On the coercivity condition in the learning of interacting particle systems

Zhongyang Li and Fei Lu

Abstract

In the learning of systems of interacting particles or agents, coercivity condition ensures identifiability of the interaction functions, providing the foundation of learning by nonparametric regression. The coercivity condition is equivalent to the strictly positive definiteness of an integral kernel arising in the learning. We show that for a class of interaction functions such that the system is ergodic, the integral kernel is strictly positive definite, and hence the coercivity condition holds true. *

Contents

1 Introduction

Consider the stochastic system of interacting particles

$$d\mathbf{X}^t = -\nabla J_\Phi(\mathbf{X}^t)dt + d\mathbf{B}^t, \tag{1.1}$$

gs

where $\mathbf{X}^t := (\mathbf{X}_1^t, \dots, \mathbf{X}_N^t) \in \mathbb{R}^{dN}$ represents the position of particle at time t, and $\mathbf{B}^t = (\mathbf{B}_1^t, \dots, \mathbf{B}_N^t)$ is a standard Brownian motion on $\mathbb{R}^{dN}$ representing the environmental noise. Here the energy potential $J_\Phi : \mathbb{R}^{dN} \to \mathbb{R}$ depends on the pairwise distances:

$$J_\Phi(\mathbf{X}) = \frac{1}{2N} \sum_{i,j=1}^{N} \Phi(|\mathbf{X}_i - \mathbf{X}_j|), \ \mathbf{X} \in \mathbb{R}^{dN},$$

*ZL: Department of Mathematics, University of Connecticut, Storrs, CT, USA 06269-1009, zhongyang.li@uconn.edu;
FL: Department of Mathematics, Johns Hopkins University, Baltimore, MD, USA, 21218; feilu@math.jhu.edu;

with $\Phi : [0, \infty) \to \mathbb{R}$. Without lost of generality, we set $\Phi(0) = 0$. It is often written in the form of

$$d\mathbf{X}_i^t = \frac{1}{N} \sum_{1 \leqslant j \leqslant N, j \neq i} \phi(|\mathbf{X}_j^t - \mathbf{X}_i^t|)(\mathbf{X}_j^t - \mathbf{X}_i^t)dt + d\mathbf{B}_i^t, \quad \text{for } i = 1, \ldots, N,$$

with $\phi(r) = \frac{\Phi'(r)}{r}$ referred as the *interaction kernel*. Examples of such systems range from particles system in physics and chemistry, granular media, to opinion dynamics in social science (see [9, 8, 7, 5] and the reference therein).

In applications of such systems, the first task is to learn the interaction kernel ϕ from trajectories of the particles. Since the values of the interaction function is under-determined from trajectory data, a fundamental issue is the identifiability of the interaction function, particularly when it has to be learned in a nonparametric fashion for generality. The following *coercivity condition* is found to be sufficient for the identifiability [4, 7, 5, 6]: for any finite dimensional hypothesis space $\mathcal{H} \subset L^2(\bar{\rho}_T)$, where $\bar{\rho}_T$ denotes the average probability density of the pairwise distance $|\mathbf{r}_{12}^t|$ with

$$\mathbf{r}_{ji}^t := \mathbf{X}_j^t - \mathbf{X}_i^t,$$

there is a constant $c_{\mathcal{H},T} > 0$ such that for all $h \in \mathcal{H}$,

$$\bar{I}_T(h) := \frac{1}{T} \int_0^T \mathbb{E}\left[h(|\mathbf{r}_{12}^t|) h(|\mathbf{r}_{13}^t|) \frac{\langle \mathbf{r}_{12}^t, \mathbf{r}_{13}^t \rangle}{|\mathbf{r}_{12}^t||\mathbf{r}_{13}^t|} \right] dt \geqslant c_{\mathcal{H},T} \|h\|_{L^2(\bar{\rho}_T)}^2. \tag{1.2}$$ eq:c_t1

We prove that the coercivity condition holds true for systems with any number of particles N and with potentials of the forms:

$$\Phi_0(r) = (a + r^\theta)^\gamma, \text{ with } a \geqslant 0, \, \theta \in (1, 2], \, \gamma \in (0, 1] \text{ such that } \gamma\theta > 1, \tag{1.3}$$ eq:Phi_0def

and when T is large. This completes an earlier result in [4], where the coercivity condition is proved either for $(\theta, \gamma) = (2, 1)$ or for systems with $N = 3$ particles, and only when the systems are stationary, by overcoming difficulties in marginalization of the high-dimensional probability density and in treating the non-equilibrium case through ergodicity.

The coercivity condition is intrinsically connected with strict positive definiteness of integral kernels, or equivalently, the positiveness of the associated integral operators. For example, the kernel associated with $\bar{I}_T(h)$ in (1.2) is

$$K_T(u, v) = \frac{\langle u, v \rangle}{|u||v|} \bar{p}_T(u, v)$$

with $\bar{p}_T(u, v) = \frac{1}{T} \int_0^T p_t(u, v)dt$, where $p_t(u, v)$ is the probability density of $(\mathbf{r}_{12}^t, \mathbf{r}_{13}^t)$, since

$$\bar{I}_T(h) = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} h(u)h(v) \frac{\langle u, v \rangle}{|u||v|} \bar{p}_T(u, v) du dv.$$

As a by product, we have identified a class of strictly positive definite integral kernels related to the interacting particle system, including $K_T(u, v)$ and $\bar{p}_T(u, v)$, as well as their counterparts for stationary densities.

Positive definite kernels play an increasingly prominent role in many applications, in particular in statistical learning with reproducing kernel Hilbert space [3]. Our results provides a new class of strictly positive definite integral kernels arising from interaction particles systems, which have potential use in sampling and kernel based-learning. Also, we introduced a technique for proving strict positive definiteness based on Müntz type theorems, and this technique may be used to establish strict positive definiteness of general integral kernels in learning problems.

The organization of the paper is as follows: in Section 2, we prove that the system of pairwise differences $(\mathbf{r}_{12}^t, \mathbf{r}_{13}^t, \ldots, \mathbf{r}_{1N}^t) \in \mathbb{R}^{d(N-1)}$ has a stationary density, and we prove in Section 3 that the system converges to the stationary density at a polynomial rate in time. In Section 4 we show that the coercivity condition holds true at the stationary density by showing that the related integral kernels are strictly positive definite. In Section 5 we show that the coercivity condition holds true for non-equilibrium systems, under additional restriction on the hypothesis space. We list in Section 6 the preliminary theory on positive definite kernels.

2 Existence of a stationary density

existStationary

Note that the center of the particles, $\mathbf{X}_c(t) =: \frac{1}{N}\sum_{i=1}^N \mathbf{X}_i^t$, satisfies

$$d\mathbf{X}_c = \frac{1}{N}\sum_{i=1}^N \mathbf{B}_i^t,$$

since $\frac{1}{N}\sum_{i=1}^N \nabla_{\mathbf{x}_i} J_\Phi(\mathbf{x}) = 0$, due to the symmetry of the interaction between the particles. Therefore, the system itself does not have a stationary distribution on $\mathbb{R}^{dN}$. However, as we show below, an equivalent system, the system for $(\mathbf{X}_1^t - \mathbf{X}_2^t, \mathbf{X}_1^t - \mathbf{X}_3^t, \ldots, \mathbf{X}_1^t - \mathbf{X}_N^t)$ (or a system of relative positions to any reference particle or to the center of the particles), is has a stationary density.

ationaryDensity

Theorem 2.1. *For $1 \leqslant i < j \leqslant N$ and the process $\mathbf{X}^t$ satisfying the system (1.1), denote*

$$\mathbf{r}_{ij}^t = \mathbf{X}_i^t - \mathbf{X}_j^t, \text{ and } r_{ij}^t = |\mathbf{r}_{ij}^t|.$$

Suppose that the function $H : \mathbb{R}^{d(N-1)} \to \mathbb{R}$

$$H(\mathbf{r}) = J_\Phi(X) = \frac{1}{N}\sum_{2\leqslant j\leqslant N} \Phi(|\mathbf{r}_{1j}|) + \frac{1}{N}\sum_{2\leqslant i<j\leqslant N} \Phi(|\mathbf{r}_{1i} - \mathbf{r}_{1j}|) \tag{2.1}$$

satisfies $\int_{\mathbb{R}^{d(N-1)}} e^{H(\mathbf{r})} d\mathbf{r} < \infty$. Then, the process $\mathbf{r}^t = (\mathbf{r}_{12}^t, \mathbf{r}_{13}^t, \ldots, \mathbf{r}_{1N}^t)^\top$ has a stationary density, and the process

$$\mathbf{Y}^t = S^{-1}\mathbf{r}^t \tag{2.2}$$

satisfies a gradient system:

$$d\mathbf{Y}^t = -\nabla_{Y^t} H(S\mathbf{Y}^t) + d\mathbf{W}^t, \tag{2.3}$$

where $\mathbf{W}^t$ *is a standard Brownian motion on* $\mathbb{R}^{(N-1)d}$*, the matrix* $S \in \mathbb{R}^{(N-1)d\times(N-1)d}$ *is an invertible matrix satisfying*

$$SS^T = A := \begin{pmatrix} 2I_d & I_d & \cdots & I_d \\ I_d & 2I_d & \cdots & I_d \\ \cdots & & & \\ I_d & I_d & \cdots & 2I_d \end{pmatrix}. \tag{2.4}$$

Remark 2.2. *The matrix* A *in* (2.4) *has an eigenvalue* $\lambda = N$ *with multiplicity* d *and an eigenvalue* $\lambda = 1$ *with multiplicity* $(N-2)d$*. Since* A *is symmetric positive definite, we can find an invertible matrix* S *satisfying* (2.4)*, for example,*

$$S = \begin{pmatrix} \sqrt{2}I_d & 0 & 0 & \dots & 0 & 0 \\ \frac{\sqrt{2}}{2}I_d & \frac{\sqrt{6}}{2}I_d & 0 & \dots & 0 & 0 \\ \frac{\sqrt{2}}{2}I_d & \frac{\sqrt{6}}{6}I_d & \frac{2\sqrt{3}}{3}I_d & \dots & 0 & 0 \\ \dots & & & & & \\ \sqrt{\frac{1}{2}}I_d & \sqrt{\frac{1}{2\cdot 3}}I_d & \sqrt{\frac{1}{3\cdot 4}}I_d & \dots & \sqrt{\frac{1}{(N-2)(N-1)}}I_d & \sqrt{\frac{N}{N-1}}I_d \end{pmatrix}. \tag{2.5}$$

