

Spectral convergence of diffusion maps: improved error bounds and an alternative normalisation

Caroline L. Wormell* Sebastian Reich†

June 3, 2020

Abstract

Diffusion maps is a manifold learning algorithm widely used for dimensionality reduction. Using a sample from a distribution, it approximates the eigenvalues and eigenfunctions of associated Laplace-Beltrami operators. Theoretical bounds on the approximation error are however generally much weaker than the rates that are seen in practice. This paper uses new approaches to improve the error bounds in the model case where the distribution is supported on a hypertorus. For the data sampling (variance) component of the error we make spatially localised compact embedding estimates on certain Hardy spaces; we study the deterministic (bias) component as a perturbation of the Laplace-Beltrami operator's associated PDE, and apply relevant spectral stability results. Using these approaches, we match long-standing pointwise error bounds for both the spectral data and the norm convergence of the operator discretisation.

We also introduce an alternative normalisation for diffusion maps based on Sinkhorn weights. This normalisation approximates a Langevin diffusion on the sample and yields a symmetric operator approximation. We prove that it has better convergence compared with the standard normalisation on flat domains, and present a highly efficient algorithm to compute the Sinkhorn weights.

1 Introduction

Many problems in data science revolve around the extraction of information about the geometry of some probability distribution given only a sample that may possibly be embedded in an ambient space of much higher dimension: examples of these problems include clustering and dimension reduction. The intrinsic geometry of such a distribution may be encoded by various weighted Laplace-Beltrami operators, from whose spectral data various desiderata can be extracted: for example, the operator's eigenfunctions may be used to define intrinsic coordinates for the support of the distribution (Coifman et al. 2005, Coifman & Lafon 2006), or may be used in spectral clustering algorithms (Nadler et al. 2006).

Diffusion maps is a widely-used algorithm to recover the relevant eigendata (Coifman et al. 2005, Coifman & Lafon 2006): the idea is to construct a particle discretisation of the evolution of a weighted Laplace-Beltrami operator \mathcal{L} over some short timestep ε . To this end, a kernel matrix K is first constructed:

$$K = \left(\frac{1}{M} k_\varepsilon(d(x^i, x^j)) \right)_{i,j=1,\dots,M}, \quad (1)$$

*School of Mathematics & Statistics, The University of Sydney, ca.wormell@gmail.com

†Department of Mathematics, University of Potsdam

where the $x^i \sim \rho dx$ are the sample points, k_ε is a symmetric probability kernel with covariance matrix εI . The kernel matrix is then normalised to be Markov (i.e. row-stochastic)

$$P = \text{diag}(Ku)^{-1}K \text{diag}(u), \quad (2)$$

for some appropriately chosen weight vector $u \in \mathbb{R}^M$.

As the sample size M is taken to infinity and the diffusion timestep ε is taken to zero with an appropriate dependence on M (Lindenbaum et al. 2017), the spectral data of P should approximate that of the Laplace-Beltrami operator semigroup $e^{\varepsilon\mathcal{L}}$, enabling reconstruction of the spectral data of the operator \mathcal{L} itself. (Indeed, this problem is often formulated as the graph Laplacian $L = \varepsilon^{-1}(P - I)$ approximating \mathcal{L} .) The Markov nature of the normalised matrix P means that the intrinsic coordinates provided by its leading eigenvectors faithfully reconstruct the intrinsic geometry of the distribution’s support (Coifman & Lafon 2006).

Standard choices of weights for these operators are of the form $\tilde{u} \equiv (K1)^{-\alpha}$, for some $\alpha \in [0, 1]$. In this case, the weighted Laplace-Beltrami operators to which the convergence occurs are

$$\check{\mathcal{L}}_\alpha \phi := \frac{1}{2}\Delta\phi + (1 - \alpha)\nabla \log \rho \cdot \nabla\phi = \frac{1}{2}\rho^{-(2-2\alpha)} \nabla \cdot (\rho^{2-2\alpha}\nabla\phi), \quad (3)$$

where ρ is the density of the distribution with respect to Lebesgue measure. The case $\alpha = 0$ (i.e. $\tilde{u} \equiv 1$) is the standard graph Laplacian normalisation; on the other hand, we recover for $\alpha = 1$ the unweighted Laplace-Beltrami operator, and for $\alpha = \frac{1}{2}$ the generator of the Langevin diffusion with invariant measure ρ (Coifman & Lafon 2006).

The last twenty years have seen a range of rigorous work establishing and bounding the convergence of diffusion maps and related methods. Because both a space and time discretisation occur, the error decomposes into two parts: a “variance” error of finite samples size M with the timestep ε held fixed, and a “bias” error from the positive timestep ε . For pointwise estimates on P , the errors associated with the two limits have been shown to be bounded respectively by $\mathcal{O}(M^{-1/2}\varepsilon^{-d/4})$ and $\mathcal{O}(\varepsilon^2)$ (Hein et al. 2005, Singer 2006). There are clear intuitions to these error rates: the first is a central limit theorem error between K and its infinite data limit, taking into account that of the M sample points, we expect $M_{\text{eff}} = \mathcal{O}(M\varepsilon^{d/2})$ to be in the effective support of the kernel; the second is a standard first-order discretisation error for a diffusion operator over timestep ε . It is natural to expect that the pointwise error of the discretisation should transfer to the spectral data: with the short timestep magnifying the errors by a factor of $\mathcal{O}(\varepsilon^{-1})$, this would yield an $\mathcal{O}(M^{-2/(8+d)})$ error for the optimal scaling of ε with M .

However, theoretical estimates for spectral data in the literature have been much weaker than this. The standard bound on the bias error in the spectral data has been the naive estimate of $\mathcal{O}(\varepsilon^{1/2})$, corresponding to the $L^p \rightarrow L^p$ operator error (Hein et al. 2005, Shi 2015, Trillos et al. 2019, Lu 2020). While the decay of the variance error as $M \rightarrow \infty$ with ε fixed has been long known as a result of the theory of Glivenko-Cantelli function classes (von Luxburg et al. 2004, 2008, Belkin & Niyogi 2007), this approach has yielded only weak quantitative bounds of $\mathcal{O}(M^{-1/2}\varepsilon^{-d-3})$ on the variance error (Shi 2015). Due to the dependence of the weights \tilde{u}_α on the sample for $\alpha \neq 0$, this approach has also largely been specialised to the graph Laplacian normalisation $\alpha = 0$. More recently optimal transport techniques have been applied to bound the variance error. These necessarily sacrifice the central limit theorem convergence in M for the much slower optimal transport rate of $\mathcal{O}((\frac{\log M}{M})^{1/d})$, but yield an overall error of $\mathcal{O}((\frac{\log M}{M})^{1/2d})$ in the eigenvalues for dimensions $d \geq 2$ (Trillos et al. 2019, Lu 2020). In Calder & Trillos (2019) these results were bootstrapped with (weaker) pointwise estimates to obtain a central limit theorem convergence in M with overall convergence rate of $\mathcal{O}((\frac{\log M}{M})^{1/d+4})$ on general manifolds. However, only completely unweighted graph Laplacians were studied, because study of weighted operators demands recursive application of the central limit theorem from the sample.

The first goal of our paper is to prove that for diffusion maps normalisations, the pointwise error bounds hold for the spectral data. This work is independent of Calder & Trillos (2019) and takes a different, more dynamical approach that defeats the recursivity problem and may in fact be applied very generally to kernel-based discretisation problems. This is because we fully carry through the pointwise convergence rates of diffusion maps discretisations to norm convergence of the discretised operators. For simplicity, we will assume the support of the measure is a flat torus $\mathbb{D} = (\mathbb{R}/L\mathbb{Z})^d$ and the sample points x^i are independent and identically distributed; we will use the standard Gaussian choice of kernel.

To achieve this goal we will apply new approaches to both the bias and variance components of the error. To bound the bias error, we will reformulate the problem as one of compact PDE evolution operators for which the perturbations are bounded from a strong norm to a weak norm, and apply the relevant spectral approximation theory (Keller & Liverani 1999). Our bounds on the variance error conservatively extend the pointwise error bound to operator errors in certain Hardy spaces via compact embedding estimates that, crucially, take advantage of the localisation of the kernel.

Combining these, we will obtain an spectral error of $\mathcal{O}(M^{-1/2}\varepsilon^{-1-d/4}(\log M\varepsilon^{-1})^{d-1/2} + \varepsilon)$: for optimal scaling $\varepsilon \sim M^{-2/(8+d)+o_M(1)}$, this gives a total error of $\mathcal{O}(M^{-2/(8+d)+o_M(1)})$. For larger dimensions $d \geq 3$, this is a major improvement over previous results for weighted Laplacians: for example, compared with Trillos et al. (2019) the accuracy is squared for $d = 8$. It is also a significant improvement on the unweighted Laplacian results of Calder & Trillos (2019). Our convergence rate for the variance error of spectral data estimates still remains weaker than variance errors observed empirically, although we believe the difference is only a small polynomial factor in ε . On the other hand, the $\mathcal{O}(\varepsilon)$ bias error bound appears optimal (from empirical results we believe this rate also carries across to curved manifolds). Our only assumptions on the sample density ρ are that it is bounded away from zero and $C^{3/2+\beta}$ Hölder for some $\beta > 0$ (i.e. a $C^{\beta'}$ first derivative for some $\beta > 1/2$).

Our theoretical approach facilitates the second goal of the paper: to propose and study a superior normalisation using Sinkhorn weights for the Langevin dynamics whose generator is

$$\mathcal{L}\phi := \tilde{\mathcal{L}}_{0.5}\phi = \frac{1}{2}\Delta\phi + \frac{1}{2}\nabla\log\rho \cdot \nabla\phi. \quad (4)$$

So-called Sinkhorn weights u , $1/(Ku)$ for a general matrix K are defined to be those making the row-stochastic matrix $P = \text{diag}(Ku)^{-1}K \text{diag}(u)$ also column-stochastic. This kind of matrix weighting problem has been studied since Sinkhorn (1964); it has seen recent interest in the context of computing entropically regularised optimal transport plans (Cuturi 2013, Altschuler et al. 2017, Feydy et al. 2019). In using Sinkhorn weights as a normalisation for diffusion maps, we will study the restricted case where the kernel matrix K is symmetric (and so one is computing a coupling of the sample's empirical measure ρ^M with itself). In this restricted case, such weights solve the (quadratic) problem

$$\text{diag}(u) = \text{diag}(Ku)^{-1}. \quad (5)$$

We will prove that, at least in the cases we consider, the Sinkhorn weights have an improved rate of convergence, with a bias error in eigendata improving to $\mathcal{O}(\varepsilon^2)$ from $\mathcal{O}(\varepsilon)$ for standard weights, while keeping the same $M \rightarrow \infty$ error rate. This means that, compared with the standard weights, a larger timestep $\varepsilon \sim M^{-2/(12+d)+o(1)}$ may be chosen with a further improved overall convergence rate of $\mathcal{O}(M^{-4/(12+d)+o(1)})$, although in practice ε has to be rather small, and thus M very large, for this convergence rate to take hold. For this convergence to hold it is only necessary that the density ρ be $C^{2+\beta}$ Hölder for $\beta > 0$.

Beyond this, the Sinkhorn normalisation has a range of advantageous and interesting properties for applications of diffusion maps. Uniquely among diffusion maps normalisations, the normalised matrix P is symmetric: its eigenvectors are therefore orthogonal with respect to the sample and they exactly perform a nonlinear principal component decomposition of the sample. Furthermore, the action of P preserves not only constant functions but also total integrals, which is of use for example in non-parametric forecasting (Berry et al. 2015).

While Sinkhorn weights must be computed iteratively, we also present an accelerated algorithm to calculate the weights that, by harnessing the symmetric nature of the problem, converges in $\mathcal{O}(1)$ matrix-vector multiplications. As a result, the use of Sinkhorn weights has minimal numerical overhead.

This paper is structured as follows. In Section 2 we define the mathematical objects used in the paper; in Section 3 we state the main theorems with a brief numerical illustration; in Section 4 we describe our accelerated Sinkhorn algorithm. We then turn to studying the convergence of relevant operators as the timestep $\varepsilon \rightarrow 0$, focussing on the more interesting case of the Sinkhorn normalisation. After stating some relevant functional-analytic results in Section 5 and describing the convergence of Sinkhorn weights as $\varepsilon \rightarrow 0$ in Section 6, we prove the necessary operator convergence result for the bias error in Section 7. We then consider the variance error, i.e. that of finite M : in Section 8 we bound the operator convergence of the kernel matrix K to a continuum limit in appropriate norms, and in Section 9 we do the same for the normalised matrix P ; in Section 10 we combine the two operator convergence results to prove the convergence of spectral data for the Sinkhorn weight case. Finally, we outline the corresponding results for standard weights in Section 11.

2 Notation

We now present some notation that will be used in the main theorems and throughout the paper.

2.1 Operators

We will use as our kernel function the periodic Gaussian kernel $k_\varepsilon(x, y) = g_{\varepsilon, L}(y - x)$:

$$g_{\varepsilon, L}(x) = \sum_{\mathbf{j} \in \mathbb{Z}^d} g_\varepsilon(x + L\mathbf{j}), \quad (6)$$

where the standard Gaussian kernel is

$$g_\varepsilon(x) = (2\pi\varepsilon)^{-d/2} e^{-\|x\|^2/2\varepsilon}. \quad (7)$$

Note that if, as is typical, the bandwidth $\sqrt{\varepsilon} \ll L$, all but one summand in (6) will be superexponentially small.

We define convolution by the periodic Gaussian kernel (6) as an operator

$$(\mathcal{C}_\varepsilon \phi)(x) = \int_{\mathbb{D}} g_{\varepsilon, L}(y - x) \phi(y) dx, \quad (8)$$

which has the semigroup property $\mathcal{C}_s \mathcal{C}_t = \mathcal{C}_{s+t}$.

In this paper we will interpolate the vectors and matrices introduced in the introduction by functions defined on the continuous domain \mathbb{D} . Our interpolation arises very naturally: the kernel

matrix K defined in (1) acting on vectors $(\phi(x^i))_{i=1,\dots,M}$ extends to the following operator

$$(\mathcal{K}_\varepsilon^M \phi)(x) := \frac{1}{M} \sum_{i=1}^M g_{\varepsilon,L}(x - x^i) \phi(x^i) = (\mathcal{C}_\varepsilon \rho^M \phi)(x), \quad (9)$$

where ρ^M is the empirical measure of the sample.

For Sinkhorn weights our weight vector u , defined in (5), then extends to the function U_ε^M given as the unique solution of

$$U_\varepsilon^M(x) (\mathcal{K}_\varepsilon^M U_\varepsilon^M)(x) \equiv 1. \quad (10)$$

Our normalised matrix then extends to the operator

$$(\mathcal{P}_\varepsilon^M \phi)(x) = U_\varepsilon^M(x) (\mathcal{K}_\varepsilon^M U_\varepsilon^M \phi)(x), \quad (11)$$

and the eigenvalues and eigenvectors (at the sample points) will be identical.

We will study a range of weighted operators of a form similar to (11) and we will write them for short in the following manner:

$$\mathcal{P}_\varepsilon^M = U_\varepsilon^M \mathcal{K}_\varepsilon^M U_\varepsilon^M.$$

In this paper we are required to consider two limits and their associated errors: the stochastic, so-called ‘‘variance’’ error as the finite sample size $M \rightarrow \infty$ for fixed timestep ε , and the deterministic, so-called ‘‘bias’’ error, in the spatial continuum limit as the timestep $\varepsilon \rightarrow 0$. We will show in Section 8 that the discrete kernel operator $\mathcal{K}_\varepsilon^M$ converges in the $M \rightarrow \infty$ data limit to a continuum kernel operator

$$(\mathcal{K}_\varepsilon \phi)(x) = \int g_\varepsilon(x - y) \phi(y) \rho(y) dy = (\mathcal{C}_\varepsilon \rho \phi)(x). \quad (12)$$

In the infinite data limit we will show in Section 9 that the U_ε^M converge to functions U_ε that satisfy a continuum version of the Sinkhorn problem

$$U_\varepsilon(x) (\mathcal{K}_\varepsilon U_\varepsilon)(x) \equiv 1. \quad (13)$$

From this we have a deterministic approximation to the semigroup $e^{\varepsilon \mathcal{L}}$

$$\mathcal{P}_\varepsilon = U_\varepsilon \mathcal{K}_\varepsilon U_\varepsilon, \quad (14)$$

to which we expect the normalised discrete operator $\mathcal{P}_\varepsilon^M$ to converge.

Because the two limits require the use of different function spaces to attain the appropriate convergence rates we will consider semi-conjugacies of our operators $\mathcal{P}_\varepsilon^M$ and \mathcal{P}_ε that will be bounded on the space of continuous functions C^0 . For concision, in this discussion we will take ‘‘ $\mathcal{A}_\varepsilon^{(M)}$ ’’ to mean ‘‘ \mathcal{A}_ε (resp. $\mathcal{A}_\varepsilon^M$)’’.

Using that $\mathcal{K}_\varepsilon^{(M)} = \mathcal{C}_{\varepsilon/2} \mathcal{K}_{\varepsilon/2}^{(M)}$ we will define the half-step weight functions

$$Y_\varepsilon^{(M)}(x) = (\mathcal{K}_{\varepsilon/2}^{(M)} U_\varepsilon^{(M)})(x) \quad (15)$$

and the half-step operators

$$\mathcal{G}_\varepsilon^{(M)} = U_\varepsilon^{(M)} \mathcal{C}_{\varepsilon/2} Y_\varepsilon^{(M)} \quad (16)$$

$$\mathcal{H}_\varepsilon^{(M)} = (Y_\varepsilon^{(M)})^{-1} \mathcal{K}_{\varepsilon/2}^{(M)} U_\varepsilon^{(M)}. \quad (17)$$

These operators $\mathcal{G}_\varepsilon^{(M)}, \mathcal{H}_\varepsilon^{(M)}$ are positive, preserve constant functions and have

$$\mathcal{P}_\varepsilon^{(M)} = \mathcal{G}_\varepsilon^{(M)} \mathcal{H}_\varepsilon^{(M)}.$$

We then define the following operators that are semi-conjugate to $(\mathcal{P}_\varepsilon^{(M)})^n$

$$\mathcal{Q}_{n,\varepsilon}^{(M)} = (\mathcal{H}_\varepsilon^{(M)} \mathcal{G}_\varepsilon^{(M)})^n. \quad (18)$$

To study the situation for the standard weights, we will define the kernel density estimate of the distribution using the sample:

$$\rho_\varepsilon^{(M)} = \mathcal{K}_\varepsilon^{(M)} \mathbf{1}$$

The weight vectors $\check{u}_\alpha := (K\mathbf{1})^{-\alpha}$ and $1/(K\check{u}_\alpha)$ then extend respectively to the functions

$$\check{U}_{\varepsilon,\alpha}^{(M)}(x) = (\rho_\varepsilon^{(M)}(x))^{-\alpha}. \quad (19)$$

$$\check{V}_{\varepsilon,\alpha}^{(M)}(x) = 1/(\mathcal{K}_\varepsilon^{(M)} \check{U}_{\varepsilon,\alpha}^{(M)})(x). \quad (20)$$

We then have the approximations to the semigroup $e^{\varepsilon \check{\mathcal{L}}_\alpha}$

$$\check{\mathcal{P}}_{\varepsilon,\alpha}^{(M)} = \check{V}_{\varepsilon,\alpha}^{(M)} \mathcal{K}_{\varepsilon,\alpha}^{(M)} \check{U}_{\varepsilon,\alpha}^{(M)},$$

and the equivalent $\check{Y}_{\varepsilon,\alpha}^{(M)}, \check{\mathcal{G}}_{\varepsilon,\alpha}^{(M)}, \check{\mathcal{H}}_{\varepsilon,\alpha}^{(M)}, \check{\mathcal{Q}}_{\varepsilon,\alpha}^{(M)}$ follow analogously.

2.2 Function spaces

We will use two different classes of function spaces to study the bias and variance error. To study the variance error, we will need spaces with very strongly compact embeddings into C^0 , specifically Hardy spaces of analytic functions. On the other hand, when considering the bias error we are comparing against the semigroup $e^{\varepsilon \mathcal{L}}$, and because of our relaxed conditions on the regularity of ρ , we can only expect the image of the semigroup to be contained in spaces of low differentiability.

To study the bias error, we will therefore make use of the scales of Sobolev spaces $W^{s,p} \subseteq L^p(\mathbb{D}, dx)$ for $s \geq 0, p \in (1, \infty]$, which each consist of function classes $[\phi]$ for which the norm

$$\|\phi\|_{W^{s,p}} := \|J^{s/2} \phi\|_{L^p},$$

is finite and well-defined, where the operator $J = I - \Delta$. For some operator \mathcal{A} that is sectorial (see Section 5) and thus for which a semigroup $e^{-t\mathcal{A}}, t \geq 0$ is defined, we define fractional powers as inverses of the injections (Henry 2006)

$$\mathcal{A}^{-s/2} := \Gamma(s/2)^{-1} \int_0^\infty t^{-s/2-1} e^{-t\mathcal{A}} dt, \quad s > 0. \quad (21)$$

The operator J is well-known to be sectorial on all $W^{s,p}$.

For integer $k \geq 0$ the space of k -times continuously differentiable functions C^k is a subset of $W^{k,\infty}$ with equivalent norms. Furthermore, for all $s' < s$, the Hölder space $C^{s'} \subseteq W^{s,\infty}$, and each $[\phi] \in W^{s,\infty}$ has an element $\phi \in C^s$: the inclusion maps between these function spaces are continuous.

On the other hand, to study the convergence of the particle discretisation (i.e. the variance error), we will use spaces of bounded analytic functions on narrow strips around the domain \mathbb{D} . We therefore define for $\zeta \geq 0$ the complex domains

$$\mathbb{D}_\zeta = \{x + iz \mid x \in \mathbb{D}, z \in [-\zeta, \zeta]^d\},$$

and the corresponding Hardy space

$$H^\infty(\mathbb{D}_\zeta) = \{\phi \in C^0(\mathbb{D}_\zeta) : \phi \text{ analytic on } \text{int } \mathbb{D}_\zeta\}$$

with norm

$$\|\phi\|_\zeta = \sup_{z \in \mathbb{D}_\zeta} |\phi(z)|.$$

Note that the Hardy space norm $\|\cdot\|_\zeta$ is always equal to or greater than $\|\cdot\|_0$, the C^0 norm on the real domain \mathbb{D} .

