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

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FPSAC'10, San Francisco, August 2010

Definition

Let $t_n \to a$. The convergence is said to be *of order* p if

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

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 $f(t) = 0$, then the iterative scheme,

$$t_{n+1} = \mathcal{N}(t_n), \quad n = 0, 1, 2, \ldots, \quad \textit{with} \quad \mathcal{N}(t) = t - \frac{f(t)}{f'(t)},$$

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 $k + 1$:

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

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

Proof (Sketch).

$a = f^{<-1>}(0) = f^{<-1>}(f(t) - f(t)) = f^{<-1>}(f(t) + u)|_{u:=-f(t)}$. $\square$

The last iteration step can also be rewritten as,

$$\mathcal{N}(t) = \sum_{\nu=0}^{k} (-1)^{\nu} \binom{\frac{f(t)}{f'(t)} D}{\nu} t,$$

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:

$$\begin{aligned} g(a) &= \sum_{\nu=0}^{\infty} (-1)^{\nu} \frac{f(t)^{\nu}}{\nu!} \left(\frac{1}{f'(t)} D \right)^{\nu} g(t) \\ &= \sum_{\nu=0}^{\infty} (-1)^{\nu} \binom{\frac{f(t)}{f'(t)} D}{\nu} g(t). \end{aligned}$$

$\square$

Typical illustrations (order $= k+1$) :

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

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

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

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

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

$$g(\ln(c)) = \sum_{\nu=0}^{\infty} (ce^{-t} - 1)^\nu \binom{D}{\nu} g(t).$$

Another illustration (order $= 2p+1$):

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

$$\frac{3}{4}\pi < t_0 < \frac{5}{4}\pi, \quad t_{n+1} = \mathcal{N}(t_n) \to \pi \quad \text{where}$$

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

Moreover,

$$g(\pi) = \sum_{\nu=0}^{\infty}(-1)^{\nu}\binom{\tan(t)D}{\nu}g(t), \quad \text{for } t \text{ near } \pi.$$

COMBINATORIAL APPROACH

Given a combinatorial species, R, the species, $A = A(X)$, of *R-enriched rooted trees* is recursively defined by

$$A = XR(A).$$

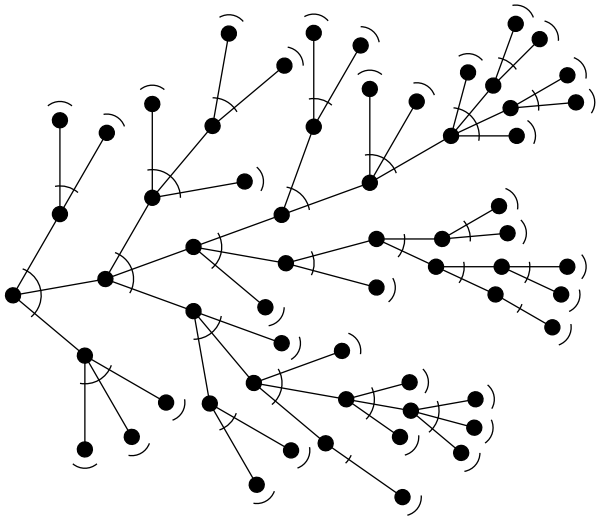


Figure: An R-enriched rooted tree ($X = \bullet$)

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 α coincides with the species A of R-enriched rooted trees on sets up to cardinality m, then

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

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

In other words,

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

Proof ($m = 6$ fixed).

- α-structures are called *light R -enriched rooted trees* .
- $(XR(\alpha) - \alpha)$-structures are called *m-broccolis* :

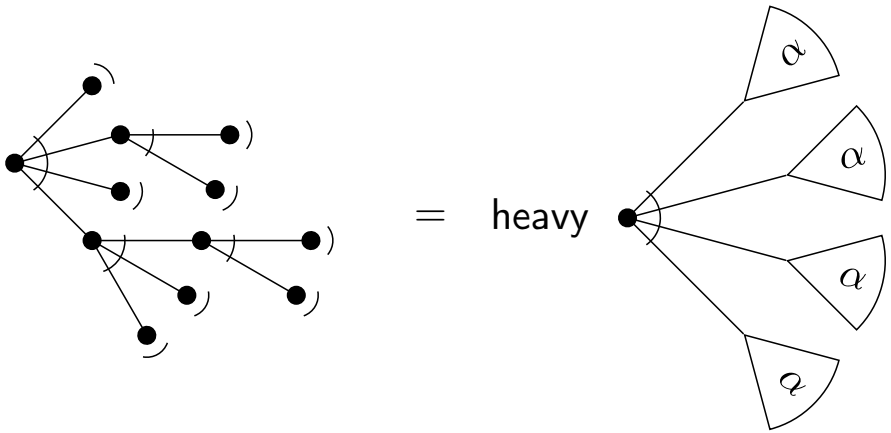


Figure: A m-broccoli for $m = 6$

- $\mathcal{D} = \frac{1}{1-XR'(T)} D$ is called an *eclosion operator* ($T = \blacktriangleleft$):