Proposition 2.3. *Let* $\mathbf{X}^t \in \mathbb{R}^{dN}$ *be the solution of* (1.1)*. The invariant density for* $(\mathbf{X}_1^t - \mathbf{X}_2^t, \mathbf{X}_1^t - \mathbf{X}_3^t)$ *has the following form*

$$p_\infty(u,v) = \frac{1}{Z} f(u,v) e^{-\frac{2}{N}[\Phi(|u|)+\Phi(|v|)+\Phi(|u-v|)]}, \tag{2.6}$$ puv

where

$$f(u,v) = \int e^{-\frac{2}{N}\left[\sum_{4\leqslant i<j}^N \Phi(|\mathbf{r}_{1i}-\mathbf{r}_{1j}|)+\sum_{l=4}^N[\Phi(|\mathbf{r}_{1l}|)+\Phi(|u-\mathbf{r}_{1l}|)+\Phi(|v-\mathbf{r}_{1l}|)]\right]} d\mathbf{r}_{14}\dots\mathbf{r}_{1N}, \tag{2.7}$$

and Z *is a normalizing constant given by*

$$Z = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(u,v)e^{-\frac{2}{N}[\Phi(|u|)+\Phi(|v|)+\Phi(|u-v|)]}dudv$$

Proof. By Lemma 2.4, the probability density

$$p_{\mathbf{Y}}(\mathbf{y}) = \frac{1}{Z_N} e^{-2H(S\mathbf{y})} \tag{2.8}$$ eq:inv_pdf

with $Z_N := \int_{\mathbb{R}^d}\dots\int_{\mathbb{R}^d} e^{-2H(S\mathbf{y})}d\mathbf{y}_1\dots d\mathbf{y}_{N-1}$, is an invariant density for (2.3). Since $\mathbf{r} = S\mathbf{y}$, by integrating $p_{\mathbf{Y}}(\mathbf{y})$ with respect to $\mathbf{r}_{14},\dots,\mathbf{r}_{1N}$, we obtain the invariant marginal density for $(\mathbf{X}_1^t - \mathbf{X}_2^t, \mathbf{X}_1^t - \mathbf{X}_3^t)$. ☐

Proof of Theorem 2.1. Note that with the notation $\mathbf{r}_{ij}^t = \mathbf{X}_i^t - \mathbf{X}_j^t$ and $r_{ij}^t = |\mathbf{r}_{ij}^t|$, the system (1.1) is equivalent to

$$d\mathbf{r}_{1i}^t = -\frac{1}{N}\left[2\phi(r_{1i}^t)\mathbf{r}_{1i}^t + \sum_{2\leqslant j\leqslant N, j\neq i}\phi(r_{1j})\mathbf{r}_{1j}^t + \phi(r_{ji})\mathbf{r}_{ji}^t\right]dt + d(\mathbf{B}_1^t - \mathbf{B}_i^t), \tag{2.9}$$

for $2 \leqslant i \leqslant N$.

The process $(\mathbf{B}_1^t - \mathbf{B}_2^t, \mathbf{B}_1^t - \mathbf{B}_3^t, \dots, \mathbf{B}_1^t - \mathbf{B}_N^t)^T$ (where T means transpose) is a $d(N-1)$-dimensional Brownian motion with mean 0 and covariance A. Then, it can be written as $S\mathbf{W}^t$, with $(\mathbf{W}^t, t \geqslant 0)$ being a standard Brownian motion on $\mathbb{R}^{d(N-1)}$.

Note that for any $2 \leqslant j \leqslant N$ and $j \neq i$, we have $\mathbf{r}_{ji}^t = \mathbf{r}_{1i}^t - \mathbf{r}_{1j}^t$. Then, with $\mathbf{b}(\mathbf{r}^t) = (\mathbf{b}_2(\mathbf{r}^t), \dots, \mathbf{b}_N(\mathbf{r}^t))^\top$, where for $2 \leqslant i \leqslant N$ we denote

$$\mathbf{b}_i(\mathbf{r}^t) = \frac{1}{N}\left[2\phi(r_{1i}^t)\mathbf{r}_{1i}^t + \sum_{2\leqslant j\leqslant N, j\neq i} \phi(r_{1j}^t)\mathbf{r}_{1j}^t + \phi(r_{ji}^t)\mathbf{r}_{ji}^t\right],$$

we may write the system (2.9) as follows:

$$d\mathbf{r}^t = -\mathbf{b}(\mathbf{r}, t)dt + S d\mathbf{W}^t. \tag{2.10}$$

Multiplying both sides of (2.10) by S^{-1}, we obtain

$$d\mathbf{Y}^t = -S^{-1}\mathbf{b}(\mathbf{r}^t)dt + d\mathbf{W}^t \tag{2.11}$$

To write it as a gradient system, note that for $2 \leqslant i \leqslant N$, we have

$$\mathbf{b}_i(\mathbf{r}) = 2\nabla_{\mathbf{r}_{1i}} H(\mathbf{r}) + \sum_{2\leqslant j\leqslant N, j\neq i} \nabla_{\mathbf{r}_{1j}} H(\mathbf{r})$$

Hence,

$$\mathbf{b}(\mathbf{r}) = \mathbf{b}(S\mathbf{Y}) = A\nabla_{\mathbf{r}} H(\mathbf{r}^t) = A[S^{-1}]^T \nabla_{\mathbf{Y}} H(S\mathbf{Y}). \tag{2.12}$$

Plugging (2.12) to (2.11), and using the equation (2.4), we obtain the gradient system (2.3).

Then, by Lemma 2.4, the process $(\mathbf{Y}^t)$ defined by the system (2.3) has a stationary density, and so does the process $(\mathbf{r}^t)$, which is a linear transformation of $\mathbf{Y}^t$. □

lemma:GradS_inv **Lemma 2.4.** *Suppose $H : \mathbb{R}^n \to \mathbb{R}$ is locally Lipschitz and that $Z = \int_{\mathbb{R}^n} e^{-\frac{2}{\sigma^2}H(x)}dx < \infty$. Then $p(x) = \frac{1}{Z}e^{-\frac{2}{\sigma^2}H(x)}$ is an invariant density to gradient system*

$$dX_t = -\nabla H(X_t)dt + \sigma dB_t,$$

where (B_t) is an n-dimensional standard Brownian motion.

Proof. It follows directly by showing that $p(x)$ is a stationary solution to the backward Kolmogorov equation, i.e.

$$\frac{\sigma^2}{2}\Delta p + \nabla \cdot (p\nabla H) = 0.$$

□

3 Convergence to the stationary density

sec:convSD

We show in this section that for a class of potentials Φ, the gradient system (2.3) is ergodic, converging to the stationary density at a polynomial rate in time.

thm:Ergodicity

Theorem 3.1. *If the potential $\Phi = \Phi_0$ given by (1.3), the system (2.3) is ergodic, converging polynomial in time to the stationary density. More precisely, if the initial condition $\mathbf{Y}^0$ has a probability density $p_0(\mathbf{y})$ satisfying*

$$\begin{aligned} &\mathbb{E}[H(S\mathbf{Y}^0)\log p_0(\mathbf{Y}^0)] < \infty, \\ &\mathbb{E}[(1+|\mathbf{Y}^0|^2)^{\frac{s}{2}}] < \infty \end{aligned} \tag{3.1}$$

eq:IC

for some $s \geqslant 2$. Then, the density $p_{\mathbf{Y}^t}(\mathbf{y})$ of $\mathbf{Y}^t$ converges to $p_{\mathbf{Y}}(\mathbf{y})$ defined in (2.8):

$$\|p_{\mathbf{Y}^t}(\mathbf{y}) - p_{\mathbf{Y}}(\mathbf{y})\|_{L^1}^2 \leqslant \frac{C}{t^\kappa} \tag{3.2}$$

eq:conv2inv

for some constant C independent of t, and

$$\kappa = \frac{s-2}{2-\theta\gamma}. \tag{3.3}$$

eq:kappa

When $\theta = 2$ and $\gamma = 1$, the potential $\Phi(r) = a + r^2$ lead to a linear system and $(\mathbf{Y}^t)$ is an Ornstein-Uhlenbeck process, and we have exponential convergence. In general, when Φ is uniformly convex, i.e. $\mathrm{Hess}_x\Phi(|x|) \geqslant \lambda I_d$, one has exponential convergence to the equilibrium for the entropy from $p_{\mathbf{Y}_t}$ to $p_{\mathbf{Y}}$ as in [2, 8]. Here we focus on the L^1 distance, because it is needed when studying the coercivity condition in Section 5. In particular, the following convergence in L^1 of the marginal density of $(\mathbf{X}_1^t - \mathbf{X}_2^t, \mathbf{X}_1^t - \mathbf{X}_3^t)$ is needed.

prop:Conv_poly

Proposition 3.2. *Let $\mathbf{X}^t$ be a solution to the system (1.1) with potential $\Phi = \Phi_0$ given by (1.3), and with initial condition satisfying (3.1). Denote by $p_t(u,v)$ the density of $(\mathbf{X}_1^t - \mathbf{X}_2^t, \mathbf{X}_1^t - \mathbf{X}_3^t)$. Then $p_t(u,v)$ converges to the stationary density $p_\infty(u,v)$ in (2.6) at a polynomial rate in t:*

$$\|p_t - p_\infty\|_{L^1} = \int_{\mathbb{R}^{2d}} |p_t(u,v) - p(u,v)| du dv \leqslant Ct^{-\kappa/2}, \tag{3.4}$$

eq:puv_conv

where C is a constant independent of t and κ is given in (3.3).

Proof. By Theorem 2.1, the process $\mathbf{Y}^t = S^{-1}\mathbf{r}^t$ with $\mathbf{r}^t = (\mathbf{X}_1^t - \mathbf{X}_2^t, \mathbf{X}_1^t - \mathbf{X}_3^t, \dots, \mathbf{X}_1^t - \mathbf{X}_N^t)$ satisfies the system (2.3). Let $p_{\mathbf{r}^t}$ be the density of $\mathbf{r}^t$, and let $p_{\mathbf{r}}$ be the corresponding stationary density. Then,

$$\begin{aligned} &\int_{\mathbb{R}^{2d}} |p_t(u,v) - p_\infty(u,v)|\, du dv \\ =& \int_{\mathbb{R}^{2d}} \left| \int_{\mathbb{R}^{d(N-3)}} p_{\mathbf{r}^t}(u,v,\mathbf{r}_{14},\dots,\mathbf{r}_{1N}) - p_{\mathbf{r}}(u,v,\mathbf{r}_{14},\dots,\mathbf{r}_{1N}) d\mathbf{r}_{14}\dots d\mathbf{r}_{1N} \right| du dv \\ \leqslant& \int_{\mathbb{R}^{d(N-1)}} |p_{\mathbf{r}^t}(u,v,\mathbf{r}_{14},\dots,\mathbf{r}_{1N}) - p_{\mathbf{r}}(u,v,\mathbf{r}_{14},\dots,\mathbf{r}_{1N})|\, d\mathbf{r}_{14}\dots d\mathbf{r}_{1N} du dv \\ =& \int_{\mathbb{R}^{d(N-1)}} \left|p_{\mathbf{Y}^t}(\mathbf{y}) - p_{\mathbf{Y}}(\mathbf{y})\right| d\mathbf{y} \leqslant |\mathrm{det} S^{-1}|\sqrt{C} t^{-\kappa/2}, \end{aligned}$$

where the last equation follows from (3.2) of Theorem 3.1. □

The proof of Theorem 3.1 is based on the following theorem in [12, Theorem 3.1].