In this paper we will assume that our measure density ρ is strictly bounded away from zero, and that it lies in the Sobolev space $W^{s,\infty}$, where $s > 3/2$ for the standard normalisation and $s > 2$ for the Sinkhorn normalisation: it is equivalent to assume that $\rho \in C^{3/2+\beta}$ (resp. $\rho \in C^{2+\beta}$) for some $\beta > 0$.

2.3 Eigendata

The generator \mathcal{L} has eigenvalues $0 = -\lambda_0 > -\lambda_1 \geq -\lambda_2 \geq \dots$, and the semigroup approximations $\mathcal{P}_\varepsilon^{(M)}$ have respective eigenvalues $1 = e^{-\varepsilon\lambda_0^{(M)}} > e^{-\varepsilon\lambda_1^{(M)}} \geq e^{-\varepsilon\lambda_2^{(M)}} \geq \dots \geq 0$. Note that the non-negativity of these eigenvalues is guaranteed via positive semi-definiteness of $\mathcal{P}_\varepsilon^{(M)}$ in $L^2(\rho^{(M)})$. We denote the corresponding eigenspaces $E_k, E_{k,\varepsilon}^{(M)}$, and merge discretised eigenspaces whose eigenvalues will converge in the limit:

$$\bar{E}_{k,\varepsilon}^{(M)} := \bigoplus_{\lambda_j = \lambda_k} E_{k,\varepsilon}^{(M)}.$$

For the standard weights we define equivalent quantities (where we have positive semi-definiteness of $\check{\mathcal{P}}_{\varepsilon,\alpha}^{(M)}$ in $L^2(\rho^{(M)}(\check{U}_{\varepsilon,\alpha}^{(M)}/\check{V}_{\varepsilon,\alpha}^{(M)})^{1/2})$).

Finally, to quantify the convergence of eigenspaces, we define the distance between vector subspaces:

$$d_{C^0}(E, F) = \max \left\{ \sup_{\phi \in B_{C^0}(1) \cap E} d_{C^0}(\phi, F), \sup_{\phi \in B_{C^0}(1) \cap F} d_{C^0}(E, \phi) \right\}.$$

3 Main results

In this paper we will deterministically bound the ‘‘variance’’ errors, which depend on the empirical measure ρ^M , exclusively via an operator error δ :

$$\delta := \left\| \mathcal{K}_{\varepsilon/2}^M - \mathcal{K}_{\varepsilon/2} \right\|_{H^\infty(\mathbb{D}_\zeta) \rightarrow C^0},$$

where $\zeta = Z_0\varepsilon^{1/2}$ for some constant Z_0 . Thus, results in terms of δ can be applied to any point sample, including weighted, dependent and deterministic samples.

When the empirical measure is an *i.i.d.* sample from the true density ρ , we have the following probabilistic bound on δ :

Theorem 3.1. *Suppose $\rho \in L^\infty$. There exist constants C_{25}, C_{26} depending only on $L, d, \|\rho\|_0, \varepsilon_0, Z_0$ such that for all $\varepsilon < \varepsilon_0$ and $c < \frac{1}{4}\|\rho\|_0 \log 2$,*

$$\mathbb{P}(\delta > c) \leq \exp \left\{ C_{25}(\log c + \log \varepsilon^{-1})^{2d+1} - C_{26}M\varepsilon^{d/2}c^2 \right\}.$$

In other words, with very high probability

$$\delta = \mathcal{O} \left(M^{-1/2} \varepsilon^{-d/4} (\log M + \log \varepsilon^{-1})^{d-1/2} \right).$$

We can now state the main theorems, on convergence of spectral data for the diffusion maps approximations:

Theorem 3.2 (Spectral convergence for standard weights). *Suppose $\rho \in C^{3/2+\beta}$, $\beta > 0$. For all $\alpha \in [0, 1]$ and $\lambda_* > 0$ there exist constants $\check{C}_{101}, \check{C}_{102}, \check{C}_{103}$ such that if $\varepsilon + \varepsilon^{-1}\delta < \check{C}_{101}$, then for $-\lambda_{k,\alpha} \geq -\lambda_*$ we have*

(a) *Convergence of eigenvalues of $\check{\mathcal{P}}_{\varepsilon,\alpha}$ and $\check{\mathcal{P}}_{\varepsilon,\alpha}^M$:*

$$\begin{aligned} |\check{\lambda}_{k,\varepsilon,\alpha} - \check{\lambda}_{k,\alpha}| &\leq \check{C}_{102}\varepsilon \\ |\check{\lambda}_{k,\varepsilon,\alpha}^M - \check{\lambda}_{k,\alpha}| &\leq \check{C}_{102}(\varepsilon + \varepsilon^{-1}\delta). \end{aligned}$$

(b) *Convergence of the respective eigenspaces:*

$$\begin{aligned} d_{C^0}(\check{\check{E}}_{k,\varepsilon,\alpha}, \check{E}_{k,\alpha}) &\leq \check{C}_{103}\varepsilon \\ d_{C^0}(\check{\check{E}}_{k,\varepsilon,\alpha}^M, \check{E}_{k,\alpha}) &\leq \check{C}_{103}(\varepsilon + \varepsilon^{-1}\delta). \end{aligned}$$

Theorem 3.3 (Spectral convergence for Sinkhorn weights). *Suppose $\rho \in C^{2+\beta}$, $\beta > 0$. For all $\lambda_* > 0$ there exist constants $C_{101}, C_{102}, C_{103}$ such that if $\varepsilon^2 + \varepsilon^{-1}\delta < C_{101}$, then for $-\lambda_k \geq -\lambda_*$ we have*

(a) *Convergence of eigenvalues of \mathcal{P}_ε and $\mathcal{P}_\varepsilon^M$:*

$$\begin{aligned} |\lambda_{k,\varepsilon} - \lambda_k| &\leq C_{102}\varepsilon^2 \\ |\lambda_{k,\varepsilon}^M - \lambda_k| &\leq C_{102}(\varepsilon^2 + \varepsilon^{-1}\delta). \end{aligned}$$

(b) *Convergence of the respective eigenspaces:*

$$\begin{aligned} d_{C^0}(\bar{E}_{k,\varepsilon}, E_k) &\leq C_{103}\varepsilon^2 \\ d_{C^0}(\bar{E}_{k,\varepsilon}^M, E_k) &\leq C_{103}(\varepsilon^2 + \varepsilon^{-1}\delta). \end{aligned}$$

An empirical comparison of the bias errors for the standard and Sinkhorn normalisations on a $C^{2+\beta}$ sampling distribution is given in Figure 1, demonstrating the optimality of the bias error bounds, and the better convergence of the Sinkhorn normalisation for $\alpha = \frac{1}{2}$.

The empirical behaviour of variance errors for a three-dimensional example is given in Figure 2. Here the variance error in the spectral data appears to have the central limit theorem convergence in the sample size M that we have shown. However, this convergence occurs in the regime $M_{\text{eff}} = M\varepsilon^{d/2} \gg 1$, i.e. up to log terms that $\delta \ll 1$: this regime is larger than that covered

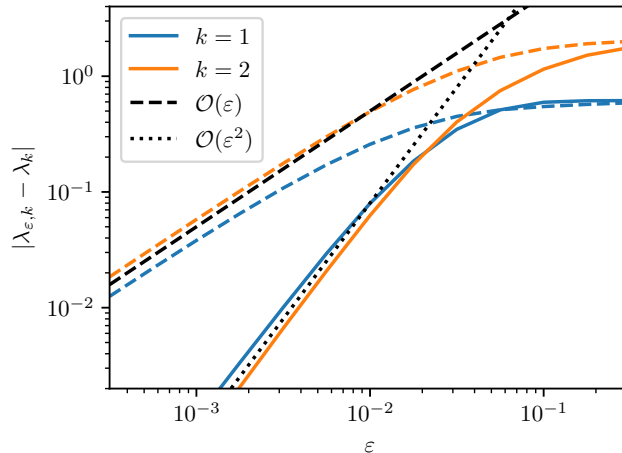


Figure 1: Bias error in eigenvalues for $C^{2.2^-}$ function density $\rho(x) = 1 + \frac{1-3^{-2.2}}{2} \sum_{j=1}^{\infty} 3^{-2.2j} \cos(3^j \cdot 2\pi x)$ on $\mathbb{D} = \mathbb{R}/\mathbb{Z}$ using a Sinkhorn normalisation (solid lines) and $\alpha = \frac{1}{2}$ standard normalisation (dashed lines). A Fourier operator discretisation with 2001 modes was used to compute the spectrum of the generator \mathcal{L} and discrete-time approximations $\mathcal{P}_\varepsilon, \check{\mathcal{P}}_{\varepsilon,1/2}$.

by our results, $\varepsilon^{-1}\delta \ll 1$. Furthermore, the dependence on the timestep ε appears to be more gentle than our results would suggest: as ε is decreased with M_{eff} fixed, the variance error in fact appears to decrease rather than increasing as $\mathcal{O}(\varepsilon^{-1})$. This is in accordance with previous observations that spectral estimates have better convergence than the pointwise estimates that our results match up to (Trillos et al. 2019, Calder & Trillos 2019).

Rather than the semigroup, one is often interested in approximating the Laplace-Beltrami operator \mathcal{L} itself via the (possibly weighted) graph Laplacian $\varepsilon^{-1}(P - I)$: as an operator, we are thus interested in

$$\mathcal{L}_\varepsilon^{(M)} := \varepsilon^{-1}(\mathcal{P}_\varepsilon^{(M)} - I),$$

and similarly for the standard weights. The eigenfunctions of these operators are the same as that of the respective $\mathcal{P}_\varepsilon^{(M)}$, thus with the same convergence. On the other hand, if we let the eigenvalues of $\mathcal{L}_\varepsilon^{(M)}$ be

$$-\check{\lambda}_{k,\varepsilon}^{(M)} = \varepsilon^{-1}(e^{-\lambda_{k,\varepsilon}^{(M)}} - I),$$

and similarly the checked equivalents for standard weights, then we also have convergence of eigenvalues.

Corollary 3.4 (Eigendata of the graph Laplacian). *For all $\alpha \in [0, 1]$ and $\lambda_* > 0$ there exist constants $C_{101}, C_{104}, \check{C}_{101}, \check{C}_{104}$ such that*

(a) *The eigenspaces of the graph Laplacians $\mathcal{L}_\varepsilon^{(M)}$ are those of the respective semigroup approximations $\mathcal{P}_\varepsilon^{(M)}$ given in Theorems 3.2 and 3.3.*

(b) *If $\rho \in C^{3/2+\beta}$ and $\varepsilon + \varepsilon^{-1}\delta < \check{C}_{101}$, then for $-\check{\lambda}_{k,\alpha} \geq -\lambda_*$ we have convergence of eigenvalues*

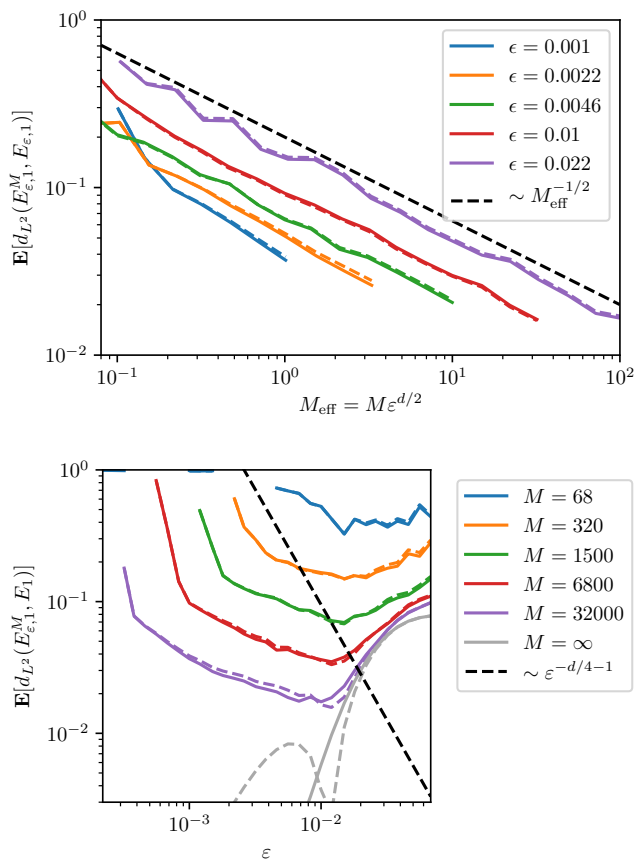


Figure 2: $L^2(\rho^M)$ error in diffusion maps estimates of eigenspace E_1 for function density $\rho(x, y, z) \propto e^{\cos 4\pi x + f(y) + f(z)}$ where $f(x) = 0.4 \cos 2\pi x + 0.12 \sin 4\pi x$ on $\mathbb{D} = (\mathbb{R}/\mathbb{Z})^3$. Sinkhorn normalisation (solid lines) and $\alpha = \frac{1}{2}$ standard normalisation (dashed lines) are compared. At top, the variance error plotted against local sample size M_{eff} for different ϵ ; at bottom the combined bias and variance error are plotted against timestep ϵ for different sample sizes M . Expectations were computed using 30 samples each. An adaptive Fourier discretisation (Olver 2019) was used to approximate the eigenfunctions of the generator \mathcal{L} and of the continuum semigroup approximations $\mathcal{P}_\epsilon, \tilde{\mathcal{P}}_{\epsilon,1/2}$.

for the standard weights

$$\begin{aligned} |\tilde{\lambda}_{k,\varepsilon,\alpha} - \check{\lambda}_{k,\alpha}| &\leq \check{C}_{104}\varepsilon, \\ |\tilde{\lambda}_{k,\varepsilon,\alpha}^M - \check{\lambda}_{k,\alpha}| &\leq \check{C}_{104}(\varepsilon + \varepsilon^{-1}\delta). \end{aligned}$$

(c) If $\rho \in C^{2+\beta}$ and $\varepsilon^2 + \varepsilon^{-1}\delta < C_{101}$, then for $-\lambda_k \geq -\lambda_*$ we have convergence of eigenvalues for the Sinkhorn weights

$$\begin{aligned} |\tilde{\lambda}_{k,\varepsilon} - \lambda_k| &\leq C_{104}\varepsilon, \\ |\tilde{\lambda}_{k,\varepsilon}^M - \lambda_k| &\leq C_{104}(\varepsilon + \varepsilon^{-1}\delta). \end{aligned}$$

Note however that for purely linear-algebraic reasons the improvement in the bias error to $\mathcal{O}(\varepsilon^2)$ for Sinkhorn weights is lost.

Our proof of the main results rely on bounds of the deviations of (powers of) our discretised half-step operators $\mathcal{G}_\varepsilon^{(M)}, \mathcal{H}_\varepsilon^{(M)}$ from their respective limits.

Thus for the Sinkhorn weights, the bias error is bounded according to the following theorem:

Theorem 3.5. *Suppose $\rho \in W^{s,\infty}$, $s > 2$, and let $S_\varepsilon(t_1, t_0)$ be the solution operator of the PDE*

$$\partial_t \phi^t = \mathcal{L}\phi^t + \nabla \hat{w}_\varepsilon^t \cdot \nabla \phi^t, \quad (22)$$

where we define $\hat{w}_\varepsilon^t := \log(\mathcal{K}_t U_\varepsilon) - \frac{1}{2} \log \rho$ for $t \in [0, \varepsilon)$ and extend ε -periodically.

Then

$$\begin{aligned} \mathcal{G}_\varepsilon &= S_\varepsilon(\varepsilon, \tfrac{1}{2}\varepsilon) \\ \mathcal{H}_\varepsilon &= S_\varepsilon(\tfrac{1}{2}\varepsilon, 0) \\ \mathcal{P}_\varepsilon &= S_\varepsilon(\varepsilon, 0) \\ \mathcal{Q}_{\varepsilon,n} &= S_\varepsilon((n + \tfrac{1}{2})\varepsilon, \tfrac{1}{2}\varepsilon). \end{aligned}$$

Furthermore, for all $T > 0$ and $\beta \in (0, \min\{s - 2, 1\})$ there exists a constant $C_{90,T,\beta}$ such that for all $0 \leq t_1 - t_0 \leq T$ and $\varepsilon \leq \varepsilon_0$,

$$\|S_\varepsilon(t_1, t_0) - e^{(t_1-t_0)\mathcal{L}}\|_{C^{3+\beta} \rightarrow C^0} \leq C_{90,T,\beta}\varepsilon^2. \quad (23)$$

If the sampling density ρ has higher regularity, we have the stronger result, which follows from a simplification of the proof of Theorem 3.5 and implies an $\mathcal{O}(\varepsilon^2)$ pointwise bias error of the Sinkhorn-weighted graph Laplacian:

Proposition 3.6. *Suppose $\rho \in W^{s,\infty}$ for $s > 4$. Then for all $\beta \in (0, 1)$ there exists a constant $C_{97,\beta}$ such that for all $t \in \mathbb{R}$, $\varepsilon \leq \varepsilon_0$,*

$$\|S_\varepsilon(t + \varepsilon, t) - e^{\varepsilon\mathcal{L}}\|_{C^{3+\beta} \rightarrow C^0} \leq C_{97,\beta}\varepsilon^3.$$

This is the best possible asymptotic rate of convergence to the semigroup for operators of the form $V_\varepsilon \mathcal{K}_\varepsilon U_\varepsilon$ for all non-uniform distributions ρ (see Remark 7.2).

Bounds on the variance error proceed from Theorem 3.1. In particular, we have the following result on the convergence of the operator $\mathcal{K}_\varepsilon^M$ (an interpolation of the kernel matrix K) to its continuum limit:

Theorem 3.7. *Let $\zeta = Z_0\varepsilon^{1/2}$. Then*

$$\|\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon\|_{H^\infty(\mathbb{D}_\zeta)} \leq e^{2dZ_0^2} \delta.$$

Note here that the imaginary-direction thickness ζ of the domain of the Hardy space $H^\infty(\mathbb{D}_\zeta)$ scales proportionally with the $\mathcal{O}(\varepsilon^{1/2})$ bandwidth of the kernel. A useful consequence of this is that it is also possible to bound the error of the k th derivative of the spatial discretisation, with a penalty in the error of $\mathcal{O}(\varepsilon^{-k/2})$.

As a consequence of Theorem 3.7, we also have operator convergence of the normalised operator $\mathcal{P}_\varepsilon^M$, which interpolates the matrix P , as well as the various auxiliary operators:

Theorem 3.8. *There exist constants Z_0, C_{37}, C_{39} such that if $\zeta = Z_0\varepsilon^{1/2}$ and $\delta \leq C_{37}$ then for all $\varepsilon \leq \varepsilon_0$ and $n \in \mathbb{N}$,*

$$\|\mathcal{P}_\varepsilon^M - \mathcal{P}_\varepsilon\|_\zeta, \|\mathcal{G}_\varepsilon^M - \mathcal{G}_\varepsilon\|_{0 \rightarrow \zeta}, \|\mathcal{H}_\varepsilon^M - \mathcal{H}_\varepsilon\|_{\zeta \rightarrow 0} \leq C_{39}\delta,$$

and

$$\|\mathcal{Q}_{\varepsilon,n}^M - \mathcal{Q}_{\varepsilon,n}\|_0 \leq C_{39}\delta n.$$

4 Numerical computation of Sinkhorn weights

While the use of Sinkhorn weights gives improved convergence in spectral data, it is necessary to calculate them iteratively: the usual Sinkhorn iteration is known to converge quite slowly in other problems, and indeed substantial efforts have been dedicated to finding ways to accelerate the convergence (Thibault et al. 2017, Altschuler et al. 2017, Feydy et al. 2019, Peyré & Cuturi 2019).

However, in our case the extra numerical work necessary to obtain the Sinkhorn weights is small, as in this section we will present a simple, general, well-conditioned algorithm to estimate the Sinkhorn weights that converges exponentially at a rate that is independent of the matrix input.

Let us first note that the traditional way that Sinkhorn weights are calculated is using so-called Sinkhorn iteration: for symmetric matrices this amounts to repeatedly iterating

$$u^{(n+1)} = 1/(Ku^{(n)}),$$

which is interpolated as

$$U^{(n+1)} = 1/\mathcal{K}_\varepsilon^M[U^{(n)}]. \quad (24)$$

As $n \rightarrow \infty$, it is well-known that $U^{(n)} \rightarrow c^{(-1)^n} U_\varepsilon^M$ for some constant $c > 0$ (Peyré & Cuturi 2019). The asymptotic rate of convergence can be bounded, since at the fixed point Sinkhorn iteration is a contraction by $\lambda_{\varepsilon,1}^M$, the second eigenvalue of the re-weighted operator $\mathcal{P}_\varepsilon^M$. This is because the Jacobian at the fixed point is conjugate to $-\mathcal{P}_\varepsilon^M$. However, from Theorem 3.3, the spectral gap $1 - \lambda_{\varepsilon,1}^M = \mathcal{O}(\varepsilon)$, so $\mathcal{O}(\varepsilon^{-1})$ iterates are needed to estimate the Sinkhorn weights to a given tolerance.

To improve this, we propose an accelerated symmetric Sinkhorn algorithm (ASSA, Algorithm 1), which harnesses the symmetry and positive definiteness of the iteration problem to accelerate the local convergence rate to $\mathcal{O}(8^{-n})$, as well as automatically removing the constant c . An iteration step of ASSA involves taking two successive Sinkhorn iterates (c.f. (24)), followed by a geometric mean of the two steps.

Data: Unweighted kernel matrix K , timestep ε , eigendata error tolerance τ
Result: Estimated Sinkhorn weight vector u with \log - L^∞ error less than $\varepsilon\tau$
 $u \leftarrow 1/\sqrt{K\mathbf{1}}$;
repeat
 $u_o \leftarrow u$;
 $v \leftarrow 1/(Ku_o)$;
 $u \leftarrow \sqrt{v/(Kv)}$;
until $\|\log(u_o/u)\|_{\ell_2} \leq \varepsilon\tau$;

Algorithm 1: Accelerated symmetric Sinkhorn algorithm (ASSA)

We can write this in the case of a kernel operator \mathcal{K} as

$$U_a^{(n)} = 1/\mathcal{K}[U^{(n)}] \quad (25)$$

$$U_b^{(n)} = 1/\mathcal{K}[U_a^{(n)}] \quad (26)$$

$$U^{(n+1)} = \sqrt{U_a^{(n)} U_b^{(n)}}. \quad (27)$$

Because the Jacobian of a Sinkhorn iteration step (24) around the fixed point U is conjugate to $-\mathcal{P} := -UKU$, the Jacobian of the ASSA step is conjugate to $-\frac{1}{2}\mathcal{P}(I - \mathcal{P})$. In our case $\mathcal{P} = \mathcal{P}_\varepsilon^M$ is a self-adjoint, positive definite Markov operator on $L^2(\rho^M)$, so its spectrum is contained in $[0, 1]$ and so the spectrum of the Jacobian is contained in $[-\frac{1}{8}, 0]$, leading to $\mathcal{O}(8^{-n})$ local rate of contraction. The geometric mean step additionally removes the constant c that is an artefact of the usual Sinkhorn algorithm. In Theorem 4.1, whose proof is in Appendix A, we show in a general setting that Algorithm 1 is guaranteed to converge for any positive initial guess, and, assuming a good initial guess, converges at the $\mathcal{O}(8^{-n})$ rate with a valid stopping condition. Around 40 ASSA iterates are typically sufficient to obtain an estimate of the Sinkhorn weight accurate to double floating point.

