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LAGRANGIAN DIFFERENTIATION, INTEGRATION, AND EIGENVALUE PROBLEMS

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SUMMARY

Calogero recently proposed a new and very powerful method for the solution of Sturm-Liouville eigenvalue problems based on Lagrangian differentiation. In this paper, I present some results of a numerical investigation of Calogero's method for physically interesting problems. I then show that one can "invert" his differentiation technique to obtain a flexible, factorially convergent Lagrangian integration scheme which should be useful in a variety of problems, e.g., solution of integral equations.

In a recent paper⁽¹⁾, Calogero proposed a new and very powerful method for the solution of Sturm-Liouville eigenvalue problems. In his approach, the operators x and d/dx in the differential equation are replaced by special $n \times n$ matrices \underline{X} and \underline{Z} , and the eigenvalues and eigenvectors are determined by matrix methods. Calogero shows that under reasonable assumptions (a subset of) the matrix eigenvalues converge factorially fast to the true eigenvalues, $|\delta\lambda_m/\lambda_m| \ll (\pi m/2n)^{n-2}$. In this paper, I present some results of a numerical investigation of Calogero's method for physically interesting problems. Its remarkable success suggested that one might "invert" the differentiation scheme to obtain a flexible, factorially convergent integration scheme useful in a variety of problems, e.g., integration with sparse data or the solution of integral or integrodifferential equations (my original motivation). I present the integration scheme and some tests of its accuracy here.

Calogero's work⁽¹⁾ is based on the observation that $n \times n$ matrix operators \underline{X} and \underline{Z} defined in terms of n arbitrary points x_1, \dots, x_n by

$$(1) \quad \underline{X}_{ij} = x_i \delta_{ij},$$

$$(2a) \quad \underline{Z}_{ij} = (x_i - x_j)^{-1}, \quad i \neq j,$$

$$(2b) \quad \underline{Z}_{i1} = \sum_{\substack{j=1 \\ j \neq i}}^n (x_i - x_j)^{-1},$$

satisfy the Heisenberg algebra of x and d/dx when acting on the finite basis $\{\underline{x}^{(m)}, m = 0, \dots, n-1\}$ with ⁽²⁻⁴⁾

$$(3) \quad \underline{x}_i^{(m)} = x_i^m / \pi_i(x_i), \quad m=0, \dots, n-1.$$

and

$$(4) \quad \pi_i(x) = \prod_{\substack{j=1 \\ j \neq i}}^n (x-x_j).$$

Specifically⁽³⁾

$$(5) \quad \underline{x} \underline{x}^{(m)} = \underline{x}^{(m+1)}, \quad 0 < m < n-2,$$

$$(6) \quad \underline{z} \underline{x}^{(m)} = m \underline{x}^{(m-1)}, \quad 0 < m < n-1.$$

These results are closely connected to Lagrangian interpolation⁽²⁾. The π 's are the Lagrange interpolation polynomials⁽⁵⁾, \underline{z} is given in terms of π by

$$(7) \quad \underline{z}_{ij} = \frac{\partial}{\partial x_i} \ln \pi_j(x_j)$$

and the \underline{x} 's give a matrix representation of the monomials x^m ,

$$(8) \quad \underline{x}^m = (\underline{\pi}(x), \underline{x}^{(m)}) = \sum_{i=1}^n x_i^m \pi_i(x) / \pi_i(x_i).$$

More generally, the (unique) polynomial of degree $n-1$ which is equal to a function $f(x)$ at x_1, \dots, x_n is

$$(9) \quad F(x) = (\underline{\pi}, \underline{F}), \quad \underline{F}_i = f(x_i) / \pi_i(x_i).$$

This polynomial approximates $f(x)$ in the sense that⁽⁵⁾

$$(10) \quad f(x) = F(x) + R_n,$$

$$(11) \quad R_n = f^{(n)}(\xi) \prod_{i=1}^n (x-x_i)/n!, \quad x_1 < \xi < x_n.$$

For functions with bounded derivatives, the Lagrange interpolation formula $f(x) = F(x)$ thus gives a factorially convergent approximation, $|R_n| < (\max |f^{(n)}(\xi)|) |x_n - x_1|^n / n!$. The formulas for Lagrangian integration⁽⁵⁾ and differentiation^(2,5) are obtained by integrating or differentiating the polynomial $F(x)$, and have similar error terms.