ttv **Theorem 3.3** ([12]). *Let $x \in \mathbb{R}^n$. Assume $W \in W^{2,\infty}_{\text{loc}}$ satisfies all the following conditions:*

(1) $\int_{\mathbb{R}^n} e^{-W(x)}dx = 1$; and

(2) there exist $U : \mathbb{R}^n \to \mathbb{R}$ and constant $a, b > 0$ such that for all $x \in \mathbb{R}^n$,

$$U(x) - a \leqslant W(x) \leqslant U(x) + b,$$

and there exist $c > 0$ and $\alpha \in (0, 2)$, such that the matrix

$$\text{Hess}[U(x)] - c(1 + |x|)^{\alpha-2} I_n$$

is a positive semi-definite, in which $Hess[U(x)]$ is the Hessian matrix for $U(x)$; and

(3) there exist $\beta > 0$, $C_0, C_1 > 0$ and $x \in \mathbb{R}^n$ satisfying

$$\nabla W(x) \cdot x \geqslant C_1|x|^\beta - C_0.$$

Let f_0 be a probability density such that

$$\int_{\mathbb{R}^n} f_0(x)[\log f_0(x) + W(x)]dx < \infty; \text{ and} \tag{3.5}$$

$$\int_{\mathbb{R}^n} f_0(x)(1 + |x|^2)^{\frac{s}{2}} dx < \infty; \text{for some } s > 2. \tag{3.6}$$

Let $f(t, \cdot)$ be a smooth solution of the Fokker-Planck equation

$$\frac{\partial f}{\partial t} = \nabla_x \cdot (\nabla_x f + f \nabla_x W)$$

with initial condition $f(0, \cdot) = f_0$. Then, there is a constant C depending on (3.5)-(3.6) and s, such that for all $t > 0$,

$$\frac{1}{2} \left\| f(t, x) - e^{-W(x)} \right\|^2_{L^1} \leqslant \int_{\mathbb{R}^n} f(t, x)[\log f(t, x) + W(x)]dx \leqslant \frac{C}{t^\kappa},$$

with $\kappa = \frac{s-2}{2-\alpha}$.

If the $W(x)$ uniformly convex, i.e. $\text{Hess}[W(x)] > cI_d$ for some $c > 0$, the convergence will be exponential in time (see [8]).

prop_ergodicity **Proposition 3.4.** *Let $n = d(N - 1)$ and*

$$W(\mathbf{y}) = H(S\mathbf{y}),$$

where $H(\cdot) : \mathbb{R}^{(N-1)d} \to \mathbb{R}$ is given by Eq.(2.1) and the matrix $S \in \mathbb{R}^{(N-1)d \times (N-1)d}$ is given by (2.5). Then, W satisfies the conditions (1)-(3) in Theorem 3.3 if the interaction potential $\Phi : \mathbb{R}^d \to \mathbb{R}$ satisfies

1. there exists $C_0, C_1, \beta > 0$ such that for all $\mathbf{r} \in \mathbb{R}^{d(N-1)}$,

$$\frac{1}{N}\left[\sum_{2\leqslant j\leqslant N} \phi(|\mathbf{r}_{1j}|)|\mathbf{r}_{1j}|^2 + \sum_{2\leqslant i<j\leqslant N} \phi(|\mathbf{r}_{ij}|)|\mathbf{r}_{ij}|^2\right] \geqslant C_1 r^{\beta} - C_0, \qquad (3.7)$$ vc2

where $\phi(r) = \frac{\Phi'(r)}{r}$;

2. there exist $c > 0$ and $\alpha \in (0, 2)$ such that for all $x \in \mathbb{R}^d$,

$$\mathrm{Hess}_x[\Phi(|x|)] - c(1 + |x|)^{\alpha-2} I_d \geqslant 0, \qquad (3.8)$$ eq:HessPhi

i.e., the matrix is positive definite, for all $x \in \mathbb{R}^d$.

Proof. We only need to verify condition (2)-(3).

For Condition (3), note that $\mathbf{r}^t = (\mathbf{r}_{12}^t, \mathbf{r}_{13}^t, \ldots, \mathbf{r}_{1N}^t) = S\mathbf{Y}^t$, when both $\mathbf{r}^t$ and $\mathbf{Y}^t$ are considered as $d(N-1) \times 1$ column vectors. Then we have

$$\nabla_{\mathbf{Y}} H(S\mathbf{Y}) \cdot \mathbf{Y} = [\nabla_{\mathbf{r}} H(\mathbf{r})]^T S S^{-1} \mathbf{r} = \nabla_{\mathbf{r}} H(\mathbf{r}) \cdot \mathbf{r}.$$

Note that with $\phi(r) := \frac{\Phi'(r)}{r}$ and with $\mathbf{r}_{ik} = \mathbf{r}_i - \mathbf{r}_k$, we can write the gradient of $H(\mathbf{r})$ in Eq.(2.1) as

$$\nabla_{\mathbf{r}_{1j}} H(\mathbf{r}) = \frac{1}{N}\phi(|\mathbf{r}_{1j}|)\mathbf{r}_{1j} + \frac{1}{N}\sum_{k=2}^{N} \phi(|\mathbf{r}_{jk}|)\mathbf{r}_{jk}, \quad \text{for } j = 2, \cdots, N. \qquad (3.9)$$ eq:gradHr

Hence we have

$$\nabla_{\mathbf{r}} H(\mathbf{r}) \cdot \mathbf{r} = \frac{1}{N}\left[\sum_{2\leqslant j\leqslant N} \phi(|\mathbf{r}_{1j}|)|\mathbf{r}_{1j}|^2 + \sum_{2\leqslant i<j\leqslant N} \phi(|\mathbf{r}_{ij}|)|\mathbf{r}_{ij}|^2\right].$$

Then Condition (3) follows from (3.7).

To prove Condition (2), note that

$$\mathrm{Hess}_{\mathbf{Y}} H(S\mathbf{Y}) = S^T \mathrm{Hess}_{\mathbf{r}} H(\mathbf{r}) S,$$

and recall that $S^T S = A$ so $S^{-T} S^{-1} = A^{-1}$ with

$$A^{-1} = \frac{1}{N}\begin{pmatrix} (N-1)I_d & -I_d & \ldots & -I_d \\ -I_d & (N-1)I_d & \ldots & -I_d \\ \vdots & \vdots & \ddots & \vdots \\ -I_d & -I_d & \ldots & (N-1)I_d \end{pmatrix} \in \mathbb{R}^{(N-1)d\times(N-1)d}.$$

Then, to show that $\mathrm{Hess}_{\mathbf{Y}} H(S\mathbf{Y}) - c(1+|\mathbf{Y}|)^{\alpha-2} I_{(N-1)d}$ is positive semi-definite, it suffices to show that

$$\mathbf{M} = \mathrm{Hess}_{\mathbf{r}} H(\mathbf{r}) - c(1 + |S^{-1}\mathbf{r}|)^{\alpha-2} A^{-1} \geqslant 0. \qquad (3.10)$$ matHA-1

Continuing from (3.9), we have

$$\nabla_{\mathbf{r}_{1i}}\nabla_{\mathbf{r}_{1j}}H(\mathbf{r}) = \frac{1}{N}\left[\delta_{ij}B_i - \delta_{i\neq j}A_{ij} + \delta_{ij}\sum_{k=2,k\neq i}^{N} A_{ik}\right],$$

where B_i and A_{ij} are $d\times d$ matrices (recalling that $\mathbf{r}_{ik} = \mathbf{r}_i - \mathbf{r}_k$) given by

$$\begin{aligned} B_i &= \nabla_{\mathbf{r}_{1i}}[\phi(|\mathbf{r}_{1i}|)\mathbf{r}_{1i}] = \phi(|\mathbf{r}_{1i}|)I_d + \frac{\phi'(|\mathbf{r}_{1i}|)}{|\mathbf{r}_{1i}|}\mathbf{r}_{1i}\otimes\mathbf{r}_{1i} = \mathrm{Hess}_{\mathbf{r}_{1i}}\Phi(|\mathbf{r}_{1i}|), \\ A_{ik} &= \nabla_{\mathbf{r}_{1i}}[\phi(|\mathbf{r}_{ik}|)\mathbf{r}_{ik}] = \phi(|\mathbf{r}_{ik}|)I_d + \frac{\phi'(|\mathbf{r}_{ik}|)}{|\mathbf{r}_{ik}|}\mathbf{r}_{ik}\otimes\mathbf{r}_{ik} = \mathrm{Hess}_{\mathbf{r}_{ij}}\Phi(|\mathbf{r}_{ij}|) \end{aligned}$$

for $i\neq k$, and where we have used the fact that $A_{ik} = -\nabla_{\mathbf{r}_{1k}}[\phi(|\mathbf{r}_{ik}|)\mathbf{r}_{ik}]$ to obtain the term $-\delta_{i\neq j}A_{ij}$. Hence, the diagonal and off-diagonal entries of the $(N-1)d\times(N-1)d$ matrix $\mathbf{M}$ in (3.10) can be written as

$$\mathbf{M} = \frac{1}{N}\begin{pmatrix} B_2 - C + \sum_{j\neq 2} D_{2j} & -D_{23} & \dots & -D_{1N'} \\ -D_{2N} & B_3 - C + \sum_{j\neq 3} D_{3j} & \dots & -D_{3N} \\ \vdots & \vdots & \ddots & \vdots \\ -D_{N2} & -D_{N3} & \dots & B_1 - C + \sum_{j\neq N} D_{Nj} \end{pmatrix}$$

with $C = c(1+|S^{-1}\mathbf{r}|)^{\alpha-2}I_d$, $D_{ij} = A_{ij} - C$.

