SPECTRAL PROPERTIES OF KERNEL MATRICES IN THE FLAT LIMIT*

SIMON BARTHELMÉ[†] AND KONSTANTIN USEVICH[‡]

Abstract. Kernel matrices are of central importance to many applied fields. In this manuscript, we focus on spectral properties of kernel matrices in the so-called "flat limit", which occurs when points are close together relative to the scale of the kernel. We establish asymptotic expressions for the determinants of the kernel matrices, which we then leverage to obtain asymptotic expressions for the main terms of the eigenvalues. A separate analysis using Kato's perturbation theory yields expressions for limiting eigenvectors, which are strongly tied to discrete orthogonal polynomials. Both smooth and finitely smooth kernels are covered, with stronger results available in the univariate case.

Key words. kernel matrices, eigenvalues, eigenvectors, radial basis functions, perturbation theory, flat limit, discrete orthogonal polynomials

AMS subject classifications. 15A18, 47A55, 47A75, 47B34, 60G15, 65D05

1. Introduction. For an ordered set of points $\mathcal{X} = (\boldsymbol{x}_1, \dots, \boldsymbol{x}_n), \, \boldsymbol{x}_k \in \Omega \subset \mathbb{R}^d$, not lying in general on a regular grid, and a kernel function $K : \Omega \times \Omega \to \mathbb{R}$, the kernel matrix K is defined as

$$\boldsymbol{K} = \boldsymbol{K}(\mathcal{X}) = \left[K(\boldsymbol{x}_i, \boldsymbol{x}_j)\right]_{i,j=1}^n.$$

These matrices occur in approximation theory (kernel-based approximation and interpolation, [26]), statistics and machine learning (Gaussian process models [35], Support Vector Machines and kernel PCA [27]).

Often, a scaling parameter ε is introduced, and the scaled kernel matrix becomes

(1)
$$\mathbf{K}_{\varepsilon} = \mathbf{K}_{\varepsilon}(\mathcal{X}) = \left[K(\varepsilon \mathbf{x}_i, \varepsilon \mathbf{x}_j) \right]_{i,j=1}^n,$$

If the kernel is a Radial Basis Function kernel (the most common case), then its value depends only on the Euclidean distance between x and y, and ε determines how quickly the kernel decays with distance.

Understanding spectral properties of kernel matrices is essential in statistical applications (e.g., for selecting hyperparameters), as well as in scientific computing (e.g., for preconditioning [11, 10]). Because the spectral properties of kernel matrices are not directly tractable in the general case, one usually needs to resort to asymptotic results. The most common form of asymptotic analysis takes $n \to \infty$. Three cases are typically considered: (a) when the distribution of points \mathcal{X} converges to some continuous measure on Ω , the kernel matrix tends in some sense to a linear operator in a Hilbert space, whose spectrum is then studied [32]; (b) recently, some authors have obtained asymptotic results in a regime where both n and the dimension d tend to infinity [8, 5, 33], using the tools of random matrix theory; (c) in a special case of \mathcal{X} lying on a regular grid, stationary kernel matrices become Toeplitz or more generally

^{*}Submitted to the editors on DATE.

Funding: This work was supported by ANR project GenGP (ANR-16-CE23-0008) and ANR project LeaFleT (ANR-19-CE23-0021-01).

 $^{^\}dagger \text{CNRS},$ Univ. Grenoble Alpes, Grenoble INP, GIPSA-lab, 38000 Grenoble, France (simon.barthelme@gipsa-lab.fr).

[‡]Université de Lorraine and CNRS, CRAN (Centre de Recherche en Automatique en Nancy), UMR 7039, Campus Sciences, BP 70239, 54506 Vandœuvre-lès-Nancy cedex, France (konstantin.usevich@univ-lorraine.fr).

multilevel Toeplitz, whose asymptotic spectral distribution are determined by their symbol (or the Fourier transform of the sequence) [14, 31, 24].

Driscoll & Fornberg [7] pioneered a new form of asymptotic analysis for kernel methods, in the context of RBF interpolation. The point set \mathcal{X} is considered fixed, with arbitrary geometry (i.e., not lying in general on a regular grid), and the scaling parameter ε approaches 0. Driscoll & Fornberg called this the "flat limit", as kernel functions become flat over the range of \mathcal{X} as $\varepsilon \to 0$. Very surprisingly, they showed that for certain kernels the RBF interpolant stays well-defined in the flat limit, and tends to the Lagrange polynomial interpolant. Later, a series of papers established similar convergence results for various types of radial functions (see [28, 22] and references therein). In particular, [28] showed that for kernels of finite smoothness the limiting interpolant is a spline rather than a polynomial.

The flat limit is interesting for several reasons. In contrast to other asymptotic analyses, it is deterministic (\mathcal{X} is fixed), and makes very few assumptions on the geometry of the point set. In addition, kernel methods are plagued by the problem of picking a scale parameter [27]. One either uses burdensome procedures like cross-validation or maximum likelihood [35] or sub-optimal but cheap heuristics like the median distance heuristic [12]. The flat limit analysis may shed some light on the problem. Finally, the results derived here can be thought of as perturbation results, in the sense that they are formally exact in the limit, but useful approximations when the scale is not too small.

Despite its importance, little was known until recently about the eigenstructure of kernel matrices in the flat limit. The difficulty comes from the fact that $K_{\varepsilon} = K(0,0)\mathbf{1}\mathbf{1}^{\mathsf{T}} + \mathcal{O}(\varepsilon)$, i.e. we are dealing with a singular perturbation problem¹.

Only recently, Wathen & Zhu [34] obtained results on the orders of eigenvalues of kernel matrices for smooth analytic radial basis kernels, based on the Courant-Fischer minimax principle. However, they did not obtain the main terms in the expansion of the eigenvalues, and their result was derived only for smooth kernels. In addition, it holds no information on the limiting eigenvectors.

In this paper, we try filling this gap by characterising both the eigenvalues and eigenvectors of kernel matrices in the flat limit. We consider both completely smooth kernels and finitely-smooth kernels. The latter (Matérn-type kernels) are very popular in spatial statistics. For establishing asymptotic properties of eigenvalues, we use the expression for the limiting determinants of K_{ε} (obtained in only for the smooth case), and Binet-Cauchy formulae. As a special case, we recover results of Wathen & Zhu, but for a wider class of kernels.

- 1.1. Overview of the results. Some of the results are quite technical, so the goal of this section is to serve as a reader-friendly summary of the contents.
 - **1.1.1.** Types of kernels. We begin with some definitions.

A kernel is called translation invariant if

$$K(\boldsymbol{x}, \boldsymbol{y}) = f(\boldsymbol{x} - \boldsymbol{y})$$

for some function f. A kernel is RBF, or stationary if, in addition, we have:

$$K(x, y) = f(x - y) = g(||x - y||_2)$$

¹ Seen from the point of view of the characteristic polynomial, the equation $\det(\mathbf{K}_{\varepsilon} + \lambda \mathbf{I}) = 0$ has a solution of multiplicity n-1 at $\varepsilon = 0$, but these roots immediately separate when $\varepsilon > 0$.

i.e. the value of the kernel depends only on the Euclidean distance between \boldsymbol{x} and \boldsymbol{y} . The function g is a radial basis function. Finally, $K(\boldsymbol{x},\boldsymbol{y})$ may be positive (semi) definite, in which case we have that for all point sets $\mathcal{X} = (\boldsymbol{x}_1,\ldots,\boldsymbol{x}_n)$, and all n > 0, the kernel matrix is positive (semi) definite.

