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RIEMANN ZEROS AND THE INVERSE PHASE PROBLEM

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Abstract

Finding a universal method of crystal structure solution and proving the Riemann hypothesis are two outstanding challenges in apparently unrelated fields. For centrosymmetric crystals however, a connection arises as the result of a statistical approach to the inverse phase problem. It is shown that parameters of the phase distribution are related to the non-trivial Riemann zeros by a Mellin transform.

Keywords

Riemann zeta function; Riemann hypothesis; crystallography; X-ray diffraction; structure factor; maximum likelihood; Mellin transform

1. Introduction

The celebrated Riemann hypothesis¹ is arguably the biggest unsolved problem in mathematics.^{2–4} The hypothesis states that all *non-trivial* zeros of the Riemann zeta function $\zeta(s)$, given for $\text{Re}(s) > 1$ by

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \frac{1}{1^s} + \frac{1}{2^s} + \frac{1}{3^s} + \cdots, \quad (1)$$

have real and equal part $\frac{1}{2}$. Here it is understood that the non-trivial zeros are distinct from the *trivial* zeros of $\zeta(s)$, which are the negative even integers ($s = -2, -4, \dots$). The validity of the Riemann hypothesis has considerable physical and mathematical implications, perhaps the most notable being Riemann's own conjecture that the fluctuations of prime numbers can be described by the complex zeros of his function.⁵

Of great importance to the X-ray crystallography community is the so-called phase problem. The phase problem has to be solved in order to determine a crystal's atomic structure from X-ray diffraction data, and arises because the intensities of the diffracted beam are proportional only to the squared moduli of the complex Fourier coefficients (structure factors) needed to reconstruct the electron density function. The challenge is then to derive the unknown phases from measured magnitudes, and for crystal structures of large molecules this requires exploiting some prior knowledge of the crystal structure,^{6,7} or by using an appropriate experimental technique (reviewed in Ref. 8). It turns out that likelihood-based algorithms return the most reliable estimate of structure factors.^{9–11}

For crystals containing an inversion centre (centrosymmetric crystals), the problem reduces to determining only the sign of each structure factor since the Fourier coefficients are real quantities. Direct methods¹² can yield a solution to the phase problem, and centrosymmetric crystals containing racemic mixtures of chiral macromolecules like proteins have been grown to this end.^{13–15} In principle however, experimental observation of phases from

centrosymmetric crystals may one day become possible to exploit resonant inelastic X-ray scattering,^{16,17} or by using magnetic reference layers as in neutron scattering.¹⁸ Structure solution based on observed phases is commonly referred to as the inverse phase problem.

Here, a likelihood function for parameters of a centrosymmetric crystal structure given a set of observed phases is derived. It is demonstrated that the best parameter estimates are related to the non-trivial zeros of the Riemann zeta function by the Mellin transform.

2. The Likelihood Function

From Read (1990),¹⁹ the conditional probability of a structure factor $\mathbf{F}$ given the value calculated from the atomic model of the crystal $\mathbf{F}_{wc}$ is

$$p(\mathbf{F}; \mathbf{F}_{wc}) = \frac{1}{\sqrt{2\pi\varepsilon\sigma_{\Delta}^2}} \exp\left(-\frac{|\mathbf{F} - \mathbf{F}_{wc}|^2}{2\varepsilon\sigma_{\Delta}^2}\right). \quad (2)$$

The conditional distribution for the true phase of $\mathbf{F}$ can be obtained by changing variables, fixing $|\mathbf{F}|$ and renormalising to yield

$$p(\varphi; |\mathbf{F}|, |\mathbf{F}_{wc}|) = \frac{1}{2} \exp\left(\frac{|\mathbf{F}||\mathbf{F}_{wc}|\cos\varphi}{\varepsilon\sigma_{\Delta}^2}\right) \operatorname{sech}\left(\frac{|\mathbf{F}||\mathbf{F}_{wc}|}{\varepsilon\sigma_{\Delta}^2}\right). \quad (3)$$