Since $D_{ij} = D_{ji}$ for all $2\leqslant i<j\leqslant N$, for any $\eta = (\eta_2,\eta_3,\dots,\eta_N)\in\mathbb{R}^{(N-1)d}$, we have

$$\begin{aligned} N\eta\mathbf{M}\eta^T &= \sum_{I=2}^{N}\langle (B_i - C)\eta_i,\eta_i\rangle + \sum_{2\leqslant i,j\leqslant N, i\neq j}\langle \mathbf{D}_{ij}\eta_i,\eta_i\rangle - \langle \mathbf{D}_{ij}\eta_i,\eta_j\rangle \\ &= \sum_{I=2}^{N}\langle (B_i - C)\eta_i,\eta_i\rangle + \sum_{2\leqslant i<j\leqslant N}\langle \mathbf{D}_{ij}(\eta_i-\eta_j),(\eta_i-\eta_j)\rangle, \end{aligned} \tag{3.11}$$

M_positiveD

where the second equality follows from the fact that D_{ij} is symmetric. Note that the eigenvalues of S are $\left\{\sqrt{\frac{k}{k-1}}\right\}_{k=2}^{N}$, so $|S^{-1}\mathbf{r}|\geqslant \frac{1}{\sqrt{2}}|\mathbf{r}|$. Since $\alpha\in(0,2)$, we have

$$(1+|S^{-1}\mathbf{r}|)^{\alpha-2} \leqslant \left(1+\frac{1}{\sqrt{2}}|\mathbf{r}|\right)^{\alpha-2} \leqslant 2^{\frac{2-\alpha}{2}}(1+|\mathbf{r}|)^{\alpha-2}$$

for each component $\mathbf{r}_i$ of $\mathbf{r} = (\mathbf{r}_1,\dots,\mathbf{r}_N)\in\mathbb{R}^{dN}$. Noticing that $\alpha>0$, we have

$$C = c(1+|S^{-1}\mathbf{r}|)^{\alpha-2}I_d \leqslant 2c(1+|\mathbf{r}_{1i}|)^{\alpha-2}I_d$$

for each $i\in\{2,3,\dots,N\}$. Hence, we have

$$\begin{aligned} B_i - C &\geqslant \mathrm{Hess}_{\mathbf{r}_{1i}}\Phi(|\mathbf{r}_{1i}|) - 2c(1+|\mathbf{r}_{1i}|)^{\alpha-2}I_d \geqslant 0, \\ D_{ij} &\geqslant \mathrm{Hess}_{\mathbf{r}_{ij}}\Phi(|\mathbf{r}_{ij}|) - 2c(1+|\mathbf{r}_{1j}|)^{\alpha-2}I_d \geqslant 0 \end{aligned}$$

for each $i,j = 2,\dots,N$. Plugging them into Eq.(3.11), we obtain that $\mathbf{M}$ is positive definite. □

lemmaPhi **Lemma 3.5.** *Let $\phi(r) := \frac{\Phi'(r)}{r}$. Then, Condition (3.7) holds if*

(i) *there exists $c_1, c_2 > 0$ such that $\phi(r) \geqslant 0$ and $\phi(r)r^2 \geqslant c_1 r^\beta - c_2$ for all $r > 0$;*

and Condition (3.8) holds if either (ii) or (iii) is true:

(ii) $\phi'(r) \geqslant 0$ and there exists $c_3 > 0$ such that $\phi(r) \geqslant c_3(1+r)^{\alpha-2}$ for all $r > 0$;

(iii) $\phi'(r) \leqslant 0$ and there exists $c_3 > 0$ such that $\phi(r) + \phi'(r)r \geqslant c_3(1+r)^{\alpha-2}$ for all $r > 0$.

Proof. Suppose (i) is true, then Condition (3.7) follows from

$$\begin{aligned}&\frac{1}{N}\left[\sum_{2\leqslant j\leqslant N} \phi(|\mathbf{r}_{1j}|)|\mathbf{r}_{1j}|^2 + \sum_{2\leqslant i<j\leqslant N} \phi(|\mathbf{r}_{ij}|)|\mathbf{r}_{ij}|^2\right] \geqslant \frac{1}{N}\sum_{2\leqslant j\leqslant N} \phi(|\mathbf{r}_{1j}|)|\mathbf{r}_{1j}|^2 \\ \geqslant& c_1 \sum_{2\leqslant j\leqslant N} |\mathbf{r}_{1j}|^\beta - c_2 \geqslant \frac{1}{N} c_1 c_\beta |\mathbf{r}|^\beta - c_2,\end{aligned}$$

where c_β is the minimum of $f(\mathbf{r}) := \sum_{2\leqslant j\leqslant N} |\mathbf{r}_{1j}|^\beta$ on the unit sphere $\{\mathbf{r} = (\mathbf{r}_{12}, \ldots, \mathbf{r}_{1N}) : \sum_{2\leqslant j\leqslant N} |\mathbf{r}_{1j}|^2 = 1\}$.

To prove Condition (3.8), note that

$$\mathrm{Hess}_x \Phi(|x|) = \nabla(\phi(|x|)x) = \phi'(|x|)\frac{x\otimes x}{|x|} + \phi(|x|)I_d.$$

Then, if (ii) is true, Condition (3.8) follows directly, since $\frac{x\otimes x}{|x|}$ is positive definite. If (iii) is true, using the fact that $I_d - \frac{x\otimes x}{|x|^2}$ is positive definite, we obtain Condition (3.8):

$$\begin{aligned}\mathrm{Hess}_x \Phi(|x|) &= \left[\phi(|x|) + \phi'(|x|)|x|\right] I_d - \phi'(|x|)|x| \left(I_d - \frac{x\otimes x}{|x|^2}\right) \\ &\geqslant \left[\phi(|x|) + \phi'(|x|)|x|\right] I_d \\ &\geqslant c_3(1+|x|)^{\alpha-2} I_d.\end{aligned}$$

□

exmp_gamma>1 **Example 3.6.** *The function $\Phi(r) = (a+r^2)^\gamma$ with $a > 0$ and $\gamma \geqslant 1$ satisfies Condition (3.7)- (3.8). To see this, note that*

$$\phi(r) = \frac{\Phi'(r)}{r} = 2\gamma(a+r^2)^{\gamma-1} \geqslant 2\gamma a^{\gamma-1},$$

and $\phi(r)r^2 \geqslant c_1 r^2 - c_2$ with $c_1 = 2\gamma a^{\gamma-1}$ and $c_2 = 0$. Therefore, Condition (3.7) holds by Lemma 3.5 (i) with $\beta = 2$. Note also that

$$\phi'(r) = 4\gamma(\gamma-1)(a+r^2)^{\gamma-2} r > 0$$

and $\phi(r) \geqslant 2\gamma a^{\gamma-1} \geqslant c_3(1+r)^{\alpha-2}$ with $c_3 = 2\gamma a^{\gamma-1}$ for any $\alpha \in (0,2)$, i.e. Lemma 3.5 (ii) hods, and so does Condition (3.8).

exmp_1 **Example 3.7.** *The function $\Phi(r) = (a + r^\theta)^\gamma$ with $a > 0$, $\gamma \in (0, 1]$, $\theta \in (1, 2]$ and $\theta\gamma > 1$ satisfies Condition (3.7)- (3.8). To see this, note that $\phi(r) = \theta\gamma(a + r^\theta)^{\gamma-1} r^{\theta-2} \geqslant 0$ and*

$$\begin{aligned}\phi(r)r^2 &= \theta\gamma(a + r^\theta)^{\gamma-1} r^\theta = \theta\gamma \left(\frac{a + r^\theta}{r^\theta}\right)^{\gamma-1} r^{\theta\gamma} \\ &= c_1 r^{\theta\gamma} + [\theta\gamma \left(\frac{r^\theta}{a + r^\theta}\right)^{1-\gamma} - c_1] r^{\theta\gamma} \geqslant c_1 r^{\theta\gamma} - c_0\end{aligned}$$

with $c_1 = \theta\gamma/2$ and with $-c_0$ being the minimum of $f(r) = \gamma[\theta \left(\frac{r^\theta}{a+r^\theta}\right)^{1-\gamma} - 1/2] r^{\theta\gamma}$ (whose maximum exists and is positive because $f(r) < 0$ for small r and $\lim_{r\to\infty} f(r) = +\infty$). Then, Condition (3.7) holds by Lemma 3.5 (i) *with $\beta = \theta\gamma$. For Condition (3.8), note that*

$$\phi'(r) = \theta\gamma(a + r^\theta)^{\gamma-2} r^{\theta-3} [\theta - 2 + \theta(\gamma - 1) r^\theta (a + r^\theta)^{\gamma-2}] \leqslant 0,$$

because $\theta \leqslant 2$ and $\gamma < 1$. Noting that $\theta - 1 + \theta(\gamma - 1) r^\theta (a + r^\theta)^{-1} \geqslant \theta - 1 + \theta(\gamma - 1) = \theta\gamma - 1 > 0$, we have

$$\begin{aligned}\phi(r) + \phi'(r)r &= \theta\gamma(a + r^\theta)^{\gamma-1} r^{\theta-2} [\theta - 1 + \theta(\gamma - 1) r^\theta (a + r^\theta)^{-1}] \\ &\geqslant \theta\gamma(\theta\gamma - 1)(a + r^\theta)^{\gamma-1} r^{\theta-2} \\ &= \theta\gamma(\theta\gamma - 1) \left(\frac{r^\theta}{a + r^\theta}\right)^{1-\gamma} \left(\frac{r}{1 + r}\right)^{\theta\gamma-2} (1 + r)^{\theta\gamma-2} \\ &\geqslant c_3 (1 + r)^{\theta\gamma-2},\end{aligned}$$

where c_3 is the minimum of the function $f(r) = \theta\gamma(\theta\gamma - 1) \left(\frac{r^\theta}{a+r^\theta}\right)^{1-\gamma} \left(\frac{r}{1+r}\right)^{\theta\gamma-2}$ (whose minimum exists and is positive because $\theta\gamma > 1$ and $\theta \leqslant 2$). Thus, Lemma 3.5 (iii) hods with $\alpha = 2\gamma$.

exmp_2 **Example 3.8.** *The function $\Phi(r) = r^\gamma$ satisfies Condition (3.7)- (3.8) only when $\gamma \in (1, 2]$. To see this, note that $\phi(r) = \gamma r^{\gamma-2}$ and $\phi(r)r^2 = \gamma r^\gamma$. Then, Lemma 3.5* (i) *holds with with $\beta = \gamma$, $c_1 = \gamma$ and $c_2 = 0$. Thus, Condition (3.7) holds for any $\gamma > 0$. For Condition (3.8), note that $\phi'(r) = \gamma(\gamma - 2) r^{\gamma-3} \leqslant 0$ when $\gamma \leqslant 2$. Also, note that*

$$\phi(r) + \phi'(r)r = \gamma r^{\gamma-2}(\gamma - 1) \geqslant \gamma(\gamma - 1)(1 + r)^{\gamma-2}.$$

Thus, Lemma 3.5 (iii) holds with $\alpha = \gamma$ and with $c_3 = \gamma(\gamma - 1) > 0$ when $\gamma \in (1, 2]$. When $\gamma > 2$, we have $\phi'(r) \geqslant 0$, but $\phi(r)/(1 + r)^{\alpha-2} = \gamma r^\gamma (1 + r)^{2-\alpha}$ has a minimum 0 over $r \in (0, inf ty)$ for any $0 < \alpha < 2$. Thus, Lemma 3.5 (ii) does not hold. Then, Condition (3.8) holds only when $\gamma \in (1, 2]$.

Proof of Theorem 3.1 . The theorem follows directly from Example 3.7-3.8, Proposition 3.4 and Theorem 3.3. □

4 Coercivity at the invariant density

sec:PD_inv

We show that for a large class of potentials Φ, the coercivity conditions holds at the invariant densities.

We consider the interaction potentials in the form of Φ_0 in (1.3), and more generally, the potentials

$$\Phi(r) = c_1\Phi_0(r) + c_2\Psi(r), \tag{4.1}$$ eq:phi_0All

where $c_1 > 0, c_2 \geqslant 0$ and $\Psi : [0,\infty) \to \mathbb{R}$ is a function such that $\Psi(|u-v|)$ is a negative definite.