All of our results are valid for stationary, positive semi-definite kernels. In addition, some are also valid for translation-invariant kernels, or even general, non-RBF kernels. For simplicity, we focus on RBF kernels in this introductory section.

An important property of an RBF kernel is its order of smoothness, which we call r throughout this paper. The definition is at first glance not very enlightening: formally, if the first p odd-order derivatives of the RBF g are zero, then r=p+1. To understand the definition, some Fourier analysis is required [30], but for the purposes of this article we will just note two consequences. When interpolating using an RBF kernel of smoothness r, the resulting interpolant is r-1 times differentiable. When sampling from a Gaussian process with covariance function of smoothness order r, the sampled process is also r-1 times differentiable (almost surely). r may equal ∞ , which is the case we call infinitely smooth. If r is finite we talk about an finitely smooth kernel. We treat the two cases separately because infinitely smooth kernels are popular, and because proofs are simpler in that case.

Finally, the points are assumed to lie in some subset of \mathbb{R}^d , and if d=1 we call this the *univariate* case, as opposed to the *multivariate* case (d>1).

1.1.2. Univariate results. In the univariate case, we can give simple closed-form expressions for the eigenvalues and eigenvectors of kernel matrices as $\varepsilon \to 0$. What form these expression take depends essentially on the smoothness order of the kernel.

We shall contrast two kernels that are at opposite ends of the smoothness spectrum. One, the squared-exponential, or Gaussian, kernel, is infinitely smooth, and is defined as:

$$K_{\varepsilon}(x,y) = \exp\left(-\varepsilon(x-y)^2\right)$$

The other has smoothness order 1, and is known as the "exponential" kernel:

$$K_{\varepsilon}(x,y) = \exp(-\varepsilon |x-y|)$$

Both kernels are RBF and positive-definite. However, the small- ε asymptotics of these two kernels are strikingly different.

In the case of the squared-exponential kernel, the eigenvalues go to 0 extremely fast, except for the first one, which goes to n. Specifically, the first eigenvalue is $\mathcal{O}(1)$, the second is $\mathcal{O}(\varepsilon^2)$, the third is $\mathcal{O}(\varepsilon^4)$, etc². Figure 1 shows the eigenvalues of the squared-exponential kernel for a fixed set \mathcal{X} of randomly-chosen nodes in the unit interval (n=10 here). The eigenvalues are shown as a function of ε , under log-log scaling. As expected from Theorem 4.2 (see also [34]), for each i, $\log \lambda_i$ is approximately linear as a function of $\log \varepsilon$. In addition, the main term in the scaling of $\log \lambda_i$ in ε (i.e., the offsets of the various lines) is also given by Theorem 4.2, and the corresponding asymptotic approximations are plotted in red. They show very good agreement with the exact eigenvalues, up to $\varepsilon \approx 1$.

Contrast that behaviour with the one exhibited by the eigenvalues of the exponential kernel. Theorem 4.5 describes the expected behaviour: the top eigenvalue is again $\mathcal{O}(1)$ and goes to n, while all remaining eigenvalues are $\mathcal{O}(\varepsilon)$. Figure 2 is the

² In fact, Theorem 4.2 guarantees the same behaviour for general kernels of sufficient smoothness.

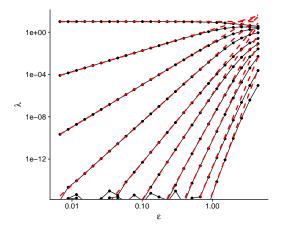


Fig. 1. Eigenvalues of the Gaussian kernel (d = 1). The set of n=20 nodes was drawn uniformly from the unit interval. In black, eigenvalues of the Gaussian kernel, for different values of ε . The dashed red curve are our small- ε expansions. Note that both axes are scaled logarithmically. The noise apparent for small ε values in the low range is due to loss of precision in the numerical computations.

counterpart of the previous figure, and shows clearly that all eigenvalues except for the top one go to 0 at unit rate. The main term in the expansions of eigenvalues determines again the offsets shown in 2, which can be computed from the eigenvalues of the centred distance matrix as shown in Theorem 4.5.

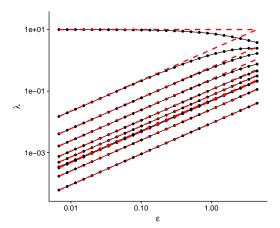


Fig. 2. Eigenvalues of the exponential kernel (d = 1). The largest eigenvalue has a slope of 0 for small ε , the others have unit slope, as in Theorem 4.4.

To sum up: except for the top eigenvalue, which behaves in the same way for both kernels, the rest scale quite differently. More generally, theorem 4.5 states that for kernels of smoothness order r < n (r = 1 for the exponential, $r = \infty$ for the Gaussian), the eigenvalues are divided into two groups. The first group is of size r, and have order 1, ε^2 , ε^4 , etc. The second group is of size n-r, and all have the same order, ε^{2r-1} .

The difference between the two kernels is also reflected in how the eigenvectors

behave. For the Gaussian kernel, the limiting eigenvectors (shown in Figure 3) are columns of the Q matrix of the QR factorization of the Vandermonde matrix (i.e., the orthogonal polynomials with respect to the discrete uniform measure on \mathcal{X}). For instance, the top eigenvector equals the constant vector $\frac{1}{\sqrt{n}}\mathbf{1}$, and the second eigenvector tor equals $\begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}^\mathsf{T} - \frac{\sum x_i}{n}$ (up to normalisation). Each successive eigenvector depends on the geometry of $\mathcal X$ via the moments $m_p(\mathcal X) = \sum_{i=1}^n x_i^p$.

In fact, this result is valid for any smooth analytic in ε kernel as shown by Theorem 8.1.

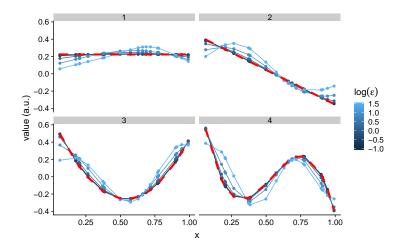


Fig. 3. First four eigenvectors of the squared-exponential kernel. We used the same set of points as in the previous two figures. In blue, eigenvectors of the Gaussian kernel, for different values of ε . The dashed red curve shows the theoretical limit as $\varepsilon \to 0$ (i.e., the first four orthogonal polynomials of the discrete measure)

In the case of finite smoothness, the two groups are associated with different groups of eigenvectors. The first group of r eigenvectors are again orthogonal polynomials. The second group are splines of order 2r-1. Convergence of eigenvectors is shown in Figure 4. This general result for the case of finite smoothness is shown in Theorem 8.3.

- 1.1.3. The multivariate case. The general, multivariate case requires more care. Polynomials continue to play a central role in the flat limit, but when d > 1they appear naturally in groups of equal degree. For instance, in d=2, we may write x = (y, z) and the first few monomials are as follows:
 - Degree 0: 1

 - Degree 1: y, z
 Degree 2: y², yz, z²
 Degree 3: y³, y²z, yz², z³

etc. Note that there is one monomial of degree 0, two monomials of degree 1, three monomials of degree 2, and so on. If d=1 there is a single monomial in each group, and here lies the essence of the difference between the univariate and multivariate cases.

