0-broccolis become $XR(0)$-structures (that is, enriched singletons, or leaves). Finally let $k \to \infty$. \qed
Corollary

Let \( R(x) = \sum_{n=0}^{\infty} r_n x^n / n! \) and \( G(x) = \sum_{n=0}^{\infty} g_n x^n / n! \). Let \( \gamma_{n,\nu} \) be the number of \( G \)-assemblies of \( R \)-enriched rooted trees on \([n]\) having exactly \( \nu \) leaves. Then, for \( \nu \geq 1 \),

\[
\sum_{n=0}^{\infty} \gamma_{n,\nu} x^n / n! \frac{r_0^\nu x^\nu}{\nu!(1 - r_1 x)^{2\nu - 1}} p_\nu(x),
\]

where \( p_\nu(x) = \omega_\nu(x, 0) \) are polynomials defined by

\[
\omega_1(x, t) = G'(t),
\]

\[
\omega_\nu(x, t) = \left( (1 - xR'(t)) \frac{\partial}{\partial t} + (2\nu - 3)xR''(t) \right) \omega_{\nu-1}(x, t).
\]

Proof.

Use induction on \( \nu \) in underlying series of the above corollary.
Examples (Some applications to generating series)

- **Ordinary rooted trees having \( \nu \) leaves \((R = E, G = X)\):**

\[
x^\nu (1 - x)^{-2\nu + 1} p_\nu (x) / \nu!,
\]

\[
p_1(x) = 1, \quad p_\nu(x) = x ((1 - x)p'_{\nu - 1}(x) + (2\nu - 3)p_{\nu - 1}(x)).
\]

- **Mobiles having \( \nu \) leaves \((R = 1 + C, G = X)\):**

\[
x^\nu (1 - x)^{-2\nu + 1} q_\nu (x) / \nu!, \quad q_\nu(x) = Q_\nu(x, 0), \quad Q_1(x, t) = 1,
\]

\[
Q_\nu(x, t) = \left( (1 - t)(1 - t - x) \frac{\partial}{\partial t} + x + (2\nu - 4)(1 - t) \right) Q_{\nu - 1}(x, t).
\]

- **Endofunctions having \( \nu \) leaves \((R = E, G = S)\):**

\[
x^\nu (1 - x)^{-2\nu + 1} \epsilon_\nu (x) / \nu!, \quad \epsilon_\nu(x) = K_\nu(x, 0), \quad K_1(x, t) = 1,
\]

\[
K_\nu(x, t) = \left( (1 - x)(1 - t) \left( x \frac{\partial}{\partial x} + \frac{\partial}{\partial t} \right) + \nu + (\nu - 3)x - (2\nu - 3)xt \right) K_{\nu - 1}(x, t).
\]