Let ρ be the marginal density of $p_\infty(u,v)$ in (2.6) with Φ defined in (4.1):

$$\rho(u) = \int p_\infty(u,v)dv. \tag{4.2}$$ eq:rho

We denote the functional in the coercivity condition as

$$I_\infty(h) := \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} h(u)\frac{\langle u,v\rangle}{|u||v|}p_\infty(u,v)h(v)dudv. \tag{4.3}$$ eq:I_infty

Theorem 4.1. *Consider the system (2.3) with the potential Φ given by (4.1) such that $p_\infty(u,v)$ in (2.6) is the stationary density. Suppose that the system start from the stationary density. Recall that ρ in (4.2) is the marginal density of p_∞. Then, the coercivity condition holds true on any finite dimensional subspace of $L^2(\rho)$. That is, for any $\mathcal{H} \subset L^2(\rho)$ that is a finite dimensional linear subspace, there exists a constant $c_{\mathcal{H}} > 0$ such that for all $h \in \mathcal{H}$,*

$$I_\infty(h) = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} h(u)\frac{\langle u,v\rangle}{|u||v|}p_\infty(u,v)h(v)dudv \geqslant c_{\mathcal{H}}\|h\|^2_{L^2(\rho)}. \tag{4.4}$$ eq:CC_infty

Proof. By Theorem 4.2 below, $I_\infty(h) \geqslant 0$ and the equality holds only when $h = 0$ everywhere. Note also that $I_\infty(h)$ is a continuous functional on $L^2(\rho)$ since by Hölder's inequality,

$$I_\infty(h) \leqslant \|h\|^2_{L^2(\rho)}.$$

Thus, (4.4) holds true with

$$c_{\mathcal{H}} = \min_{h\in\mathcal{H},\, \|h\|^2_{L^2(\rho)}=1} I_\infty(h),$$

when $\mathcal{H} \in L^2(\rho)$ is a finite dimensional linear subspace. □

The above coercivity condition is based on the following theorem:

main **Theorem 4.2.** *Let $p_\infty(u,v)$ be the density function in (2.6) with Φ defined as (4.1). Let $I_\infty(h)$ be the functional defined in (4.3). Then,*

$$I_\infty(h) = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} h(u)\frac{\langle u,v\rangle}{|u||v|}p_\infty(u,v)h(v)dudv \geqslant 0$$

for any $h \in L^2(\mathbb{R}^d,\rho)$ with ρ defined in (4.2), and $I_\infty(h) = 0$ only when $h = 0$ almost everywhere.

Theorem 4.2 is equivalent to that the integral kernel $\frac{\langle u,v\rangle}{|u||v|}p_\infty(u,v)$ in the definition of $I_\infty(h)$ is strictly positive definite. To prove this, we start with a few technical results about positive definite integral kernels.

We introduce the following notation to simplify the expression of the marginalization in $I_\infty(h)$. For any function $\Phi : \mathbb{R}^+ \to \mathbb{R}$, we denote

$$\begin{aligned} D_\Phi^{\triangle}(u,v) &= \Phi(|u|) + \Phi(|v|) - \Phi(|u-v|); \\ D_\Phi^{\square}(u,v) &= \Phi(|u|) + \Phi(|v|) - \Phi(|u-v|) - \Phi(0). \end{aligned} \tag{4.5}$$

eq:triangle_box

Then, for the function Φ in (4.1), we have

$$\begin{aligned} &\Phi(|u|) + \Phi(|v|) + \Phi(|u-v|) \\ =& -[\Phi(|u|) + \Phi(|v|) - \Phi(|u-v|)] + \Phi(|u|) + \Phi(|v|) \\ =& -c_1 D_{\Phi_0}^{\triangle}(u,v) - c_2 D_\Psi^{\square}(u,v) + c_2\Psi(0) + \Phi(|u|) + \Phi(|v|). \end{aligned} \tag{4.6}$$

eq:phi_decomp

Recall that $p_\infty(u,v)$ in (2.6) is

$$p_\infty(u,v) = \frac{1}{Z} f(u,v) e^{-\frac{2}{N}[\Phi(|u|)+\Phi(|v|)+\Phi(|u-v|)]},$$

where

$$f(u,v) = \int e^{-\frac{2}{N}\left[\sum_{4\leqslant i<j}^N \Phi(|\mathbf{r}_{1i}-\mathbf{r}_{1j}|) + \sum_{l=4}^N [\Phi(|\mathbf{r}_{1l}|)+\Phi(|u-\mathbf{r}_{1l}|)+\Phi(|v-\mathbf{r}_{1l}|)]\right]} d\mathbf{r}_{14}\ldots\mathbf{r}_{1N}.$$

For any fixed $\mathbf{r}_{14}, \mathbf{r}_{15}, \ldots, \mathbf{r}_{1N}$, let

$$\overline{h}_{\mathbf{r}}(u) = h(u) e^{-\frac{4}{N}\Phi(|u|) - \frac{2}{N}\sum\limits_{4\leqslant l\leqslant N}\Phi(|u-\mathbf{r}_{1l}|) - \frac{1}{N}\sum\limits_{4\leqslant i<j\leqslant N}\Phi(|\mathbf{r}_{1i}-\mathbf{r}_{1j}|) - \frac{1}{N}\sum\limits_{4\leqslant l\leqslant N}\Phi(|\mathbf{r}_{1l}|)}. \tag{4.7}$$

Then, combining (4.6) and (4.7), we have

$$\begin{aligned} I_\infty(h) &= \frac{1}{Z}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^{(N-3)d}} \overline{h}_{\mathbf{r}}(u)\overline{h}_{\mathbf{r}}(v)\frac{\langle u,v\rangle}{|u||v|} e^{\frac{2}{N}[\Phi(|u|)+\Phi(|v|)-\Phi(|u-v|)]} d\mathbf{r}_{14}\cdots d\mathbf{r}_{1N}\,du\,dv \\ &= \frac{1}{Z} e^{\frac{2c_2}{N}\Psi(0)} \int_{\mathbb{R}^{(N-1)d}} \overline{h}_{\mathbf{r}}(u)\overline{h}_{\mathbf{r}}(v)\frac{\langle u,v\rangle}{|u||v|} e^{\frac{2}{N}[c_1 D_{\Phi_0}^{\triangle}(u,v) + c_2 D_\Psi^{\square}(u,v)]} d\mathbf{r}_{14}\cdots d\mathbf{r}_{1N}\,du\,dv. \end{aligned} \tag{4.8}$$

eq:I_triangle_b

The following lemma shows that $D_{\Phi_0}^{\triangle}(u,v)$ and $D_\Psi^{\square}(u,v)]$ are positive definite.

lm:triangeBox

Lemma 4.3. *Let $\Phi : \mathbb{R}^+ \to \mathbb{R}$ be a function and consider the functions $D_\Phi^{\triangle}(u,v)$ and $D_\Phi^{\square}(u,v)$ defined in (4.5).*

(i) If $\Phi(|u-v|)$ is negative definite, then $D_\Phi^{\square}(u,v)$ is positive definite.

(ii) If in addition that $\Phi(0) \geqslant 0$, then $D_\Phi^{\triangle}(u,v)$ is positive definite.

In particular, Φ_0 defined in (1.3) is negative definite and $\Phi_0(0) \geqslant 0$, so $D_{\Phi_0}^{\triangle}(u,v)$ is positive definite.

Proof. Applying Theorem 6.4 to the function $\psi(u,v) = \Phi(|u-v|)$, we obtain that both $D_\Phi^{\square}(u,v)$ and $D_\Phi^{\triangle}(u,v)$ are positive definite.

To show that $D^{\triangle}_{\Phi_0}(u,v)$ is positive definite, we need to show that $\Phi_0(u-v)$ is negative definite. By Theorem 6.6, it suffices to show that $\psi(u,v) = a + |u-v|^2$ is negative definite. Note that $\psi(u,v)$ is symmetric and for any $\{c_1, c_2, \ldots, c_n\} \in \mathbb{R}$ with $\sum_{j=1}^n c_j = 0$,

$$\begin{aligned}\sum_{j,k=1}^{n} c_j c_k \psi(u_j, u_k) &= \sum_{j,k=1}^{n} c_j c_k \left[a + |u_j|^2 + |u_k|^2 - 2\langle u_j, u_k\rangle\right] \\ &= -2 \sum_{j,k=1}^{n} c_j c_k \langle u_j, u_k\rangle = -2|\sum_j c_j u_j|^2 \leqslant 0,\end{aligned}$$

for any $\{u_1, u_2, \ldots, u_n\} \in \mathbb{R}^d$. Thus, $\psi(u,v) = a + |u-v|^2$ is negative definite. □

The proof of Theorem 4.2 relies on the fact that the polynomials are dense in a class of weighted $L^2(\mu)$ spaces, as in the following lemma:

poly **Lemma 4.4.** [11, Lemma 1.1] *Let μ be a measure on $\mathbb{R}^d$ satisfying*

$$\int e^{c\|x\|} d\mu(x) < \infty$$

for some $c > 0$, where $\|x\| = \sum_{j=1}^d |x_j|$. Then the polynomials are dense in $L^2(\mu)$.

rop_powerKernel **Proposition 4.5.** *For Φ_0 in (1.3) with $\gamma \in (0,1)$ and $h_{\mathbf{r}} : \mathbb{R}^d \to \mathbb{R}$ defined in (4.7), let*

$$I_{\mathbf{r}} := \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} h_{\mathbf{r}}(u) h_{\mathbf{r}}(v) \frac{\langle u, v\rangle}{|u||v|} \left[\Phi_0(|u|) + \Phi_0(|v|) - \Phi_0(|u-v|)\right] du dv.$$

Then, $I_{\mathbf{r}} \geqslant 0$ and $I_{\mathbf{r}} = 0$ if and only if $h = 0$ almost everywhere.

Proof. From the expression (1.3), we obtain

$$I_{\mathbf{r}} = I_1 + I_2;$$

where

$$\begin{aligned} I_1 :&= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} h_{\mathbf{r}}(u) h_{\mathbf{r}}(v) \frac{\langle u, v\rangle}{|u||v|} \left[(a + |u|^\theta)^\gamma + (a + |v|^\theta)^\gamma - (2a + |u|^\theta + |v|^\theta)^\gamma\right] du dv; \\ I_2 :&= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} h_{\mathbf{r}}(u) h_{\mathbf{r}}(v) \frac{\langle u, v\rangle}{|u||v|} \left[(2a + |u|^\theta + |v|^\theta)^\gamma - (a + |u-v|^\theta)^\gamma\right] du dv. \end{aligned}$$

By Lemma 6.8 and Lemma 6.9, $(a + |u|^\theta)^\gamma + (a + |v|^\theta)^\gamma - (2a + |u|^\theta + |v|^\theta)^\gamma$ is positive definite as a function of (u,v), therefore $I_1 \geqslant 0$.

