2D Fourier series

2D function with periodicity vectors $\vec{a}_1$ and $\vec{a}_2$:

$$f(\vec{r}) = \sum_{-K\le k\le K} \sum_{-L\le l\le L} F_{k,l} \exp\left[\mathrm{i}2\pi \left(k\vec{b}_1 + l\vec{b}_2\right)\vec{r}\right], \tag{1}$$

with reciprocal vectors $\vec{b}_j$ defined by $\vec{a}_i\vec{b}_j = \delta_{ij}$.

For a real function, this can be rewritten

$$\begin{aligned} f(\vec{r}) = \sum_{k=0}^{K}\sum_{l=0}^{L} & A_{k,l}\cos\left(2\pi k\vec{b}_1\vec{r}\right)\cos\left(2\pi l\vec{b}_2\vec{r}\right) \\ & + B_{k,l}\cos\left(2\pi k\vec{b}_1\vec{r}\right)\sin\left(2\pi l\vec{b}_2\vec{r}\right) \\ & + C_{k,l}\sin\left(2\pi k\vec{b}_1\vec{r}\right)\cos\left(2\pi l\vec{b}_2\vec{r}\right) \\ & + D_{k,l}\sin\left(2\pi k\vec{b}_1\vec{r}\right)\sin\left(2\pi l\vec{b}_2\vec{r}\right), \end{aligned} \tag{2}$$

where the real coefficients are given by

$$\begin{aligned} A_{k,l} &= \frac{(2-\delta_{k0})(2-\delta_{l0})}{4}\left(F_{k,l} + F_{-k,l} + F_{k,-l} + F_{-k,-l}\right), \\ B_{k,l} &= \mathrm{i}\frac{(2-\delta_{k0})(2-\delta_{l0})}{4}\left(F_{k,l} + F_{-k,l} - F_{k,-l} - F_{-k,-l}\right), \\ C_{k,l} &= \mathrm{i}\frac{(2-\delta_{k0})(2-\delta_{l0})}{4}\left(F_{k,l} + F_{-k,l} + F_{k,-l} + F_{-k,-l}\right), \\ D_{k,l} &= \frac{(2-\delta_{k0})(2-\delta_{l0})}{4}\left(-F_{k,l} + F_{-k,l} + F_{k,-l} - F_{-k,-l}\right). \end{aligned}$$

Fitting

Without symmetry

We fit the coefficient $F_{k,l}$ of the Fourier series to the dataset $f(\vec{r}_i) = f_i$. The least square fitting corresponds to the minimization of the cost function

$$C(F_{k,l}) = \sum_i \left|f(\vec{r}_i) - f_i\right|^2.$$

The minimization leads to the linear equations

$$\sum_{m,n} A_{kl,mn} F_{m,n} = B_{kl}, \tag{3}$$

where the matrix A and the vector B are defined by

$$\begin{aligned} A_{kl,mn} &= \sum_i e_{kl}^{i*} e_{mn}^{i} \\ B_{kl} &= \sum_i e_{kl}^{i*} f^{i}, \end{aligned}$$

with

$$e_{kl}^{i} = \exp\left[\mathrm{i}2\pi\left(k\vec{b}_1 + l\vec{b}_2\right)\vec{r}_i\right].$$

With symmetry operations

The function f obeys the set of symmetry operations $(R_s, \vec{u}_s)$:

$$f(R_s\vec{r} + \vec{u_s}) = f(\vec{r}), \qquad \forall\vec{r}.$$

To fit its coefficients, we consider the symmetrized function

$$\tilde{f}(\vec{r}) = \sum_{-\tilde{K}\leq k\leq\tilde{K}} \sum_{-\tilde{L}\leq l\leq\tilde{L}} \tilde{F}_{k,l} \frac{1}{S} \sum_s \exp\left[\mathrm{i}2\pi \left(k\vec{b}_1 + l\vec{b}_2\right) (R_s\vec{r} + \vec{u}_s)\right], \tag{4}$$

with S the total number of symmetry operations. The least-square fitting leads to the same linear equations as system (3), with the matrix A and the vector B now defined from the quantity

$$e^i_{kl} = \frac{1}{S} \sum_s \exp\left[\mathrm{i}2\pi \left(k\vec{b}_1 + l\vec{b}_2\right) (R_s\vec{r_i} + \vec{u}_s)\right].$$

The symmetrized Fourier series (4) can be written back in a regular series like (1) using the relation

$$\tilde{F}_{k,l} \frac{1}{S} \exp\left[\mathrm{i}2\pi \left(k\vec{b}_1 + l\vec{b}_2\right) (R_s\vec{r} + \vec{u}_s)\right] = F_{m,n} \exp\left[\mathrm{i}2\pi \left(m\vec{b}_1 + n\vec{b}_2\right) \vec{r}\right],$$

where

$$\begin{aligned} m =& \left(k\vec{b}_1 + l\vec{b}_2\right) R_s\vec{a}_1, \\ n =& \left(k\vec{b}_1 + l\vec{b}_2\right) R_s\vec{a}_2, \\ F_{m,n} =& \tilde{F}_{k,l} \frac{1}{S} \exp\left[\mathrm{i}2\pi \left(k\vec{b}_1 + l\vec{b}_2\right) \vec{u}_s\right]. \end{aligned}$$