In infinitely smooth kernels like the squared-exponential, as shown in [34], there are as many eigenvalues of order $\mathcal{O}(\varepsilon^{2k})$ as there are monomials of degree k in dimension d: for instance, there are 4 monomials of degree 3 in dimension 2, and so 4

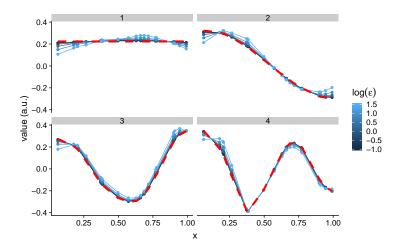


FIG. 4. First four eigenvectors of the exponential kernel. The same set of nodes is used as in fig. 3. In blue, the eigenvectors of the kernel, for different values of ε . The dashed red curve shows the theoretical limit as $\varepsilon \to 0$. From Theorem 8.3, these are (1) the vector $\frac{1}{\sqrt{n}}$ and (2-4) the first three eigenvectors of $\left(\mathbf{I} - \frac{\mathbf{1}\mathbf{1}^\mathsf{T}}{n}\right) \mathbf{D}_{(1)} \left(\mathbf{I} - \frac{\mathbf{1}\mathbf{1}^\mathsf{T}}{n}\right)$.

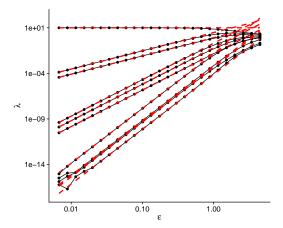


Fig. 5. Eigenvalues of the squared-exponential kernel in the multivariate case (d = 2). The set of n=10 nodes was drawn uniformly from the unit square. In black, eigenvalues of the Gaussian kernel, for different values of ε . The dashed red curve are our small- ε expansions. Eigenvalues appear in groups of different orders, recognisable here as having the same slopes as $\varepsilon \to 0$. A single eigenvalue if of order $\mathcal{O}(1)$. Two eigenvalues are of order $\mathcal{O}(\varepsilon^2)$, as many as there are monomials of degree 1 in two dimensions. Three eigenvalues are of order $\mathcal{O}(\varepsilon^4)$, as many as there are monomials of degree 2 in two dimensions, etc.

eigenvalues of order $\mathcal{O}(\varepsilon^8)$. An example is shown on fig. 5. In finitely-smooth kernels like the exponential kernel, there are r successive groups of eigenvalues with order $\mathcal{O}(1)$, $\mathcal{O}(\varepsilon^2)$, ..., up to $\mathcal{O}(\varepsilon^{2r-2})$. Following that, all remaining eigenvalues have order $\mathcal{O}(\varepsilon^{2r-1})$, just like in the one-dimensional case.

We show in Theorem 6.2, that the main terms of these eigenvalues in each group can be computed from the QR factorization of the Vandermonde matrix and a Schur complement associated with the Wronskian matrix of the kernel. In the finite smooth-

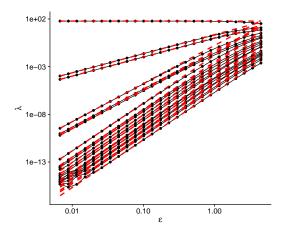


FIG. 6. Eigenvalues of a finitely smooth kernel in d=2. Here we picked a kernel with smoothness index r=3 (the exponential kernel has order r=1). The set of n=20 nodes was drawn uniformly from the unit square. The first r=3 groups of eigenvalues have the same behaviour as in the squared-exponential kernel: one is $\mathcal{O}(1)$, two are $\mathcal{O}(\varepsilon^2)$, three are $\mathcal{O}(\varepsilon^4)$. All the rest are $\mathcal{O}(\varepsilon^5)$.

ness case, the same expansions are valid until the smoothness order, and the last group of eigenvalues is given by the eigenvalues of the projected distance matrix, as in the one-dimensional case.

Finally, in the multivariate case, we also fully characterise the eigenprojectors. In a nutshell, the subspaces associated with each group of eigenvalues are spanned by orthogonal polynomials of a certain order. The eigenvectors are the subject of a conjecture given in section 8, which we believe to be quite solid.

1.2. Overview of tools used in the paper. For finding the orders of the eigenvalues, as in [34], we use the Courant-Fisher minimax principle (more precisely, Theorem 3.3 proved in [15]). However, unlike [34], we do not use directly the results of Micchelli [23], but rather rotate the kernel matrices using the Q factor in the QR factorization of the Vandermonde matrix, and find the expansion of rotated matrices from the Taylor expansion of the kernel.

The key results are the expansions for the determinants of K_{ε} , which use the expansions of rotated kernel matrices. Our results on determinants (Theorems 4.1, 4.4, 6.1, and 6.3) generalize those of Lee & Micchelli [21]. The next key observation is that principal submatrices of K_{ε} are also kernel matrices, hence the results on determinants imply the results on expansions elementary symmetric polynomials of eigenvalues (via the correspondence between elementary symmetric polynomials, see Theorem 3.1, and the Binet-Cauchy formula). Finally, the main terms of the eigenvalues can be retrieved from the main terms of the elementary symmetric polynomials, as shown in Lemma 3.4. An important tool for the multivariate and finite smoothness case is Lemma 3.10 on low-rank perturbation of elementary symmetric polynomials that we could not find elsewhere in the literature

To study the properties of the eigenvectors, we employ Kato's perturbation theory for linear operators [18]. In our case we are dealing with the Hermitian matrices, and many results of [18] simplify: a summary is given in Section 7. The central aspect of Kato's method involves a process of successive reductions: K_{ε} has a single non-null eigenvalue, associated with the eigenvector $\frac{1}{\sqrt{n}}\mathbf{1}$. However, we need to extract infor-

mation on the remaining n-1 others. To do so, we shall project K_{ε} on the space orthogonal to the first eigenvectors: in that subspace, a top eigenvector emerges, associated with an eigenvalue of order ε^2 . We project again on the orthogonal subspace, another eigenvector emerges, etc. An example of the process of reduction is shown below, where the multiplicity of the 0-th eigenvalue is put in parentheses.

If d > 1, eigenvectors emerge in groups, as we will see, but the process is similar. For example, if d=2, at the ℓ -th reduction step, a group of $\ell+1$ eigenvalues and eigenvectors will appear as shown below:

where k is the smallest number such that $n-{k+2 \choose 2}>0$

- 1.3. Organisation of the paper. In an attempt to make the paper readerfriendly, it is organized as follows. In Section 2 we recall the main terminology for 1D kernels. In Section 3 we gather well-known (or not so well known) results on eigenvalues, determinants, elementary symmetric polynomials and their perturbations, which are key tools used in the paper. Section 4 contains the main results on determinants or eigenvalues in the univariate (d=1) case. While these results are special cases of the multivariate case (d > 1), the latter is burdened with heavier notation due to the complexity of dealing with multivariate polynomials. In addition, it requires a number of technical assumptions on the arrangement of points, which are typical for multivariate polynomial interpolation. To get a gist of the results and techniques, the reader is advised to first consult the case d = 1. In Section 5, we introduce all the needed notation to handle the multivariate case. Section 6 contains the main results of the paper on determinants and eigenvalues in their full generality. In Section 7, we provide a brief summary on analytic perturbation theory, before proving the results on eigenvectors in Section 8.
- 2. Background and main notation: the one-dimensional case. This section contains main definitions and examples of kernels in 1D case. We assume that the kernel function $K: \Omega \times \Omega \to \mathbb{R}$ is in the class $\mathcal{C}^{(\ell,\ell)}(\Omega)$, $\Omega = (-a;a)$, i.e. all the partial derivatives $\frac{\partial^2}{\partial x^i \partial y^j} K$ exist and are continuous for $0 \le i, j \le \ell$ on $\Omega \times \Omega$. We will often need the following short-hand notation for partial derivatives

$$K^{(i,j)} \stackrel{\text{def}}{=} \frac{\partial^{i+j}}{\partial x^i \partial y^j} K,$$

and we introduce the so-called Wronskian matrix

(3)
$$\mathbf{W}_{k,k} \stackrel{\text{def}}{=} \begin{bmatrix} \frac{K^{(0,0)}(0,0)}{0!0!} & \cdots & \frac{K^{(0,k)}(0,0)}{0!k!} \\ \vdots & & \vdots \\ \frac{K^{(k,0)}(0,0)}{k!0!} & \cdots & \frac{K^{(k,k)}(0,0)}{k!k!} \end{bmatrix}.$$

