Nuttall's compact formula

March 2006

The present file is http://www.math.ucl.ac.be/˜magnus/num3/nuttallc.pdf

1. Preludium.

Let ρ be a weight function of support s. The Padé $[n-1/n]$ rational approximation to $f(z) = \int_s \dfrac{\rho(t)\,dt}{z-t} \sim \dfrac{m_0}{z} + \dfrac{m_1}{z^2} + \cdots$ about $z=\infty$ is $\dfrac{\nu_n(z)}{p_n(z)}$ of degrees $n-1$ and n such that $f(z) - \dfrac{\nu_n(z)}{p_n(z)} = O\left(\dfrac{1}{z^{2n+1}}\right)$, when $z\to\infty$, or

$$q_n(z) := p_n(z)f(z) - \nu_n(z) = O\left(\frac{1}{z^{n+1}}\right).$$

Remark that $p_n(z)f(z) = \displaystyle\int_s \frac{[p_n(z)-p_n(t)\ +p_n(t)]\rho(t)\,dt}{z-t}$, that the part involving $p_n(z)-p_n(t)$ is a polynomial of degree $\leqslant n-1$ in z, and that what remains is at most $O(1/z)$: this means that we just encountered the numerator polynomial ν_n and the remainder q_n:

$$\nu_n(z) = \int_s \frac{[p_n(z)-p_n(t)]\rho(t)\,dt}{z-t}\ ,\ q_n(z) = \int_s \frac{p_n(t)\rho(t)\,dt}{z-t},$$

and that this latter $q_n(z)$ is only $O(1/z^{n+1})$ amounts to the ***orthogonality*** of p_n and all polynomials of degree $<n$ with respect to ρ.

2. Thema.

Let $\{b_0,\dots,b_{n-1}\}$ be a basis of the space $\mathscr{P}_{n-1}$ of polynomials of degree $\leqslant n-1$, and $\mathcal{R}$ an operator. We consider a matrix representation $R_{i,j} = \langle b_i|\mathcal{R}|b_j\rangle$, where $\langle\ \ \rangle$ is tha scalar product $\langle f|g\rangle = \int_s f(t)g(t)\rho(t)\,dt$. The matrix R of finite order n does not tell everything on the operator $\mathcal{R}$, it only allows to recover the orthogonal projection (***Galerkin*** approximation [2]) on $\mathscr{P}_{n-1}$ of $\mathcal{R}r$, where r is also in $\mathscr{P}_{n-1}$. So, if the expansion r in the b_i's basis is $r=\sum_k \alpha_k b_k$,

$$R\begin{bmatrix}\alpha_0\\ \vdots\\ \alpha_{n-1}\end{bmatrix} = \begin{bmatrix}\langle b_0|\mathcal{R}|r\rangle\\ \vdots\\ \langle b_{n-1}|\mathcal{R}|r\rangle\end{bmatrix}\ , r = [b_0\cdots b_{n-1}]R^{-1}\begin{bmatrix}\langle b_0|\mathcal{R}|r\rangle\\ \vdots\\ \langle b_{n-1}|\mathcal{R}|r\rangle\end{bmatrix}.$$

Well, for a fixed z, let $\mathcal{R}$ be z times identity minus the multiplication operator by the variable, that is, $\mathcal{R}f(t) = (z-t)f(t)$. Let us take $r(t) = \dfrac{p_n(z)-p_n(t)}{z-t}$, then $\mathcal{R}r(t) = p_n(z)-p_n(t)$ which is reduced to the constant $p_n(z)$ when it comes to orthogonal projections on $\mathscr{P}_{n-1}$:

$$\nu_n(z) = \langle r|1\rangle = p_n(z)[\langle b_0|1\rangle\cdots\langle b_{n-1}|1\rangle]R^{-1}\begin{bmatrix}\langle b_0|1\rangle\\ \vdots\\ \langle b_{n-1}|1\rangle\end{bmatrix}\ ,$$

or

$$\frac{\nu_n(z)}{p_n(z)} = \langle r|1\rangle = [\langle b_0|1\rangle \cdots \langle b_{n-1}|1\rangle] R^{-1} \begin{bmatrix} \langle b_0|1\rangle \\ \vdots \\ \langle b_{n-1}|1\rangle \end{bmatrix} , \tag{1}$$

the Nuttall's compact formula [1]. Of course $p_n(z)$ is (a constant times) the determinant of R, i.e., det $[z\langle b_i|b_j\rangle - \langle b_i|b_{j+1}\rangle]$.

Remark also that if $b_k = p_k$, the basis of orthonormal polynomials, R is $zI - J$, where J is the jacobi tridiagonal matrix of recurrence coefficients.