Theorem 4.1. *Suppose μ is a measure and \mathcal{K} a positive operator that is bounded, positive semi-definite and self-adjoint on $L^2(\mu)$ and bounded on $L^\infty(\mu)$.*

Let U solve the Sinkhorn problem for this operator, and let $U^{(n)}$ be the n th iterate of the accelerated symmetric Sinkhorn algorithm (25 – 27) with $U^{(0)} > 0$. Then

(a) *(Global convergence) For all $n \geq 0$ and $U^{(0)} > 0$,*

$$\|\log U^{(n)} - \log U\|_{L^\infty(\mu)} \leq 2 \left(\theta \frac{1+\theta}{2}\right)^n \|\log U^{(0)} - \log U\|_{L^\infty(\mu)},$$

where $\theta < 1$ is the worst-case contraction rate of standard Sinkhorn iteration, given in the proof (64).

(b) *(Local convergence rate) If $\|\log U^{(0)} - \log U\|_{L^\infty(\mu)} \leq k < 0.1$, then if $k'' := ke^{4k}(2 + \frac{1}{2}ke^{4k}) < \frac{3}{8}$, the faster convergence holds*

$$\|\log U^{(n)} - \log U\|_{L^2(\mu)} \leq \left(\frac{1}{8} + k''\right)^n \|\log U^{(0)} - \log U\|_{L^2(\mu)}.$$

(c) *(Stopping condition) Under the conditions of part (b),*

$$\|\log U^{(n)} - \log U\|_{L^2(\mu)} \leq \left(1 - \left(\frac{1}{8} + k''\right)^{-1}\right)^{-1} \|\log U^{(n)} - \log U^{(n-1)}\|_{L^2(\mu)}.$$

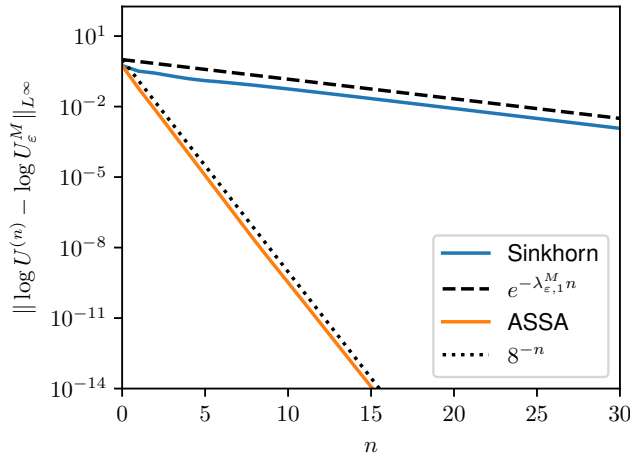


Figure 3: Convergence of standard Sinkhorn iteration (blue) and ASSA (orange) for an $M = 3000$ sample from the standard normal distribution in dimension 3 with kernel parameter $\varepsilon = 0.5$.

Proposition 4.2. *The empirical measure $\rho^{(M)}$ and kernel operator $\mathcal{K}_\varepsilon^{(M)}$ respectively satisfy the conditions for Theorem 4.1.*

Note that when μ is a discrete measure (e.g. $\mu = \rho^M$) we can recover bounds on the L^∞ norm using norm equivalence:

$$\|\cdot\|_{L^\infty(\rho^M)} \leq M^{-1/2} \|\cdot\|_{L^2(\rho^M)}.$$

It is also possible to relax the positive semi-definiteness constraint on the kernel operator \mathcal{K} , as long as the negative spectrum of the weighted operator \mathcal{P} is far away from -1 .

Because the only steps in ASSA are standard Sinkhorn iteration and a geometric mean, ASSA is very well-conditioned, and can be expected to perform well in more general circumstances, including for samples on curved manifolds and from distributions with non-compact support: in Figure 3 fast convergence of ASSA is shown for a Gaussian sampling distribution.

As an initial value for iteration we use the standard $\alpha = \frac{1}{2}$ right-hand weight $U^{(0)} = (\mathcal{K}_\varepsilon^M \mathbf{1})^{-1/2}$. According to the following proposition, when $\varepsilon, \delta \ll 1$, this guess should be close enough to the Sinkhorn weight that the fast local convergence rate takes hold immediately.

Proposition 4.3 (ASSA initialisation). *There exist constants C_{120}, C_{121} independent of M, ε such that if $\delta < C_{120}$ and $\varepsilon \leq \varepsilon_0$, then*

$$\|\log(\mathcal{K}_\varepsilon^M \mathbf{1})^{-1/2} - \log U_\varepsilon^M\|_{L^\infty(\rho^M)} \leq C_{121}(\delta + \varepsilon),$$

where $(\mathcal{K}_\varepsilon^M \mathbf{1})^{-1/2}$ is the initial condition for ASSA.

These results are proven in Appendix A.

5 Function space results

Before we study the $\varepsilon \rightarrow 0$ operator limit, we state some useful results in functional analysis.

Recall from Section 2.2 that we defined scales of fractional Sobolev spaces $W^{s,p}$ of functions ϕ for which $J^s \phi \in L^p$, where the sectorial Bessel operator $J := I - \Delta$.

A sufficient condition for a Banach space operator $\mathcal{A} : B \rightarrow B$ to be *sectorial* is that its spectrum is confined to a left open half-plane and there exists $C < \infty$ such that for λ in the complement of this half-plane

$$\|(\lambda + \mathcal{A})^{-1}\|_B \leq C|\lambda|^{-1}.$$

The operators J and $\tilde{J} := I - 2\mathcal{L}$ are both well-known to be sectorial on $L^p = W^{0,p}$ provided that our measure density $\rho \in C^{1+\beta}$. The Bessel operator J is also sectorial on $W^{s,p}$ for all positive s .

From Theorem 1.4.8 in Henry (2006) and using that ∇ is bounded as an operator from $W^{s+1,p} \rightarrow W^{s,p}$, we have by induction that $\tilde{J} = I - 2\mathcal{L}$ is a sectorial operator on $W^{r,p}$, $r \leq s$, $p > 1$ and that for $\beta \in [0, 1]$, $\tilde{J}^{\beta/2}$ is bounded as an operator $W^{r+\beta,p} \rightarrow W^{r,p}$, $r \leq s$; the condition for this to hold is that multiplication by $J^{1/2} \log \rho$ is bounded on $W^{r,p}$, $r \leq s$: this is assured by the Leibniz rule for fractional derivatives $J^{\beta/2}$ (Bourgain & Li 2014, Li 2019), provided $\rho \in W^{s,p}$ and $s \geq 1$.

Standard results, for instance in Chapter 1 of Henry (2006), and the aforementioned Leibniz rule, give the following, as well as analogues for $\tilde{\mathcal{L}}_\alpha$:

Proposition 5.1. *Suppose that $\rho \in W^{s,\infty}$ for $s \geq 1$. Then for all $p \in (1, \infty]$:*

- *There exist constants K_p^∇ such that for all $r \geq 0$*

$$\|\nabla\|_{W^{r+1,p} \rightarrow W^{r,p}}, \|\nabla \cdot\|_{W^{r+1,p} \rightarrow W^{r,p}} \leq K_p^\nabla;$$

- *For all $0 \leq q \leq r \leq s$ there exists a constant $K_{p;r,s}^\times$ such that for all $\phi \in W^{r,p}$, $\psi \in W^{s,\infty}$,*

$$\|\phi\psi\|_{W^{r,p}} \leq K_{p;q,r,s}^\times \|\phi\|_{W^{r,p}} \|\psi\|_{W^{s,\infty}};$$

- *For all $r < s - 2$, there exists $K_{p;r}$ such that*

$$\|\mathcal{L}\|_{W^{r+2,p} \rightarrow W^{r,p}} \leq K_{p;r};$$

- *For all $s < k + \beta$, $\beta \in (0, 1)$, there exists $K_{k+\beta,s}^C$ such that the norm of the inclusion map $C^{k+\beta} \rightarrow W^{s,\infty}$ is bounded by $K_{k+\beta,s}^C$.*

- *For all $q \leq r \leq s$ and all $T > 0$ there exists $K_{p;q,r}^T$ such that for $t \in [0, T]$*

$$\|e^{t\mathcal{L}}\|_{W^{q,\infty} \rightarrow W^{r,\infty}} \leq t^{-(r-q)/2} K_{p;q,r}^T;$$

- *There exists a $a > 0$ such that for all $q \leq r \leq s$ and all $T > 0$ there exists $\tilde{K}_{p;q,r}^T$ such that for $t \in [0, T]$*

$$\|e^{t\mathcal{L}}|_{Z \cap W^{q,\infty}}\|_{W^{q,\infty} \rightarrow W^{r,\infty}} \leq t^{-(r-q)/2} e^{-at} \tilde{K}_{p;q,r}^T,$$

where the \mathcal{L} -invariant subspace

$$Z = \left\{ \phi \in L^\infty : \int_{\mathbb{D}} \phi \rho \, dx = 0 \right\}. \quad (28)$$

6 Convergence of Sinkhorn weights as $\varepsilon \rightarrow 0$

Our convergence analysis requires an understanding the behaviour of the continuum limit Sinkhorn weights U_ε . These satisfy the equation (13), which in this section we will find useful to formulate as

$$U_\varepsilon^{-1} = \mathcal{C}_\varepsilon(\sigma^2 U_\varepsilon), \quad (29)$$

where \mathcal{C}_ε is convolution with the Gaussian kernel $g_{\varepsilon,L}$ and $\sigma^2 := \rho$. We expect U_ε to converge to $\sigma^{-1} = \rho^{-1/2}$ as $\varepsilon \rightarrow 0$, but because the kernel $g_{\varepsilon,L}$ becomes singular as $\varepsilon \rightarrow 0$ this is not trivial.

We consider this problem by formulating U_ε as the fixed point (up to constant scaling) of Sinkhorn iteration:

$$U^{(n+1)} = 1/(\mathcal{C}_\varepsilon(\sigma^2 U^{(n)})) \quad (30)$$

Since for fixed $\varepsilon > 0$ the operator $\mathcal{C}_\varepsilon \sigma^2$ is uniformly positive, Sinkhorn iteration is a contraction on the cone of positive functions and thus for all initial conditions $U_0 > 0$ the convergence holds (Sinkhorn 1964)

$$U^{(2n)} \rightarrow cU_\varepsilon, U^{(2n+1)} \rightarrow c^{-1}U_\varepsilon$$

for some $c > 0$ depending on $U^{(0)}$. Note that while the iteration (30) in the $\varepsilon \rightarrow 0$ limit has 2-periodic dynamics for all initial conditions, we do recover a fixed point $U_0 = \rho^{-1/2} = \sigma^{-1}$ that is the solution of the Sinkhorn problem (29) for $\varepsilon = 0$.

Motivated by the log-space formulation of cone metrics we set

$$w^{n\varepsilon} = (-1)^n \log \sigma U^{(n)},$$

so that

$$w^{(2n+1)\varepsilon} = \mathcal{N}_\varepsilon w^{2n\varepsilon} \quad (31)$$

$$w^{(2n+2)\varepsilon} = -\mathcal{N}_\varepsilon(-w^{2n\varepsilon}), \quad (32)$$

where the nonlinear semigroup $(\mathcal{N}_t)_{t \geq 0}$ is given by

$$\mathcal{N}_t \phi = \log(\sigma^{-1} \mathcal{C}_t(\sigma e^\phi)).$$

Using that $\frac{d}{dt} \mathcal{C}_t = \frac{1}{2} \Delta \mathcal{C}_t$ it is straightforward to show that the infinitesimal generator of \mathcal{N}_t is given by

$$\left. \frac{d}{dt} \mathcal{N}_t \phi \right|_{t=0} = \frac{1}{2} \Delta \phi + \frac{1}{2} |\nabla \phi|^2 + \frac{\nabla \sigma}{\sigma} \cdot \nabla \phi + \frac{\Delta \sigma}{2\sigma}.$$

By using \mathcal{N}_t to interpolate (31 – 32) in time, we can thus write Sinkhorn iteration as a nonlinear PDE

$$\partial_t w^t = \mathcal{L} w^t + (-1)^{\lfloor \varepsilon^{-1} t \rfloor} \left(\frac{1}{2} |\nabla w^t|^2 + \frac{\Delta \sigma}{2\sigma} \right). \quad (33)$$

Note that this PDE can be decomposed as a sum of an autonomous linear part, in fact the limiting generator of the diffusion maps problem \mathcal{L} , with a non-autonomous, rapidly oscillating nonlinear part that has time integral zero. Consequently, we can apply averaging results to this system as $\varepsilon \rightarrow 0$. This will give us convergence of w^t and thus U_ε :

Theorem 6.1. *Suppose $\rho \in W^{s,\infty}$, $s \geq 2$.*

Then the PDE (33) has a unique limit cycle w_ε^t with $w_\varepsilon^{t+\varepsilon} = -w_\varepsilon^t$ and $w_\varepsilon^0 = \log \rho^{1/2} + \log U_\varepsilon$.

Furthermore for all $0 \leq r < s + 1$,

$$\limsup_{\varepsilon \rightarrow 0} \sup_t \|w_\varepsilon^t\|_{W^{r,\infty}} = 0,$$

and

$$\lim_{\varepsilon \rightarrow 0} \|\log U_\varepsilon - \log \rho^{-1/2}\|_{W^{r,\infty}} = 0.$$

This has the following immediate corollary:

Corollary 6.2. *Suppose $\rho \in W^{s,\infty}$, $s \geq 2$. Then there exists a constant C_{68} such that for all $\varepsilon \leq \varepsilon_0$*

$$\sup_{\varepsilon \leq \varepsilon_0} \|U_\varepsilon\|_{C^3} \leq C_{68} < \infty$$

and for all $r < s + 1$ a constant $C_{69,r}$ such that that for all $\varepsilon \leq \varepsilon_0$

$$\sup_{\varepsilon \leq \varepsilon_0} \sup_t \|w_\varepsilon^t\|_{W^{r,\infty}} \leq C_{69,r} < \infty.$$

The uniform bounds on the $(2\varepsilon$ -periodic) limit cycle w_ε^t are of particular use to us, because $w_\varepsilon^t = (-1)^{\lfloor t/\varepsilon \rfloor} w_\varepsilon^t$: that is, up to a periodic change of sign, it is the same as the ε -periodic drift error term in the time discretisation of diffusion maps (22).

Remark 6.3. *By applying instead Theorem 1.1 of Ilyin (1998), one can show that as $\varepsilon \rightarrow 0$, the solution of the Sinkhorn iteration PDE (33), w^t , converges to an averaging limit*

$$\partial_t \bar{w}^t = \mathcal{L} \bar{w}^t$$

over finite time scales (c.f. the Monge-Ampere PDE derived for non-symmetric Sinkhorn iteration in Berman (2017)). As a result, one recovers the asymptotic rate of (standard) Sinkhorn iteration

$$\lim_{n \rightarrow \infty} \frac{-\log \|U^{(n)} - U_\varepsilon\|}{n} = -\lambda_1 \varepsilon,$$

where $-\lambda_1$ is the first non-zero eigenvalue of the Langevin dynamics \mathcal{L} .

Proof of Theorem 6.1. This amounts to checking the conditions of Theorem 1.2 of Ilyin (1998). Due to the invariance of constant functions under Sinkhorn iteration we will project our PDE (33) onto the subspace of zero mean functions Z defined in (28). We thus consider

$$\partial_t w^t = \mathcal{L} w^t + \mathcal{F}(w^t, \varepsilon^{-1}t) + \mathcal{X}(\varepsilon^{-1}t), \quad (34)$$

where

$$\begin{aligned} \mathcal{F}(\phi, \tau) &= (-1)^{\lfloor \tau \rfloor} \frac{1}{2} (I - \mathcal{Z}) (|\nabla \phi|^2) \\ \mathcal{X}(\tau) &= (-1)^{\lfloor \tau \rfloor} (I - \mathcal{Z}) \left(\frac{\Delta \sigma}{2\sigma} \right), \end{aligned}$$

and the projection operator

$$(\mathcal{Z}\phi)(x) := \int_{\mathbb{D}} \phi(y) \rho(y) \, dy.$$

Suppose $r \geq s - 1$ (the result will then follow immediately for $r < s - 1$). Set Banach spaces $E = W^{r,\infty} \cap Z$, $F = W^{r-1,\infty} \cap Z$, $X = W^{s-2,\infty} \cap Z$ and $\mathcal{E} = Z$.

Proposition 5.1 implies the various conditions on the linear operator \mathcal{L} and the averaged semigroup $e^{\mathcal{L}t}$ required for Theorem 1.2 of Ilyin (1998). We also have that the nonlinear part $\mathcal{F} : E \times \mathbb{R} \rightarrow F$ is Lipschitz on bounded subsets of E and the driver \mathcal{X} has range in X . Both are locally integrable over τ . As a result, we have that the attractor of (34) converges in the strong space E uniformly to the attractor of $\partial_t w^t = \mathcal{L}w^t$ in E , i.e. zero. In other words, if $\{w_\varepsilon^{t,\mathcal{Z}}\}_{t \in \mathbb{R}}$ is this attractor (which by the convergence of Sinkhorn iteration is necessarily a unique limit cycle), then

$$\limsup_{\varepsilon \rightarrow 0} \sup_t \|w_\varepsilon^{t,\mathcal{Z}}\|_E = 0.$$

If we let w_ε^t be the solution of the unprojected PDE (33) corresponding to the true Sinkhorn weights with $w_\varepsilon^{n\varepsilon} = (-1)^n \log \sigma U_\varepsilon$, then for all t one has $w_\varepsilon^{t+\varepsilon} = -w_\varepsilon^t$; furthermore if $w_\varepsilon^{t,\mathcal{Z}}$ is the attractor (necessarily a limit cycle) of the projected PDE (34) then

$$w_\varepsilon^t - w_\varepsilon^{t,\mathcal{Z}} = \mathcal{Z}w_\varepsilon^t = \int_{\mathbb{D}} w_\varepsilon^t \rho \, dy.$$

From (33) and using that $\nabla w_\varepsilon^t = \nabla w_\varepsilon^{t,\mathcal{Z}}$ we find that

$$\sup_{\varepsilon \leq \varepsilon_0} \|\partial_t \mathcal{Z}w_\varepsilon^t\| = \sup_{\varepsilon \leq \varepsilon_0} \left| \int_{\mathbb{D}} \left(\frac{1}{2} |\nabla w_{t,\mathcal{Z}}|^2 + \frac{\Delta \sigma}{2\sigma} \right) \rho \, dx \right| < \infty.$$

Then using that $\mathcal{Z}w_\varepsilon^{t+\varepsilon} = \frac{1}{2}(\mathcal{Z}w_\varepsilon^{t+\varepsilon} - \mathcal{Z}w_\varepsilon^t)$ implies that

$$\limsup_{\varepsilon \rightarrow 0} \sup_t \|w_\varepsilon^t - w_\varepsilon^{t,\mathcal{Z}}\|_{W^{r,\infty}} \rightarrow 0,$$

giving us what is required. \square

Because w_ε^t is up to a time-varying change of sign the drift term in the temporally-discretised PDE (22), we will find it useful to make some more specific estimates on w_ε^t to prove the operator convergence in the next section. In particular, we will show that $w_\varepsilon^t = \mathcal{O}(\varepsilon)$, and that w_ε^t is symmetric in time up to $\mathcal{O}(\varepsilon^2)$.

Lemma 6.4. *Suppose $\rho \in W^{s,\infty}$, $s > 2$ and w_ε^t is as in Theorem 6.1. Then for all $r \in [2, s+1]$ there exist $C_{70,r}, C_{71,r}$ such that for all $\varepsilon \leq \varepsilon_0$, $t \in [0, \varepsilon]$*

$$\|w_\varepsilon^t\|_{W^{r-2,\infty}} \leq \frac{1}{2} C_{71,r} \varepsilon \tag{35}$$

and

$$\|J^{-r^*/2}(w_\varepsilon^t + w_\varepsilon^{\varepsilon-t})\|_{W^{r-4+r^*,\infty}} \leq C_{70,r} \varepsilon^2, \tag{36}$$

where $r^* = \max\{4 - r, 0\}$.

Proof of Lemma 6.4. Making use of Corollary 6.2 and Proposition 5.1, we have that

$$\|\partial_t w_\varepsilon^t\|_{W^{r-2,\infty}} \leq \frac{1}{2} K_{\infty;r-2} C_{69,r} + K_{\infty;:,r-2,r-1,r-1}^\times (K_{\infty}^\nabla C_{69,r-1})^2 + \left\| \frac{\Delta \rho^{1/2}}{2\rho^{1/2}} \right\|_{W^{r-2,\infty}} \leq C_{72,r}$$

From Theorem 6.1 we have that $w_\varepsilon^t = -w_\varepsilon^{t-\varepsilon}$, and so as a result

$$\sup_{t \in [0, \varepsilon]} \|w_\varepsilon^t\|_{W^{r-2,\infty}} = \sup_{t \in [0, \varepsilon]} \frac{1}{2} \|w_\varepsilon^t - w_\varepsilon^{t-\varepsilon}\|_{W^{r-2,\infty}} \leq \frac{1}{2} C_{72,r} \varepsilon,$$

as required for (35).