2.1. Translational kernels. Let us consider an important example of translational kernels, defined as

$$K(x,y) = \varphi(x-y).$$

We assume that $\varphi \in \mathcal{C}^{2r}(-2a,2a)$; hence, φ has a Taylor expansion around 0

$$\varphi(t) = \alpha_0 + \alpha_1 t + \alpha_2 t^2 + \dots + \alpha_{2r} t^{2r} + o(t^{2r}), \text{ where } \alpha_k \stackrel{\text{def}}{=} \frac{\varphi^{(k)}(0)}{k!}.$$

Therefore $K \in \mathcal{C}^{r,r}(\Omega \times \Omega)$ and its derivatives at 0 are

(4)
$$\frac{K^{(i,j)}(0,0)}{i!j!} = \frac{(-1)^j \phi^{(i+j)}(0)}{i!j!} = (-1)^j \binom{i+j}{j} \alpha_{i+j},$$

i.e., the Wronskian matrix has the form:

$$\mathbf{W}_{k,k} = \begin{bmatrix} \alpha_0 & -\alpha_1 & \alpha_2 & -\alpha_3 & \cdots \\ \alpha_1 & -2\alpha_2 & 3\alpha_3 & -4\alpha_4 & \cdots \\ \alpha_2 & -3\alpha_3 & 6\alpha_4 & -10\alpha_5 & \cdots \\ \alpha_3 & -4\alpha_4 & 10\alpha_5 & -20\alpha_6 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}.$$

A special case of the translational kernels are smooth RBFs, which will be considered in the next subsection. The simplest example is the Gaussian kernel with

$$\varphi(t) = \exp(-t^2) = 1 - t^2 + \frac{t^4}{2!} - \frac{t^6}{3!} + \cdots,$$

i.e. for all integer $\nu \geq 0$

$$\alpha_{2\nu} = \frac{(-1)^{\nu}}{\nu!}, \quad \alpha_{2\nu+1} = 0.$$

In this case, the Wronskian matrix becomes

$$\boldsymbol{W}_{k,k} = \begin{bmatrix} 1 & 0 & -1 & 0 & \cdots \\ 0 & 2 & 0 & -2 & \cdots \\ -1 & 0 & 3 & 0 & \cdots \\ 0 & -2 & 0 & -\frac{10}{3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}.$$

2.2. RBF kernels with finite smoothness. We consider the case when

(5)
$$K(x,y) = f(|x-y|).$$

We put following the assumptions on f:

- $f \in C^{2r}(-2a, 2a)$;
- the highest derivative of odd order is not zero $f^{(2r-1)}(0) \neq 0$;
- the lower derivatives with odd order vanish, i.e., $f^{(2\ell-1)}(0) = 0$ for $\ell < r$.

If the function f(t) satisfies these assumptions, then r is called the order of smoothness of K. Note that f admits a Taylor expansion

(6)
$$f(t) = f_0 + f_2 t^2 + \dots + f_{2r-2} t^{2r-2} + t^{2r-1} (f_{2r-1} + \mathcal{O}(t)).$$

where $f_k = f^{(k)}(0)/k!$ is a shorthand notation for the scaled derivative at 0. For example, for the exponential kernel $\exp(-|x-y|)$, we have $f_0 = 1$ and $f_1 = -1$, so the smoothness order is r = 1. For the C^2 Matern kernel $(1 + |x-y|) \exp(-|x-y|)$, we have $f_0 = 1$, $f_1 = 0$, $f_2 = -1/2$, $f_3 = 1/3$, so the smoothness order is r = 2.

Using (6) we may write the scaled kernel matrix as

(7)
$$\mathbf{K}_{\varepsilon} = f_0 \mathbf{D}_{(0)} + f_2 \varepsilon^2 \mathbf{D}_{(2)} + \dots + f_{2r-2} \varepsilon^{2r-2} \mathbf{D}_{(2r-2)} + \varepsilon^{2r-1} f_{2r-1} \mathbf{D}_{(2r-1)} + \mathcal{O}(\varepsilon).$$

where matrix $\mathbf{D}_{(k)} = \left[|x_i - x_j|^k \right]_{i,j}$ is the *k*-th Hadamard power of the Euclidean distance matrix $\mathbf{D}_{(1)}$ (see the next subsection).

2.3. Vandermonde matrices, distance matrices and their properties. First, we denote by $V_{\leq k}$ is the Vandermonde matrix up to degree k

(8)
$$\mathbf{V}_{\leq k} = \begin{bmatrix} 1 & x_1 & \cdots & x_1^k \\ \vdots & & \vdots \\ 1 & x_n & \cdots & x_n^k \end{bmatrix},$$

which has rank $\min(n, k+1)$ if the nodes are distinct. In particular, the matrix $V_{\leq n-1}$ is square and invertible for distinct nodes.

For even k, the Hadamard powers $D_{(k)}$ of the distance matrix can be expressed via the columns of the Vandermonde matrix using the binomial expansion

(9)
$$\mathbf{D}_{(2\ell)} = \sum_{j=0}^{2\ell} (-1)^j \binom{2\ell}{j} \mathbf{v}_j \mathbf{v}_{2\ell-j}^\mathsf{T},$$

where $\boldsymbol{v}_k \stackrel{\text{def}}{=} \begin{bmatrix} x_1^k & \cdots & x_n^k \end{bmatrix}^\mathsf{T}$ are columns of Vandermonde matrices. Therefore, rank $\boldsymbol{D}_{(2\ell)} = \min(2\ell+1,n)$ if all points x_k are distinct.

Moreover, (9) gives a way to rewrite the expansion (7) in the following form

(10)
$$K_{\varepsilon} = \sum_{\ell=0}^{r-1} \varepsilon^{2j} \underbrace{V_{\leq 2\ell} W_{/2\ell} V_{\leq 2\ell}^{\mathsf{T}}}_{f_{2\ell} D_{(2\ell)}} + \varepsilon^{2r-1} f_{2r-1} D_{(2r-1)} + \mathcal{O}(\varepsilon^{2r}),$$

where $\mathbf{W}_{/s} \in \mathbb{R}^{(s+1) \times (s+1)}$ has nonzero elements only on its antidiagonal:

(11)
$$\left(\mathbf{W}_{s} \right)_{j+1,s-j+1} \stackrel{\text{def}}{=} f_{s} (-1)^{j} {s \choose j}.$$

For example,

$$W_{/2} = f_2 \begin{bmatrix} 0 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & 0 \end{bmatrix}.$$

In fact, from (4), non-zero elements of $W_{/s}$ are scaled derivatives of the kernel:

$$\left(\mathbf{W}_{\diagup s} \right)_{j+1,s-j+1} = \frac{K^{(j,s-j)}(0,0)}{j!(s-j)!};$$

this justifies the notation $W_{/2\ell}$ (i.e., an antidiagonal of the Wronskian matrix).

On the other hand, for k odd, the matrices $\mathbf{D}_{(k)}$ exhibit an entirely different set of properties. Of most interest here is conditional positive-definitess, which guarantees that the distance matrices are positive definite when projected on a certain subspace. The following result appears eg. in [9], ch. 8, but follows directly from an earlier paper by Micchelli [23].