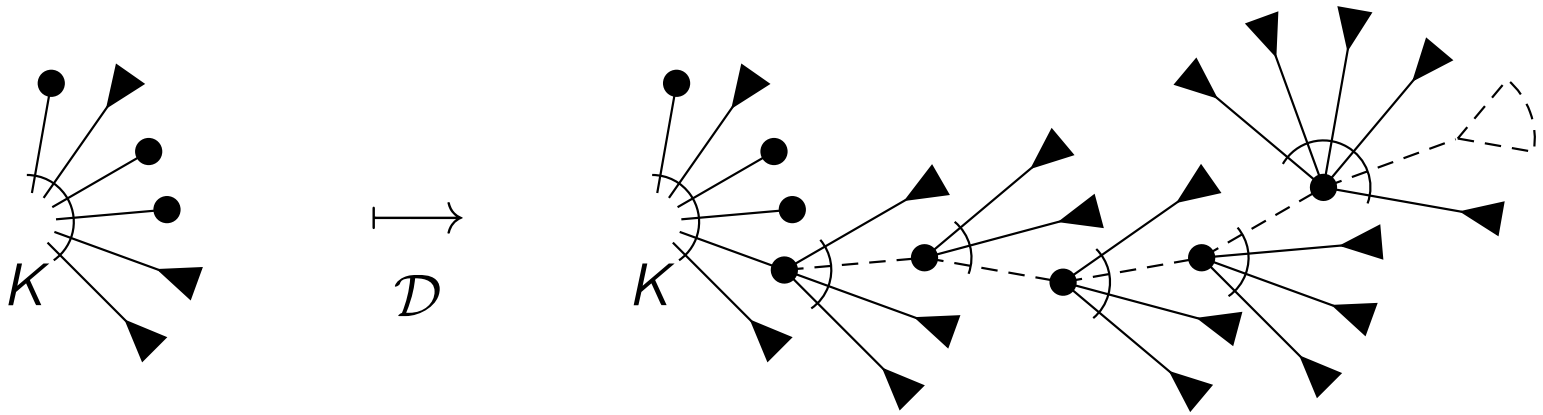
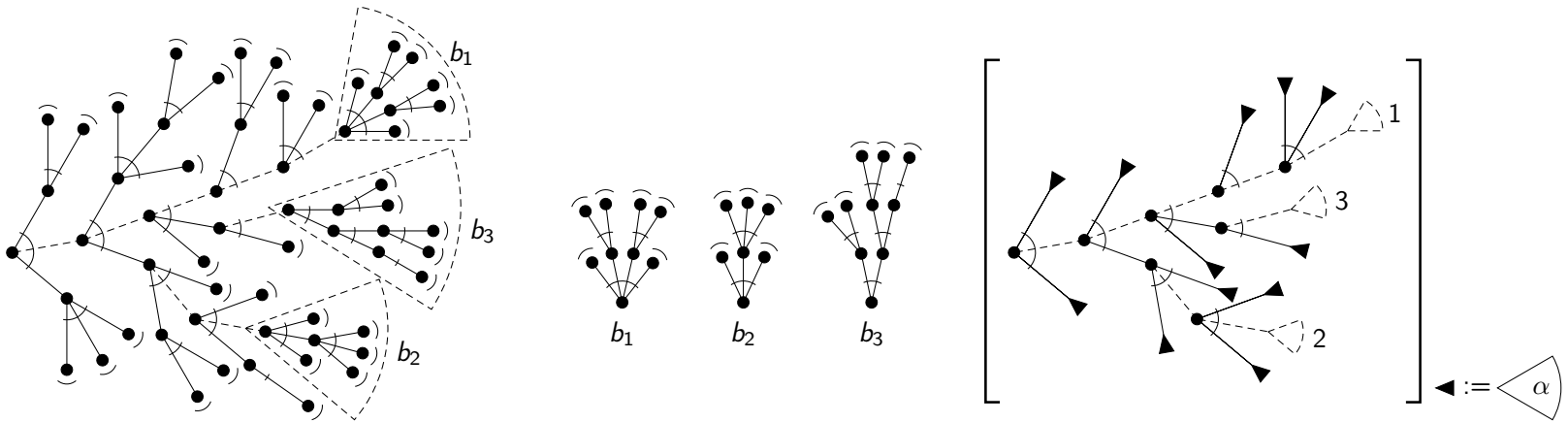


Figure: The eclosion operator $\mathcal{D}$ applied to a species $K(X, T)$

Now let τ be an A-structure on a set of size $\leq (k+1)(m+1)$. Let ν be the number of broccolis contained in τ. Then $0 \leq \nu \leq k$. Number arbitrarily these broccolis from 1 to ν 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 $\mathfrak{S}_\nu$ acts on these structures.

$\square$

Corollary

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

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

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

Proof.

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

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* ν *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*

$$\begin{aligned} \omega_1(x,t) &= G'(t), \\ \omega_\nu(x,t) &= \left((1-xR'(t))\frac{\partial}{\partial t} + (2\nu-3)xR''(t)\right)\omega_{\nu-1}(x,t). \end{aligned}$$

Proof.

Use induction on ν in underlying series of the above corollary. $\square$

Examples (Some applications to generating series)

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

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

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

- *Mobiles having ν 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 ν leaves* $(R = E, G = S)$:

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

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