To obtain (36), we will want to take the second derivative in time: however, for $r \in (2, 4)$ we do not have enough regularity in our function spaces to do that, so we will introduce an inverse fractional derivative $J^{-r^*/2}$ to compensate. In particular, we have that for $t \in (0, \varepsilon)$,

$$\begin{aligned}\partial_{tt}J^{-r^*/2}w^t &= \partial_t J^{-r^*/2} \partial_t w^t \\ &= \frac{1}{2} \partial_t J^{-r^*/2} (-Jw^t + w^t + \nabla \log \rho \cdot \nabla w^t + \nabla \partial_t w^t \cdot \nabla w^t + \Delta \sigma / \sigma) \\ &= -\frac{1}{2} J^{1-r^*/2} \partial_t w^t + \frac{1}{2} J^{-r^*/2} \partial_t w^t + \frac{1}{2} J^{-r^*/2} \nabla (\log \rho + 2w^t) \cdot \nabla \partial_t w^t,\end{aligned}$$

and as a result this second time derivative is uniformly bounded in $W^{r-4+r^*, \infty}$:

$$\begin{aligned}\|\partial_{tt}J^{-r^*/2}w^t\|_{W^{r-4+r^*, \infty}} &\leq \frac{1}{2} C_{72,r} + \frac{1}{2} C_{69,r} + \\ &\quad \frac{1}{2} K_{\infty; r-4+r^*, r-1, r-3}^\times (K_\infty^\nabla)^2 C_{72,r} (\|\log \rho\|_{W^{r-1, \infty}} + 2C_{69, r-1}) \\ &=: \frac{1}{2} C_{70,r}.\end{aligned}$$

Thus, by applying Taylor's theorem,

$$\left\| J^{-r^*/2} \left(w_\varepsilon^t + w_\varepsilon^{\varepsilon-t} - 2w_\varepsilon^{\varepsilon/2} \right) \right\|_{W^{r-4+r^*, \infty}} \leq \sup_{t \in [0, \varepsilon]} \|\partial_{tt}J^{-r^*/2}w^t\|_{W^{r-4+r^*, \infty}} \varepsilon^2 \leq \frac{1}{2} C_{70,r} \varepsilon^2. \quad (37)$$

Since $w_\varepsilon^0 = -w_\varepsilon^\varepsilon$, by setting $t = 0$ in (37) we have

$$\|2J^{-r^*/2}w_\varepsilon^{\varepsilon/2}\|_{W^{r-4+r^*, \infty}} \leq \frac{1}{2} C_{70,r} \varepsilon^2. \quad (38)$$

Recombining this with (37) we obtain the necessary result. \square

Remark 6.5. *Since from (38) we have for $s > 4$ (i.e. $\rho \in C^{4+\beta}$) that*

$$\|\mathcal{K}_{\varepsilon/2} U_\varepsilon - \rho^{1/2}\|_{L^\infty} = \mathcal{O}(\varepsilon^2),$$

the Sinkhorn problem can be used to perform second-order non-parametric estimation on the density ρ .

7 Deterministic convergence of operators

Recall from (14) that the deterministic approximation to the semigroup is

$$\mathcal{P}_\varepsilon = U_\varepsilon \mathcal{K}_\varepsilon U_\varepsilon.$$

In this section, we will harness our results on the Sinkhorn weight U_ε from the previous section to Theorem 3.5 on convergence of \mathcal{P}_ε to the semigroup $e^{\varepsilon \mathcal{L}}$. Before this, we will make some remarks on the rate of convergence to the semigroup.

Remark 7.1. *For the Sinkhorn normalisation the bias error convergence is of second order in the timestep ε , unlike the first-order convergence for standard weights (c.f. Proposition 11.3). This is actually a result of the self-adjointness of the normalised operator.*

To be more specific (and to outline the strategy of the proof of Theorem 3.5), we can write the action of \mathcal{P}_ε as solving the PDE (22), which we recall here,

$$\begin{aligned}\phi^0 &= \phi \\ \partial_t \phi^t &= \mathcal{L} \phi^t + \nabla \hat{w}_\varepsilon^t \cdot \nabla \phi^t,\end{aligned} \quad (39)$$

so that $\phi^\varepsilon = \mathcal{P}_\varepsilon \phi$, where recall that the discrepancy in drift compared with the semigroup is

$$\hat{w}_\varepsilon^t = \log(\mathcal{K}_t U_\varepsilon) - \frac{1}{2} \log \rho, \quad t \in [0, \varepsilon].$$

Note that because the Sinkhorn normalisation (13) is required to be symmetric,

$$\hat{w}_\varepsilon^0 = \log U_\varepsilon + \frac{1}{2} \log \rho = - \lim_{t \uparrow \varepsilon} \hat{w}_\varepsilon^t.$$

If $\phi, \rho, U_\varepsilon$ are of sufficiently high regularity, for small ε we can average the PDE (39) over $t \in [0, \varepsilon]$:

$$\partial_t \phi^t \approx \mathcal{L} \phi^t + \nabla \left(\varepsilon^{-1} \int_0^\varepsilon \hat{w}_\varepsilon^t \, d\tau \right) \cdot \nabla \phi^t.$$

The averaged drift can then be approximated using the trapezoidal rule with

$$\varepsilon^{-1} \int_0^\varepsilon \hat{w}_\varepsilon^t \, d\tau = \frac{1}{2} (\hat{w}_\varepsilon^0 + \lim_{t \uparrow \varepsilon} \hat{w}_\varepsilon^t) + \mathcal{O}(\varepsilon^2) = \mathcal{O}(\varepsilon^2).$$

As a result the operator \mathcal{P}_ε should closely approximate $e^{\varepsilon \mathcal{L}}$, as required.

Remark 7.2. The $\mathcal{O}(\varepsilon^3)$ rate of convergence $\mathcal{P}_\varepsilon \rightarrow e^{\varepsilon \mathcal{L}}$ is in general the best possible for operators of the form $V_\varepsilon \mathcal{K}_\varepsilon U_\varepsilon$. We can best see this by comparing the re-weighted operators for $n = 1$:

$$\sigma V_\varepsilon \mathcal{K}_\varepsilon U_\varepsilon \sigma^{-1} = V_\varepsilon \sigma e^{\varepsilon \frac{1}{2} \Delta} \sigma U_\varepsilon$$

and

$$\sigma e^{\varepsilon \mathcal{L}} \sigma^{-1} = e^{\varepsilon (\frac{1}{2} \Delta - \frac{1}{2} \sigma^{-1} \Delta \sigma)},$$

where $\sigma = \rho^{1/2}$. Taking a power series in ε and writing each side in the form

$$\sum_{k \geq 0} \left(\frac{1}{2^k} \Delta^k + \sum_{j=0}^{k-1} (\beta_{j,k} \Delta^j + \nabla \beta_{j,k} \cdot \nabla \Delta^{j-1}) \right) \varepsilon^k,$$

we see that for the $\beta_{k-1,k}$ coefficients to match it is necessary that

$$\left. \frac{\partial}{\partial \varepsilon} (V_\varepsilon + U_\varepsilon) \right|_{\varepsilon=0} = - \frac{1}{2(k-1)!} \sigma^{-2} \Delta \sigma.$$

Unless $\Delta \sigma \equiv 0$, i.e. $\sigma = \rho^{1/2}$ is constant, then this can only hold simultaneously for $k = 1, 2$: an $\mathcal{O}(\varepsilon^3)$ error between $e^{\varepsilon \mathcal{L}}$ and $V_\varepsilon \mathcal{K}_\varepsilon U_\varepsilon$ is thus the best possible (and hence we expect also an $\mathcal{O}(\varepsilon^2)$ error for the spectral data).

To prove Theorem 3.5, we will require the following result:

Proposition 7.3. Suppose $\rho \in W^{s,\infty}$, $s > 2$. Then for all $T > 0$, $\beta \in (0, \min\{s-2, 1\})$, there exists a constant $C_{89,T,\beta}$ such that for all $|t_1 - t_0| \leq T$,

$$\|S_\varepsilon(t_1, t_0)\|_{C^{3+\beta}} \leq C_{89,T,\beta}.$$

Proof of Proposition 7.3. From Corollary 6.2, we have for all $r < s + 1$ an ε -uniform bound on the $W^{r,\infty}$ norm of $w_\varepsilon^t = (-1)^{\lfloor t/\varepsilon \rfloor} \hat{w}_\varepsilon^t$. We therefore also have uniform in ε bounds on the $C^{3+\beta}$ norm of $\frac{1}{2} \log \rho + \hat{w}_\varepsilon^t$ for $2 + \beta < s$. We can thus apply Theorem 1.2 of Lorenzi (2000) to (22) to obtain relevant uniform bounds on $\|S_\varepsilon(t_1, t_0)\|_{C^{2+\beta}}$. By observing that (22) implies that

$$\partial_t \partial_{x_i} \phi^t = \mathcal{L} \partial_{x_i} \phi^t + \nabla \partial_{x_i} \left(\frac{1}{2} \log \rho + w^t \right) \cdot \nabla \phi^t, \quad (40)$$

we can then re-apply Lorenzi (2000) to obtain bounds on $\|S_\varepsilon(t_1, t_0)\|_{C^{3+\beta}}$. \square

We now prove Theorem 3.5.

Proof of Theorem 3.5. The definitions of $\mathcal{G}_\varepsilon, \mathcal{H}_\varepsilon, \mathcal{P}_\varepsilon, \mathcal{Q}_{\varepsilon,n}$ follow immediately by observing that for $0 \leq t_0 < t_1 \leq \varepsilon$,

$$S_\varepsilon(t_1, t_0) \phi = (\mathcal{K}_{t_1} U_\varepsilon)^{-1} \mathcal{C}_{t_1-t_0} ((\mathcal{K}_{t_0} U_\varepsilon) \phi).$$

Writing $S_0(t_1, t_0) = e^{(t_1-t_0)\mathcal{L}}$, the discrepancy in the errors is

$$S_\varepsilon(t_1, t_0) - S_0(t_1, t_0) = \int_{t_0}^{t_1} S_0(t_1, \tau) \nabla \hat{w}_\varepsilon^\tau \cdot \nabla S_\varepsilon(\tau, t_1) d\tau. \quad (41)$$

We can then bound

$$\begin{aligned} \|S_\varepsilon(t_1, t_0) - S_0(t_1, t_0)\|_{C^{3+\beta} \rightarrow L^\infty} &\leq (t_1 - t_0) \sup_{\tau \in [0, \varepsilon]} (\|S_0(t_1, \tau)\|_{L^\infty} K_{\infty;0,0,1}^\times K_\infty^\nabla \|\hat{w}_\varepsilon^\tau\|_{W^{1,\infty}} \times \\ &\quad K_\infty^\nabla \|S_\varepsilon(\tau, t_0)\|_{C^{3+\beta} \rightarrow W^{1,\infty}}) \\ &\leq \varepsilon K_{\infty;0,0,1}^\times (K_\infty^\nabla)^2 C_{71,1} \varepsilon \|S_\varepsilon(\tau, t_0)\|_{C^{3+\beta} \rightarrow W^{1,\infty}} \varepsilon \\ &\leq \varepsilon K_{\infty;0,0,1}^\times (K_\infty^\nabla)^2 C_{71,1} K_{3+\beta,1}^C C_{89,T,\beta} \varepsilon^2, \end{aligned}$$

where in the second-last inequality we used that $\hat{w}_\varepsilon^t = (-1)^{\lfloor t/\varepsilon \rfloor} w_\varepsilon^t$, and then Lemma 6.4, and in the last inequality Proposition 7.3.

Using that $S_\varepsilon(t_1, t_0) L^\infty \subset C^0$ and that the $C^{3+\beta}$ norm dominates the $W^{1,\infty}$ norm, we obtain (23) for $t_1 - t_0 < \varepsilon$.

We can use the previous result to reduce from all $0 < t_1 - t_0 < T$ to the case where $t_1 - t_0$ is a multiple of ε : mathematically, this is because if $m = \lfloor (t_1 - t_0)/\varepsilon \rfloor$, then we have

$$\begin{aligned} &\|S_\varepsilon(t_1, t_0) - S_0(t_1, t_0)\|_{C^{3+\beta} \rightarrow L^\infty} \\ &\leq \|S_\varepsilon(t_1, t_0 + m\varepsilon)\|_{L^\infty} \|S_\varepsilon(t_0 + m\varepsilon, t_0) - S_0(t_0 + m\varepsilon, t_0)\|_{C^{3+\beta} \rightarrow L^\infty} \\ &\quad + \|S_\varepsilon(t_1, t_0 + m\varepsilon) - S_0(t_1, t_0 + m\varepsilon)\|_{C^{3+\beta} \rightarrow L^\infty} \|S_0(t_0 + m\varepsilon, t_0)\|_{C^{3+\beta}} \\ &\leq \|S_\varepsilon(t_0 + m\varepsilon, t_0) - S_0(t_0 + m\varepsilon, t_0)\|_{C^{3+\beta} \rightarrow L^\infty} \\ &\quad + K_{\infty;3,3}^T \|S_\varepsilon(t_1, t_0 + m\varepsilon) - S_0(t_1, t_0 + m\varepsilon)\|_{C^{3+\beta} \rightarrow L^\infty}. \end{aligned}$$

At the same time, simply applying the previous argument to $t_1 - t_0 = m\varepsilon$ will give an error of size $\mathcal{O}(\varepsilon)$ instead of $\mathcal{O}(\varepsilon^2)$: we need to average over a cycle of w_ε^t . The aim is to move all the $\nabla \hat{w}_\varepsilon^\tau \cdot \nabla$ drift operators in (41) in a period of \hat{w}_ε^τ to the same point in time, and show that their average is small (c.f. Ilyin (1998), Chapter 7 of Henry (2006)).

To move the drift operators in time we will use that

$$\begin{aligned} \left\| \frac{d}{d\tau} S_\varepsilon(\tau, t_0) \right\|_{C^{3+\beta} \rightarrow W^{1,\infty}} &= \|\mathcal{L} + \nabla w_\varepsilon^\tau \cdot \nabla\|_{W^{3,\infty} \rightarrow W^{1,\infty}} K_{3+\beta,3}^C \|S_\varepsilon(\tau, t_0)\|_{C^{3+\beta}} \\ &\leq (K_{\infty;3} + K_{\infty;1,1,1}^\times C_{71,2} (K_\infty^\nabla)^2 \varepsilon_0) K_{3+\beta,3}^C C_{89,T,\beta} := C_{92,T,\beta}, \end{aligned}$$

so that if $\bar{t} = s + \varepsilon \lfloor \varepsilon^{-1}(\tau - t_0) \rfloor$,

$$\|S_\varepsilon(\tau, t_0) - S_\varepsilon(\bar{t}, t_0)\|_{C^{3+\beta} \rightarrow W^{1,\infty}} \leq C_{92,T,\beta} \varepsilon,$$

and so using Lemma 6.4,

$$\|S_0(t_1, \tau) \nabla \hat{w}_\varepsilon^\tau \cdot \nabla (S_\varepsilon(\tau, t_0) - S_\varepsilon(\bar{t}, t_0))\|_{C^{3+\beta} \rightarrow L^\infty} \leq (K_\infty^\nabla)^2 C_{71,1} C_{92,T,\beta} \varepsilon.$$

To change the length of the S_0 part, we use that, for any $r \in (3, \min\{s+1, 4\})$,

$$\begin{aligned} \left\| \frac{d}{d\tau} S_0(t_1, \tau) \right\|_{W^{r-2, \infty} \rightarrow L^\infty} &= \|\mathcal{L}\|_{W^{2, \infty} \rightarrow L^\infty} \|S_0(t_1, \tau)\|_{W^{r-2, \infty} \rightarrow W^{2, \infty}} \\ &\leq K_{\infty;0} (t_1 - \tau)^{r/2-2} K_{\infty;r-2,2}^T, \end{aligned}$$

so by integrating we have

$$\|S_0(t_1, \tau) - S_0(t_1, \bar{t})\|_{W^{r-2, \infty} \rightarrow L^\infty} \leq K_{\infty;0} K_{\infty;r-2,2}^T \left(\frac{\tau}{2} - 1\right)^{-1} \left((t_1 - \bar{t})^{r/2-1} - (t_1 - \varepsilon - \bar{t})^{r/2-1} \right) \varepsilon.$$

We can then bound the remaining part as

$$\|\nabla \hat{w}_\varepsilon^\tau \cdot \nabla S_\varepsilon(\bar{t}, t_0)\|_{C^{3+\beta} \rightarrow W^{r-2, \infty}} \leq C_{89,T,\beta} K_{3+\beta,3}^C K_{\infty;r-2,r-2,2}^\times (K_\infty^\nabla)^2 C_{71,r-2}.$$

As a result, for some constant $C_{93,T,\beta}$ we have

$$\begin{aligned} &\|S_0(t_1, \tau) \nabla \hat{w}_\varepsilon^\tau \cdot \nabla S_\varepsilon(\tau, t_1) - S_0(t_1, \bar{t}) \nabla \hat{w}_\varepsilon^\tau \cdot \nabla S_\varepsilon(\bar{t}, t_1)\|_{C^{3+\beta} \rightarrow L^\infty} \\ &\leq C_{93,T,\beta} \left((t_1 - \bar{t})^{r/2-1} - (t_1 - \varepsilon - \bar{t})^{r/2-1} \right) \varepsilon, \end{aligned}$$

and so using (41),

$$\begin{aligned} &\|S_\varepsilon(t_0 + m\varepsilon, t_0) - S_0(t_0 + m\varepsilon, t_0)\|_{C^{3+\beta} \rightarrow L^\infty} \\ &\leq C_{93,T,\beta} \max\{m\varepsilon, (m\varepsilon)^{r/2-1}\} \varepsilon^2 + \sum_{n=0}^{m-1} \left\| e^{(m-n)\varepsilon \mathcal{L}} \nabla \bar{w}_\varepsilon \cdot \nabla S_\varepsilon(t_0 + n\varepsilon, t_0) \right\|_{C^{3+\beta} \rightarrow L^\infty}, \quad (42) \end{aligned}$$

where

$$\bar{w}_\varepsilon := \int_{t_0}^{t_0+\varepsilon} w_\varepsilon^t dt.$$

Then, using that

$$\int_{t_0}^{t_0+\varepsilon} \hat{w}_\varepsilon^t dt = \int_0^\varepsilon w_\varepsilon^t dt = \int_0^{\varepsilon/2} (w_\varepsilon^t + w_\varepsilon^{\varepsilon-t}) dt,$$

we have from Lemma 6.4 that, for $r \in (3, \min\{4, s\})$,

$$\|J^{-(4-r)/2} \bar{w}_\varepsilon\|_{L^\infty} \leq \frac{1}{2} C_{70,r} \varepsilon^3.$$

This means that \bar{w}_ε , a function in $W^{r,\infty}$, is particularly small in the negative Sobolev norm $W^{r-4,\infty}$. To avoid dealing with negative Sobolev spaces, which particularly due to the endpoint parameter of integrability $p = \infty$ are complex to negotiate, we make an excursion into spaces associated with $\infty > p \gg 1$, where we can easily apply dual norms to get the result we would like.

If we let $p \in (1, \infty)$ and set $q^{-1} = 1 - p^{-1}$, then we have that for $\phi \in W^{3, \infty}$,

$$\left\| e^{(m-n)\varepsilon\mathcal{L}/2} \nabla \bar{w}_\varepsilon \cdot \nabla \phi \right\|_{L^p} = \sup_{\|\psi\|_q=1} \int_{\mathbb{D}} \psi e^{(m-n)\varepsilon\mathcal{L}} \nabla \bar{w}_\varepsilon \cdot \nabla \phi \, dx.$$

Since $e^{(m-n)\varepsilon\mathcal{L}/2} = e^{\frac{1}{2}(t-\bar{t})\mathcal{L}}$ is a symmetric kernel operator with respect to the measure $\rho \, dx$, this and integration by parts give that

$$\int_{\mathbb{D}} \psi e^{(m-n)\varepsilon\mathcal{L}/2} \nabla \bar{w}_\varepsilon \cdot \nabla \, dx = - \int_{\mathbb{D}} \bar{w}_\varepsilon g \, dx, \quad (43)$$

where

$$g := \nabla \cdot \left(e^{(m-n)\varepsilon\mathcal{L}} \rho^{-1} \psi \right) \rho \nabla \phi.$$

This term can be bounded in the $W^{4-r, q}$ norm with liberal use of Proposition 5.1, by using that

$$\left\| \nabla \cdot \left(e^{(m-n)\varepsilon\mathcal{L}/2} \rho^{-1} \psi \right) \rho \nabla \phi \right\|_{W^{4-r, q}} \leq K_q^\nabla K_{q; 5-r, 5-r, 2}^\times \left\| e^{(m-n)\varepsilon\mathcal{L}/2} \rho^{-1} \psi \right\|_{W^{5-r, q}} K_\infty^\nabla \|\phi\|_{W^{3, \infty}}$$

and

$$\left\| e^{(m-n)\varepsilon\mathcal{L}/2} \rho^{-1} \psi \right\|_{W^{5-r, q}} \leq K_{q; 5-r, 5-r, 3}^\times \|\rho\|_{W^{2, \infty}} K_{q; 0, 5-r}^T ((m-n)\varepsilon/2)^{-(5-r)/2} \|\rho^{-1}\|_\infty.$$

Thus, there exist constants $C_{94, T, p, r}$ such that for all $(m-n)\varepsilon \leq T$,

$$\|g\|_{W^{4-r, q}} \leq C_{94, T, p} ((m-n)\varepsilon)^{-(5-r)/2}.$$

Returning to (43), we obtain that

$$\int_{\mathbb{D}} \bar{w}_\varepsilon g \, dx = \int_{\mathbb{D}} (J^{-(4-r)/2} \bar{w}_\varepsilon) (J^{(4-r)/2} g) \, dx,$$

using firstly that $J^{-(r-2)/2} J J^{(4-r)/2}$ is the identity, secondly that from (21), $J^{-(r-2)/2}$ is a symmetric kernel operator, and finally integration by parts. Using this we can deduce that

$$\begin{aligned} \int_{\mathbb{D}} \bar{w}_\varepsilon g \, dx &\leq \|J^{-(4-r)/2} \bar{w}_\varepsilon\|_{L^p} \|g\|_{W^{4-r, q}} \\ &\leq |\mathbb{D}|^{1/p} \|J^{-(4-r)/2} \bar{w}_\varepsilon\|_{L^\infty} C_{94, T, p, r} ((m-n)\varepsilon)^{-(5-r)/2} \\ &\leq L^{d/p} \frac{1}{2} C_{70, r} \varepsilon^3 C_{94, T, p, r} ((m-n)\varepsilon)^{-(5-r)/2} \\ &:= C_{95, T, p, r} ((m-n)\varepsilon)^{-(5-r)/2} \varepsilon^3. \end{aligned}$$

As a result, we can say that

$$\left\| e^{(m-n)\varepsilon\mathcal{L}/2} \nabla \bar{w}_\varepsilon \cdot \nabla S_\varepsilon(t_0 + n\varepsilon, t_0) \right\|_{W^{3, \infty} \rightarrow L^p} \leq C_{95, T, p, r} ((m-n)\varepsilon)^{-(5-r)/2} \varepsilon^3. \quad (44)$$

To obtain (42) from (44), it remains to obtain a bound on the rest of the action of the semigroup $\|e^{(m-n)\varepsilon\mathcal{L}/2}\|_{L^p \rightarrow L^\infty}$. Recalling the definition of the Gaussian kernel (7), we use the Gaussian upper estimate (Liskevich & Semenov 2000) that for $t \leq T$,

$$(e^{t\mathcal{L}/2} \phi)(x) \leq C_{96} \int g_{C_{97}t}(x-y) \phi(y) \, dy$$

for some C_{96}, C_{97} depending on $\|\nabla \log \rho\|_{L^\infty}, L, d, T$, to get that

$$\|e^{t\mathcal{L}/2}\phi\|_{L^\infty} \leq C_{96}\|g_{C_{97}t/2}\|_{L^q}\|\phi\|_{L^p} \leq C_{96}q^{-d/2q}(C_{97}t/2)^{-d/p}\|\phi\|_{L^p} := C_{98,p}t^{-d/p}\|\phi\|_{L^p}.$$

Then, applying also Proposition 7.3 for the norm of $S_\varepsilon(t_0 + n\varepsilon, t_0)$, we have

$$\left\|e^{(m-n)\varepsilon\mathcal{L}}\nabla\bar{w}_\varepsilon \cdot \nabla S_\varepsilon(t_0 + n\varepsilon, t_0)\right\|_{W^{3,\infty} \rightarrow L^\infty} \leq C_{98,p}C_{95,T,p,r}K_{3+\beta,3}^C C_{89,T,\beta}((m-n)\varepsilon)^{-(5-r)/2-d/p}\varepsilon^3. \quad (45)$$

Fixing r and choosing $p > 2d/(r-3)$ we have $(5-r)/2+d/p < 1$ and thus there exists a constant $C_{96,T,\beta}$ such that for $m\varepsilon \leq T$,

$$\sum_{n=0}^{m-1} \left\|e^{(m-n)\varepsilon\mathcal{L}}\nabla\bar{w}_\varepsilon \cdot \nabla S_\varepsilon(t_0 + n\varepsilon, t_0)\right\|_{W^{3,\infty} \rightarrow L^\infty} \leq C_{96,T,\beta}\varepsilon^2.$$

Combining this with (42) gives us (23) for $t_1 = t_0 + m\varepsilon$ as required. \square

8 Convergence of kernel operator in finite data approximation

We now turn to the ‘‘variance’’ error, i.e. the convergence of the finite data approximation as the sample size $M \rightarrow \infty$. In this section we begin by showing the convergence of the discretised Gaussian kernel $\mathcal{K}_\varepsilon^M$ to the continuum limit \mathcal{K}_ε . We prove convergence first pointwise for fixed functions, then extend to convergence in norm on fixed functions, and then finally to norm-convergence of operators.