3. **Variations.**

If $\begin{bmatrix} \alpha_0 \\ \vdots \\ \alpha_{n-1} \end{bmatrix}$ is $R^{-1} \begin{bmatrix} \langle b_0|1\rangle \\ \vdots \\ \langle b_{n-1}|1\rangle \end{bmatrix}$, then $\left[\begin{array}{c|ccc} 0 & \langle b_0|1\rangle & \cdots & \langle b_{n-1}|1\rangle \\ \hline \langle b_0|1\rangle & & & \\ \vdots & & \mathrm{R} & \\ \langle b_{n-1}|1\rangle & & & \end{array}\right] \left[\begin{array}{c} -1 \\ \hline \alpha_0 \\ \vdots \\ \alpha_{n-1} \end{array}\right] = \left[\begin{array}{c} \nu_n(z)/p_n(z) \\ \hline 0 \\ \vdots \\ 0 \end{array}\right]$,

so $\nu_n(z) = -\dfrac{p_n(z)}{\det R} \left|\begin{array}{c|ccc} 0 & \langle b_0|1\rangle & \cdots & \langle b_{n-1}|1\rangle \\ \hline \langle b_0|1\rangle & & & \\ \vdots & & \mathrm{R} & \\ \langle b_{n-1}|1\rangle & & & \end{array}\right|$ or also

$q_n(z) = p_n(z)f(z) - \nu_n(z) = \dfrac{p_n(z)}{\det R} \det \left[\begin{array}{c|ccc} f(z) & \langle b_0|1\rangle & \cdots & \langle b_{n-1}|1\rangle \\ \hline \langle b_0|1\rangle & & & \\ \vdots & & \mathrm{R} & \\ \langle b_{n-1}|1\rangle & & & \end{array}\right]$, but this does not suggest the $O(z^{-n-1})$ behaviour for large z. However, the latter matrix can be written as $\left\langle \begin{bmatrix} 1 \\ (z-t)b_0 \\ \vdots \\ (z-t)b_{n-1} \end{bmatrix} \middle| \dfrac{1}{z-t} \middle| \begin{bmatrix} 1 & (z-t)b_0 & \dots & (z-t)b_{n-1} \end{bmatrix} \right\rangle$, and considering that $1, (z-t)b_0(t), \dots, (z-t)b_{n-1}(t)$ are linear combinations of $b_0(t), \dots, b_n(t)$: $\begin{bmatrix} 1 \\ (z-t)b_0 \\ \vdots \\ (z-t)b_{n-1} \end{bmatrix} = T \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_n \end{bmatrix}$, so that

$$q_n(z) = \text{constant } det \left\langle \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_n \end{bmatrix} \middle| \frac{1}{z-t} \middle| \begin{bmatrix} b_0 & b_1 & \dots & b_n \end{bmatrix} \right\rangle = \text{const. } \det[\langle b_i|(z-t)^{-1}|b_j\rangle]_{i,j=0}^{n},$$

which is Pierre's formula [4].

4. **References.**

[1] J. Nuttall, The connection of Padé approximants with stationary variational principles and the convergence of certain Padé approximants (pp. 219–230) in *The Padé approximant in theoretical physics*, edited by George A. Baker, Jr. and John L. Gammel. Mathematics in Science and Engineering, Vol. 71. Academic Press, New York-London, 1970.

[2] O. Goscinski, E. Brändas (Quantum Chemistry Group, University of Uppsala, Uppsala, Sweden), Padé approximants to physical properties via inner projections, *International Journal of Quantum Chemistry* Volume **5**, Issue 2 , Pages 131 – 156 Published Online: 1 Sep 2004 Copyright ©1971 John Wiley & Sons, Inc.
Save Title to My Profile Set E-Mail Alert
Sponsored in part by the Swedish Natural Sciences Research Council and in part by the Air Force Office of Scientific Research (OSR) Through the European Office of Aerospace Research (OAR) United States Air Force under Grant EOOAR-70-0073. Abstract
The [N, M] Padé approximants to functions formally associated to power series expanssions are expressed in terms of expectation values of inverse matrices. These formulae, which can be derived by the inner-projection technique, lead to a simple analysis of the properties of serveral approximation methods and their inter-relationships, in particular Gaussian integration, continued factorization and Padé approximations, which are of current interest in the calculation of physical properties. A relation with Fredholm integral equations and expansions of the resolvent is also discussed. The use of operator inequalities in a systematic fashion is particularly convenient when both the function being approximated and the coefficients of the power series have physically meaningful expressions as moments of operators.

[3] G. Turchetti, PADE APPROXIMANTS, STJELTJES FUNCTIONS. AND VARIATIONAL PROPERTIES ... Nuttal's formula we quote another compact formula to compute PA we shall prove later, ... `www-sop.inria.fr/miaou/anap03/ Pade_Turchetti_Porquerolles.ps`

[4] P. van Moerbeke, Random matrices II: orthogonal polynomials and non-linear PDE, sém. non linéaire UCLouvain/KULeuven, March 2006.

[5] ? [PDF] Pade approximants and closed form solutions of the KdV and MKdV ... is Nutall's compact formula [10] for the. [N/N]. Pade approximant to the series (19); it involves the. first 2N perturbation terms. ... `heldref.metapress.com/index/K5W77L2121247165.pdf`