Title
FEJER MEANS IN FOURIER SYNTHESIS. A NOTE

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Fejér means in Fourier synthesis. A note.

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The partial sums of the Fourier series for a non-constant, non-negative function may assume negative values. However, the Fejér means of that function are everywhere positive, and this provides an additional test for acceptability of the Fourier synthesis of an electron density function.

Consider the function ρ,

$$\rho(x,y,z) = \sum_k \sum_\ell \sum_m F_{k,\ell,m} \exp\left[i(kx + \ell y + mz)\right] .$$

Taking ρ to be of period 2π in each variable is no restriction of generality. The partial sums of ρ are

$$S_{K,L,M}(x,y,z) = \sum_{k=-K}^{K} \sum_{\ell=-L}^{L} \sum_{m=-M}^{M} F_{k,\ell,m} \exp\left[i(kx + \ell y + mz)\right] ,$$

and the Fejér means of ρ are

$$\sigma_{K,L,M}(x,y,z) = (K+1)^{-1}(L+1)^{-1}(M+1)^{-1} \sum_{k=0}^{K} \sum_{\ell=0}^{L} \sum_{m=0}^{M} S_{k,\ell,m}(x,y,z).$$

The function ρ is everywhere non-negative if and only if the Fejér mean $\sigma_{k,\ell,m}$ is everywhere positive for each k, ℓ, and m (Zygmund 1959, p. 314). This is equivalent to the Karle and Hauptman (1950) formulation in terms of positive definite forms. Thus when ρ is a synthesized electron density function a negative value for some Fejér mean implies that the value of some Fourier coefficient appearing in that mean is incorrect. Note that if ρ is to be calculated by evaluating partial sum of its Fourier series then evaluation of the Fejér means is easy.

Since for continuous ρ the Fejér means converge to ρ (Zygmund 1959, p. 304), although generally slower than converging partial sums, approximation to the electron density function by positive functions is feasible. Finally, the maximum of each Fejér mean is a lower bound for the maximum of ρ (Zygmund 1959, p. 303).

References

Karle, J. and H. Hauptman (1950). Acta Cryst. 3, 181.

Zygmund, A. (1959). Trigonometric Series, Vol. II. Cambridge, University Press.

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