LEMMA 2.1. For a distinct node set \mathcal{X} of size $n > r \geq 1$, we let \mathbf{B} be a full column rank matrix such that $\mathbf{B}^{\mathsf{T}}\mathbf{V}_{\leq r-1} = 0$. Then the matrix $(-1)^r\mathbf{B}^{\mathsf{T}}\mathbf{D}_{(2r-1)}\mathbf{B}$ is positive definite.

For instance, if r = 1, we may pick any basis \boldsymbol{B} orthogonal to the constant vector $\boldsymbol{1}$, and the lemma implies that $(-1)\boldsymbol{B}^{\mathsf{T}}\boldsymbol{D}_{(1)}\boldsymbol{B}$ has n-1 positive eigenvalues. We note for future reference that the result generalises almost unchanged to the multivariate case

- **3.** Determinants and elementary symmetric polynomials. In this paper, we will heavily use the elementary symmetric polynomials of eigenvalues, and we collect in this section some useful (more or less known) facts about them.
- 3.1. Eigenvalues, principal minors and elementary symmetric polynomials. The k-th elementary symmetric polynomial of $\lambda_1, \ldots, \lambda_n$ is defined as:

(12)
$$e_k(\lambda_1, \dots, \lambda_n) = \sum_{\substack{|\mathcal{Y}|=k\\\mathcal{Y}\subset\{1,\dots,n\}}} \prod_{i\in\mathcal{Y}} \lambda_i,$$

i.e., the sum is running over all subsets of size k of $\{1, \ldots, n\}$. In particular, $e_1(\lambda_1, \ldots, \lambda_n) = \sum_{i=1}^n \lambda_i$, $e_2(\lambda_1, \ldots, \lambda_n) = \sum_{i < j} \lambda_i \lambda_j$, and $e_n(\lambda_1, \ldots, \lambda_n) = \prod_{i=1}^n \lambda_i$.

Next, we consider the elementary symmetric polynomials applied to eigenvalues of matrices, and define (with some abuse of notation):

$$e_k(\mathbf{A}) \stackrel{\text{def}}{=} e_k(\lambda_1(\mathbf{A}), \dots, \lambda_n(\mathbf{A})).$$

Then the first and the last polynomials are the trace and determinant of ${\bf A}$:

$$e_1(\mathbf{A}) = \operatorname{Tr} \mathbf{A}, \quad e_n(\mathbf{A}) = \det \mathbf{A}.$$

This fact is a special case of a more general result on sums of principal minors.

Theorem 3.1 ([15, Theorem 1.2.12]).

(13)
$$e_k(\mathbf{A}) = \sum_{\substack{\mathcal{Y} \subset \{1, \dots, n\} \\ |\mathcal{Y}| = k}} \det(\mathbf{A}_{\mathcal{Y}, \mathcal{Y}})$$

where $\mathbf{A}_{\mathcal{Y},\mathcal{Y}}$ is a submatrix of \mathbf{A} with rows and columns indexed by \mathcal{Y} , i.e. the sum runs over all principal minors of size $k \times k$.

REMARK 3.2. The scaled symmetric polynomials $(-1)^k e_k(\mathbf{A})$ are the coefficients of the characteristic polynomial $\det(t\mathbf{I} - \mathbf{A})$ at the coefficient t^{n-k} .

We also recall a useful bound on smallest eigenvalues, which is a direct corollary of the Courant-Fischer "min-max" principle.

THEOREM 3.3 ([15, Theorem 4.3.21]). Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be symmetric, and its eigenvalues arranged in non-increasing order $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. If there exist an m-dimensional subspace $\mathcal{L} \subset \mathbb{R}^n$ and a constant c_1 such that

$$\frac{\boldsymbol{u}^{\mathsf{T}} \boldsymbol{A} \boldsymbol{u}}{\boldsymbol{u}^{\mathsf{T}} \boldsymbol{u}} \le c_1,$$

for all $u \in \mathcal{L} \setminus \{0\}$, then the smallest m eigenvalues are bounded as

$$\lambda_n \le \lambda_{n-1} \le \dots \le \lambda_{n-m+1} \le c_1.$$

3.2. Orders of elementary symmetric polynomials. Next, we assume that $\lambda_1(\varepsilon), \ldots, \lambda_n(\varepsilon)$ are functions of some small parameter ε and we are interested in the orders of the corresponding elementary symmetric polynomials

$$e_s(\varepsilon) \stackrel{\text{def}}{=} e_s(\lambda_1(\varepsilon), \dots, \lambda_n(\varepsilon)), \quad 1 \le s \le n,$$

as $\varepsilon \to 0$. The following obvious observation will be important.

Lemma 3.4. Assume that

$$\lambda_1(\varepsilon) = \mathcal{O}(\varepsilon^{L_1}), \ \lambda_2(\varepsilon) = \mathcal{O}(\varepsilon^{L_2}), \ \dots, \ \lambda_n(\varepsilon) = \mathcal{O}(\varepsilon^{L_n}),$$

as $\varepsilon \to 0$ and $0 \le L_1 \le \cdots \le L_n$ are some integers. Then it holds that

$$e_1(\varepsilon) = \mathcal{O}(\varepsilon^{L_1}), \ e_2(\varepsilon) = \mathcal{O}(\varepsilon^{L_1 + L_2}), \ \dots, \ e_n(\varepsilon) = \mathcal{O}(\varepsilon^{L_1 + \dots + L_n}).$$

Proof. The proof follows from the definition of e_s the fact that the product $f(\varepsilon) = \mathcal{O}(\varepsilon^a)$ and $g(\varepsilon) = \mathcal{O}(\varepsilon^b)$ is of the order $f(\varepsilon)g(\varepsilon) = \mathcal{O}(\varepsilon^{a+b})$.

We will need a refinement of Lemma 3.4 concerning the main terms of such functions.

LEMMA 3.5. Suppose that $\lambda_1(\varepsilon), \ldots, \lambda_n(\varepsilon)$ have the form

(14)
$$\lambda_1(\varepsilon) = \varepsilon^{L_1}(\widetilde{\lambda}_1 + \mathcal{O}(\varepsilon)), \dots, \lambda_n(\varepsilon) = \varepsilon^{L_n}(\widetilde{\lambda}_n + \mathcal{O}(\varepsilon)),$$

for some integers $0 \le L_1 \le \cdots \le L_r$. Then

1. The elementary symmetric polynomials have the form

(15)
$$e_{1}(\varepsilon) = \varepsilon^{L_{1}}(\widetilde{e}_{1} + \mathcal{O}(\varepsilon))$$

$$e_{2}(\varepsilon) = \varepsilon^{L_{1} + L_{2}}(\widetilde{e}_{2} + \mathcal{O}(\varepsilon))$$

$$\vdots$$

$$e_{n}(\varepsilon) = \varepsilon^{L_{1} + \dots + L_{n}}(\widetilde{e}_{n} + \mathcal{O}(\varepsilon)).$$

2. If either s = n or $L_s < L_{s+1}$, the main term \tilde{e}_s can be expressed as

$$\widetilde{e}_s = \widetilde{\lambda}_1 \cdots \widetilde{\lambda}_s$$
.