Note also that for $0 < \gamma < 1$,

$$z^\gamma = \frac{\gamma}{\Gamma(1-\gamma)} \int_0^\infty (1 - e^{-\lambda z}) \frac{d\lambda}{\lambda^{\gamma+1}},$$

where $\Gamma(1-\gamma) = \int_0^\infty x^{-\gamma} e^{-x} dx$ is the Gamma function. Then, with $C_\gamma := \frac{\gamma}{\Gamma(1-\gamma)}$, and with the notation

$$D^{\triangle}_{\psi}(u,v) = |u|^\theta + |v|^\theta - |u-v|^\theta \tag{4.9}$$ D_psi

for the function $\psi(u) = |u|^\theta$ as in (4.5), we have

$$
\begin{aligned}
I_2 &= C_\gamma \int_0^\infty \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} h_{\mathbf{r}}(u)h_{\mathbf{r}}(v)\frac{\langle u,v\rangle}{|u||v|}\left[e^{-\lambda(a+|u-v|^\theta)} - e^{-\lambda(2a+|u|^\theta+|v|^\theta)}\right] dudv\frac{d\lambda}{\lambda^{\gamma+1}}\\
&= C_\gamma \int_0^\infty \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} h_{\mathbf{r}}(u)h_{\mathbf{r}}(v)\frac{\langle u,v\rangle}{|u||v|}e^{-\lambda(|u|^\theta+|v|^\theta+a)}[e^{2\lambda D_\psi^\triangle(u,v)} - e^{-\lambda a}]dudv\frac{d\lambda}{\lambda^{\gamma+1}}\\
&= C_\gamma \int_0^\infty \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} h_{\mathbf{r}}(u)h_{\mathbf{r}}(v)\frac{\langle u,v\rangle}{|u||v|}e^{-\lambda(|u|^\theta+|v|^\theta+a)}e^{2\lambda D_\psi^\triangle(u,v)}dudv\frac{d\lambda}{\lambda^{\gamma+1}}, \qquad (4.10)
\end{aligned}
$$

eq:I2_theta

where the last equality follows from the fact that

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} h_{\mathbf{r}}(u)h_{\mathbf{r}}(v)\frac{\langle u,v\rangle}{|u||v|}e^{-\lambda(|u|^2+|v|^2+a)}e^{-\lambda a}dudv = 0$$

due to symmetry.

Consider first the case when $\theta = 2$. Note that $D_\psi^\triangle(u,v) = \langle u,v\rangle$. We have, by the Taylor expansion of $e^{2\lambda D_\psi^\triangle(u,v)}$,

$$
\begin{aligned}
I_2 &= C_\gamma \sum_{k=0}^\infty \int_0^\infty e^{-\lambda a}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\left[\frac{h_{\mathbf{r}}(u)e^{-\lambda|u|^2}}{|u|}\right]\left[\frac{h_{\mathbf{r}}(v)e^{-\lambda|v|^2}}{|v|}\right]\frac{(2\lambda)^k\langle u,v\rangle^{k+1}}{k!}dudv\frac{d\lambda}{\lambda^{\gamma+1}}\\
&= C_\gamma \sum_{\substack{i_1,\dots,i_d\geqslant 0,\\ k=i_1+\dots+i_d\geqslant 1}} \int_0^\infty e^{-\lambda a}\frac{(2\lambda)^{k-1}k}{i_1!\cdot\ldots\cdot i_d!}\left|\int_{\mathbb{R}^d}\frac{h_{\mathbf{r}}(u)e^{-\lambda|u|^2}u_1^{i_1}\cdot\ldots u_d^{i_d}}{|u|}du\right|^2\frac{d\lambda}{\lambda^{\gamma+1}}. \qquad (4.11)
\end{aligned}
$$

ig

Hence we have $I_{\mathbf{r}} \geqslant 0$, and $I_{\mathbf{r}} = 0$ only when for all the $i_1,\dots,i_d \geqslant 0$, $i_1+\dots+i_d \geqslant 1$, and almost every $\lambda \geqslant 0$,

$$\int_{\mathbb{R}^d}\frac{h_{\mathbf{r}}(u)e^{-\lambda|u|^2}u_1^{i_1}\cdot\ldots u_d^{i_d}}{|u|}du = 0.$$

Then, by Lemma 4.4, $I_{\mathbf{r}} = 0$ if and only if $h = 0$ almost everywhere in $\mathbb{R}^d$.

Next, consider the case when $\theta \in (1,2)$. Note first that $D_\psi^\triangle(u,v)$ with $\psi(u) = |u|^\theta$ is positive definite by Lemma 4.3, so is its powers. Then, continuing from (4.10), we have

$$
\begin{aligned}
I_2 &\geqslant C_\gamma \int_0^\infty \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} h_{\mathbf{r}}(u)h_{\mathbf{r}}(v)\frac{\langle u,v\rangle}{|u||v|}e^{-\lambda(|u|^\theta+|v|^\theta+a)}D_\psi^\triangle(u,v)dudv\frac{d\lambda}{\lambda^{\gamma+1}}\\
&= C_\gamma e^{-\lambda a}\int_0^\infty \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \widetilde{h}_{\mathbf{r}}(u)\widetilde{h}_{\mathbf{r}}(v)\frac{\langle u,v\rangle}{|u||v|}(|u|^{2\gamma}+|v|^{2\gamma}-|u-v|^{2\gamma})dudv\frac{d\lambda}{\lambda^{\gamma+1}},
\end{aligned}
$$

where $\widetilde{h}_{\mathbf{r}}(u) := h_{\mathbf{r}}(u)e^{-\lambda|u|^\theta}$ and in the equality, we rewrite $D_\psi^\triangle(u,v) = |u|^{2\gamma}+|v|^{2\gamma}-|u-v|^{2\gamma}$ with $\gamma = \theta/2$. This returns to the above case when $\theta = 2$. □

Proof of Theorem 4.2 . Note first that $D_{\Phi_0}^\triangle(u,v)$ and $D_\Psi^\square(u,v)]$ are positive definite by Lemma 4.3. We prove the theorem by separating it into the following cases:

- Case I: $\gamma = 1$ and $\theta \in (0,2]$;
- Case II: $\gamma \in (0,1)$ and $\theta \in (1,2]$

Case I: when $\gamma = 1$ and $\theta = (1,2]$. We detail only the case $\theta = 2$, and the proof for case when $\theta \in (1,2)$ is similar to those in Proposition 4.5 by using Gamma function. Note that $D^{\triangle}_{\Phi_0}(u,v) = 2\langle u,v\rangle$. With $Z_1 = \frac{1}{Z}e^{\frac{2c_2}{N}\Psi(0)+\frac{2c_1 a}{N}}$, we have

$$I_\infty(h) \quad = \quad Z_1 \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^{(N-3)d}} \overline{h}_{\mathbf{r}}(u)\overline{h}_{\mathbf{r}}(v)\frac{\langle u,v\rangle}{|u||v|}e^{\frac{4c_1\langle u,v\rangle}{N}}e^{\frac{2c_2}{N}D^{\square}_{\Psi}(u,v)}d\mathbf{r}_{14}\cdots d\mathbf{r}_{1N}dudv.$$

Since $D^{\square}_{\Psi}(u,v)$ is positive definite, and so is any power of it by Theorem 6.2(2). Thus,

$$\begin{aligned} I_\infty(h) &= Z_1 \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^{(N-3)d}} \overline{h}_{\mathbf{r}}(u)\overline{h}_{\mathbf{r}}(v)\frac{\langle u,v\rangle}{|u||v|}e^{\frac{4c_1\langle u,v\rangle}{N}} \\ &\quad \times \sum_{k=0}^{\infty}\frac{1}{k!}\left[\frac{2c_2}{N}D^{\square}_{\Psi}(u,v)\right]^k d\mathbf{r}_{14}\cdots d\mathbf{r}_{1N}dudv \\ &\geqslant Z_1 \int_{\mathbb{R}^d}\int_{\mathbb{R}^{(N-3)d}} \overline{h}_{\mathbf{r}}(u)\overline{h}_{\mathbf{r}}(v)\frac{\langle u,v\rangle}{|u||v|}e^{\frac{4c_1\langle u,v\rangle}{N}}d\mathbf{r}_{14}\cdots d\mathbf{r}_{1N}dudv. \end{aligned}$$

Expanding the term $e^{\frac{4c_1\langle u,v\rangle}{N}}$ into polynomials, we have

$$\begin{aligned} I_\infty(h) &\geqslant Z_1 \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^{(N-3)d}} \overline{h}_{\mathbf{r}}(u)\overline{h}_{\mathbf{r}}(v)\frac{1}{|u||v|}\sum_{k=0}^{\infty}\frac{(4c_1)^k\langle u,v\rangle^{k+1}}{k!N^k}d\mathbf{r}_{14}\cdots d\mathbf{r}_{1N}dudv \\ &= Z_1 \int_{\mathbb{R}^{(N-3)d}} \sum_{\substack{i_1,\ldots,i_d\geqslant 0,\\ k=i_1+\ldots+i_d\geqslant 1}} \frac{(4c_1/N)^{k-1}k}{i_1!\ldots i_d!}\left|\int_{\mathbb{R}^d}\frac{\overline{h}_{\mathbf{r}}(u)u_1^{i_1}\cdots u_d^{i_d}}{|u|}du\right|^2 d\mathbf{r}_{14}\cdots d\mathbf{r}_{1N}. \end{aligned} \tag{4.12}$$

eq:h*1

Hence $I_\infty(h) \geqslant 0$ and $I_\infty(h) = 0$ if and only if for any $i_1+\ldots+i_d \geqslant 1$, $i_1,\ldots,i_d \geqslant 0$, and almost every $(\mathbf{r}_{14},\ldots\mathbf{r}_{1N}) \in \mathbb{R}^{(N-3)d}$

$$\int_{\mathbb{R}^d}\frac{\overline{h}_{\mathbf{r}}(u)u_1^{i_1}\cdots u_d^{i_d}}{|u|}du = 0.$$

From the expression (4.7) and Lemma 4.4, we obtain that $I_\infty(h) = 0$ if and only if $h = 0$ almost everywhere.

