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On the Spectral Gap of a Square Distance Matrix

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Abstract We consider a square distance matrix which arises from a preconditioned Jacobian matrix for the numerical computation of the Cahn–Hilliard problem. We prove strict negativity of all but one associated eigenvalues. This solves a conjecture in Christieb et al. (J Comput Phys 257:193–215, 2014).

Keywords Distance matrix · Eigenvalue · Solvability

1 Introduction

In [2], Christlieb et al. developed a novel computational framework for phase field models from energy gradient flows. For the Cahn–Hilliard model, a key step in the asymptotic results obtained therein is concerned with the solvability of a preconditioned Jacobian matrix. More specifically, the authors formulated the following conjecture (see [2, p. 204]):

Conjecture 1 *If* $\{x_i\}$, $i = 1, 2, \ldots, M$ *are distinct points in [0,1) and the entries* b_{ij} *of the* $M \times M$ *matrix B are given by*

$$b_{ij} = d_{ij} - d_{ij}^2,$$

Dedicated to Ya.G. Sinai on occasion of his 80th birthday.

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where d_{ij} are the distances between points x_i and x_j, taken either as absolute value or the periodic interval, then the matrix PBP has $M-1$ strictly negative eigenvalues. Here P is the projection onto the subspace orthogonal to constant vectors.

Note that $B^T = B$, $P^T = P$ and hence PBP are symmetric matrices. The purpose of this note is to prove Conjecture 1. For more background on the numerical analysis of phase field type models, we refer to the introduction of [2]. For more recent developments in this area, see [4,5] and the references therein. See also [1] for additional implications of Conjecture 1 for many particle systems interacting with inter-particle energies given by b_{ij}. One should note that in the zero-temperature statistical physics of n-rigid particles, a closely related issue is whether or not a three body (i.e. the third virial expansion) term is require to described an ordered state, or whether two body terms are sufficient. For instance take particle coordinates x_j and θ_j for $1 \leq j \leq n$, the probability density for a dilute gas can be expanded out with a virial expansion in the spirit of Onsager:

$$P(x_1, \theta_1, x_2, \theta_2, \ldots, x_n, \theta_n) = \text{Const} \cdot \sum_{i \neq j} H(x_i, \theta_i, x_j, \theta_j)$$

where $H = 1$ if the particles i, j overlap and 0 if they do not. Looking at the marginal distribution obtained by integrating over the spatial coordinates x_i, x_j etc. one has

$$P(\theta_1, \theta_2, \ldots, \theta_n) \propto \sum_{i,j} W(\theta_i - \theta_j),$$

where W = excluded volume. These angles $0 \leq \theta_j < 2\pi$, which means the periodic case is practically very important and not just a theoretical artifact on numerical solvers that require a finite domain. Maximizing the probability, in the large N limit will likely have a trivial solution where the theta's are uniformly distributed on the circle. If the generalized distance matrix obtained by W satisfies the spectral gap condition in the paper then it is likely that three body terms are required. One of the first models for rigid rods where the generalized distance function would be periodic can be found in [6] (Onsager used $W(\theta) \propto |\sin(\theta)|$).

2 Main Theorem

To prove Conjecture 1, we first prove the following main theorem.

Theorem 2.1 *Let $M \geq 2$ and $\{x_i\}_{i=1}^M$ be distinct points in [0,1). Suppose f: $\mathbb{R} \to \mathbb{R}$ is a 1-periodic, symmetric function $f(-x) = f(x)$, with $Fourier$ expansion*

$$f(z) = \sum_{k \in \mathbb{Z}} f_k e^{2\pi k i z}$$

such that $\sum_{k \in \mathbb{Z}} |f_k| < \infty$ and

$$f_k < 0, \qquad \forall\, 0 \neq k \in \mathbb{Z}.$$

Then for any $\xi = (\xi_1, \xi_2, \ldots, \xi_M) \in \mathbb{R}^M$ with $\sum_{i=1}^M \xi_i = 0$ and $\xi \neq (0, 0, \ldots, 0)$, we have

$$\xi^T B \xi \leq -\alpha_B |\xi|^2 < 0,$$

where the matrix B is given by $B_{ij} = f(x_i - x_j)$ and $\alpha_B > 0$ is a constant depending on $(M, \{x_i\}_{i=1}^M, \{f_k\}_{k=1}^{M-1})$.