In particular, if s > 1 and $\widetilde{e}_{s-1} \neq 0$, then the main term $\widetilde{\lambda}_s$ can be found as

$$\widetilde{\lambda}_s = \frac{\widetilde{e}_s}{\widetilde{e}_{s-1}}.$$

Proof. 1. By definition, the e.s.p. can be expanded as

$$(16) \qquad e_{s}(\varepsilon) = \sum_{1 \leq t_{1} < \dots < t_{s} \leq n} \prod_{j=1}^{s} \varepsilon^{L_{t_{j}}} (\widetilde{\lambda}_{t_{j}} + \mathcal{O}(\varepsilon))$$

$$= \varepsilon^{L_{1} + \dots + L_{s}} \Big(\sum_{\substack{1 \leq t_{1} < \dots < t_{s} \leq n \\ L_{1} + \dots + L_{s} = L_{t_{1}} + \dots + L_{t_{s}}}} \prod_{j=1}^{s} \widetilde{\lambda}_{t_{j}} + \mathcal{O}(\varepsilon) \Big),$$

which follows from the fact that $L_{t_1} + \cdots + L_{t_s}$ is minimized at $t_j = j$.

2. The case s = n is obvious, because there is only one possible tuple (t_1, \ldots, t_s) . Consider the case $L_s < L_{s+1}$, $1 \le s < n$. If $t_s > s$, then the sum is increased

$$L_1 + \cdots + L_s < L_{t_1} + \cdots + L_{t_s}$$

hence
$$(1, \ldots, s)$$
 is the only possible choice for (t_1, \ldots, t_s) in (16).

We also need a generalization of Lemma 3.5 to the case of a group of equal L_k .

LEMMA 3.6. As in Lemma 3.5, we assume that $\lambda_1(\varepsilon), \ldots, \lambda_n(\varepsilon)$ have the form (14) and the corresponding $e_k(\varepsilon)$ have the form (15), for some $0 \le L_1 \le \cdots \le L_n$, and define $L_0 = -1$, $L_{n+1} = +\infty$, for an easier treatment of border cases.

If for $0 \le m \le n - s$, there is a separated group of m functions

$$\lambda_{s+1}(\varepsilon), \ldots, \lambda_{s+m}(\varepsilon)$$

of repeating degrees, i.e.

$$(17) L_s < L_{s+1} = \dots = L_{s+m} < L_{s+m+1},$$

then the main terms \widetilde{e}_{s+k} , $1 \leq k \leq m$ in (15), are connected with e.s.p. of the main terms $\widetilde{\lambda}_{s+k}$, $1 \leq k \leq m$ as follows:

$$\widetilde{e}_{s+k} = \begin{cases} e_k(\widetilde{\lambda}_{s+1}, \dots, \widetilde{\lambda}_{s+m}), & s = 0, \\ \widetilde{\lambda}_1 \cdots \widetilde{\lambda}_s e_k(\widetilde{\lambda}_{s+1}, \dots, \widetilde{\lambda}_{s+m}) = \widetilde{e}_s e_k(\widetilde{\lambda}_{s+1}, \dots, \widetilde{\lambda}_{s+m}), & s > 0. \end{cases}$$

In particular, if s > 1 and $\tilde{e}_s \neq 0$, the e_k for the main terms of the group are equal to

$$e_k(\widetilde{\lambda}_{s+1},\ldots,\widetilde{\lambda}_{s+m}) = \frac{\widetilde{e}_{s+k}}{\widetilde{e}_s},$$

hence $\widetilde{\lambda}_{s+1}, \ldots, \widetilde{\lambda}_{s+m}$ are the roots of the polynomial (see Remark 3.2)

$$q(\lambda) = \widetilde{e}_s \lambda^m - \widetilde{e}_{s+1} \lambda^{m-1} + \widetilde{e}_{s+2} \lambda^{m-2} + \dots + (-1)^m \widetilde{e}_{s+m}.$$

Proof. When (17) is satisfied, we need to find

$$\widetilde{e}_{s+k} = \sum_{\substack{1 \leq t_1 < \dots < t_{s+k} \leq n \\ L_1 + \dots + L_{s+k} = L_{t_1} + \dots + L_{t_{s+k}}}} \prod_{j=1}^{s+k} \widetilde{\lambda}_{t_j}$$

where, as in the previous case, the minimum sum $L_{t_1} + \cdots + L_{t_{s+k}}$ is achieved by

$$L_1 + \cdots + L_s + L_{s+1} + \cdots + L_{s+k}$$
,

and the sum increases if $t_s > s$ or if $t_{s+k} > s+m$. Therefore, $(t_1, \ldots, t_s) = (1, \ldots, s)$ and the main term becomes

$$\widetilde{e}_{s+k} = \prod_{i=1}^{s} \widetilde{\lambda}_i \left(\sum_{s+1 \le t_{s+1} < \dots < t_{s+k} \le s+m} \prod_{j=1}^{k} \widetilde{\lambda}_{t_{s+j}} \right).$$

Remark 3.7. Assumptions in Lemmas 3.5 to 3.6 can be relaxed (when expansions (14) are valid up to a certain order), but we keep the current statement for simplicity.

3.3. On eigenvalues of parameter-dependent matrices. For determining the orders of eigenvalues, we will need the following simple corollary of Theorem 3.3 about the orders of the eigenvalues.

LEMMA 3.8. Suppose that $K(\varepsilon) \in \mathbb{R}^{n \times n}$, defined in a neighbourhood of 0, is positive semidefinite and its eigenvalues are ordered as

$$\lambda_1(\varepsilon) \ge \lambda_2(\varepsilon) \ge \cdots \ge \lambda_n(\varepsilon) \ge 0.$$

Suppose that there exists a matrix $U \in \mathbb{R}^{n \times m}$, $U^{\mathsf{T}}U = I_m$, such that

(18)
$$\boldsymbol{U}^{\mathsf{T}}\boldsymbol{K}(\varepsilon)\boldsymbol{U} = \mathcal{O}(\varepsilon^{L})$$

in a neighborhood of 0. Then the last m eigenvalues of $K(\varepsilon)$ are of order at most L

$$\lambda_i(\varepsilon) = \mathcal{O}(\varepsilon^L), \text{ for } n - m < j \le n.$$

Proof. Assumption (18) and equivalence of matrix norms implies that

$$\|\boldsymbol{U}^{\mathsf{T}}\boldsymbol{K}(\varepsilon)\boldsymbol{U}\|_{2} \leq C\varepsilon^{L}.$$

for some constant C. Hence, we have that for any $z \in \mathbb{R}^m \setminus \{0\}$,

$$\frac{\boldsymbol{z}^{\mathsf{T}}\boldsymbol{U}^{\mathsf{T}}\boldsymbol{K}(\varepsilon)\boldsymbol{U}\boldsymbol{z}}{\boldsymbol{z}^{\mathsf{T}}\boldsymbol{U}^{\mathsf{T}}\boldsymbol{U}^{\mathsf{T}}\boldsymbol{z}} \leq \|\boldsymbol{U}^{\mathsf{T}}\boldsymbol{K}(\varepsilon)\boldsymbol{U}\|_{2} \leq C\varepsilon^{L}.$$

By choosing the range of U as \mathcal{L} and applying Theorem 3.3, we complete the proof. \square Finally, we recall a classic results on eigenvalues for analytic perturbations.

THEOREM 3.9 ([18, Ch. II, Theorem 1.10]). Let $K(\varepsilon)$ be a real symmetric $n \times n$ matrix depending analytically on ε in the neighborhood of 0. Then all the eigenvalues $\lambda_k(\varepsilon)$, $1 \le k \le n$ can be chosen analytic; moreover, the orthogonal projectors $P_k(\varepsilon)$ on the corresponding rank-one eigenspaces can be also chosen analytic, so that

$$m{K}(arepsilon) = \sum_{k=1}^n \lambda_k(arepsilon) m{P}_k(arepsilon)$$

is the eigenvalue decomposition of $K(\varepsilon)$ in a neighborhood of 0.