Case II: when $\gamma \in (0,1)$ and $\theta \in (1,2]$. Noticing that

$$\Phi(|u|)+\Phi(|v|)-\Phi(|u-v|)-c_2\Psi(0) = c_1 D^{\triangle}_{\Phi_0}(u,v)+c_2 D^{\square}_{\Psi}(u,v)$$

is positive definite and so are its powers, we have

$$\begin{aligned} I &\geqslant e^{\frac{2c_2}{N}\Psi(0)}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^{(N-3)d}} \overline{h}_{\mathbf{r}}(u)\overline{h}_{\mathbf{r}}(v)\frac{\langle u,v\rangle}{|u||v|} \\ &\quad \frac{2}{N}\left[\Phi(|u|)+\Phi(|v|)-\Phi(|u-v|)-c_2\Psi(0)\right]d\mathbf{r}_{14}\cdots d\mathbf{r}_{1N}dudv \\ &= e^{\frac{2c_2}{N}\Psi(0)}(I_3+I_4), \end{aligned}$$

where

$$
\begin{aligned}
I_3 &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^{(N-3)d}} \overline{h}_{\mathbf{r}}(u)\overline{h}_{\mathbf{r}}(v)\frac{\langle u,v\rangle}{|u||v|}\frac{2c_1}{N}D^{\triangle}_{\Phi_0}(u,v)d\mathbf{r}_{14}\cdots d\mathbf{r}_{1N}dudv,\\
I_4 &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^{(N-3)d}} \overline{h}_{\mathbf{r}}(u)\overline{h}_{\mathbf{r}}(v)\frac{\langle u,v\rangle}{|u||v|}\frac{2c_2}{N}D^{\square}_{\Psi}(u,v)d\mathbf{r}_{14}\cdots d\mathbf{r}_{1N}dudv.
\end{aligned}
$$

Note that $I_4 \geqslant 0$ by the positive definiteness of $D^{\square}_{\Psi}(u,v)$. We may write

$$
I_3 = e^{\frac{2c_2}{N}\Psi(0)}\int_{\mathbb{R}^{(N-3)d}} I_{\mathbf{r}} d\mathbf{r}_{14}\cdots d\mathbf{r}_{1N},
$$

where

$$
I_{\mathbf{r}} = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \overline{h}_{\mathbf{r}}(u)\overline{h}_{\mathbf{r}}(v)\frac{\langle u,v\rangle}{|u||v|}\frac{2c_1}{N}D^{\triangle}_{\Phi_0}(u,v)dudv
$$

By Proposition 4.5, we obtain that $I_{\mathbf{r}} \geqslant 0$, and $I_{\mathbf{r}} = 0$ if and only if $h_{\mathbf{r}} = 0$ almost everywhere on $\mathbb{R}^d$. Hence we have $I_3 \geqslant 0$, and $I_3 > 0$ for all $h \neq 0$. Then the theorem follows. ☐

The major effort in the above proof of Theorem 4.2 is to deal with the inner product term $\frac{\langle u,v\rangle}{|u||v|}$ in the definition of $I_\infty(h)$. When the inner product is removed, the above proof directly implies that $p_\infty(u,v)$ is strictly positive definite. The following lemma shows that the function $f(u,v)$ in (2.7), which is part of $p_\infty(u,v)$, is also strictly positive definite.

lm:fuv_pd

Lemma 4.6. *Let $\Phi : \mathbb{R}^d \to \mathbb{R}$ be a continuous function.*

1. *For any fixed $\mathbf{r}_{14}, \mathbf{r}_{15}, \ldots, \mathbf{r}_{1N} \in \mathbb{R}^d$,*

$$
g_{\mathbf{r}}(u,v) := \sum_{4\leqslant i<j\leqslant N}\Phi(|\mathbf{r}_{1i}-\mathbf{r}_{1j}|) + \sum_{1\leqslant l\leqslant N}\left[\Phi(|\mathbf{r}_{1l}|)+\Phi(|u-\mathbf{r}_{1l}|)+\Phi(|v-\mathbf{r}_{1l}|)\right],
$$

as a function of (u,v) is negative definite.

2. *The function $f(u,v) : \mathbb{R}^d\times\mathbb{R}^d \to \mathbb{R}$, as defined in (2.7), is strictly positive definite.*

Proof. We first prove Part (1). First note that $g_{\mathbf{r}}(u,v) = g_{\mathbf{r}}(v,u)$. Moreover, for any real numbers $\{c_i\}_{i=1}^k$ satisfying $\sum_{i=1}^k c_i = 0$, we have

$$
\sum_{i=1}^k\sum_{j=1}^k c_ic_jg_{\mathbf{r}}(u_i,u_j) = 0.
$$

Then, following from Definition 6.1, the function $g_{\mathbf{r}}(u,v)$ is negative definite.

The strict positive definiteness of $f(u,v)$ follows from the fact that for any fixed $(\mathbf{r}_{14}, \mathbf{r}_{15}, \ldots, \mathbf{r}_{1N})$, the integrand $e^{-\frac{2}{N}g_{\mathbf{r}}(u,v)}$ is strictly positive definite as a function of (u,v) since by Part (1), $g_{\mathbf{r}}(u,v)$ is negative definite. ☐

5 Coercivity of mean densities

:coercivityMean

Let $\mathbf{X}^t \in \mathbb{R}^d$ be the solution of (1.1). Let $p_t(u,v)$ be the density function for $(\mathbf{X}_1 - \mathbf{X}_2, \mathbf{X}_1 - \mathbf{X}_3)$ at time t, and correspondingly, with $p_\infty(u,v)$ being the stationary density. We show in this section that the coercivity condition holds true on a class of finite dimensional spaces $\mathcal{H} \in L^2(\rho_T)$ on $[0,T]$ when T is large, where ρ_T is the marginal density of the mean density of $p_t(u,v)$ on $[0,T]$, that is,

$$\bar{p}_T(u,v) = \frac{1}{T}\int_0^T p_t(u,v)dt, \quad \bar{\rho}_T(u) = \int_{\mathbb{R}^d} \bar{p}_T(u,v)dv. \tag{5.1}$$

eq:meanPDF

:coercivityMean

Theorem 5.1. *Consider the system (2.3) with the potential Φ given by (4.1) and with initial condition satisfying (3.1). Let $\bar{\rho}_T$ and $I_\infty(h)$ be defined as in (5.1) and (4.3), respectively. Then, the coercivity condition holds true on any finite-dimensional function space $\mathcal{H} \subset L^2(\bar{\rho}_T)$ such that*

$$S_{\mathcal{H}} := \sup_{0\neq h\in\mathcal{H}} \frac{\|h\|_\infty^2}{I_\infty(h)} < \infty, \tag{5.2}$$

S_H

when $T > (1+4S_{\mathcal{H}})T_{c,\mathcal{H}}$ with $T_{c,\mathcal{H}} := (8CNS_{\mathcal{H}}^2)^{1/\kappa}$, where κ is defined in (3.3), ρ_T is defined in (5.1), and $\|h\|_\infty = \sup_{u\in\mathbb{R}^d}|h(u)|$. That is, there exists a constant $c_{\mathcal{H},T} > 0$ such that for all $h \in \mathcal{H}$,

$$\bar{I}_T(h) := \frac{1}{T}\int_0^T \int_{\mathbb{R}^d} h(u)\frac{\langle u,v\rangle}{|u||v|}p_t(u,v)h(v)dudv \geqslant c_{\mathcal{H},T}\|h\|^2_{L^2(\bar{\rho}_T)}.$$

Remark 5.2. *(i) Condition (5.2) is in fact a strong version of the coercivity condition with respect to the uniform norm at the stationary density: it is equivalent to*

$$I_\infty(h) \geqslant S_{\mathcal{H}}^{-1}\|h\|_\infty^2, \text{ for all } h \in \mathcal{H}.$$

By requiring more regularity (uniform norm versus $L^2(\rho)$) at the stationary density, we gain coercivity in time. (ii) An analytical verification of Condition (5.2) is often out of reach except the Gaussian case, since the stationary measure p_∞ involves a marginalization of a non-Gaussian distribution. One may obtain a glimpse of the condition on h from (4.12) and (4.11), and may require that

$$S_{\mathcal{H}} := \sup_{0\neq h\in\mathcal{H}} \frac{\|h\|_\infty^2}{\|h\|_*^2} < \infty,$$

by assuming that $I_\infty(h)$ is bounded from below by $\|h\|_*^2$ given by

$$\|h\|_*^2 := \sum_{\substack{i_1,\ldots,i_d\geqslant 0,\\ k=i_1+\ldots+i_d\geqslant 1}} \int_0^\infty e^{-\lambda a}\frac{(2\lambda)^{k-1}k}{i_1!\cdot\ldots\cdot i_d!}\left|\int_{\mathbb{R}^d}\frac{h(u)e^{-\lambda|u|^2}u_1^{i_1}\cdot\ldots\cdot u_d^{i_d}}{|u|}du\right|^2\frac{d\lambda}{\lambda^{\gamma+1}}.$$

(iii) On the other hand, in practice, this condition can be numerically verified because

$$I_\infty(h) = \mathbb{E}_\infty\left[h(\mathbf{r}_{12})h(\mathbf{r}_{13})\frac{\langle\mathbf{r}_{12},\mathbf{r}_{13}\rangle}{|\mathbf{r}_{12}||\mathbf{r}_{13}|}\right]$$

and the expectation can be approximated by samples from data.

Lemma 5.3. *For each nonzero $h \in L^2(\bar{\rho})$, if*

$$t > T_{c,h} := C^{\frac{1}{\kappa}} \left(\frac{2\|h\|_\infty^2}{I_\infty(h)} \right)^{\frac{2}{\kappa}} < \infty, \tag{5.3}$$

then

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} h(u) \frac{\langle u, v \rangle}{|u||v|} p_t(u,v) h(v) du dv \geqslant \frac{1}{2} I_\infty(h)$$

If

$$T \geqslant \left(1 + \frac{4\|h\|_\infty^2}{I_\infty(h)}\right) T_{c,h} \tag{5.4}$$

then

$$\frac{1}{T} \int_0^T \int_{\mathbb{R}^d} h(u) \frac{\langle u, v \rangle}{|u||v|} p_t(u,v) h(v) du dv \geqslant \frac{\|h\|_\infty^2}{I_\infty(h) + 4\|h\|_\infty^2} I_\infty(h).$$

Proof. We first prove Part (1). Note that by Proposition 3.2,

$$\begin{aligned} & \left| \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} h(u) \frac{\langle u, v \rangle}{|u||v|} (p_t(u,v) - p_\infty(u,v)) h(v) du dv \right| \\ \leqslant \quad & \|h\|_\infty^2 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} |p_t(u,v) - p_\infty(u,v)| \, du dv \leqslant \|h\|_\infty^2 C t^{-\kappa/2}. \end{aligned}$$

Hence,

$$\begin{aligned} & \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} h(u) \frac{\langle u, v \rangle}{|u||v|} p_t(u,v) h(v) du dv \\ \geqslant \quad & I_\infty(h) - \left| \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} h(u) \frac{\langle u, v \rangle}{|u||v|} \left[p_t(u,v) - p_\infty(u,v) \right] h(v) du dv \right| \\ \geqslant \quad & I_\infty(h) - \|h\|_\infty^2 C t^{-\kappa/2}. \end{aligned} \tag{5.5}$$

If (5.3) holds, we have

$$I_\infty(h) \geqslant 2\|h\|_\infty^2 C t^{-\kappa/2}.$$

Then Part I follows from (5.5).