Calogero's procedure in ref. 1 is to map the differential equation⁽⁶⁾

$$(12) \quad Aw(x) = [a_2(x) \frac{d^2}{dx^2} + a_1(x) \frac{d}{dx} + a_0(x)]w(x) = \lambda w(x), \quad a < x < b,$$

to the matrix equation

$$(13) \quad \underline{Aw} = [\underline{a_2(X)Z^2} + \underline{a_1(X)Z} + \underline{a_0(X)}]w = \underline{\lambda}w$$

by the substitutions $x \rightarrow \underline{X}$, $d/dx \rightarrow \underline{Z}$, with $x_1, \dots, x_n \in (a, b)$. For operators A with polynomial eigenfunctions, the n eigenvalues $\hat{\lambda}_j, j=1, \dots, n$ of \underline{A} are equal to the lowest n eigenvalues λ_j of A ⁽⁷⁾, and the eigenfunctions are related by $\underline{w} = w(x_1)/\pi_1(x_1)$, $w(x) = (\underline{\pi}(x), \underline{w})$, $j=1, \dots, n$. It is therefore plausible that the matrix equation will also give good approximations for some of the lowest eigenvalues and eigenvectors of A for more general problems. Calogero in fact estimates the rate of convergence of eigenvalues of A to corresponding eigenvalues of \underline{A} , with the result quoted above.

There are some subtleties in this procedure which cause complications in practice. The matrices \underline{a}_1 are usually not polynomial and carry \underline{w} off any finite basis $\{\underline{x}^{(m)}\}$. There is consequently no reason to expect all of the n eigenvalues of \underline{A} to converge to eigenvalues of A . Furthermore, for the \underline{a}_1 real (the usual case), \underline{A} is real but not symmetric and can have pairs of complex conjugate eigenvalues which do not correspond to any of the (real) eigenvalues of a self adjoint Sturm-Liouville operator. As a result, only a subset of the $\hat{\lambda}$'s may actually converge to eigenvalues of A . However, when this subset is properly ordered, we find that $\hat{\lambda}_j \rightarrow \lambda_j$ where $\lambda_1 < \lambda_2 < \dots < \lambda_n$ are the $n' < n$ lowest eigenvalues of A . These $\hat{\lambda}$'s are easy to pick out of the complete set $\{\hat{\lambda}\}$ because of their rapid convergence and subsequent stability as n is increased.

In Table I, I illustrate the remarkable power of Calogero's method using the Bessel functions $J_l(j_{l,n}r)$ for r on $[0,1]$ with $j_{l,n}$ the n th zero of $J_l(x)$. I impose the boundary conditions $J_l = r^l, r \rightarrow 0$, and $J_l(j_{l,n}) = 0$ explicitly by writing the Bessel function as

$$(14) \quad J_l(j_{l,n}r) = r^l(1-r^2)w_l(r^2),$$

change to $z = r^2$ as a new variable, and obtain an equation for \underline{w} of the form in eq. (13) with

$$(15) \quad \underline{a}_2 = -4\underline{x}, \underline{a}_1 = -4(l+1)\underline{1} + 8\underline{x}/(1-\underline{x}), \underline{a}_0 = 4(l+1)/(1-\underline{x}).$$

As may be seen from Table I, the convergence of the eigenvalue $\hat{j}_{0,k}$ to $j_{0,k} = \lambda_{0,k}^{1/2}$ is extremely rapid. For example, $\hat{j}_{0,1}$ is accurate to twenty-two figures for $n = 15$, while $\hat{j}_{0,10}$ is accurate to 3.4% for $n =$

20 even though there are only two points to define each of the ten loops of $J_0(j_{0,10}r)$. The results for $\hat{j}_{1,k}$ and $\hat{j}_{2,k}$ are similar.

I have also tested Calogero's method for the physically-interesting problem of the radial Schrödinger equation with the Coulomb-plus-linear potential used to fit the mass spectra of bound $c\bar{c}$ and $b\bar{b}$ systems (charmonium and upsilonium)⁽⁹⁾

$$(16) \quad V(r) = -\frac{a}{r} + br.$$

The method I have used is appropriate for a large class of confining interactions⁽¹⁰⁾. It involves extracting both the dominant exponential factor in the radial wave function for $r \rightarrow \infty$ and the factor r^l which appears for $r \rightarrow 0$, and changing variables to eliminate irrational powers of r in the resulting wave equation. Specifically, I write $R_l(r)$ as

$$(17) \quad R_l(r) = \exp\left(-\frac{2}{3} (mqb)^{1/2} r^{3/2}\right) r^l w(x), \quad x = 2r^{1/2},$$

and apply Calogero's procedure to the equation for $w(x)$ using n equally spaced points which extend beyond the (estimated) classical turning point. The results of the calculation for charmonium are given in Table II. The ground state (1S) energy for a 20×20 matrix is accurate to (a ridiculous) 1 eV out of 0.36 GeV, while the 5S and 5P levels are accurate to 0.4% ($l=0$) and 0.1% ($l=1$). The calculation (and that in Table I) required 0.76 sec per l value on a CDC Cyber 175, and is sufficiently fast that one can contemplate adjustment of the potential point-by-point in fitting the observed energies.