3.4. Saddle point matrices and elementary symmetric polynomials. In this subsection, we will be interested in determinants and elementary symmetric polynomials for so-called saddle point matrices [2]. Let $V \in \mathbb{R}^{n \times r}$ be a full column rank matrix. For a matrix $A \in \mathbb{R}^{n \times n}$, we define the *saddle-point matrix* as

$$\begin{bmatrix} \boldsymbol{A} & \boldsymbol{V} \\ \boldsymbol{V}^\mathsf{T} & 0 \end{bmatrix}.$$

Consider a full QR decomposition of $V \in \mathbb{R}^{n \times r}$, i.e.

$$(19) \hspace{1cm} \boldsymbol{V} = \boldsymbol{Q}\boldsymbol{R} = \boldsymbol{Q}_{\mathsf{thin}}\boldsymbol{R}_{\mathsf{thin}}, \quad \boldsymbol{Q} = \begin{bmatrix} \boldsymbol{Q}_{\mathsf{thin}} & \boldsymbol{Q}_{\perp} \end{bmatrix}, \quad \boldsymbol{R} = \begin{bmatrix} \boldsymbol{R}_{\mathsf{thin}} \\ \boldsymbol{0} \end{bmatrix},$$

where $Q \in \mathbb{R}^{n \times n}$, $Q_{\perp} \in \mathbb{R}^{n \times (n-r)}$, $Q^{\mathsf{T}}Q = I$, R_{thin} is upper-triangular, and $Q_{\perp}^{\mathsf{T}}V = 0$.

LEMMA 3.10. For any $\mathbf{A} \in \mathbb{R}^{n \times n}$ and $\mathbf{V} \in \mathbb{R}^{n \times r}$, it holds that

$$\det \begin{bmatrix} \boldsymbol{A} & \boldsymbol{V} \\ \boldsymbol{V}^\mathsf{T} & 0 \end{bmatrix} = (-1)^r \det(\boldsymbol{V}^\mathsf{T} \boldsymbol{V}) \det(\boldsymbol{Q}_\perp^\mathsf{T} \boldsymbol{A} \boldsymbol{Q}_\perp) = (-1)^r (\det \boldsymbol{R}_\mathsf{thin})^2 \det(\boldsymbol{Q}_\perp^\mathsf{T} \boldsymbol{A} \boldsymbol{Q}_\perp),$$

where the matrices R_{thin} and Q_{\perp} are given in the QR decomposition given in (19). The proof of Lemma 3.10 is contained in Appendix A.

We will also also need to evaluate the elementary symmetric polynomials of matrices of the form $Q_{\perp}^{\mathsf{T}} A Q_{\perp}$. For a power series (or a polynomial)

$$a(t) = a_0 + a_1 t + \dots + a_N t^N + \dots,$$

we use the following notation, standard in combinatorics, for its coefficients:

$$[t^r] \{a(t)\} \stackrel{\text{def}}{=} a_r = \frac{1}{r!} \left(\frac{d^r}{dt^r} a(t) \right) \Big|_{t=0}.$$

With this notation, the following lemma on low-rank perturbations of A holds true.

LEMMA 3.11. Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ and $\mathbf{V} \in \mathbb{R}^{n \times r}$, with the QR decomposition of \mathbf{V} given as before by eq. (19). Then

$$[t^r] \{e_k(\boldsymbol{A} + t\boldsymbol{V}\boldsymbol{V}^\mathsf{T})\} = \det(\boldsymbol{V}^\mathsf{T}\boldsymbol{V})e_{k-r}(\boldsymbol{Q}_{\perp}^\mathsf{T}\boldsymbol{A}\boldsymbol{Q}_{\perp}).$$

In particular, if k = n, we get

$$[t^r] \left\{ \det(\boldsymbol{A} + t\boldsymbol{V}\boldsymbol{V}^\mathsf{T}) \right\} = \det(\boldsymbol{V}^\mathsf{T}\boldsymbol{V}) \det(\boldsymbol{Q}_\perp^\mathsf{T}\boldsymbol{A}\boldsymbol{Q}_\perp) = (-1)^r \det \begin{bmatrix} \boldsymbol{A} & \boldsymbol{V} \\ \boldsymbol{V}^\mathsf{T} & 0 \end{bmatrix}$$

The proof of Lemma 3.11 is also contained in Appendix A.

Remark 3.12. Alternative expressions for perturbations of elementary symmetric polynomials are available in [16, Theorem 2.16], and [17, Corollary 3.3], but they do not lead directly to the compact expression in Lemma 3.11 that we need.

4. Results in the 1D case.

4.1. Smooth kernels. We begin this section by generalizing the result of [21, Corollary 2.9] on determinants of scaled kernel matrix K_{ε} in the smooth case.

THEOREM 4.1. Let $K \in \mathcal{C}^{(n,n)}(\Omega \times \Omega)$ be the kernel function. Then for small ε , 1. the determinant of \mathbf{K}_{ε} from (1) has the expansion

$$\det(\boldsymbol{K}_{\varepsilon}) = \varepsilon^{n(n-1)} (\det(\boldsymbol{V}_{\leq n-1})^2 \det \boldsymbol{W}_{n-1,n-1} + \mathcal{O}(\varepsilon)).$$

2. if K_{ε} are positive semidefinite, then eigenvalues have orders

$$\lambda_k(\varepsilon) = \mathcal{O}(\varepsilon^{2(k-1)}).$$

While the proof of 1) is given in [21, Corollary 2.9], and the proof of 2) for the RBF analytic kernels is contained in [34], we provide a short proof of Theorem 4.1 in Subsection 4.3, which also illustrates the main ideas behind other proofs in the paper.

Theorem 4.1, together with Theorem 3.1 allows us to find the main terms of the eigenvalues for analytic-in-parameter K_{ε} .

THEOREM 4.2. Let $K \in \mathcal{C}^{(n,n)}(\Omega)$ be the kernel such that K_{ε} symmetric positive semidefinite and analytic in ε in the neighbourhood of 0. Then for $k \leq n$ it holds that

$$\lambda_k = \varepsilon^{2(k-1)}(\widetilde{\lambda}_k + \mathcal{O}(\varepsilon)),$$

where the main terms satisfy

(20)
$$\widetilde{\lambda}_1 \dots \widetilde{\lambda}_s = \det(\mathbf{V}_{\leq s-1}^\mathsf{T} \mathbf{V}_{\leq s-1}) \det(\mathbf{W}_{s-1,s-1}).$$

Proof. First, due to analyticity and Theorem 4.1, we have that expansions (14) are valid for $L_k = 2(k-1)$. Second, the submatrices of K_{ε} are also kernel matrices (of smaller size), which, in turn can be found from Theorem 4.1. More precisely,

$$e_{s}(\boldsymbol{K}_{\varepsilon}) = \sum_{1 \leq k_{1} < \dots < k_{s} \leq n} \det(\boldsymbol{K}_{\varepsilon}(x_{k_{1}}, \dots, x_{k_{s}}))$$

$$= \varepsilon^{s(s-1)} \det \boldsymbol{W}_{s-1, s-1} \sum_{1 \leq k_{1} < \dots < k_{s} \leq n} (\det \boldsymbol{V}_{\leq s-1}(x_{k_{1}}, \dots, x_{k_{s}}))^{2} + \mathcal{O}(\varepsilon)$$

$$(21) \qquad = \varepsilon^{s(s-1)} \det \boldsymbol{W}_{s-1, s-1} \det(\boldsymbol{V}_{\leq s-1}^{\mathsf{T}} \boldsymbol{V}_{\leq s-1}) + \mathcal{O}(\varepsilon),$$

where the last but one equality follows from Theorem 4.1, and the last equality follows from the Binet-Cauchy formula.

Finally, we employ Lemma 3.5 on relations between the main terms in (14) and (15).