Recall from (9 – 12) that we defined the operators \mathcal{K}_ε and $\mathcal{K}_\varepsilon^M$ as

$$(\mathcal{K}_\varepsilon\phi)(x) = \int g_{\varepsilon,L}(x-y)\phi(y)\rho(y)dy \quad (46)$$

and

$$(\mathcal{K}_\varepsilon^M\phi)(x) = \frac{1}{M} \sum_{i=1}^M g_{\varepsilon,L}(x-x^i)\phi(x^i). \quad (47)$$

Since the $\{x_i\}$ are sampled from the measure ρ , the continuous operator $\mathcal{K}_\varepsilon\phi$ is the expectation of the discretised operator $\mathcal{K}_\varepsilon^M\phi$ with respect to this sampling. Because the discretised operator is the sum of independent random variables $g_{\varepsilon,L}(x-x^i)\phi(x^i)$, it is therefore natural to try to construct central limit theorems.

The basic result we will use for this purpose is the following general result that provides strong quantitative control on the tail probabilities:

Lemma 8.1. *Consider an i.i.d. collection of bounded, centred random variables X_i . Then if $\mathbb{E}[X^2] \leq \nu$ and $c \leq 2 \log 2\nu/\|X\|_0$,*

$$\mathbb{P}\left(\left|\frac{1}{M} \sum_{i=1}^M X_i\right| > c\right) \leq 2e^{-Mc^2/4\nu}.$$

Proof. We have the Chernoff bound

$$\mathbb{P}\left(\frac{1}{M} \sum_{i=1}^M X_i > c\right) \leq \min_t e^{-Mct} \mathbb{E}[e^{tX}]^M.$$

The second derivative of $\mathbb{E}[e^{tX}]$, the moment generating function of X , can be bounded

$$\frac{d^2}{dt^2}\mathbb{E}[e^{tX}] = \mathbb{E}[X^2 e^{tX}] \leq \nu e^{t\|X\|_{L^\infty}},$$

and therefore using Taylor's theorem and that $\mathbb{E}[X] = 0$,

$$\mathbb{E}[e^{tX}] \leq 1 + \frac{1}{2}t^2\nu e^{t\|X\|_{L^\infty}} \leq e^{\frac{1}{2}t^2\nu e^{t\|X\|_{L^\infty}}}.$$

Consequently,

$$\mathbb{P}\left(\frac{1}{M}\sum_{i=1}^M X_i > c\right) \leq \min_t e^{-Mct}\mathbb{E}[e^{tX}]^M \leq \min_t e^{-Mct + \frac{1}{2}Mt^2\nu e^{t\|X\|_{L^\infty}}}.$$

If we set $t = c/2\nu$, we have by stipulation that $e^{t\|X\|_{L^\infty}} \leq 2$ and so

$$\mathbb{P}\left(\frac{1}{M}\sum_{i=1}^M X_i > c\right) \leq e^{-Mc^2/4\nu}.$$

The lower bound follows similarly, giving the required bound. \square

To deal with the fact that we are using the periodised Gaussian kernel $g_{\varepsilon,L}$ rather than the standard one g_ε , we will require the following proposition:

Proposition 8.2. *Define the increasing functions of ε*

$$\begin{aligned}\gamma_{\varepsilon,L} &= \sum_{j \in \mathbb{Z}} e^{-j^2 L^2 / 2\varepsilon}, \\ \gamma'_{\varepsilon,L} &= \sum_{j=1}^{\infty} (2j+1)L\varepsilon^{-1/2} e^{-(2j-1)^2 L^2 / 8\varepsilon}.\end{aligned}$$

Then for all $x \in [-L/2, L/2]^d$,

$$\begin{aligned}g_{\varepsilon,L}(x) &\leq (1 + \gamma_{\varepsilon,L})^d g_\varepsilon(x), \\ \sup g_{\varepsilon,L} &\leq \gamma_{\varepsilon,L}^d g_\varepsilon(0), \\ \text{Lip } g_{\varepsilon,L} &\leq \gamma'_{L,\varepsilon,d} \text{Lip } g_\varepsilon,\end{aligned}$$

where

$$\gamma'_{L,\varepsilon,d} := e^{-1} + d\gamma'_{\varepsilon,L}\gamma_{\varepsilon,L}^{d-1}.$$

The next lemma, on pointwise evaluation of the operators we are interested in, follows from Lemma 8.1.

Lemma 8.3. *For all $\phi \in C^0$, $c \leq \|\rho\|_0 \log 2$ and $x \in \mathbb{D}$,*

$$\mathbb{P}\left(|(\mathcal{K}_\varepsilon^M \phi)(x) - (\mathcal{K}_\varepsilon \phi)(x)| > c\|\phi\|_0\right) \leq 2 \exp\left\{-\frac{Mc^2}{4\gamma_{\varepsilon,L}^d (2\pi\varepsilon)^{-d/2} \|\rho\|_0}\right\}.$$

Proof of Lemma 8.3. Equations (46 – 47) and the independent sampling of the x^i from ρ mean that $(\mathcal{K}_\varepsilon^M \phi)(x)$ is a sum of *i.i.d.* centred, bounded random variables:

$$(\mathcal{K}_\varepsilon^M \phi)(x) = \frac{1}{M} \sum_{i=1}^M \mathfrak{g}_x(x^i),$$

where

$$\mathfrak{g}_x(y) = g_{\varepsilon,L}(x-y)\phi(x^i) - \mathbb{E}_y[g_{\varepsilon,L}(x-y)\phi(y)].$$

The sup-norm of this function is bounded as

$$\|\mathfrak{g}_x\|_0 \leq 2\|g_{\varepsilon,L}(x-\cdot)\phi(\cdot)\|_0 \leq 2(2\pi\varepsilon)^{-d/2}\gamma_{\varepsilon,L}^d\|\phi\|_0,$$

and the L^2 norm as

$$\begin{aligned} \mathbb{E}[\mathfrak{g}_x^2] &\leq \mathbb{E}_y[g_{\varepsilon,L}(x-y)^2\phi(y)^2] \\ &= \int g_{\varepsilon,L}(x-y)^2\phi(y)^2\rho(y)dy \\ &\leq (2\pi\varepsilon)^{-d/2}\gamma_{\varepsilon,L}^d\|\phi\|_0^2\|\rho\|_0. \end{aligned}$$

From an application of Lemma 8.1 the result then follows. \square

By using the compactness of our domain \mathbb{D} we can extend this to bounds on the function norms:

Lemma 8.4. *There exist constants C_0, C_1 depending only on $L, d, \|\rho\|_0, \varepsilon_0$ such that for all $\varepsilon < \varepsilon_0$, $\phi \in C^0$ and $c < \|\rho\|_0 \log 2$,*

$$\mathbb{P}(\|(\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon)\phi\|_0 > 2c\|\phi\|_0) \leq 2C_1c^{-d}\varepsilon^{-d(d+1)/2} \exp\{-C_0M\varepsilon^{d/2}c^2\}.$$

Proof of Lemma 8.4. Firstly, we have the deterministic bound that

$$\text{Lip}(\mathcal{K}_\varepsilon - \mathcal{K}_\varepsilon^M)\phi \leq \text{Lip } \mathcal{K}_\varepsilon\phi + \text{Lip } \mathcal{K}_\varepsilon^M\phi \leq 2\text{Lip } g_\varepsilon\|\phi\|_0 = 2\varepsilon^{-1/2}(2\pi\varepsilon)^{-d/2}\gamma'_{L,\varepsilon,d}\|\phi\|_0. \quad (48)$$

Now, define the finite subset of the domain $\mathbb{D} = [0, L]^d$

$$S_\xi = \{(\xi n_1, \dots, \xi n_d) : n_1, \dots, n_d = 0, \dots, \lceil L/\xi \rceil - 1\}.$$

No point in \mathbb{D} is more than $\sqrt{d}\xi$ away from an element of S_ξ , and S_ξ contains no more than $(L/\xi + 1)^d$ points.

By applying Lemma 8.3 and a union bound, we obtain that for all $x \in S_\xi$

$$\mathbb{P}\left(\sup_{x \in S_\xi} |(\mathcal{K}_\varepsilon^M \phi)(x) - (\mathcal{K}_\varepsilon \phi)(x)| > c\|\phi\|_0\right) \leq 2(L/\xi + 1)^d \exp\{-C_0M\varepsilon c^2\},$$

where the constant

$$C_0 := \frac{1}{4}\gamma_{\varepsilon_0,L}^{-d}(2\pi)^{d/2}\|\rho\|_0^{-1}.$$

Using the Lipschitz bound (48) we can then say that

$$\begin{aligned} \mathbb{P}\left(\sup_{x \in \mathbb{D}} |(\mathcal{K}_\varepsilon^M \phi)(x) - (\mathcal{K}_\varepsilon \phi)(x)| > (c + 2\varepsilon^{-1/2}(2\pi\varepsilon)^{-d/2}\sqrt{d}\gamma'_{L,\varepsilon,d}\xi)\|\phi\|_0\right) \\ \leq 2(L/\xi + 1)^d \exp\{-C_0M\varepsilon^{d/2}c^2\}. \end{aligned}$$

Setting

$$\xi = \frac{c\varepsilon^{1/2}(2\pi\varepsilon)^{d/2}\gamma'_{L,\varepsilon,d}}{2\sqrt{d}}$$

we obtain

$$\mathbb{P}(\|(\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon)\phi\|_0 > 2c\|\phi\|_0) \leq 2 \left(\frac{2L\sqrt{d}\varepsilon^{-1/2}(2\pi\varepsilon)^{-d/2}}{c\gamma'_{L,\varepsilon,d}} + 1 \right)^d \exp\{-C_0M\varepsilon^{d/2}c^2\},$$

which requiring that $\varepsilon \leq \varepsilon_0$ and setting

$$C_1 = \left(2L\sqrt{d}(2\pi)^{-d/2}/\gamma'_{L,\varepsilon_0,d} + \varepsilon_0^{(d+1)/2}\|\rho\|_0 \log 2 \right)^d$$

gives the required bound. \square

We would now like to extend this result to convergence as operators. Recall that we defined for $\zeta > 0$ the complex domains

$$\mathbb{D}_\zeta = \{x + iz \mid x \in \mathbb{D}, z \in [-\zeta, \zeta]^d\},$$

so that $\mathbb{D} \subset \mathbb{D}_\zeta \subset (\mathbb{C}/L\mathbb{Z})^d$; we also defined the Hardy spaces

$$H^\infty(\mathbb{D}_\zeta) = \{\phi \in C^0(\mathbb{D}_\zeta) : \phi \text{ analytic on } \text{int } \mathbb{D}_\zeta\}$$

with $\|\cdot\|_\zeta$ being the $C^0(\mathbb{D}_\zeta)$ norm. In Theorems 3.1 and 3.7 (presented in Section 3) we show that when the size of ζ scales with the kernel bandwidth $\sqrt{\varepsilon}$, $\mathcal{K}_\varepsilon^M$ converges in operator norm to \mathcal{K}_ε .

To extend from function-wise convergence to uniform convergence across all functions, we will again make use of a compactness argument: this time, the compact embedding of $H^\infty(\mathbb{D}_\zeta)$ in $C^0(\mathbb{D})$. This choice allows us to obtain good operator convergence bounds in the strong space $H^\infty(\mathbb{D}_\zeta)$ as, Gaussian convolution \mathcal{C}_ε maps the weak space $C^0(\mathbb{D})$ into the strong space $H^\infty(\mathbb{D}_\zeta)$ with an $\mathcal{O}(1)$ penalty in norm, provided that ζ is $\mathcal{O}(\varepsilon^{1/2})$ (see Proposition 8.8).

However, this scaling restriction on ζ , which arises from the width of the Gaussian kernel, leads to a complication. The larger complex domain \mathbb{D}_ζ is only a relatively small extension of the real domain \mathbb{D} , which means that a covering of $H^\infty(\mathbb{D}_\zeta)$ requires a number of $C^0(\mathbb{D})$ balls that is exponentially large in $\varepsilon^{-1/2}$ and thus jeopardises the Central Limit Theorem bounds obtained in Lemma 8.4.

However, we can use the Gaussian kernel's localisation to our advantage, as the values of $\mathcal{K}_\varepsilon^M\phi(x)$, $\mathcal{K}_\varepsilon\phi(x)$ more or less depend only on values of ϕ inside a ball slightly larger than $\mathcal{O}(\varepsilon^{1/2})$. We thus divide our domain \mathbb{D} up into small, overlapping cubes \mathcal{E} of this size: the complex ζ -fattening \mathcal{E}_ζ is a sufficiently large extension of \mathcal{E} and on each of these cubes we therefore have acceptable covering numbers.

We will make use of the following quantitative compactness result, proved in Appendix B:

Proposition 8.5. *Let $\mathcal{E} \subset \mathbb{D}$ be a hypercube of side length $2\ell \geq 2\zeta/\eta_0$ and, \mathcal{E}_ζ the closed ζ -fattening of \mathcal{E}*

$$\mathcal{E}_\zeta = \{x \in \mathbb{D}_\zeta : d(x, \mathcal{E}) \leq \zeta\}.$$

There exist constants C_{11}, C_{12} dependent only on η_0, d such that for each $\xi \in (0, \frac{1}{2})$ there exists a set $\mathcal{S}_\xi^{\ell, \zeta}$ such that for every function $\phi \in H^\infty(\mathcal{E}_\zeta)$ with $\|\phi\|_{H^\infty(\mathcal{E}_\zeta)} \leq 1$,

$$\sup_{\psi \in \mathcal{S}_\xi^{\ell, \zeta}} \|\phi - \psi\|_{C^0(\mathcal{E})} \leq \xi, \tag{49}$$

and the cardinality of $\mathcal{S}_\xi^{\ell, \zeta}$ is bounded by

$$|\mathcal{S}_\xi^{\ell, \zeta}| \leq e^{(C_{11} \log \xi^{-1} + C_{12} \log(\zeta^{-1} \ell))(\zeta^{-1} \ell \log \xi^{-1})^d}.$$

Using Proposition 8.5 we can prove central limit theorem-style bounds on the operator norm of $\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon$ from a strong space associated with a larger cube \mathcal{E} to a weak space associated with a smaller cube E .

Proposition 8.6. *Let \mathcal{E} be as in Proposition 8.7 and let E be a hypercube of side length $2l < 2\ell$ centred inside \mathcal{E} . Then there exist positive constants C_{12}, C_{13}, C_{14} dependent only on $\|\rho\|_0, d, L, \eta_0, \varepsilon_0$ such that for $c \leq \|\rho\|_0 \log 2$,*

$$\begin{aligned} & \mathbb{P} \left(\|(\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon) \mathbb{1}_E\|_{H^\infty(\mathcal{E}_\zeta) \rightarrow C^0(E)} \geq 3c \|\phi\|_0 \right) \\ & \leq \exp \left\{ (C_{13} \log \varepsilon^{-1} + C_{14} \log c^{-1} + C_{12} \log(\ell/\zeta))^{d+1} (\ell/\zeta)^d - \frac{Mc^2}{4(2\pi\varepsilon)^{-d/2} \|\rho\|_0} \right\}. \end{aligned}$$

Proof of Proposition 8.6. The proof proceeds analogously to the proof of Lemma 8.4.

Let $\mathcal{S}_\xi^{\ell, \zeta}$ be as in Proposition 8.5. The difference between the operators can be bounded deterministically by

$$\|\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon\|_0 \leq \|\mathcal{K}_\varepsilon^M\|_0 + \|\mathcal{K}_\varepsilon\|_0 \leq 2\gamma_{\varepsilon, L}^d (2\pi\varepsilon)^{-d/2}$$

and so, using (49),

$$\sup_{\psi \in \mathcal{S}_\xi^{\ell, \zeta}} \left\| (\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon) \mathbb{1}_E (\|\phi\|_\zeta^{-1} \phi - \psi) \right\|_{C^0(E)} \leq 2\gamma_{\varepsilon, L}^d (2\pi\varepsilon)^{-d/2} \xi \quad (50)$$

for all ϕ in the unit ball of $H^\infty(\mathcal{E}_\zeta)$.

On the other hand, we can apply Lemma 8.4 and a union bound to show that

$$\mathbb{P} \left(\sup_{\psi \in \mathcal{S}_\xi^{\ell, \zeta}} \|(\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon) \mathbb{1}_E \psi\|_0 > 2c \right) \leq |\mathcal{S}_\xi^{\ell, \zeta}| C_1 c^{-d} \varepsilon^{-d(d+1)/2} \exp \left\{ -C_0 M \varepsilon^{d/2} c^2 \right\}. \quad (51)$$

By combining (50 – 51) and setting $\xi = (2\pi\varepsilon)^{d/2} c / 2\gamma_{\varepsilon, L}^d$ we obtain that

$$\mathbb{P} \left(\sup_{\|\phi\|_{H^\infty(\mathcal{E}_\zeta)} \leq 1} \|(\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon) \mathbb{1}_E \phi\|_0 > 3c \right) \leq |\mathcal{S}_{(2\pi\varepsilon)^{d/2} c / 2\gamma_{\varepsilon, L}^d}^{\ell, \zeta}| C_1 c^{-d} \varepsilon^{-d(d+1)/2} \exp \left\{ -C_0 M \varepsilon^{d/2} c^2 \right\},$$

which using that $\varepsilon \leq \varepsilon_0$, $\ell/\zeta \geq \eta_0$ and $c \leq \|\rho\|_0 \log 2$ and the bound on $\mathcal{S}_\xi^{\ell, \zeta}$ in Proposition 8.5 gives the required bound. \square

We can also make a deterministic bound on the error that this restriction to the larger cube \mathcal{E} introduces relative to the full diffusion:

Proposition 8.7. *Let \mathcal{E}, E be as in Proposition 8.6. Then*

$$\|(\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon) \mathbb{1}_{\mathbb{D} \setminus E}\|_{H^\infty(\mathbb{D}_\zeta) \rightarrow C^0(E)} \leq 2(1 + \gamma_{\varepsilon, L})^d (2\pi\varepsilon)^{-d/2} e^{-(\ell-l)^2/2\varepsilon}.$$

Proof of Proposition 8.7. For $x \in E$,

$$\begin{aligned} |\mathcal{K}_\varepsilon^M \mathbb{1}_{\mathbb{D} \setminus \mathcal{E}} \phi(x)| &\leq \frac{1}{M} \sum_{i=1}^M |g(x - x^i)| \mathbb{1}_{\mathbb{D} \setminus \mathcal{E}}(x^i) \|\phi\|_0 \\ &\leq \sup_{y \in \mathbb{D} \setminus \mathcal{E}} g(x - y) \|\phi\|_0 \\ &\leq (2\pi\varepsilon)^{-d/2} (1 + \gamma_{\varepsilon, L})^d e^{-(\ell-l)^2/2\varepsilon} \|\phi\|_0. \end{aligned}$$

Similarly,

$$|\mathcal{K}_\varepsilon \mathbb{1}_{\mathbb{D} \setminus \mathcal{E}} \phi(x)| \leq (2\pi\varepsilon)^{-d/2} (1 + \gamma_{\varepsilon, L})^d e^{-(\ell-l)^2/2\varepsilon} \|\phi\|_0$$

Combining these results and using that $\|\cdot\|_0 \leq \|\cdot\|_\zeta$ we obtain what is required. \square

This is enough for us to prove Theorem 3.1

Proof of Theorem 3.1. Set

$$\ell = 2l = \sqrt{8\varepsilon \min\{1, \log(2(1 + \gamma_{\varepsilon, L})^d c^{-1} (2\pi\varepsilon)^{-d/2})\}}.$$

From Proposition 8.7 we thus have

$$\|(\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon) \mathbb{1}_{\mathbb{D} \setminus \mathcal{E}}\|_{H^\infty(\mathbb{D}_\zeta) \rightarrow C^0(E)} \leq c.$$