If φ^o denotes the observed phase, the distribution $p(\varphi^o; |\mathbf{F}|, |\mathbf{F}_{wc}|)$ is related to $p(\varphi; |\mathbf{F}|, |\mathbf{F}_{wc}|)$ by a simple substitution

$$p(\varphi^o; |\mathbf{F}|, |\mathbf{F}_{wc}|) = \frac{1}{2} \exp\left(\frac{|\mathbf{F}||\mathbf{F}_{wc}|\cos\varphi^o}{\varepsilon\sigma_{\Delta}^2}\right) \operatorname{sech}\left(\frac{|\mathbf{F}||\mathbf{F}_{wc}|}{\varepsilon\sigma_{\Delta}^2}\right). \quad (4)$$

It is important to note that the phase of each structure factor for a centrosymmetric crystal may only take the values $\varphi = 0$ or $\varphi = \pi$.

The product of $p(\varphi^o; |\mathbf{F}|, |\mathbf{F}_{wc}|)$ over all structure factors with indices $\mathbf{h}$ is then interpreted as the likelihood function

$$\mathcal{L}(\varphi^o; |\mathbf{F}_{wc}|, \sigma_{\Delta}^2) = \prod_{\mathbf{h}} p(\varphi^o; |\mathbf{F}|, |\mathbf{F}_{wc}|), \quad (5)$$

but as usual it is more convenient to work with the log-likelihood

$$LLK = \log \mathcal{L}(\varphi^o; |\mathbf{F}_{wc}|, \sigma_{\Delta}^2). \quad (6)$$

The partial derivatives of LLK taken with respect to the parameters $|\mathbf{F}_{wc}|$ and σ_{Δ}^2 are given by

$$\frac{\partial LLK}{\partial |\mathbf{F}_{wc}|} = \sum_{\mathbf{h}} \frac{|\mathbf{F}|}{\varepsilon\sigma_{\Delta}^2} \left[\cos\varphi^o - \tanh\left(\frac{|\mathbf{F}||\mathbf{F}_{wc}|}{\varepsilon\sigma_{\Delta}^2}\right) \right], \quad (7)$$

and

$$\frac{\partial LLL}{\partial \sigma_{\Delta}^2} = - \sum_h \frac{|\mathbf{F}||\mathbf{F}_{wc}|}{\varepsilon(\sigma_{\Delta}^2)^2} \left[\cos \varphi^o - \tanh \left(\frac{|\mathbf{F}||\mathbf{F}_{wc}|}{\varepsilon \sigma_{\Delta}^2} \right) \right]. \quad (8)$$

The goal of the crystallographer is to find the zeros of the functions (7) and (8), and choose $|\mathbf{F}_{wc}|$ and σ_{Δ}^2 from these such that the extremum is a maximum.

3. Appearance of the Riemann Zeros

For a continuous function $f: \mathbb{R}^+ \rightarrow \mathbb{R}$, the Mellin transform $\hat{f}$ of f is defined to be

$$\hat{f}(s) = \int_0^{\infty} x^{s-1} f(x) dx. \quad (9)$$

This integral transform exists in some complex strip $\{s: a < \text{Re}(s) < b\}$ that contains the imaginary axis.

Since φ^o can only equal zero or π , the expression contained within square brackets in both (7) and (8) has the identity

$$\cos \varphi^o - \tanh \left(\frac{|\mathbf{F}||\mathbf{F}_{wc}|}{\varepsilon \sigma_{\Delta}^2} \right) = \cos \varphi^o \left[1 - \tanh \left(\frac{|\mathbf{F}||\mathbf{F}_{wc}| \cos \varphi^o}{\varepsilon \sigma_{\Delta}^2} \right) \right]. \quad (10)$$

