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Note

Analytic Inversion of Nine-Point Poisson Operator

The analytic inversion of finite-difference Poisson operators has been extended from the five-point operator [1] to the nine-point operator, taken in the form [2]

$$\begin{pmatrix} 1 & 4 & 1 \\ 4 & -20 & 4 \\ 1 & 4 & 1 \end{pmatrix} \left(\Phi - \frac{h^2}{12} \nabla^2 \Phi \right) \approx 6h^2 \nabla^2 \Phi.$$

The potentials due to a solitary negative gaussian unit charge at the origin (top left corner) are

1.0472	3.6276	5.0208	5.8355
	(−.0117)	(−.0048)	(−.0011)
	4.3392	5.2502	5.9419
	(+.0067)	(+.0014)	(−.0000)
		5.7195	6.2046
		(+.0007)	(+.0003)
			6.5299
			(+.0002)

The bracketed numbers indicate by how much these potentials exceed the ideal, $\Phi = \ln(\text{distance}^2) + \text{constant}$, and they are about one order of magnitude smaller than for the five-point operator. The "constant" differs from that for the five-point operator by $\ln(3/2)$; see below.

The potential zero is chosen so that at the origin, one has only the contribution $4\pi/12$ associated with the $(h^2/12)\,\nabla^2$ term. Elsewhere, for row and column indices n, m and with $\xi = \exp(i\pi/6)$,

$$\Phi_n^{(m)} = 4\mathrm{Re} \int_0^1 \left(1 - \left[\frac{(\tau - \xi^2)(\tau + \xi^{*2})}{(\tau + \xi^2)(\tau - \xi^{*2})} \right]^n \left[\frac{(\tau - \xi)(\tau - \xi^*)}{(\tau + \xi)(\tau + \xi^*)} \right]^m \right) \frac{d\tau}{2\tau},$$

to be deduced by making a few changes in the analysis presented in Ref. [1]. (Specifically, the expression for $K + 1/K$ becomes $(10 - 4\cos 2\pi k/N)/(2 + \cos 2\pi k/N)$, a multiplier $(4 + K + 1/K)/6$ accompanies the recurring quantity $1/(K - 1/K)$, the square root $\sqrt{2t^2 + 1}$ is replaced by $\sqrt{(4t^2/3) + 1}$, $\sqrt{2}$ becomes $\sqrt{3}$ in the formulas connecting t with τ, $\sqrt{i}$ becomes $e^{i\pi/3}$ in the expression for $e^{i\theta}$ but it becomes $e^{i\pi/6}$ in the last formula for K.) Symmetry in n, m is nontrivial.

Evaluation of the integral gives $\Phi_0^{(1)} = 2\pi/\sqrt{3}$, and further along the top line one can use the definitions

$$E_0 = \Phi_0^{(1)}, \qquad E_1 = \Phi_0^{(2)} - \Phi_0^{(1)}, \qquad E_m = \Phi_0^{(m+1)} - \Phi_0^{(m)} \cdots$$

which obey the recurrence relation

$$(m+1)(E_{m+1} - 7E_m) = m(7E_m - E_{m-1}) - 24,$$

to be deduced by differentiating the function

$$24(\tau^2 - \tau\sqrt{3} + 1)^m (1 - \tau^2)/(\tau^2 + \tau\sqrt{3} + 1)^{m+1}.$$

(Hence $\Phi_0^{(2)} = 16\pi/\sqrt{3} - 24$, $\Phi_0^{(3)} = 162\pi/\sqrt{3} - 288$, etc.) An asymptotic solution is $E_m = [2/(m + 1/2)] + o(m^{-3})$ for the gradients between grid points.

Having created the top line, one applies the nine-point operator first at the origin to deduce. $\Phi_1^{(1)} = 6\pi - 8\pi/\sqrt{3}$ and then elsewhere along the top line to get the values on the first line below. Using symmetry about the diagonal and using the nine-point operator everywhere else to the right of the diagonal, one can then fill in the rest of the table. The value of the constant along with the logarithm was found empirically to be $2\gamma + \ln 12$ (γ = Euler's constant) as against $2\gamma + \ln 8$ for the five-point operator. The form of the constant, $2\gamma + \ln$ (integer), was guessed. The integer 12 fitted so well as to leave no doubt about its correctness. However, a general proof could not be found. Nor was it possible to prove without exception that the multipliers of $2\pi/\sqrt{3}$ in the analytic expressions for the potentials must always be integers: the multipliers of π obviously are, and the remaining contributions to the analytic expressions for $\Phi_n^{(m)}$ are rational.

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References

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