The success of Calogero's method for differentiation and differential equations suggests that an "inverse" method related to Lagrangian integration might be useful for numerical integration and the solution of integral equations. In the remainder of the paper I will develop a simple matrix procedure for Lagrangian integration and sketch how it might be applied. My derivations will be given elsewhere in more detail.

I begin with the expressions

$$(18a) \quad f(x) = \int_{x_1}^x g(x') dx', \quad f(x_1) = 0,$$

$$(18b) \quad g(x) = \frac{df}{dx}(x).$$

The Lagrangian matrix representation of the second equation is⁽²⁾

$$(19) \quad \underline{g} = \underline{Z} \underline{f}, \quad \underline{f}_j = f(x_j)/\pi_j(x_j),$$

with $g(x) = (\underline{\pi}(x), \underline{g})$. The matrix \underline{Z} is singular and cannot be inverted in eq. (19) to obtain the integral f from g . In particular \underline{Z} annihilates the constant vector $\underline{x}^{(0)}$, eq. (6), so has a vanishing determinant (zero is in fact the n -fold-degenerate eigenvalue of \underline{Z}).

However, \underline{Z} can be written as

$$(20) \quad \underline{Z} = \underline{L} \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & \underline{Z} \end{array} \right) \underline{R}.$$

where the matrices \underline{L} and \underline{R} are nonsingular,

$$(21) \quad \underline{L} = \left(\begin{array}{c|ccc} 1 & -1 & -1 & \dots \\ \hline 0 & & 1 & \dots \end{array} \right), \quad \underline{R} = \left(\begin{array}{c|c} \pi_1 & 0 \\ \hline -\pi/\pi_2 & 1 \\ \hline -\pi_1/\pi_n & \dots \end{array} \right).$$

$\pi_j \equiv \pi_j(x_j)$, $j = 1, \dots, n$, and the $(n-1) \times (n-1)$ matrix $\underline{\hat{Z}}$ is the restriction of \underline{Z} to the indicated block,

$$(22) \quad \underline{\hat{Z}}_{ij} = \underline{Z}_{ij}, \quad i, j = 2, \dots, n.$$

The matrix $\underline{\hat{Z}}$ is invertible and $\underline{\hat{Z}}^{-1}$ is the matrix analog of the integral operator in eq. (18a). Thus, multiplying eq. (19) by \underline{L}^{-1} , using the representation for \underline{Z} in eq. (20), and imposing the boundary condition $\underline{f}_1 = 0$ from eq. (18a), one finds that eq. (19) is equivalent to the $(n-1)$ -dimensional equation

$$(23) \quad \underline{\hat{g}} = \underline{\hat{Z}} \underline{\hat{f}}$$

where $\underline{\hat{f}} = \begin{pmatrix} 0 \\ \underline{f} \end{pmatrix}$, $\underline{\hat{g}} = \begin{pmatrix} 0 \\ \underline{g} \end{pmatrix}$, and

$$(24) \quad \underline{\hat{f}} = \underline{\hat{Z}}^{-1} \underline{\hat{g}}.$$

Since the projection $(\underline{\pi}(x), \underline{f})$ gives the Lagrange interpolation polynomial for $f(x)$, eq. (24) and the boundary condition $\underline{f}_1 = 0$ give the integration formula (exact for polynomials $g(x)$ with degree $< n-2$)

$$(25) \quad f(x) = \int_{x_1}^x g(x') dx' = (\underline{\pi}(x), \underline{\hat{Z}}^{-1} \underline{\hat{g}}), \quad \underline{\hat{g}}_j = g(x_j)/\pi_j(x_j).$$

This is an open-endpoint formula; g is needed only at the $n-1$ points $x_2 \dots x_n$, while $\underline{\hat{Z}}$ involves all n points x_1, \dots, x_n .

By taking differences of the expression in eq. (25) for different choices of $x \in \{x_j\}$ I obtain the formulas

$$(26a) \quad \int_{x_l}^{x_{l+m}} g(x) dx = \sum_{k=2}^n (A_{l+m,k} - A_{l,k}) g(x_k),$$

$$(26b) \quad A_{j,k} = \pi_j(x_j) (\hat{Z}^{-1})_{jk} / \pi_k(x_k).$$

Eq. (26a) is the usual Lagrange integration formula⁽⁵⁾ and has an error term R_n bounded by

$$(27) \quad |R_n| < \frac{1}{(n-1)!} \max |g^{(n-1)}(y)| M^n, \quad x_l < y < x_{l+m}, \quad M = x_{l+m} - x_l.$$

More generally for arbitrary a and b in the interval $[x_1, x_n]$,

$$(28) \quad \int_a^b g(x) dx = (\hat{\pi}(b) - \hat{\pi}(a)) \hat{Z}^{-1} \hat{g}.$$