Making use of this property, each term in Eqs. (7) and (8) becomes of the form

$$f_{a,p,v}(x) = apx^v [1 - \tanh(ax^p)], \quad (11)$$

where the variable x and quantities a, p, v are to be chosen appropriately when one is transforming (7) or (8) with respect to $|\mathbf{F}_{wc}|$ or σ_{Δ}^2 . From Eq. (6.4) in Ref. 20, the Mellin transform of $\varphi(x) = ap[1 - \tanh(ax)]$ is given by

$$\hat{\phi}(z) = \frac{p \Gamma(z) (1 - 2^{1-z})}{(2a)^{z-1}} \zeta(z), \quad \text{Re}(z) > 0. \quad (12)$$

Using the general formula that the Mellin transform of any function $f(x) = x^v \varphi(x^p)$ is

$$\hat{f}(z) = \frac{1}{p} \hat{\phi} \left(\frac{z+v}{p} \right), \quad p > 0, \quad (13)$$

or

$$\hat{f}(z) = -\frac{1}{p} \hat{\phi} \left(\frac{z+v}{p} \right), \quad p < 0, \quad (14)$$

it can be confirmed that the Mellin transform of Eq. (11) is

$$\hat{f}_{a,k}(s) = (-1)^k \frac{\Gamma(s) (1 - 2^{1-s})}{(2a)^{s-1}} \zeta(s), \quad (15)$$

where

$$s = \frac{z+v}{p}. \quad (16)$$

For the relevant values of v and p , the condition $\text{Re}(z) > 0$ includes $\text{Re}(s) = \frac{1}{2}$.

From above, the Mellin transforms of Eqs. (7) and (8) are given by

$$\mathcal{M}(s) = (-1)^k \sum_{\mathbf{h}} \frac{\Gamma(s) (1 - 2^{1-s})}{(2a)^{s-1}} \zeta(s), \quad (17)$$

where $a = |\mathbf{F}| \cos \varphi^o / \varepsilon \sigma_{\Delta}^2$, $k = 0$ for Eq. (7) and $a = |\mathbf{F}| |\mathbf{F}_{wc}| \cos \varphi^o$, $k = 1$ for Eq. (8). It follows that this function can be minimized by selecting each $s_{\mathbf{h}}$ from the non-trivial Riemann zeros, or from the set $s_n = 1 + 2n / \log 2$ ($n = \pm 1, \pm 2, \dots$) when the Riemann zeta function is analytic and finite there.

It is possible to exploit a functional property of the Mellin transform when searching for a single value of s that minimises the entire function (e.g. corresponding to a single value of σ_{Δ}^2). For any function $f(x)$ and finite $\mathbf{h}$ such that

$$f(x) = \sum_{\mathbf{h}} \lambda_{\mathbf{h}} g(\mu_{\mathbf{h}} x), \quad (18)$$

it is a simple matter to confirm the Mellin transform of $f(x)$ is

$$\hat{f}(s) = \hat{g}(s) \sum_{\mathbf{h}} \lambda_{\mathbf{h}} \mu_{\mathbf{h}}^{-s}, \quad (19)$$

where $\hat{g}(s)$ is the Mellin transform of $g(x)$. By taking $\mu_{\mathbf{h}} = 1/a$, $\mathbf{h}$ and

$$g(x) = g(\sigma_{\Delta}^2) = \frac{1}{(\sigma_{\Delta}^2)^2} \left[1 - \tanh \left(\frac{1}{\sigma_{\Delta}^2} \right) \right], \quad (20)$$

the Mellin transform of (8) is

$$\mathcal{M}(s) = - \frac{\Gamma(s) (1 - 2^{1-s})}{2^{s-1}} \zeta(s) \sum_{\mathbf{h}} \left(\frac{|\mathbf{F}|^2 \cos \varphi^o}{\varepsilon} \right)^{s-1}. \quad (21)$$

It follows that (21) vanishes if one is to take s equal to any non-trivial Riemann zero.

4. Concluding Remarks

The log-likelihood for the inverse phase problem can be maximized in Mellin space by the non-trivial zeros of the Riemann zeta function. The Riemann hypothesis implies these lie on

the critical strip $\frac{1}{2} + it$. Until development of a method to directly measure phase information this observation is of purely theoretical interest, but may be envisaged to one day have a practical application to crystal structure solution.

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