Now we prove Part (2). Note that

$$\begin{aligned} \bar{I}_T(h) \quad &= \quad \frac{1}{T} \left[\int_0^{T_c} \int_{\mathbb{R}^d} h(u) \frac{\langle u, v \rangle}{|u||v|} p_t(u,v) h(v) du dv + \int_{T_c}^T \int_{\mathbb{R}^d} h(u) \frac{\langle u, v \rangle}{|u||v|} p_t(u,v) h(v) du dv \right] \\ &\geqslant \quad \frac{1}{T} \left[\frac{1}{2} I_\infty(h)(T - T_c) - \|h\|_\infty^2 T_c \right]. \end{aligned} \tag{5.6}$$

If (5.4) holds, we have

$$\frac{1}{2} I_\infty(h)(T - T_c) \geqslant 2\|h\|_\infty^2 T_c$$

and

$$T - T_c \geqslant \frac{4\|h\|_\infty^2}{I_\infty(h) + 4\|h\|_\infty^2} T$$

Then

$$\bar{I}_T(h) \geqslant I_\infty(h)\frac{1}{4T}(T - T_c) \geqslant \frac{\|h\|_\infty^2}{I_\infty(h) + 4\|h\|_\infty^2} I_\infty(h).$$

Then Part (2) follows. □

Proof of Theorem 5.1. We show first that $\bar{I}_T(h) > 0$ when $h \neq 0$ in $L^2(\bar{\rho}_T)$. Note that if $t > T_{c,\mathcal{H}}$, equivalently, $t^{-\kappa/2} < \frac{1}{2}(CS_{\mathcal{H}})^{-1}$, we have $1 - CS_{\mathcal{H}} t^{-\kappa/2} \geqslant 1/2$. Then, it follows from (5.5) that

$$\begin{aligned}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} h(u)\frac{\langle u, v\rangle}{|u||v|}p_t(u,v)h(v)dudv &\geqslant I_\infty(h)(1 - \|h\|_\infty^2 C t^{-\kappa/2}) \\ &\geqslant I_\infty(h)(1 - S_{\mathcal{H}} t^{-\kappa/2}) \geqslant \frac{1}{2} I_\infty(h).\end{aligned}$$

Hence, as in (5.6), we have,

$$\begin{aligned}\bar{I}_T(h) &\geqslant I_\infty(h)\frac{1}{T}\left[\frac{1}{2}(T - T_{c,\mathcal{H}}) - S_{\mathcal{H}}^2 T_{c,\mathcal{H}}\right] \\ &\geqslant I_\infty(h)\frac{1}{4T}(T - T_{c,\mathcal{H}}) \geqslant I_\infty(h)\frac{4S_{\mathcal{H}}}{1 + 4S_{\mathcal{H}}}.\end{aligned}$$

where in the last two inequalities we used the facts that $T - T_{c,\mathcal{H}} > 4S_{\mathcal{H}} T_{c,\mathcal{H}}$ and $\frac{T - T_{c,\mathcal{H}}}{T} > \frac{4S_{\mathcal{H}}}{1+4S_{\mathcal{H}}}$, both following directly from that $T > (1 + 4S_{\mathcal{H}})T_{c,\mathcal{H}}$. By Theorem 4.2, $I_\infty(h) = 0$ only if $h = 0$ almost everywhere. Thus, $\bar{I}_T(h) > 0$ when $h \neq 0$ in $L^2(\bar{\rho}_T)$.

Next, to prove the coercivity condition, suppose on the contrary it does not hold, that is, there exists a sequence of nonzero functions $\{h_n\} \subset \mathcal{H}$ such that $\frac{\bar{I}_T(h_n)}{\|h_n\|_{L^2(\rho)}^2} \to 0$. Since $\mathcal{H}$ is finite dimensional, the normalized sequence $\bar{h}_n = \frac{h_n}{\|h_n\|_{L^2(\rho_T)}}$ has a convergence subsequence. Denote the limit by $\bar{h}$. Then, we have $\bar{I}_T(\bar{h}) = 0$ and $\|\bar{h}\|_{L^2(\rho_T)} = 1$, a contradiction. □

6 Appendix: positive definite kernels

sec:append

In this section, we review the definitions of positive and negative definite kernels, as well as their basic properties. The following definition is a real version of the definition in [1, p.67].

def_spd

Definition 6.1. *Let X be a nonempty set. A function $\phi : X \times X \to \mathbb{R}$ is called a (real) positive definite kernel if and only if it is symmetric (i.e. $\phi(x, y) = \phi(y, x)$) and*

$$\sum_{j,k=1}^{n} c_j c_k \phi(x_j, x_k) \geqslant 0 \tag{6.1}$$

for all $n \in \mathbb{N}$*,* $\{x_1, \ldots, x_n\} \subset X$ *and* $\mathbf{c} = (c_1, \ldots, c_n) \in \mathbb{R}^n$*. The function* ϕ *is called strictly positive definite if the equality holds only when* $\mathbf{c} = \mathbf{0} \in \mathbb{R}^n$*. We call the function* ϕ *a (real) negative definite kernel if and only if it is symmetric and*

$$\sum_{j,k=1}^{n} c_j c_k \phi(x_j, x_k) \leqslant 0 \tag{6.2}$$

for all $n \geqslant 2$*,* $\{x_1, \ldots, x_n\} \in X$ *and* $\{c_1, \ldots, c_n\} \in \mathbb{R}$ *with* $\sum_{j=1}^{n} c_j = 0$*.*

Remark. In the definition of positive definiteness in [1, p.67], a function $\phi : X \times X \to \mathbb{C}$ is positive definite if and only if

$$\sum_{j,k=1}^{n} c_j \bar{c}_k \phi(x_j, x_k) \geqslant 0 \tag{6.3}$$

for all $n \in \mathbb{N}$, $\{x_1, \ldots, x_n\} \in X$ and $\{c_1, \ldots, c_n\} \in \mathbb{C}$, where $\bar{c}$ denotes the complex conjugate of a complex number c. It is straightforward to check that when ϕ is real-valued and symmetric, the definitions (6.1) and (6.3) are equivalent. Similarly, In the definition of negative definiteness in [1, p.67], a function $\phi : X \times X \to \mathbb{C}$ is negative definite if and only if it is Hermitian (i.e. $\phi(x, y) = \overline{\phi(y, x)}$) and

$$\sum_{j,k=1}^{n} c_j \bar{c}_k \phi(x_j, x_k) \leqslant 0 \tag{6.4}$$

for all $n \geqslant 2$, $\{x_1, \ldots, x_n\} \in X$ and $\{c_1, \ldots, c_n\} \in \mathbb{C}$ with $\sum_{j=1}^{n} c_j = 0$. We can again check that when ϕ is real-valued, the definitions (6.2) and (6.4) are equivalent. In this paper, we only consider real-valued, symmetric kernels.

t52 **Theorem 6.2** (Properties of positive definite kernels)**.** *Suppose that* $k, k_1, k_2 : \mathcal{X} \times \mathcal{X} \subset \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ *are positive definite kernels. Then*

1. $c_1 k_1 + c_2 k_2$ *is positive definite, for* $c_1, c_2 \geqslant 0$
2. $k_1 k_2$ *is positive definite. ([1, p.69])*
3. $\exp(k)$ *is positive definite. ([1, p.70])*
4. $k(f(u), f(v))$ *is positive definite for any map* $f : \mathbb{R}^d \to \mathbb{R}^d$
5. *Inner product* $\langle u, v\rangle = \sum_{j=1}^{d} u_j v_j$ *is positive definite ([1, p.73])*
6. $f(u)f(v)$ *is positive definite for any function* $f : \mathcal{X} \to \mathbb{R}$ *([1, p.69]).*
7. *If* $k(u, v)$ *is measurable and integrable, then* $\iint k(u, v)\,du\,dv \geqslant 0$ *([10, p.524])*

pdm **Theorem 6.3.** [1, Theorem 3.1.17] Let $\phi : X \times X \to \mathbb{R}$ be symmetric. Then ϕ is positive definite if and only if

$$\det(\phi(x_j, x_k)_{j,k \leqslant n}) \geqslant 0$$

for all $n \in \mathbb{N}$ and all $\{x_1, \ldots, x_n\} \subseteq X$.

tpn **Theorem 6.4.** [1, Lemma 3.2.1] Let X be a nonempty set, $x_0 \in X$ and let $\psi : X \times X \to \mathbb{R}$ be a symmetric kernel. Put $\phi(x,y) := \psi(x,x_0) + \psi(y,x_0) - \psi(x,y) - \psi(x_0,x_0)$. Then ϕ is positive definite if and only if ψ is negative definite. If $\psi(x_0,x_0) \geqslant 0$, then $\phi_0(x,y) = \psi(x,x_0) + \psi(y,x_0) - \psi(x,y)$ is positive definite if and only if ψ is negative definite.

t53 **Theorem 6.5.** *Let X be a nonempty set and let $\psi : X \times X \to \mathbb{R}$ be a kernel. Then ψ is negative definite if and only if $\exp(-t\psi)$ is positive definite for all $t > 0$.*

Proof. The complex version of this theorem is proved in Theorem 3.2.2 of of [1]. The real version can be proved in a similar way. □

t54 **Theorem 6.6.** *If $\psi : X \times X \to \mathbb{R}$ is negative definite and $\psi(x,x) \geqslant 0$, then so are ψ^α for $0 < \alpha < 1$ and $\log(1+\psi)$.*

Proof. The complex version of this theorem is proved in Theorem 3.2.10 of [1]. The real version can be proved in a similar way. □

t55 **Theorem 6.7.** [1, Proposition 3.3.2] Let X be nonempty and $\psi : X \times X \to \mathbb{C}$ be negative definite. Assume $\{(x,y) \in X \times X, \psi(x,y) = 0\} = \{(x,x) : x \in X\}$, then $\sqrt{\psi}$ is a metric on X.

l22 **Lemma 6.8.** *Let*

$$\phi(x,y) = x^\gamma + y^\gamma - (x+y)^\gamma. \tag{6.5}$$

When $\gamma \in (0,1)$, $\phi(x,y)$ is positive definite on $[0,\infty) \times [0,\infty)$.

Proof. Let $\psi_\gamma(x,y) = (x+y)^\gamma$. Then $\psi_1(x,y) = x + y$ is negative definite. By Theorem 6.6, for $\gamma \in (0,1)$, $\psi_\gamma(x,y)$ is negative definite since $\psi_\gamma(x,x) \geqslant 0$, when $x \geqslant 0$. Then

$$\phi(x,y) = \psi_\gamma(x,0) + \psi_\gamma(0,y) - \psi_\gamma(x,y)$$

is positive definite by Theorem 6.4. □

l23 **Lemma 6.9.** *Let $\phi(x,y)$ be defined as in (6.5). Let $g : \mathbb{R}^d \to [0,\infty)$ be a function. Then*

$$\tilde{\phi}(u,v) = \phi(g(u), g(v))$$

is positive definite on $\mathbb{R}^d \times \mathbb{R}^d$.

Proof. For any $c_1, \ldots, c_n \in \mathbb{R}$ and $u_1, \ldots, u_n \in \mathbb{R}^d$, let $x_i = g(u_i)$. Then we have

$$\sum_{i,j=1}^n c_i c_j \tilde{\phi}(u_i,u_j) = \sum_{i,j=1}^n c_i c_j \phi(g(u_i), g(u_j)) = \sum_{i,j=1}^n c_i c_j \phi(x_i,x_j) \geqslant 0,$$

by the positive definiteness of ϕ in Lemma 6.8. Then the lemma follows. □

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