Combining this with Proposition 8.6 and using that $\ell/\zeta \leq C_{16} \log(c^{-1}\varepsilon^{-1})$ we have

$$\begin{aligned} \mathbb{P}(\|(\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon) \mathbb{1}_{\mathcal{E}}\|_{H^\infty(\mathcal{E}_\zeta) \rightarrow C^0(E)} \geq 4c \|\phi\|_0) \\ \leq \exp\left\{(C_{17} \log \varepsilon^{-1} + C_{18} \log c^{-1})^{d+1} \log(c^{-1}\varepsilon^{-1})^d - \frac{Mc^2}{4(2\pi\varepsilon)^{-d/2} \|\rho\|_0}\right\}. \end{aligned}$$

The full domain \mathbb{D} can be covered by $\lceil L/l \rceil^d \leq (1 + L/\sqrt{8\varepsilon})^d$ hypercubes of side-length l . Thus

$$\mathbb{P}(\|(\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon) \mathbb{1}_{\mathcal{E}}\|_{H^\infty(\mathcal{E}_\zeta) \rightarrow C^0(\mathbb{D})} \geq 4c \|\phi\|_0) \leq \exp\left\{C_{20} (\log(2\varepsilon c)^{-1})^{2d+1} - C_0 M \varepsilon^{d/2} c^2\right\}, \quad (52)$$

which by relabelling $4c \rightarrow c$ and $\varepsilon \rightarrow \varepsilon/2$, and setting $C_{26} = 2^{-d/2} C_0/64$ gives us (3.1), as required. \square

The remaining necessary ingredient for the proof of Theorem 3.7 is a bound taking one from the weak space back into the strong space. Recall the definition of the Gaussian kernel operator (8):

$$\mathcal{C}_\varepsilon \phi(x) = \int_{\mathbb{D}} g_{\varepsilon, L}(x - y) \phi(y) \, dy.$$

Then the following proposition holds:

Proposition 8.8. *For all $\phi \in C^0(\mathbb{D})$,*

$$\|\mathcal{C}_\varepsilon \phi\|_\zeta \leq e^{d\zeta^2/2\varepsilon} \|\phi\|_0.$$

Proof of Proposition 8.8. Extending ϕ periodically to \mathbb{R}^d , we find that

$$\begin{aligned}\|\mathcal{C}_\varepsilon\phi\|_\zeta &= \sup_{x \in \mathbb{D}, z \in [-\zeta, \zeta]^d} \left| \int_{\mathbb{R}^d} (2\pi\varepsilon)^{-d/2} e^{-(x-y+iz)^2/2\varepsilon} \phi(y) \, dy \right| \\ &\leq \sup_{x \in \mathbb{D}, z \in [-\zeta, \zeta]^d} \int_{\mathbb{R}^d} (2\pi\varepsilon)^{-d/2} e^{-\Re \sum_{j=1}^d (x_j - y_j + iz_j)^2/2\varepsilon} \|\phi\|_0 \, dy \\ &= \sup_{z \in [-\zeta, \zeta]^d} e^{|z|^2/2\varepsilon} \|\phi\|_0,\end{aligned}$$

giving the required result. \square

Proof of Theorem 3.7. We can decompose

$$\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon = \mathcal{C}_{\varepsilon/2}(\mathcal{K}_{\varepsilon/2}^M - \mathcal{K}_{\varepsilon/2}),$$

where we recall that \mathcal{C}_ε is convolution by a Gaussian of variance ε . Combining Proposition 8.8 and Theorem 3.1, we obtain the necessary bound in the H^∞ norm. \square

9 Convergence of the weighted operator in finite data approximation

We now turn to the normalised operator $\mathcal{P}_\varepsilon^M$. We must first bound the convergence of the function U_ε^M solving the discretised Sinkhorn problem (10) converges to the continuum limit U_ε solving (13). To apply uniform bounds on U_ε and $(I - \mathcal{P}_\varepsilon)^{-1}$ in the C^0 norm to Hardy spaces, we will find the following proposition, whose proof is in Appendix C useful:

Proposition 9.1. *Suppose that $\phi > 0$. Then if $\zeta = Z_0\varepsilon^{1/2}$ with*

$$Z_0 \leq \frac{\pi}{8d} (\|\phi\|_0 \|\phi^{-1}\|_0 \|\rho\|_0 \|\rho^{-1}\|_0)^{-2},$$

then if $\psi = 1/(\mathcal{K}\phi)$, the bounds in the Hardy norm hold

$$\begin{aligned}\|\psi\|_\zeta &\leq 2\|\phi^{-1}\|_0 \\ \|\psi^{-1}\|_\zeta &\leq e^{2dZ_0^2} \|\rho\|_0 \|\phi\|_0.\end{aligned}$$

As an immediate consequence we have

Proposition 9.2. *If $\zeta = Z_0\varepsilon^{1/2}$ with $Z_0 \leq \pi(\|\rho\|_0 \|\rho^{-1}\|_0 C_{68}^2)^{-2}/8d$, where C_{68} is defined in Theorem 6.1, then*

$$\|U_\varepsilon\|_\zeta \leq 2C_{68}^{-1}, \quad (53)$$

We will also find the following proposition useful:

Proposition 9.3. *There exists a constant C_{48} such that for all $\varepsilon < \varepsilon_0$ and Z_0 as in Proposition 9.2, then*

$$\|(I + \mathcal{P}_\varepsilon)^{-1}\|_\zeta \leq C_{48}. \quad (54)$$

To prove this proposition we require the following result, whose proof is in Appendix C.

Lemma 9.4. *There exists a constant C_{40} such that for all $\varepsilon \leq \varepsilon_0$,*

$$\|(I + \mathcal{P}_\varepsilon)^{-1}\|_0 \leq C_{40}.$$

Proof of Proposition 9.3. We decompose

$$(I - \mathcal{P}_\varepsilon)^{-1} = I + \mathcal{P}_\varepsilon(I - \mathcal{P}_\varepsilon)^{-1}.$$

We then have for $\phi \in H^\infty(\mathbb{D}_\zeta)$ that

$$\|\mathcal{P}_\varepsilon(I - \mathcal{P}_\varepsilon)^{-1}\phi\|_\zeta \leq \|U_\varepsilon\|_\zeta \|D_\varepsilon\|_{0 \rightarrow \zeta} \|U_\varepsilon\|_0 \|(I - \mathcal{P}_\varepsilon)^{-1}\|_0 \|\phi\|_0,$$

which by an application of Proposition 9.2 and Lemma 9.4 gives

$$\|\mathcal{P}_\varepsilon(I - \mathcal{P}_\varepsilon)^{-1}\phi\|_\zeta \leq 2C_{68}^2 e^{2dZ_0^2} C_{40} \|\phi\|_0.$$

Using that $\|\cdot\|_0 \leq \|\cdot\|_\zeta$ we obtain the required result. \square

We can now prove convergence of the Sinkhorn weight as the number of particles $M \rightarrow \infty$:

Lemma 9.5. *Suppose Z_0 is as in Proposition 9.2. There exist constants C_{37}, C_{38} such that if $\delta \leq C_{37}$ then*

$$\|U_\varepsilon^M - U_\varepsilon\|_\zeta, \|Y_\varepsilon^M - Y_\varepsilon\|_0, \|(Y_\varepsilon^M)^{-1} - (Y_\varepsilon)^{-1}\|_0 \leq C_{38}\delta,$$

where $\zeta = Z_0\varepsilon^{1/2}$.

Proof of Lemma 9.5. We can rewrite (13 – 10) as

$$\begin{aligned} U_\varepsilon(x) (\mathcal{K}_\varepsilon U_\varepsilon)(x) &\equiv 1 \\ U_\varepsilon^M(x) (\mathcal{K}_\varepsilon^M U_\varepsilon^M)(x) &\equiv 1. \end{aligned}$$

If for $\theta \in [0, 1]$ we set

$$\mathcal{K}_\varepsilon^\theta := (1 - \theta)\mathcal{K}_\varepsilon + \theta\mathcal{K}_\varepsilon^M$$

then we obtain a one-parameter family of Sinkhorn weight functions U_ε^θ solving

$$U_\varepsilon^\theta(x) (\mathcal{K}_\varepsilon^\theta U_\varepsilon^\theta)(x) \equiv 1. \tag{55}$$

The existence and uniqueness of the U_ε^θ follow from the positivity of the operator $\mathcal{K}_\varepsilon^\theta$, on $L^\infty(\mathbb{D})$ for $\theta \in [0, 1)$ and on $L^\infty(\{x^i\}_{i=1\dots M})$ for $\theta = 1$.

Furthermore, because

$$\frac{d}{d\theta} \mathcal{K}_\varepsilon^\theta = \mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon$$

is a bounded operator on H_ζ^∞ , we can apply the implicit function theorem to (55) as long as U_ε^θ stays in H_ζ^∞ , so that

$$\frac{d}{d\theta} \log U_\varepsilon^\theta = -(I + U_\varepsilon^\theta \mathcal{K}_\varepsilon^\theta U_\varepsilon^\theta)^{-1} U_\varepsilon^\theta(x) ((\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon) U_\varepsilon^\theta)(x).$$

We have from Propositions 9.2 and 9.3 that $\|U_\varepsilon\|_\zeta \leq 2C_{68}$, and $\|(I - \mathcal{P}_\varepsilon)^{-1}\|_\zeta \leq C_{48}$, and from Theorem 3.7 that $\|\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon\|_\zeta \leq e^{2dZ_0^2} \delta$. Note that since \mathcal{P}_ε has 1 as an eigenvalue, $C_{48} \geq 1/2$.

If $B(\theta) := \|\log U_\varepsilon^\theta - \log U_\varepsilon\|_\zeta$, then

$$B'(\theta) \leq \left\| \frac{d}{d\theta} \log U_\varepsilon^\theta \right\|_\zeta \leq C_{48} (1 - C_{48} \|U_\varepsilon^\theta \mathcal{K}_\varepsilon^\theta U_\varepsilon^\theta - \mathcal{P}_\varepsilon\|_\zeta)^{-1} e^{2dZ_0^2} \delta \|U_\varepsilon^\theta\|_\zeta.$$

Because $\|U_\varepsilon^\theta\|_\zeta \leq 2C_{68}e^{B(\theta)}$,

$$B'(\theta) \leq \frac{4C_{68}^2 C_{48} e^{2dZ_0^2} \delta e^{2B(\theta)}}{1 - 4C_{68}^2 C_{48} (\|\mathcal{K}_\varepsilon^\theta\|_\zeta B(\theta) (e^{2B(\theta)} + e^{B(\theta)} + e^{2dZ_0^2} \delta e^{B(\theta)}))}$$

and because $\|\mathcal{K}_\varepsilon^\theta\|_\zeta \leq \|\mathcal{K}_\varepsilon\|_\zeta + \theta e^{2dZ_0^2} \delta \leq 1 + e^{2dZ_0^2} \delta$,

$$B'(\theta) \leq \frac{4C_{68}^2 C_{48} e^{2dZ_0^2} \delta e^{2B(\theta)}}{1 - 4C_{68}^2 C_{48} (2(1 + e^{2dZ_0^2} \delta) B(\theta) e^{2B(\theta)} + e^{2dZ_0^2} \delta e^{B(\theta)})}.$$

Thus, as long as $B(\theta) \leq \min\{e^{2dZ_0^2} \delta, C_{30}\}$ and $\delta \leq C_{31}/(4C_{68}^2 C_{48} e^{2dZ_0^2}) =: C_{35}$ for some fixed constants C_{30}, C_{31}, C_{32} ,

$$B'(\theta) \leq C_{32} 4C_{68}^2 C_{48} e^{2dZ_0^2} \delta$$

and thus

$$\|\log U_\varepsilon - \log U_\varepsilon^M\|_\zeta \leq B(1) \leq C_{32} 4C_{68}^2 C_{48} e^{2dZ_0^2} \delta.$$

Furthermore, for some fixed constant C_{33} ,

$$\begin{aligned} \|U_\varepsilon^M - U_\varepsilon\|_\zeta &\leq \|U_\varepsilon\|_\zeta \left(e^{\|\log U_\varepsilon - \log U_\varepsilon^M\|_\zeta} - 1 \right) \\ &\leq C_{33} 8C_{68}^3 C_{48} e^{2dZ_0^2} \delta \\ &\leq C_{33} 8C_{68}^3 C_{48} e^{2dZ_0^2} \delta =: C_{34} \delta, \end{aligned}$$

as required.

To prove the second part, we use the definition of $Y_\varepsilon^{(M)}$ in (15) to say that

$$Y_\varepsilon^M - Y_\varepsilon = (\mathcal{K}_{\varepsilon/2}^M - \mathcal{K}_{\varepsilon/2}) U_\varepsilon^M - \mathcal{K}_{\varepsilon/2} (U_\varepsilon^M - U_\varepsilon)$$

and so

$$\|Y_\varepsilon^M - Y_\varepsilon\|_0 \leq (2C_{68} + C_{35} + C_{34}) \delta =: C_{36} \delta.$$

Furthermore,

$$(Y_\varepsilon^M)^{-1} - (Y_\varepsilon)^{-1} = \frac{Y_\varepsilon^{-2} (Y_\varepsilon^M - Y_\varepsilon)}{1 - Y_\varepsilon^{-1} (Y_\varepsilon - Y_\varepsilon^M)}$$

and so using that

$$\|Y_\varepsilon^{-1}\|_0 \leq \|\rho^{-1}\|_0 \|U_\varepsilon^{-1}\|_0 \leq \|\rho^{-1}\|_0 \|\rho U_\varepsilon\|_0 = \|\rho^{-1}\|_0 \|\rho\|_0 C_{68},$$

we have that provided that $\delta < \min\{C_{35}, (C_{36} \frac{1}{2} \|\rho^{-1}\|_0 \|\rho\|_0 C_{68})^{-1}\} =: C_{37}$,

$$\|(Y_\varepsilon^M)^{-1} - (Y_\varepsilon)^{-1}\|_0 \leq 2(\|\rho^{-1}\|_0 \|\rho\|_0 C_{68})^2 C_{36} \delta =: C_{38} \delta.$$

Readjusting $C_{38} = \max\{C_{34}, C_{36}, C_{38}\}$, we have what is required. \square

The convergence of the Sinkhorn-weighted operator then follows in Theorem 3.8, which we prove here:

Proof of Theorem 3.8. We can decompose

$$\mathcal{P}_\varepsilon^M - \mathcal{P}_\varepsilon = U_\varepsilon^M (\mathcal{K}_\varepsilon^M - \mathcal{K}_\varepsilon) U_\varepsilon^M + U_\varepsilon^M \mathcal{K}_\varepsilon (U_\varepsilon^M - U_\varepsilon) + (U_\varepsilon^M - U_\varepsilon) \mathcal{K}_\varepsilon U_\varepsilon.$$

Using Lemma 9.5, Propositions 9.2 and 9.3 and that $\|\mathcal{K}_\varepsilon\|_\zeta \leq \|\rho\|_0$ we have that

$$\begin{aligned} \|\mathcal{P}_\varepsilon^M - \mathcal{P}_\varepsilon\|_\zeta &\leq ((2C_{68} + C_{38}C_{37})^2 C_{38} + (2C_{68} + C_{38}C_{37})\|\rho\|_0 C_{38} + \\ &\quad C_{38}\|\rho\|_0 2C_{68}) e^{2dZ_0^2} \delta, \\ &=: C_{39}\delta \end{aligned}$$

for some constant C_{39} .

The corresponding bounds for the half-step operators $\mathcal{G}_\varepsilon^M$, $\mathcal{H}_\varepsilon^M$ and the semi-conjugate operator $\mathcal{Q}_{\varepsilon,1}^M$ arise similarly, with an appropriate adjustment of C_{39} ; this extends to general $\mathcal{Q}_{\varepsilon,n}^M = (\mathcal{Q}_{\varepsilon,1}^M)^n$ by using that $\mathcal{Q}_{\varepsilon,1}^M$, $\mathcal{Q}_{\varepsilon,n}$ are row-stochastic and thus have unit C^0 norm. \square

10 Convergence of spectral data

We can now combine our ‘‘bias’’ and ‘‘variance’’ operator errors to understand the convergence of the spectral data. Instead of the operator $\mathcal{P}_\varepsilon^{(M)} = \mathcal{G}_\varepsilon^{(M)}\mathcal{H}_\varepsilon^{(M)}$ we will consider the semi-conjugacies $\mathcal{Q}_{\varepsilon,1}^{(M)} = \mathcal{H}_\varepsilon^{(M)}\mathcal{G}_\varepsilon^{(M)}$, so that we can use the function space C^0 consistently across the two limits. The outline of our attack is standard (Keller & Liverani 1999): we will first establish the convergence of resolvents in a strong space-to-weak space operator norm sense, and then use this to bound the error in the discretised operators’ spectrum, and in spectral projection operators (and thus eigenspaces).

While the variance error $\mathcal{Q}_{\varepsilon,n}^M - \mathcal{Q}_{\varepsilon,n}$ is just a perturbation in operator norm (from Theorem 3.8), the bias error $\mathcal{Q}_{\varepsilon,n} - e^{n\varepsilon\mathcal{L}}$ is only small from the strong space $C^{3+\beta}$ into the weak space C^0 . To obtain convergence of resolvents we must therefore quantify the regularising behaviour of the operators $\mathcal{Q}_{\varepsilon,n}$ from the weak space into the strong space:

Proposition 10.1. *Suppose $\rho \in W^{s,\infty}$, $s > 2$, and $\beta \in (0, \min\{s - 2, 1\})$. For all $\tilde{T} > 0$ there exists a constant $C_{100,\beta}$ depending on \tilde{T}, ρ, β such that for all $\varepsilon \leq \varepsilon_0$, $n\varepsilon \geq \tilde{T}$*

$$\|\mathcal{Q}_{\varepsilon,n}\|_{C^0 \rightarrow C^{3+\beta}} \leq C_{100},$$

where $\mathcal{Q}_{\varepsilon,n}$ is defined in (18).

Proof. For $\tilde{T} \leq n\varepsilon \leq \tilde{T} + \varepsilon_0$ this is a Schauder estimate (Knerr 1980), which can be extended from $C^{2+\beta}$ to $C^{3+\beta}$ along the lines of Proposition 7.3. For larger n , this follows by using that $\|\mathcal{Q}_{\varepsilon,1}\|_{C^0} = 1$. \square

Let us denote the resolvent of an operator \mathcal{A} as

$$R_\lambda(\mathcal{A}) := (\lambda I - \mathcal{A})^{-1}.$$

We have the following bound on the resolvent of our semigroup in the C^0 norm:

Proposition 10.2. *For all $\tilde{T} > 0$ there exists a constant C_{99} depending on \tilde{T}, ρ such that for $t > \tilde{T}$*

$$\|R_\lambda(e^{t\mathcal{L}})\|_{C^0} \leq |\lambda|^{-1} (1 + C_{99}d(\lambda, e^{t\sigma(\mathcal{L})})).$$

Proof. Using that $\|\cdot\|_{C^0} \geq \|\cdot\|_{L^2(\rho)}$ we have

$$\|R_\lambda(e^{t\mathcal{L}})\|_{C^0} \leq |\lambda|^{-1} (1 + \|e^{t\mathcal{L}}\|_{L^2(\rho) \rightarrow C^0} \|R_\lambda(e^{t\mathcal{L}})\|_{L^2(\rho)}).$$

Upper Gaussian estimates on $e^{\tilde{T}\mathcal{L}}$ (Liskevich & Semenov 2000) mean that we can bound

$$\|e^{t\mathcal{L}}\|_{L^2(\rho)\rightarrow C^0} \leq \|e^{\tilde{T}\mathcal{L}}\|_{L^2(\rho)\rightarrow C^0} \|e^{(t-\tilde{T})\mathcal{L}}\|_{L^2(\rho)} = \|e^{\tilde{T}\mathcal{L}}\|_{L^2(\rho)\rightarrow C^0} =: C_{99}.$$

Furthermore, since $e^{t\mathcal{L}}$ is normal in $L^2(\rho)$ with spectrum $\sigma(e^{t\mathcal{L}}) = e^{t\sigma(\mathcal{L})}$, the resolvent's norm is bounded by the distance to the spectrum

$$\|R_\lambda(e^{t\mathcal{L}})\|_{L^2(\rho)} = d(\lambda, e^{t\sigma(\mathcal{L})}),$$

giving us what is required. \square

The following result then allows us to extend the previous bound to resolvents of the discretised operators:

Lemma 10.3. *Suppose $n\varepsilon \in [\tilde{T}, T]$, and let the quantities*

$$\begin{aligned} X_1 &= |\lambda|^{-2}(1 + C_{99}d(\lambda, e^{t\sigma(\mathcal{L})}))C_{90,T}, \\ X_2 &= 1 + |\lambda|^{-1}(1 + C_{99}d(\lambda, e^{t\sigma(\mathcal{L})})), \\ X_3 &= |\lambda|^{-1}C_{39}T\varepsilon^{-1}\delta X_2. \end{aligned}$$

Then if $\delta < C_{39}$,

(a) *If $C_{100}X_1 \leq 1$, then $R_\lambda(\mathcal{Q}_{\varepsilon,n})$ is bounded in C^0 and*

$$\|R_\lambda(\mathcal{Q}_{\varepsilon,n}) - R_\lambda(e^{\mathcal{L}n\varepsilon})\|_{C^{3+\beta}\rightarrow C^0} \leq \frac{X_2}{1 - C_{100}X_1}X_1.$$

(b) *If $C_{100}X_1 + X_3 \leq 1$, then $R_\lambda(\mathcal{Q}_{\varepsilon,n}^M)$ is bounded in C^0 and*

$$\|R_\lambda(\mathcal{Q}_{\varepsilon,n}^M) - R_\lambda(\mathcal{Q}_{\varepsilon,n})\|_{C^0} \leq \frac{|\lambda|^{-1}\tilde{X}_1X_3}{(1 - C_{100}X_1 - X_3)(1 - C_{100}X_1)}.$$

Proof of Lemma 10.3. By algebraic manipulations we have both that

$$R_\lambda(\mathcal{Q}_{\varepsilon,n}) = \lambda^{-1}(I + \mathcal{Q}_{\varepsilon,n}R_\lambda(\mathcal{Q}_{\varepsilon,n})) \quad (56)$$

and

$$R_\lambda(\mathcal{Q}_{\varepsilon,n}) = R_\lambda(e^{\mathcal{L}n\varepsilon}) + \lambda\mathcal{X}_1R_\lambda(\mathcal{Q}_{\varepsilon,n}), \quad (57)$$

where the operator

$$\mathcal{X}_1 = \lambda^{-1}R_\lambda(e^{\mathcal{L}n\varepsilon})(\mathcal{Q}_{\varepsilon,n} - e^{\mathcal{L}n\varepsilon}).$$

By substituting (57) into (56), we then have that

$$(I - \mathcal{X}_1\mathcal{Q}_{\varepsilon,n})R_\lambda(\mathcal{Q}_{\varepsilon,n}) = \lambda^{-1}\mathcal{X}_2,$$

where

$$\mathcal{X}_2 := I + \mathcal{Q}_{\varepsilon,n}R_\lambda(e^{\mathcal{L}n\varepsilon}).$$

We then have using Theorem 3.5 that

$$\begin{aligned} \|\mathcal{X}_1\|_{C^{3+\beta}\rightarrow C^0} &\leq |\lambda|^{-1}\|R_\lambda(e^{\mathcal{L}n\varepsilon})\|_{C^0}\|\mathcal{Q}_{\varepsilon,n} - e^{\mathcal{L}n\varepsilon}\|_{C^{3+\beta}\rightarrow C^0} \leq X_1, \\ \|\mathcal{X}_2\|_{C^0} &\leq 1 + \|R_\lambda(e^{\mathcal{L}n\varepsilon})\|_{C^0}\|\mathcal{Q}_{\varepsilon,n}\|_{C^0} \leq X_2, \end{aligned}$$

so, using Proposition 10.1, if $C_{100}X_1 < 1$ then

$$\|R_\lambda(\mathcal{Q}_{\varepsilon,n})\|_{C^0} \leq \frac{|\lambda|^{-1}X_2}{1 - C_{100}X_1} < \infty. \quad (58)$$

Then, substituting (56) instead into (57) and rearranging, we obtain that

$$(I - \mathcal{X}_1\mathcal{Q}_{\varepsilon,n})(R_\lambda(\mathcal{Q}_{\varepsilon,n}) - R_\lambda(e^{\mathcal{L}n\varepsilon})) = \mathcal{X}_1\mathcal{X}_2$$

so that again if $C_{100}X_1 < 1$,

$$\|R_\lambda(\mathcal{Q}_{\varepsilon,n}) - R_\lambda(e^{\mathcal{L}n\varepsilon})\|_{C^{3+\beta} \rightarrow C^0} \leq \frac{X_2}{1 - C_{100}X_1} X_1,$$

as required for (a).