Remark 2.2 It follows easily that the matrix PBP has eigenvalue 0 with eigenvector $(1, \dots, 1)$, and other $M-1$ eigenvalues are strictly negative.

Remark 2.3 There exists a plethora of 1-periodic functions whose Fourier coefficients (for $k \neq 0$) are explicitly given and have definite sign. For example, the nth Bernoulli polynomial has the expansion

$$B_n(z) = -\frac{n!}{(2\pi i)^n} \sum_{k\neq 0} \frac{e^{2\pi k i z}}{k^n}.$$

In particular for $n = 2, 4$ and $z \in [0, 1]$:

$$B_2(z) = z^2 - z + \frac{1}{6},$$
$$B_4(z) = z^4 - 2z^3 + z^2 - \frac{1}{30}.$$

The Bernoulli polynomials play an important role in the discrepancy theory of integration lattices for quasi Monte Carlo methods (cf. [3] and the references therein). It is a remarkable fact that the function $f(z) = z - z^2$ (which is essentially the same as $-B_2(z)$ since the constant $\frac{1}{6}$ does not matter in view of mean-zero conditions) also show up in the square distance matrix in Conjecture 1.

Proof of Theorem 2.1. For any non-zero vector $\xi = (\xi_1, \xi_2, \dots, \xi_M)$ with $\sum_{i=1}^M \xi_i = 0$, we compute

$$\begin{aligned}
\xi^T B\xi &= \sum_{i,j=1}^M \xi_i\xi_j f(x_i - x_j) \\
&= \sum_{i,j=1}^M \sum_{k\in\mathbb{Z}} f_k \xi_i \xi_j e^{2\pi i k(x_i - x_j)} \\
&= \sum_{k\in\mathbb{Z}} f_k \left| \sum_{i=1}^M \xi_i e^{2\pi i k x_i} \right|^2.
\end{aligned}$$

Denote $\omega_i = e^{2\pi i x_i}$ and note that[1] $\omega_i \neq \omega_j$ if $i \neq j$. Consider the matrix equation:

$$\begin{pmatrix} 1 & \dots & 1 \\ \omega_1 & \dots & \omega_M \\ \vdots & \vdots & \vdots \\ \omega_1^{M-1} & \dots & \omega_M^{M-1} \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \xi_M \end{pmatrix} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_M \end{pmatrix}.$$

Note that the coefficient matrix $\Omega = (\omega_j^{i-1})_{1\leq i,j\leq M}$ is the usual Vandermonde matrix which is nonsingular thanks to the fact that $(\omega_i)_{1\leq i\leq M}$ are distinct (Recall $\det(\Omega) = \prod_{1\leq i<j\leq M}(\omega_j - \omega_i)$). It then follows that

$$\sum_{1\leq k\leq M-1} (-f_k) \left| \sum_{j=1}^M \xi_j e^{2\pi i k x_j} \right|^2 \geq c_1 \cdot \min_{1\leq k\leq M-1} (-f_k) \cdot \sum_{j=1}^M \xi_j^2,$$

[1] Here we used the fact that $x_i \in [0, 1)$. In particular we do not allow the situation $x_{i_0} = 0, x_{j_0} = 1$ for some i_0, j_0.

where $c_1 > 0$ is a constant depending only on (M, $\{x_i\}_{i=1}^M$). Note that for $k = 0$, $\sum_{i=1}^M \xi_i = 0$ by assumption and the value of f_0 does not affect the sum $\xi^T B\xi$. The desired conclusion then follows. □

In practice it is often desirable to have a criterion on the negative-definiteness of the function f without explicitly computing Fourier coefficients. The following "Pólya"-type proposition gives a sufficient condition which can already yield a proof of Conjecture 1. The proof of Conjecture 1 in Sect. 3 is based on an explicit computation.

Proposition 2.4 *Suppose* $f : \mathbb{R} \to \mathbb{R}$ *is* 1*-periodic, even and continuous. If* f *is concave on the interval* [0, 1]*, then*

$$f_k \le 0, \quad \forall\, 0 \ne k \in \mathbb{Z},$$

where f_k *is the kth Fourier coefficient. If furthermore* $f \in C^2([0,1])$ *and for some* $\alpha > 0$*,*

$$\min_{0\le x\le 1} f''(x) \le -\alpha < 0, \tag{2.1}$$

then there are constants $c_1, c_2 > 0$*, such that*

$$\frac{c_2}{k^2} \le -f_k \le \frac{c_1}{k^2}, \qquad \forall\, 0 \ne k \in \mathbb{Z}. \tag{2.2}$$

Remark 2.5 For Conjecture 1, note that $f(x) = x - x^2$ for $0 \le x \le 1$ which clearly satisfies $-f'' = 2$. Many more explicit examples can be easily constructed without appealing to the representation of Fourier series. It should also be clear from (2.2) that concavity is only a sufficient (but not necessary) condition for non-positivity. One explicit counterexample is the Bernoulli polynomial $B_4(z)$ mentioned before.