The advantage of the present approach to Lagrangian integration is its flexibility. It is easy using matrix methods to change n and the selected points $\{x_j\}$ during a calculation. Thus for equally spaced points, eq. (28) is a Newton-Cotes integration formula exact for polynomials of degree $< n-2$, while for $a=x_1=0, b=1$, and x_2, \dots, x_n the $n-1$ zeros of $P_{n-1}(2x-1)$, eq. (28) gives Gauss' integration formula and is exact for polynomials of degree $< 2n-3$. Furthermore, the rate of convergence of the Lagrangian approximation to the exact integral can be greatly enhanced by increasing n as the number of points used in the integration is increased. For example, the value of $S_1(x)$

$-\int_0^x (\sin x/x) dx$ is given correctly to 1×10^{-5} by eq. (26a) with $n = 12$ equally spaced points $\{x\} \{-1, 0, \dots, 10\}$ (11 point Newton-Cotes

integration) and to $< 1 \times 10^{-10}$ for $n = 20$; to obtain the same accuracy with Simpson's rule requires ~ 25 (~ 435) points. Some preliminary calculations also show that these results can be quite useful in the numerical solution of integral equations.

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REFERENCES AND FOOTNOTES

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2. F. Calogero, Lett. Nuovo Cimento 35, 273 (1982), erratum, Lett. Nuovo Cimento 36, 447 (1983).
3. F. Calogero, J. Math. Phys. 22, 919 (1981).
4. The vector $\underline{x}^{(m)}$, $m = 0, 1, \dots$, is denoted by $\underline{v}^{(m+1)}$ in ref. 3. With our labeling m is precisely the degree of the monomial x^m represented by $\underline{x}^{(m)}$.
5. See, for example, W.E. Milne, Numerical Calculus, Princeton University Press, 1949, Chap. 3.
6. We assume that the boundary conditions in the original Sturm-Liouville problem have been imposed explicitly in writing eq. (12). The functions $a_i(x)$ are generally singular at $x = a, b$, and $w(x)$ and \underline{v} are required only to be finite at those points (1).

7. We suppose here that the eigenvalues λ_j of A are real and are ordered so that $\lambda_1 < \lambda_2 < \dots < \lambda_n < \dots$.
8. M. Abramowitz and I.A. Stegun, Handbook of Mathematical Functions, Dover, 1972, Table 9.5.
9. K.J. Miller and M.G. Olsson, Phys. Rev. D 25, 2383 (1982). I would like to thank L.J. Nickisch for calculating the "exact" values in Table II using Miller's band matrix method with a 200x200 matrix.
10. A useful test case for checking the accuracy of the matrix programs is the radial oscillator. After the substitution

$$R_\ell(r) = \exp(-\frac{1}{2} r^2) r^\ell w(r^2)$$

and a change of variables from r to $x = r^2$, we obtain the matrix equation

$$[-4X Z^2 + (4X - (4\ell+6)1) Z + (2\ell+9)1] \underline{w} = \hat{\lambda} \underline{w}$$

with exact integer eigenvalues $\hat{\lambda} = \lambda = 4n + 2\ell - 1$, $n = 1, 2, \dots$,
 $\ell = 0, 1, \dots$

TABLE I

Zeros of the Bessel functions calculated using Calogero's method.
Results given to more than 10 figures are accurate to ± 1 in the last
figure given.

k	$j_{0,k}$, exact ⁽⁸⁾	$j_{0,k}$, n = 15	$j_{0,k}$, n = 20
1	2.40482 55577	2.40482 55576 95772 76862 17	
2	5.52007 81103	5.52007 81103 86310 65	
3	8.65372 79129	8.65372 79129 1 11012
4	11.79153 44391	11.79153 4468	11.79153 44390 1429
5	14.93091 77086	14.93093 5	14.93091 77085
6	18.07106 39679	18.0732	18.07106 4005
7	21.21163 66299	21.0256	21.21164 66
8	24.35247 15308	24.98	24.35309
9	27.49347 91320	27.60	27.515
10	30.63460 64684	-	30.74

TABLE II

The energies $E_{n,l}$ of the lowest states in charmonium calculated using Calogero's method for the potential $V(r) = -a/r + br$, $a = 0.49$, $b = 0.17 \text{ GeV}^2$, $m_c = 1.35 \text{ GeV}$ (⁹).

N	$E_{n,0}$ (GeV)		$E_{n,1}$ (GeV)	
	"Exact"(⁹)	$20 \times 20, r_{\max} = 9 \text{ GeV}^{-1}$	"Exact"(⁹)	$20 \times 20, r_{\max} = 12 \text{ GeV}^{-1}$
1	0.3643	0.3643	0.7720	0.7720
2	0.9505	0.9505	1.2292	1.2292
3	1.3862	1.3862	1.6155	1.6155
4	1.7592	1.7594	1.9605	1.9606
5	2.0948	2.1035	2.2773	2.2797