For part (b), we have that

$$(R_\lambda(\mathcal{Q}_{\varepsilon,n}^M) - R_\lambda(\mathcal{Q}_{\varepsilon,n}))(I - (\mathcal{Q}_{\varepsilon,n}^M - \mathcal{Q}_{\varepsilon,n})R_\lambda(\mathcal{Q}_{\varepsilon,n})) = R_\lambda(\mathcal{Q}_{\varepsilon,n})(\mathcal{Q}_{\varepsilon,n}^M - \mathcal{Q}_{\varepsilon,n})R_\lambda(\mathcal{Q}_{\varepsilon,n}).$$

We also have from Theorem 3.8 that

$$\|\mathcal{Q}_{\varepsilon,n}^M - \mathcal{Q}_{\varepsilon,n}\|_{C^0} \leq C_{39}n\delta \leq C_{39}T\varepsilon^{-1}\delta,$$

and so, using (58),

$$\|(\mathcal{Q}_{\varepsilon,n}^M - \mathcal{Q}_{\varepsilon,n})R_\lambda(\mathcal{Q}_{\varepsilon,n})\|_{C^0} \leq \frac{X_3}{1 - C_{100}X_1}.$$

Consequently if

$$X_3 + C_{100}X_1 < 1,$$

then

$$\|R_\lambda(\mathcal{Q}_{\varepsilon,n}^M) - R_\lambda(\mathcal{Q}_{\varepsilon,n})\|_{C^0} \leq \frac{|\lambda|^{-1}X_2X_3}{(1 - C_{100}X_1 - X_3)(1 - C_{100}X_1)}$$

and in particular, $R_\lambda(\mathcal{Q}_{\varepsilon,n}^M)$ is bounded. \square

Using Lemma 10.3, we can prove Theorem 3.3:

Proof of Theorem 3.3. Fix T and set $\tilde{T} = T + 2\varepsilon_0$ and $n = \lceil \tilde{T}/\varepsilon \rceil$.

The eigenvalues of $\mathcal{Q}_{\varepsilon,n}^{(M)}$ are $e^{n\varepsilon\lambda_{k,\varepsilon}^{(M)}}$, and the eigenvalues of $e^{\mathcal{L}n\varepsilon}$ are $e^{n\lambda_k}$. On $[e^{-T\lambda_*}, 1]$, the logarithm function is bi-Lipschitz, so bounds on the errors in the eigenvalues of $\mathcal{Q}_{\varepsilon,n}^{(M)}$ translate to the bounds necessary for the theorem.

By considering the constants in Lemma 10.3 we find that for ε^2 and $\varepsilon^{-1}\delta$ sufficiently small, the resolvents $R_\lambda(\mathcal{Q}_{\varepsilon,n})$, $R_\lambda(\mathcal{Q}_{\varepsilon,n}^M)$ are bounded respectively for

$$\begin{aligned} d(\lambda, \sigma(e^{\mathcal{L}n\varepsilon})) &< C_{103}\varepsilon^2, \\ d(\lambda, \sigma(\mathcal{Q}_{\varepsilon,n}^M)) &< C_{104}(\varepsilon^2 + \varepsilon^{-1}\delta). \end{aligned}$$

This bounds the distances between the spectra of $\mathcal{Q}_{\varepsilon,n}^{(M)}$ and of $e^{\mathcal{L}n\varepsilon}$. Furthermore, if $C_{104}(\varepsilon^2 + \delta)$ is smaller than r , which we define to be half the smallest gap between distinct eigenvalues and between the eigenvalues and $e^{-\varepsilon\lambda_*}$, then by considering the rank of the relevant spectral projections, the multiplicities are preserved.

For part (b), we will use the spectral projections, $\Pi_k, \Pi_{k,\varepsilon}^{(M)}$, where Π_k is the $L^2(\rho)$ -orthogonal projection onto E_k , and

$$\Pi_{k,\varepsilon}^{(M)} := \frac{r}{2\pi} \int_0^{2\pi} R_{e^{-nk\lambda_k + r e^{i\theta}}(\mathcal{Q}_{\varepsilon,n}^{(M)})} d\theta. \quad (59)$$

When $C_{103}(\varepsilon^2 + \delta) < r$, then $\Pi_{k,\varepsilon}^{(M)}$ are projections onto the finite-dimensional spaces $\mathcal{H}_\varepsilon^{(M)} \bar{E}_{k,\varepsilon}^{(M)}$.

Choose $\beta \in (0, \min\{s-2, 1\})$, where s is such that $\rho \in W^{s,\infty}$. Lemma 10.3 and equation (59) give us that

$$\|\Pi_{k,\varepsilon}^M - \Pi_k\|_{C^{3+\beta} \rightarrow C^0} \leq C_{105}(\varepsilon^2 + \varepsilon^{-1}\delta).$$

If $\phi \in E_k$ with $\|\phi\|_{C^0} = 1$, then

$$\begin{aligned} \|e^{\varepsilon\mathcal{L}/2}\Pi_k\phi - \mathcal{G}_\varepsilon^M \Pi_{k,\varepsilon}^M \phi\|_{C^0} &\leq \|(e^{\varepsilon\mathcal{L}/2} - \mathcal{G}_\varepsilon^M)\Pi_k\phi - \mathcal{G}_\varepsilon^M(\Pi_k - \Pi_{k,\varepsilon}^M)\phi\|_{C^0} \\ &\leq \left(\|e^{\varepsilon\mathcal{L}/2} - \mathcal{G}_\varepsilon\|_{C^{3+\beta} \rightarrow C^0} + \|\mathcal{G}_\varepsilon - \mathcal{G}_\varepsilon^M\|_{C^0} \right) \|\Pi_k\|_{C^{3+\beta}} \\ &\quad + C_{105}(\varepsilon^2 + \varepsilon^{-1}\delta) \|\phi\|_{C^{3+\beta}} \\ &\leq \left(C_{90,T}\varepsilon^2 + C_{39}\delta \right) \|\Pi_k\|_{C^{3+\beta}} + C_{105}(\varepsilon^2 + \varepsilon^{-1}\delta) \|\phi\|_{C^{3+\beta}}, \end{aligned}$$

where in the last line we used Theorems 3.5 and 3.8.

We know that Π_k is bounded on $C^{3+\beta}$ (independent of M, ε), and that E_k is a finite-dimensional subspace of $C^{3+\beta}$ and thus the C^0 and $C^{3+\beta}$ norms are equivalent, so that then

$$\begin{aligned} \|e^{\varepsilon\mathcal{L}/2}\Pi_k\phi - \mathcal{G}_\varepsilon^M \Pi_{k,\varepsilon}^M \phi\|_{C^0} &\leq C_{106}(\varepsilon^2 + \varepsilon^{-1}\delta) \|\phi\|_{C^0} \\ &\leq e^{\lambda_*\varepsilon/2} C_{106}(\varepsilon^2 + \varepsilon^{-1}\delta) e^{-\lambda_k\varepsilon/2} \|\phi\|_{C^0}, \end{aligned}$$

Now, $e^{\varepsilon\mathcal{L}/2}\Pi_k\phi = e^{-\lambda_k\varepsilon/2}\phi$, and $\mathcal{G}_\varepsilon^M \Pi_{k,\varepsilon}^M \phi \in \bar{E}_{k,\varepsilon}^M$, so

$$d(\phi, \bar{E}_{k,\varepsilon}^M) \leq C_{107}(\varepsilon^2 + \varepsilon^{-1}\delta).$$

As a result of Lemma 1 in Osborn (1975), we have what we need for $\bar{E}_{k,\varepsilon}^M$; the equivalent for $\bar{E}_{k,\varepsilon}$ holds similarly. \square

Proof of Corollary 3.4. The difference between the graph Laplacian eigenvalues and the semi-group eigenvalues can be bounded

$$\begin{aligned} |\tilde{\lambda}_{k,\varepsilon}^{(M)} - \lambda_{k,\varepsilon}^{(M)}| &= \varepsilon^{-1} |e^{-\varepsilon\lambda_{k,\varepsilon}^{(M)}} + 1 - \varepsilon\lambda_{k,\varepsilon}^{(M)}| \\ &\leq \frac{1}{2}\varepsilon^{-1}(\varepsilon\lambda_{k,\varepsilon}^{(M)})^2 \\ &\leq \frac{1}{2}\lambda_*^2\varepsilon \leq C_{105}\varepsilon, \end{aligned}$$

where in the second-last inequality we used from the proof of Theorem 3.3 that $-\lambda_{k,\varepsilon}^{(M)}$ is forced to be greater than $-\lambda_*$. Combining this bound with Theorem 3.3(a) gives part (b); part (a) follows similarly from Theorem 3.2(a). \square

11 Results for standard weights

In this section we will sketch the proof of Theorem 3.2 on the convergence of spectral data for standard weights. For the most part this closely follows the argument for the Sinkhorn weights,

however it is somewhat simpler in that the weights are explicitly given, and the bias error is only first-order in the timestep so the averaging argument is not necessary.

We will again study the bias error by interpolating $\check{\mathcal{P}}_{\varepsilon,\alpha}$ in time as a PDE. We begin by bounding the associated drift term: as with the Sinkhorn weights, we will need to venture into bounding the norm of inverse derivatives of the drift terms.

Proposition 11.1. *Suppose $\rho \in W^{s,\infty}$, $s > \frac{3}{2}$ and let $r^* = \max\{0, 2 - s\}$. Then there exists a constant $C_{132,s}$ such that for all $\varepsilon \geq 0$,*

$$\|J^{-s^*/2} \log \rho_\varepsilon - \log \rho\|_{W^{s-2+r^*,\infty}} \leq C_{132,s}\varepsilon.$$

Proof. Because J and Δ commute and $\|e^{t\Delta}\|_{L^\infty} \leq 1$, for all t

$$\|\rho_t\|_{W^{s,\infty}} = \|e^{t\Delta/2}\rho\|_{W^{s,\infty}} \leq \|\rho\|_{W^{s,\infty}}.$$

Consequently if we set $\omega^t := J^{-s^*/2} \log \rho_t$, then because $\rho_t \geq \inf \rho$,

$$\|\omega^t\|_{W^{s+r^*,\infty}} = \|\log \rho_t\|_{W^{s,\infty}} \leq C_{131,s}$$

for some $C_{131,s}$. Then, because

$$\partial_t \omega^t = \frac{1}{2} \Delta \omega^t + \frac{1}{2} J^{-s^*/2} |\nabla J^{r^*/2} \omega^t|^2,$$

there exists $C_{132,s}$ such that for all $t \in [0, \varepsilon_0]$,

$$\|\partial_t \omega^t\|_{W^{s-2+r^*,\infty}} \leq C_{132,s},$$

and so

$$\|J^{-s^*/2}(\log \rho_\varepsilon - \log \rho)\|_{W^{s-2+r^*,\infty}} = \|\omega_\varepsilon - \omega_0\|_{W^{s-2+r^*,\infty}} \leq C_{132,s}\varepsilon,$$

as required. \square

Proposition 11.2. *Suppose $\rho \in W^{s,\infty}$, $s > \frac{3}{2}$. Let $\check{w}_{\varepsilon,\alpha}^t = \log(\mathcal{K}_{\varepsilon\{t/\varepsilon\}} \check{U}_{\varepsilon,\alpha}) - (1 - \alpha) \log \rho$, and let $r^* = \max\{0, 2 - s\}$. Then there exists a constant $C_{135,s}$ such that for all $\varepsilon \in [0, \varepsilon_0]$,*

$$\|J^{-s^*/2} \check{w}_{\varepsilon,\alpha}^t\|_{W^{s-2+r^*,\infty}} \leq C_{135,s}\varepsilon.$$

Proof. Because $\rho_\varepsilon \leq \inf \rho$, we know that for all $\varepsilon \in [0, \varepsilon_0]$,

$$\|\rho \check{U}_{\varepsilon,\alpha}\|_{W^{s,\infty}} = \|\rho \rho_\varepsilon^{-\alpha}\|_{W^{s,\infty}} \leq C_{134,s}$$

for some constant $C_{134,s}$. As in Proposition 11.1 this gives us uniform boundedness of $J^{-s^*/2} \check{w}_{\varepsilon,\alpha}^t$ in $W^{s+r^*,\infty}$, and so by a similar argument we obtain the required result. \square

The following proposition bounds the convergence of the continuum operator $\check{\mathcal{P}}_{\varepsilon,\alpha}$ as $\varepsilon \rightarrow 0$. In this case an averaging result is not necessary: we only need to bound the drift term.

Proposition 11.3. *Suppose $\rho \in W^{s,\infty}$, $s > \frac{3}{2}$, and let $\check{S}_{\varepsilon,\alpha}(t_1, t_0)$ be the solution operator of the PDE*

$$\partial_t \phi^t = \check{\mathcal{L}}_\alpha \phi^t + \nabla \check{w}_t^{\varepsilon,\alpha} \cdot \nabla \phi^t, \quad (60)$$

where $\check{w}_t^{\varepsilon,\alpha} := \log(\mathcal{K}_{\varepsilon\{t/\varepsilon\}} \rho_\varepsilon^{-\alpha}) - (1 - \alpha) \log \rho$.

Then

$$\begin{aligned}\check{\mathcal{G}}_{\varepsilon,\alpha} &= \check{S}_{\varepsilon,\alpha}(\varepsilon, \tfrac{1}{2}\varepsilon) \\ \check{\mathcal{H}}_{\varepsilon,\alpha} &= \check{S}_{\varepsilon,\alpha}(\tfrac{1}{2}\varepsilon, 0) \\ \check{\mathcal{P}}_{\varepsilon,\alpha} &= \check{S}_{\varepsilon,\alpha}(\varepsilon, 0) \\ \check{\mathcal{Q}}_{\varepsilon,n} &= \check{S}_{\varepsilon,\alpha}((n + \tfrac{1}{2})\varepsilon, \tfrac{1}{2}\varepsilon).\end{aligned}$$

Furthermore, for all $T > 0$, $\beta \in (\frac{1}{2}, \min\{1, s-1\})$ there exists a constant $\check{C}_{90,T,\beta,\alpha}$ such that for all $0 \leq t_1 - t_0 \leq T$ and $\varepsilon \leq \varepsilon_0$,

$$\|\check{S}_{\varepsilon,\alpha}(t_1, t_0) - e^{(t_1-t_0)\check{\mathcal{L}}_\alpha}\|_{C^{2+\beta} \rightarrow C^0} \leq \check{C}_{90,T,\beta,\alpha}\varepsilon. \quad (61)$$

Proof. The first part is as in the proof of Theorem 3.5.

From Proposition 11.2 we have that for $r \in (\frac{3}{2}, \min\{2, s\})$,

$$\|J^{-r^*/2-1}\nabla\check{w}_{\varepsilon,\alpha}^t\|_{W^{s-2+r^*,\infty}} \leq K^\nabla C_{135,r}\varepsilon,$$

where $r^* = \max\{0, 2-r\}$.

We then have that for $\beta \in (\frac{1}{2}, \min\{1, r-1\})$,

$$\begin{aligned}\|\check{S}_{\varepsilon,\alpha}(t_1, t_0) - e^{(t_1-t_0)\check{\mathcal{L}}_\alpha}\|_{C^{2+\beta} \rightarrow C^0} \\ \leq \int_{t_0}^{t_1} \|e^{(\tau-t_0)\check{\mathcal{L}}_\alpha}\nabla\check{w}_t^\varepsilon \cdot \nabla\|_{W^{r,\infty} \rightarrow C^0} \|S_\varepsilon(t_1, \tau)\|_{C^{2+\beta} \rightarrow W^{r,\infty}} d\tau.\end{aligned} \quad (62)$$

By passing through L^p spaces so as to consider the adjoint and thus implicitly pass into negative Sobolev spaces, as in the proof of Theorem 3.5, we find that there exist $\eta < 2$ and $C_{136,r,\beta}$ such that

$$\|e^{(t_1-\tau)\check{\mathcal{L}}_\alpha}\nabla\check{w}_t^\varepsilon \cdot \nabla\|_{W^{r,\infty} \rightarrow C^0} \|S_\varepsilon(\tau, t_0)\|_{C^{2+\beta} \rightarrow W^{r,\infty}} \leq C_{136,r,\beta}\varepsilon^2(t_1-\tau)^{-\eta/2},$$

which by integrating (62) gives the necessary result. \square

When ρ has higher regularity, we have the following tighter result, comparable to Proposition 3.6:

Proposition 11.4. *Suppose $\rho \in W^{s,\infty}$ for $s > 3$. Then for all $\alpha \in [0, 1]$, $\beta \in (0, 1)$ there exists a constant $\check{C}_{97,\alpha,\beta,T}$ such that for all $t_0 \leq t_1$, $\varepsilon \leq \varepsilon_0$,*

$$\|\check{S}_{\varepsilon,\alpha}(t_1, t_0) - e^{(t_1-t_0)\check{\mathcal{L}}_\alpha}\|_{C^{1+\beta} \rightarrow C^0} \leq \check{C}_{97,\alpha,\beta}(t_1-t_0)\varepsilon.$$

We now consider the variance error. The following proposition follows directly from Proposition 9.1 and Theorem 3.7.

Proposition 11.5. *There exists Z_0 such that if $\zeta = Z_0\varepsilon^{1/2}$, then for all $\varepsilon \in [0, \varepsilon_0]$,*

$$\begin{aligned}\|\rho_\varepsilon\|_\zeta &\leq e^{2dZ_0}\|\rho\|_0 \\ \|\rho_\varepsilon^{-1}\|_\zeta &\leq 2\|\rho^{-1}\|_0 \\ \|\rho_\varepsilon^M - \rho_\varepsilon\|_\zeta &\leq e^{2dZ_0}\delta.\end{aligned} \quad (63)$$

Using that $\check{U}_{\varepsilon,\alpha} = \rho_\varepsilon^{-\alpha}$ and another application of Proposition 9.1 allows us to bound the weights:

Proposition 11.6. *There exists Z_0 such that if $\zeta = Z_0\varepsilon^{1/2}$, then there exists a constant C_{140} such that for all $\varepsilon \in [0, \varepsilon_0]$, $\alpha \in [0, 1]$,*

$$\|\check{U}_{\varepsilon, \alpha}\|_{\zeta}, \|1/\check{U}_{\varepsilon, \alpha}\|_{\zeta}, \|\check{V}_{\varepsilon, \alpha}\|_{\zeta}, \|1/\check{V}_{\varepsilon, \alpha}\|_{\zeta} \leq C_{140}.$$

By combining these estimates with (63), we obtain that

Proposition 11.7. *There exist constants $\check{Z}_0, \check{C}_{37}, \check{C}_{38}$ such that for all $\varepsilon \in [0, \varepsilon_0]$, $\alpha \in [0, 1]$, if $\delta \leq \check{C}_{37}$ then*

$$\|\check{U}_{\varepsilon, \alpha}^M - \check{U}_{\varepsilon, \alpha}\|_{\zeta}, \|\check{V}_{\varepsilon, \alpha}^M - \check{V}_{\varepsilon, \alpha}\|_{\zeta}, \|\check{Y}_{\varepsilon, \alpha}^M - \check{Y}_{\varepsilon, \alpha}\|_0, \|(\check{Y}_{\varepsilon, \alpha}^M)^{-1} - (\check{Y}_{\varepsilon, \alpha})^{-1}\|_0 \leq \check{C}_{38}\delta,$$

where $\zeta = \check{Z}_0\varepsilon^{1/2}$.

The next proposition then follows along the lines of Theorem 3.8:

Proposition 11.8. *There exist $\check{Z}_0, \check{C}_{39}$ such that if $\check{\zeta} = Z_0\varepsilon^{1/2}$ and $\delta \leq \check{C}_{37}$ then for all $\varepsilon \leq \varepsilon_0$ and $n \in \mathbb{N}$,*

$$\|\check{\mathcal{P}}_{\varepsilon, \alpha}^M - \check{\mathcal{P}}_{\varepsilon, \alpha}\|_{\zeta}, \|\check{\mathcal{G}}_{\varepsilon, \alpha}^M - \check{\mathcal{G}}_{\varepsilon, \alpha}\|_{0 \rightarrow \zeta}, \|\check{\mathcal{H}}_{\varepsilon, \alpha}^M - \check{\mathcal{H}}_{\varepsilon, \alpha}\|_{\zeta \rightarrow 0} \leq \check{C}_{39}\delta,$$

and

$$\|\check{\mathcal{Q}}_{\varepsilon, \alpha, n}^M - \check{\mathcal{Q}}_{\varepsilon, \alpha, n}\|_0 \leq \check{C}_{39}\delta n.$$

Using Propositions 11.3 and 11.8, the proof of Theorem 3.2 then follows by analogy with Theorem 3.3.