Proof of Proposition 2.4. Easy to check that $f_k = f_{-k}$. Since for $k \ge 1$,

$$f_k = \int_0^1 f(x)\cos(2\pi kx)dx = \sum_{j=0}^{k-1}\int_{\frac{j}{k}}^{\frac{j+1}{k}} f(x)\cos(2\pi kx)dx$$
$$= \sum_{j=0}^{k-1}\frac{1}{k}\int_0^1 f\left(\frac{y+j}{k}\right)\cos(2\pi y)dy,$$

it suffices to prove the case $k = 1$. Observe

$$\int_0^1 f(x)\cos(2\pi x)dx$$
$$= \int_0^{\frac{1}{4}}\left(f(x) + f(1-x) - f\left(\frac{1}{2}-x\right) - f\left(\frac{1}{2}+x\right)\right)\cos(2\pi x)dx.$$

To prove non-positivity, it then suffices to show for any $0 < x_0 < \frac{1}{4}$,

$$f(x_0) + f(1-x_0) - f\left(\frac{1}{2}-x_0\right) - f\left(\frac{1}{2}+x_0\right) \le 0.$$

Assume first $f \in C^2((0,1))$. Then by concavity $f'' \le 0$ on (0, 1). Easy to check that

$$f(1-x_0) - f\left(\frac{1}{2}-x_0\right) - \left(f\left(\frac{1}{2}+x_0\right) - f(x_0)\right)$$
$$= \int_0^{\frac{1}{2}}\left(f'\left(\frac{1}{2}-x_0+\theta\right) - f'(x_0+\theta)\right)d\theta \le 0.$$

In the general case (without C^2 assumption), note that for fixed x_0, we can suitably mollify the function f to have a sequence $f_\epsilon \to f$ with $f_\epsilon'' \le 0$ on $(\frac{x_0}{2}, 1 - \frac{x_0}{2})$. The argument is obvious.

We now turn to (2.2). The upper bound follows from integration by parts. For the lower bound, by using (2.1) and the preceding computation (applied to the function $f(\frac{y+j}{k})$), we have for $k \ge 1$,

$$
\begin{aligned}
-f_k &\ge \sum_{j=0}^{k-1} \frac{1}{k} \int_0^{\frac{1}{4}} \frac{\alpha}{k^2} \cdot \left(\frac{1}{2} - 2x_0\right) \cdot \frac{1}{2} \cos(2\pi x_0) dx_0 \\
&\ge \frac{\text{const} \cdot \alpha}{k^2}.
\end{aligned}
$$

□

3 Proof of Conjecture 1

First observe that to prove Conjecture 1, we only need to consider the action of B on the subspace of vectors $\xi = (\xi_1, \ldots, \xi_M)$ with the property $\sum_{i=1}^M \xi_i = 0$. It suffices to prove that the matrix operator $-B$ is strictly positive definite in this subspace. As stated in the statement of Conjecture 1, we shall discuss two cases of the distance function.

Periodic Case: In this case we have $f(z) = |z| - z^2$ for $-\frac{1}{2} \le z \le \frac{1}{2}$. It is not difficult to compute for $0 \ne k \in \mathbb{Z}$,

$$
\begin{aligned}
f_k &= \int_{-\frac{1}{2}}^{\frac{1}{2}} \left(|z| - z^2\right) e^{2\pi i k z}\, dz \\
&= 2 \int_0^{\frac{1}{2}} \left(z - z^2\right) \cos(2\pi k z)\, dz \\
&= -\frac{1}{2\pi^2 k^2}.
\end{aligned}
$$

Thus by Theorem 2.1, we conclude that the matrix PBP has $M - 1$ strictly negative eigenvalues.