A Proof of Theorem 4.1 and Proposition 4.3

Proof of Theorem 4.1. In this proof, we will find it useful to define the functions $l^{(n)} = \log U^{(n)} - \log U$, and similarly $l_a^{(n)}, l_b^{(n)}$.

We begin by proving (a) using Birkhoff cones. Let Λ^+ be the set of positive, bounded functions on the support of μ , and let d_{Λ^+} be the projective cone Hilbert metric on Λ^+/\mathbb{R}^+

$$d_{\Lambda^+}(\phi, \psi) := \sup \log \frac{\phi}{\psi} - \inf \log \frac{\phi}{\psi} \leq 2\|\log \phi - \log \psi\|_{L^\infty}.$$

Then it is well-known (Peyré & Cuturi 2019) that if

$$\theta := \tanh \left(\frac{1}{4} \sup_{x, y \in \text{supp } \mu} d_{\Lambda^+}(\mathcal{K}\delta_x, \mathcal{K}\delta_y) \right) < 1, \quad (64)$$

then by the Birkhoff cone theorem, for any $\phi \in \Lambda^+$

$$d_{\Lambda^+}(1/\mathcal{K}[\phi], U) = d_{\Lambda^+}(\mathcal{K}[\phi], \mathcal{K}[U]) \leq \theta d_{\Lambda^+}(\phi, U).$$

This gives the contraction rate of standard Sinkhorn iteration.

However, one can also check for any $\phi, \psi \in \Lambda^+$,

$$d_{\Lambda^+}(\sqrt{\phi\psi}, U) \leq \frac{1}{2}(d_{\Lambda^+}(\phi, U) + d_{\Lambda^+}(\psi, U)).$$

Applying this to (25 – 27) gives that

$$d_{\Lambda^+}(U^{(n+1)}, U) \leq \frac{1}{2}(\theta^2 + \theta)d_{\Lambda^+}(U^{(n)}, U).$$

Finally, since

$$e^{l^{(n)}} = \sqrt{e^{l_a^{(n-1)}} / \mathcal{P}e^{l_a^{(n-1)}}},$$

where we recall that $e^{l_a^{(n-1)}} = U_a^{(n-1)} / U$, and furthermore since

$$\int (\mathcal{P}e^{l_a^{(n)}} - e^{l_a^{(n)}}) d\mu = 0,$$

we find that

$$\sup l^{(n)} \geq 0 \geq \inf l^{(n)}$$

so

$$\|\log U^{(n)} - \log U\|_{L^\infty} \leq d(U^{(n)}, U),$$

giving us what we need.

We now consider the local convergence rate. To use the spectral properties of the normalised operator $\mathcal{P} := UKU$ we will pass to the $L^2(\mu)$ norm.

Using that $\|l^{(0)}\|_{L^\infty} \leq k$, then by the previous part, for all n

$$\|l^{(n)}\|_{L^\infty} \leq 2k,$$

and the same holds for $l_a^{(n)}, l_b^{(n)}$. Consequently, taking logarithms of exponentials of these functions is Lipschitz with constant e^{2k} ; furthermore, for any function l with $\|l\|_{L^\infty} \leq 2k$,

$$\|e^l - l\|_{L^2} \leq ke^{2k}\|l\|_{L^2},$$

and so since $\|\mathcal{P}\|_{L^\infty} = \|\mathcal{P}\|_{L^2} = 1$,

$$\|e^{\mathcal{P}l} - \mathcal{P}e^l\|_{L^2} \leq \|e^{\mathcal{P}l} - \mathcal{P}l\|_{L^2} + \|\mathcal{P}(l - e^l)\|_{L^2} \leq 2ke^{2k}\|l\|_{L^2}.$$

Since $l_a^{(n)} = -\log(\mathcal{P}e^{l^{(n)}})$,

$$\begin{aligned} \|l_a^{(n)} + \mathcal{P}l^{(n)}\|_{L^2} &\leq e^{2k}\|e^{-l_a^{(n)}} - e^{-\mathcal{P}l^{(n)}}\|_{L^2} \\ &= e^{2k}\|\mathcal{P}e^{-l^{(n)}} - e^{-\mathcal{P}l^{(n)}}\|_{L^2} \\ &\leq k'\|l^{(n)}\|_{L^2}, \end{aligned}$$

where $k' = ke^{4k}$. Similarly,

$$\|l_b^{(n)} - (\mathcal{P})^2 l^{(n)}\|_{L^2} \leq k'\|l_a^{(n)}\|_{L^2} + \|l_a^{(n)} - \mathcal{P}l^{(n)}\|_{L^2} \leq k'(2 + k')\|l^{(n)}\|_{L^2}$$

Then, since $l^{(n+1)} = \frac{1}{2}(l_a^{(n)} + l_b^{(n)})$,

$$\|l^{(n+1)} - \frac{1}{2}\mathcal{P}(I - \mathcal{P})l^{(n)}\|_{L^2} \leq k''\|l^{(n)}\|_{L^2}, \quad (65)$$

where $k'' = k'(2 + \frac{1}{2}k')$.

Now, \mathcal{P} is a Markov operator which is self-adjoint in $L^2(\mu)$ and, furthermore, positive semi-definite on this space as \mathcal{K} is and U is positive. As a consequence, the spectrum of \mathcal{P} is a subset of $[0, 1]$. Hence, the spectrum of $\frac{1}{2}\mathcal{P}(I - \mathcal{P})$ is contained in $[-\frac{1}{8}, 0]$, and so its $L^2(\mu)$ norm is bounded by $\frac{1}{8}$. We thus have

$$\|l^{(n)}\|_{L^2} \leq \left(\frac{1}{8} + k'(2 + \frac{1}{2}k')\right)^n \|l^{(0)}\|_{L^2} \leq \left(\frac{1}{8} + k''\right)^n \|l^{(0)}\|_{L^\infty}.$$

To prove part (c), we use (65), so that

$$\|l^{(n+1)} - l^{(n)}\|_{L^2} \geq \|(I + \frac{1}{2}\mathcal{P}(1 - \mathcal{P}))l^{(n)}\|_{L^2} - k''\|l^{(n)}\|_{L^2} \geq (\frac{7}{8} - k'')\|l^{(n)}\|_{L^2} \geq \frac{\frac{7}{8} - k''}{\frac{1}{8} + k''}\|l^{(n+1)}\|_{L^2},$$

□

Proof of Proposition 4.3. This proposition is a consequence of bounds in the rest of the paper. We have from Theorem 3.7 that

$$\|\mathcal{K}_\varepsilon^M 1 - \mathcal{K}_\varepsilon 1\|_{L^\infty} \leq e^{2d\zeta^2} \delta.$$

It is a standard result on Gaussian kernels that

$$\|\mathcal{K}_\varepsilon 1 - \rho\|_{L^\infty} = \|(C_\varepsilon - I)\rho\|_{L^\infty} \leq \frac{1}{2}\varepsilon\|\rho\|_{W^{2,\infty}}.$$

Lemma 9.5 gives us that if $\delta \leq C_{37}$ then

$$\|U_\varepsilon^M - U_\varepsilon\|_{L^\infty} \leq C_{38}\delta.$$

As a result of Theorem 6.1 and Lemma 6.4,

$$\|\log U_\varepsilon - \log \rho^{-1/2}\|_{L^\infty} \leq C_{71,2}\varepsilon.$$

These results together mean that there exist constants C_{120}, C_{121} such that if $\delta < C_{120}$ and $\varepsilon < \varepsilon_0$,

$$\|\log((\mathcal{K}_\varepsilon^M 1)^{-1/2}) - \log U_\varepsilon^M\|_{L^\infty} \leq C_{121}(\delta + \varepsilon),$$

as required. □

B Proof of Proposition 8.5

Proof of Proposition 8.5. Let $z_\mathcal{E}$ be the centre of \mathcal{E} , set $\eta = \operatorname{arcsinh}(\zeta/\ell) < \eta_0$ and define \mathbb{T}_η^d as the complex η -fattening of the hyper-torus \mathbb{T}^d :

$$\mathbb{T}_\eta^d = ((\mathbb{R} + i[-\eta, \eta])/2\pi\mathbb{Z})^d$$

Define the map $\tau : \mathbb{T}_\eta^d \rightarrow \mathcal{E}_\zeta$

$$\tau(z) = \ell \cos z + z_\mathcal{E}.$$

Now the Hardy space $H^\infty(\mathcal{E}_\zeta)$ is isometrically embedded in the Hardy space of bounded, even analytic functions on \mathbb{T}_η^d , $H_{\text{even}}^\infty(\mathbb{T}_\eta^d)$, via the map $C_\tau : \phi \mapsto \phi \circ \tau$. This map is also an isometric embedding of $C^0(\mathcal{E})$ into $C^0(\mathbb{T}^d)$.

The Hardy space $H_{\text{even}}^\infty(\mathbb{T}_\eta^d)$ in turn is a subset of another Hardy space $H_{\text{even}}^2(\mathbb{T}_\eta^d)$, consisting of even analytic functions on \mathbb{T}_η^d that are bounded with respect to the norm

$$\|\phi\|_{H_{\text{even}}^2(\mathbb{T}_\eta^d)}^2 = (4\pi)^{-d} \int_{\partial\mathbb{T}_\eta^d} |\phi(z)|^2 dz.$$

Furthermore, $\|\phi\|_{H_{\text{even}}^2(\mathbb{T}_\eta^d)} \leq \|\phi\|_{H_{\text{even}}^\infty(\mathbb{T}_\eta^d)}$, so the image of the unit ball $C_\tau B_{H^\infty(\mathcal{E}_\zeta)}(0, 1)$ is contained in the unit ball of $H_{\text{even}}^\infty(\mathbb{T}_\eta^d)$.

On $H_{\text{even}}^2(\mathbb{T}_\eta^d)$ we have the compactness result:

Proposition B.1. *The unit ball in $H_{\text{even}}^2(\mathbb{T}_\eta^d)$ may be covered by $C^0(\mathbb{T}^d)$ balls with centres a the finite set \hat{S}_ξ^η , and for $\eta \in (0, \eta_0)$ and $\xi \in (0, 1/2)$ there exist constants C_9, C_{10} depending only on η_0, d such that*

$$|\hat{S}_\xi^\eta| \leq e^{(C_9 \log \xi^{-1} + C_{10} \log \eta^{-1})(\eta^{-1} \log \xi^{-1})^d}$$

As a result, we can cover $B := C_\tau B_{H^\infty(\mathcal{E}_\zeta)}(0, 1)$ by C^0 balls centred at the points in $\hat{S}_{\xi/2}^\eta$. It does not necessarily hold that $\hat{S}_{\xi/2}^\eta \subset B$, but because the diameter of a $\xi/2$ -ball is bounded by ξ , around each $\xi/2$ ball that intersects B we can choose a ξ -ball with a centres inside B . From the injectivity of the isometry C_τ we get the desired set $S_{\xi, \zeta}^{\ell, \eta}$. \square

Proof of Proposition B.1. The functions

$$b_k(z) = \prod_{j=1}^d \cosh 2k_j \eta^{-1/2} \cos k_j z_j$$

for $k \in \mathbb{N}^d$ form an orthonormal basis of $H_{\text{even}}^2(\mathbb{T}_\eta^d)$.

Furthermore,

$$\|b_k(z)\|_{C^0(\mathbb{T}^d)} \leq \prod_{j=1}^d \cosh 2k_j \eta^{-1/2} \leq 2^{d/2} e^{\sum k_j \eta}.$$

Let us construct \hat{S}_ξ^η so that a $\xi/2$ -fattening of the subspace spanned by basis elements $\{b_k\}_{\sum k_j \leq k^*}$ for some k^* covers the Hardy space ball, and then construct a lattice of functions inside this subspace.

If we set

$$k^* = \max\{d + 2 \log(2^{2+d} \sqrt{d/2\pi} \xi^{-2})/\eta, 2 + 2d/\eta\} \leq C_5 \eta^{-1} \log \xi^{-1},$$

for some positive constant C_5 dependent only on d, η_0 , we can choose

$$\hat{S}_\xi^\eta = \left\{ \sum_{\sum k_j \leq k^*} w_k b_k \mid w_k \in \left[-2^{-d/2} e^{-\sum k_j \eta}, 2^{-d/2} \eta^{-\sum k_j \eta} \right] \cap (\xi(k^*)^{-d/2}/2)\mathbb{Z} \right\}.$$

A crude bound on the size of this set gives that

$$\begin{aligned} |\hat{S}_\xi^\eta| &\leq (2^{4-d/2} (k^*)^{d/2} \xi^{-1} + 1)^{(k^*)^d} \\ &\leq (C_8 \xi^{-1} \eta^{-d/2} (\log \xi^{-1})^{d/2})^{(C_5 \eta^{-1} \log \xi)^d} \\ &\leq e^{(C_9 \log \xi^{-1} + C_{10} \log \eta^{-1})(\eta^{-1} \log \xi^{-1})^d} \end{aligned}$$

for positive constants (dependent only on d, η_0) C_8, C_9, C_{10} . \square

C Proof of Proposition 9.1 and Lemma 9.4

Proof of Proposition 9.1. The second equation is a simple application of Proposition 8.8.

For the first equation we can say that

$$\psi(z)^{-1} = \int_{\mathbb{R}^d} g_\varepsilon(z - y) \rho(y) \phi(y) \, dy$$

and consequently,

$$\begin{aligned}\|\psi\|_{\zeta}^{-1} &= \inf_{z \in \mathbb{D}_{\zeta}} \left| \int_{\mathbb{R}^d} g_{\varepsilon}(z-y) \rho(y) \phi(y) \, dy \right| \\ &= \inf_{x \in \mathbb{D}, s \in [-\zeta, \zeta]^d} \left| \int_{\mathbb{R}^d} e^{(|s|^2/2 + is \cdot (x-y))/\varepsilon} g_{\varepsilon}(x-y) \rho(y) \phi(y) \, dy \right|.\end{aligned}$$

Using that $\phi > 0$ on the real domain \mathbb{D} and that $|e^{iw} - 1| \leq |w|$ for real w , we have then that

$$\|\psi\|_{\zeta}^{-1} \geq \inf_{x \in \mathbb{D}, s \in [-\zeta, \zeta]^d} e^{|s|^2/2\varepsilon} \left((\mathcal{K}_{\varepsilon}\phi)(x) - \left| \int_{\mathbb{R}^d} g_{\varepsilon}(x-y) \varepsilon^{-1} (s \cdot (x-y)) \rho(y) \phi(y) \, dy \right| \right).$$

Using that

$$\|g_{\varepsilon}(x)s \cdot x\|_{L^1(\mathbb{R}^d, dx)} \leq \sqrt{2\varepsilon/\pi} |s| \leq \sqrt{2\varepsilon/\pi} \sqrt{d\zeta^2} \leq \sqrt{2dZ_0/\pi\varepsilon},$$

we have

$$\|\psi\|_{\zeta}^{-1} \geq \|\mathcal{K}_{\varepsilon}\phi\|_0 - \sqrt{2dZ_0/\pi} \|\rho\|_0 \|\phi\|_0.$$

Because

$$\|\mathcal{K}_{\varepsilon}\phi\|_0^{-1} \leq \|\rho^{-1}\|_0 \|\phi^{-1}\|_0,$$

our assumption on Z_0 gives us the required bound. \square

Proof of Lemma 9.4. Consider the following forward equation on the domain \mathbb{D} for $t \in [0, \varepsilon]$:

$$\partial_t \phi^t = \mathcal{L}\phi^t + \nabla \hat{w}_{\varepsilon}^t \cdot \nabla \phi^t, \quad (66)$$

recalling that

$$e^{\hat{w}_{\varepsilon}^t} = \rho^{-1} e^{\frac{1}{2}t\Delta}(U_{\varepsilon}\rho). \quad (67)$$

We have from Theorem 3.5 that $\mathcal{P}_{\varepsilon}^m$ is given by

$$\mathcal{P}_{\varepsilon}\phi = S_{\varepsilon}(m\varepsilon, 0)\phi(y) \, dy,$$

where the solution operator $S_{\varepsilon}(t_1, t_0)$ is a kernel operator. We can thus use PDE results to study the functional behaviour of $\mathcal{P}_{\varepsilon}$.

We divide the operator

$$(I + \mathcal{P}_{\varepsilon})^{-1} = I - \mathcal{P}_{\varepsilon} + (I - \mathcal{P}_{\varepsilon}^{2n^*})^{-1} \sum_{n=2}^{2n^*+1} (-1)^n \mathcal{P}_{\varepsilon}^n, \quad (68)$$

where $n^* = \lceil (2\varepsilon^{-1}) \rceil$, and consider in turn the norms of $(I - \mathcal{P}_{\varepsilon}^{2n^*})^{-1}$ and $\mathcal{P}_{\varepsilon}^{2n+2} - \mathcal{P}_{\varepsilon}^{2n+1}$.

We have from Corollary 6.2 that

$$\sup_t \|\log \rho + \hat{w}_{\varepsilon}^t\|_0 \leq \|\log \rho\|_0 + C_{69,0},$$

and consequently Gaussian lower estimates on the fundamental solution from Theorem 1 of Liskevich & Semenov (2000)¹ imply that there exists a constant $C_{41} \in (0, 1)$ depending on $L, d, C_{68}, \|\rho\|_0, \text{Lip} \log \rho, \varepsilon_0$ such that for all bounded non-negative functions ϕ ,

$$\inf S(2n^*\varepsilon, 0)\phi \geq C_{41} \|\phi\|_{L^{\infty}},$$

¹Here as usual we use that we can extend $\mathbb{D} = (\mathbb{R}/LZ)^d$ to \mathbb{R}^d in the natural way.

where we recall that $2n^*\varepsilon \in [1, 1 + 2\varepsilon_0]$. The Sinkhorn balancing (13) makes \mathcal{P}_ε bistochastic, so $\|\mathcal{P}_\varepsilon\|_0 = 1$: if $\|\phi\|_0 = 1$ and $\int_{\mathbb{D}} \phi dx = 0$ then

$$\mathcal{P}_\varepsilon^{2n^*} \phi = \mathcal{P}_\varepsilon^{2n^*} \phi^+ - \mathcal{P}_\varepsilon^{2n^*} \phi^- = (\mathcal{P}_\varepsilon^{2n^*} \phi^+ - C_{41}) - (\mathcal{P}_\varepsilon^{2n^*} \phi^- - C_{41}),$$

where $\phi^+, \phi^- \geq 0$ are the positive and negative parts of ϕ respectively.

Since the two bracketed quantities are non-negative, we have

$$\|\mathcal{P}_\varepsilon^{2n^*} \phi\|_0 \leq \max \left\{ \sup \mathcal{P}_\varepsilon^{2n^*} \phi^+ - C_{41}, \sup \mathcal{P}_\varepsilon^{2n^*} \phi^- - C_{41} \right\} = \|\mathcal{P}_\varepsilon \phi\|_0 - C_{41} = 1 - C_{41}.$$

Thus,

$$\|\mathcal{P}_\varepsilon^{2n^*}\|_0 \leq 1 - C_{41} < 1$$

and so

$$\|(I - \mathcal{P}_\varepsilon^{2n^*})^{-1}\|_0 \leq C_{41}^{-1}.$$

On the other hand, we have the Schauder estimate from Theorem 1 of Knerr (1980) that there exists a constant C_{42} depending on $d, L, \varepsilon_0, C_{68}$ such that for $0 < t_0 < t_1 < 1 + 2\varepsilon_0$ and $\mathcal{A} \in \{\Delta, \nabla\}$,

$$\|\mathcal{A}S_\varepsilon(t_1, 0)\phi - \mathcal{A}S_\varepsilon(t_0, 0)\phi\|_0 \leq C_{42}s^{-(1+\beta/2)}(t_1 - t_0)^{\beta/2}\|\phi\|_0.$$

Since \hat{w}_ε^t is ε -periodic, we can apply these equations with the evolution of S_ε (66) to say that for $t \in [0, 1 + \varepsilon_0]$,

$$\left\| \frac{\partial}{\partial t} S_\varepsilon(t + \varepsilon, 0)\phi - \frac{\partial}{\partial t} S_\varepsilon(t, 0)\phi \right\|_0 \leq 2C_{42}t^{-(1+\beta/2)}\varepsilon^{\beta/2}\|\phi\|_0.$$

As a result,

$$\begin{aligned} \left\| \frac{1}{2}(\mathcal{P}_\varepsilon^{2n+2} - 2\mathcal{P}_\varepsilon^{2n+1} + \mathcal{P}_\varepsilon^{2n}) \right\| &= \left\| \frac{1}{2} \int_{2n\varepsilon}^{(2n+1)\varepsilon} \left(\frac{\partial}{\partial t} S_\varepsilon(t + \varepsilon, 0) - \frac{\partial}{\partial t} S_\varepsilon(t, 0) \right) dt \right\| \\ &\leq C_{42}(2n\varepsilon)^{-(1+\beta/2)}\varepsilon^{1+\beta/2} \\ &= C_{42}(2n)^{-(1+\beta/2)} \end{aligned}$$

Since, recalling (68),

$$\sum_{n=2}^{2n^*+1} (-1)^n \mathcal{P}_\varepsilon^n = \frac{1}{2}(-\mathcal{P}_\varepsilon^{2n^*+2} + \mathcal{P}_\varepsilon^2) + \sum_{n=1}^{n^*} \frac{1}{2}(\mathcal{P}_\varepsilon^{2n+2} - 2\mathcal{P}_\varepsilon^{2n+1} + \mathcal{P}_\varepsilon^{2n}),$$

we have

$$\left\| \sum_{n=2}^{2n^*+1} (-1)^n \mathcal{P}_\varepsilon^n \right\|_0 \leq 1 + C_{42}2^{-(1+\beta/2)}(1 + 2/\beta)$$

and so

$$\|(I + \mathcal{P}_\varepsilon)^{-1}\|_0 \leq 2 + C_{41}^{-1} \left(1 + C_{42}2^{-(1+\beta/2)}(1 + 2/\beta) \right) =: C_{40}$$

as required. \square

Acknowledgement. This research has been partially funded by Deutsche Forschungsgemeinschaft (DFG, German Science Foundation) - SFB 1294/1 - 318763901.

CLW would like to thank Jakiw Pidstrigach, Daniel Daners, David Lee and Harry Crimmins for helpful discussions.

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