Absolute Value Case: In this case we recall

$$b_{ij} = d_{ij} - d_{ij}^2, \quad d_{ij} = |x_i - x_j|.$$

Since $x_i \ne x_j \in [0, 1)$, we have $|x_i - x_j| < 1$. We can then regard

$$f(z) = |z| - z^2, \ |z| < 1,$$

and view f as a 2-periodic function on $\mathbb{R}$ with the fundamental domain $[-1, 1]$. One can then write down a Fourier expansion :

$$f(z) = \sum_{k \in \mathbb{Z}} f_k e^{k\pi i z}, \ |z| < 1$$

and verify for $k \ne 0$,

$$f_k = -\frac{1}{\pi^2 k^2} \left(1 + (-1)^k\right).$$

Note that $f_k < 0$ for $0 \neq k \in 2\mathbb{Z}$. We then have

$$\xi^T B\xi = \sum_{k\in 2\mathbb{Z}} f_k \left|\sum_{i=1}^{M} \xi_i e^{ik\pi x_i}\right|^2$$
$$= \sum_{\tilde{k}\in \mathbb{Z}} f_{2\tilde{k}} \left|\sum_{i=1}^{M} \xi_i e^{i2\tilde{k}\pi x_i}\right|.$$

The rest of the argument is then similar to the periodic case before. We omit the details.

4 Characterization of f

The following theorem provides a converse to Theorem 2.1. It is deeply connected with the usual Bochner Theorem in probability theory. The novelty here is the semi-positivity on a subspace of co-dimension one.

Theorem 4.1 *Let $f : \mathbb{R} \to \mathbb{R}$ be 1-periodic, symmetric ($f(x) = f(-x)$) and continuous. Suppose for any $M \geq 2$, any distinct points $(x_j)_{j=1}^M \in [0, 1)$, and any $\xi = (\xi_1, \ldots, \xi_M) \in \mathbb{R}^M$ orthogonal to the constant vector, it holds that*

$$\sum_{i,j=1}^{M} f(x_i - x_j)\xi_i\xi_j \geq 0.$$

Then for any $0 \neq k \in \mathbb{Z}$, we have

$$f_k \geq 0,$$

where f_k is the kth Fourier coefficient of f.

Remark 4.2 The function f above plays the role of the usual characteristic function ϕ in standard Bochner type theorems. It should be noted that in "Bochner" case, one usually only assumes the continuity of $\phi = \phi(t)$ at $t = 0$, and deduce the continuity of ϕ on $\mathbb{R}$ from positivity definiteness. It is certainly possible to relax our continuity assumption on f in Theorem 4.1 along similar lines. However for the sake of simplicity we will not dwell on this subtle issue here.

Remark 4.3 A natural question worth further exploring is the characterization of f satisfying semi-positivity on subspaces of finite or even infinite co-dimension. This is connected with nonlinear optimization problems with constraints (cf. [1]). Yet another possibility is to investigate the spectrum of bilinear forms generated from "singular" two-body type interaction potentials such as Lennard–Jones.

Lemma 4.4 *Under the same assumptions on f as in Theorem 4.1, we have for any $0 \neq k \in \mathbb{Z}$,*

$$\int_0^1 \int_0^1 f(x-y)\cos(2\pi kx)\cos(2\pi ky)dxdy \geq 0,$$
$$\int_0^1 \int_0^1 f(x-y)\sin(2\pi kx)\sin(2\pi ky)dxdy \geq 0.$$

Proof of Lemma 4.4. For each integer $N > |k|$, note that

$$\sum_{l=0}^{N-1} e^{\frac{2\pi ikl}{N}} = 0.$$

One can then choose $x_l = \frac{l-1}{N}$, $\xi_l = \cos(2\pi kx_l)$ (resp. $\xi_l = \sin(2\pi kx_l)$), $l = 1, \ldots, N$ and send N to infinity to get the result. Note that the continuity of f is used in the last approximation step. □

Proof of Theorem 4.1. Easy to check that $f_k = f_{-k} \in \mathbb{R}$. By using periodicity of f, we write for $0 \neq k \in \mathbb{Z}$:

$$\begin{aligned}
f_k &= \int_0^1 f(x)\cos(2\pi kx)dx \\
&= \int_0^1 f(x-y)\cos(2\pi k(x-y))dx \\
&= \int_0^1\int_0^1 f(x-y)\cos(2\pi k(x-y))dxdy \\
&= \int_0^1\int_0^1 f(x-y)(\cos(2\pi kx)\cos(2\pi ky) + \sin(2\pi kx)\sin(2\pi ky))dxdy \geq 0,
\end{aligned}$$

where in the last step we used Lemma 4.4. □

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