COROLLARY 4.3. If $1 < s \le n$, det $W_{s-2,s-2} \ne 0$ and points in \mathcal{X} distinct, then the main term of the s-th eigenvalue can be obtained as

(22)
$$\widetilde{\lambda}_s = \frac{\det(\mathbf{V}_{\leq s-1}^\mathsf{T} \mathbf{V}_{\leq s-1})}{\det(\mathbf{V}_{\leq s-2}^\mathsf{T} \mathbf{V}_{\leq s-2})} \cdot \frac{\det(\mathbf{W}_{s-1,s-1})}{\det(\mathbf{W}_{s-2,s-2})}.$$

In particular, if det $W_{n-2,n-2} \neq 0$, then all the eigenvalues are given by (22). Moreover, the individual ratios in (22) can be computed in the following way:

$$\frac{\det(\boldsymbol{V}_{\leq s-1}^{\mathsf{T}}\boldsymbol{V}_{\leq s-1})}{\det(\boldsymbol{V}_{\leq s-2}^{\mathsf{T}}\boldsymbol{V}_{\leq s-2})} = ((\boldsymbol{V}_{\leq s-1}^{\mathsf{T}}\boldsymbol{V}_{\leq s-1})^{-1})_{s,s}^{-1} = R_{s,s}^{2},$$

where $R_{s,s}$ is the last ((s,s)-th) diagonal element of the $\mathbf{R}_{\mathsf{thin}} \in \mathbb{R}^{s \times s}$ matrix in the thin QR decomposition of $\mathbf{V}_{< s-1}$. Similarly,

$$\frac{\det(\boldsymbol{W}_{s-1,s-1})}{\det(\boldsymbol{W}_{s-2,s-2})} = ((\boldsymbol{W}_{s-1,s-1})^{-1})_{s,s}^{-1} = C_{s,s}^2,$$

where $C_{s,s}$ is the last diagonal element of the Cholesky factor of $W_{s-1,s-1} = CC^{\mathsf{T}}$.

Proof. The statements follow from Theorem 4.2, Lemma 3.5 and Cramer's rule.□

4.2. Finite smoothness. Next, we provide an analogue of Theorem 4.1 for an RBF kernel with the order of smoothness r, which is smaller or equal to the number of points (i.e., Theorem 4.1 cannot be applied.).

THEOREM 4.4. For an RBF kernel (5) with order of smoothness $r \leq n$,

1. the determinant can be expressed as

$$\det(\mathbf{K}_{\varepsilon}) = \varepsilon^{n(2r-1)-r^2} \left(\widetilde{k} + \mathcal{O}(\varepsilon) \right),\,$$

where the main term is given by

(23)
$$\widetilde{k} = (-1)^r \det \mathbf{W}_{r-1,r-1} \det \begin{bmatrix} f_{2r-1} \mathbf{D}_{(2r-1)} & \mathbf{V}_{\leq r-1} \\ \mathbf{V}_{\leq r-1}^\mathsf{T} & 0 \end{bmatrix},$$

(24)
$$\widetilde{k} = \det \boldsymbol{W}_{r-1,r-1} \det(\boldsymbol{V}_{\leq r-1}^{\mathsf{T}} \boldsymbol{V}_{\leq r-1}) \det(f_{2r-1} \boldsymbol{Q}_{\perp}^{\mathsf{T}} \mathbf{D}_{(2r-1)} \boldsymbol{Q}_{\perp}),$$

where $\mathbf{Q}_{\perp} \in \mathbb{R}^{n \times (n-r)}$ is the semi-orthogonal matrix such that $\mathbf{Q}_{\perp}^{\mathsf{T}} \mathbf{V}_{\leq r-1} = 0$ (e.g., the matrix \mathbf{Q}_{\perp} in the full QR decomposition (19) of $\mathbf{V} = \mathbf{V}_{\leq r-1}$).

2. The eigenvalues have the orders

$$\lambda_s(\varepsilon) = \begin{cases} \mathcal{O}(\varepsilon^{2(s-1)}), & s \le r, \\ \mathcal{O}(\varepsilon^{2r-1}), & s > r. \end{cases}$$

The proof of Theorem 4.4 again is postponed to Subsection 4.4 in order to present a more straightforward corollary on eigenvalues.

As an example, we have for r = 1 (exponential kernel):

(25)
$$\det(\mathbf{K}_{\varepsilon}) = -\varepsilon^{n-1} n K(0,0) \det \begin{bmatrix} \mathbf{D}_{(1)} & \mathbf{1} \\ \mathbf{1}^{\mathsf{T}} & 0 \end{bmatrix},$$

where ${\bf 1}$ denotes a vector with all entries equal to 1.

Combining Lemma 3.6 with Theorem 4.4, we get the following result.

THEOREM 4.5. Let K be the kernel function satisfying the assumptions of Theorem 4.4, and also \mathbf{K}_{ε} be positive semidefinite and analytic in ε . Then it holds that 1. The main terms of first r eigenvalues $\widetilde{\lambda}_1, \ldots, \widetilde{\lambda}_r$ satisfy (20), for $1 \leq s \leq r$. In particular, if $1 < s \leq r$, det $\mathbf{W}_{s-2,s-2} \neq 0$, then $\widetilde{\lambda}_s$ is given by (22).

2. If det $W_{r-1,r-1} \neq 0$ and $V_{\leq r-1}$ is full rank, $\widetilde{\lambda}_{r+1}, \ldots, \widetilde{\lambda}_n$ are the eigenvalues of

$$f_{2r-1}(\boldsymbol{Q}_{\perp}^{\mathsf{T}}\mathbf{D}_{(2r-1)}\boldsymbol{Q}_{\perp}).$$

4.3. Proofs for 1D smooth case. We need the following technical lemma.

Lemma 4.6. For any upper triangular matrix $\mathbf{R} \in \mathbb{R}^{(k+1)\times(k+1)}$ it holds that

$$\boldsymbol{\Delta}^{-1} \boldsymbol{R} \boldsymbol{\Delta} = \operatorname{diag}(\boldsymbol{R}) + \mathcal{O}(\varepsilon),$$

where diag(\mathbf{R}) is the diagonal part of \mathbf{R} and $\mathbf{\Delta} = \mathbf{\Delta}_k(\varepsilon) \in \mathbb{R}^{(k+1)\times(k+1)}$ is defined as

(26)
$$\boldsymbol{\Delta}_{k}(\varepsilon) \stackrel{def}{=} \begin{bmatrix} 1 & & & \\ & \varepsilon & & \\ & & \ddots & \\ & & & \varepsilon^{k} \end{bmatrix}, \quad \operatorname{diag}(\boldsymbol{R}) = \begin{bmatrix} R_{1,1} & & & \\ & \ddots & & \\ & & R_{k+1,k+1} \end{bmatrix}$$

Proof. A direct calculation gives

$$\boldsymbol{\Delta}^{-1} \boldsymbol{R} \boldsymbol{\Delta} = \begin{bmatrix} R_{1,1} & \varepsilon R_{1,2} & \cdots & \varepsilon^k R_{1,k+1} \\ 0 & R_{2,2} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \varepsilon R_{k,k+1} \\ 0 & \cdots & 0 & R_{k+1,k+1} \end{bmatrix}.$$

Proof of Theorem 4.1. We will use a special form of Maclaurin expansion (i.e. the Taylor expansion at 0) for bivariate functions, differentiable with respect to a "rectangular" set of multi-indices. Let us take $x,y\in\Omega$ and apply first the Maclaurin expansion first with respect to x

$$K(x,y) = K(0,y) + x \frac{\partial K}{\partial x}(0,y) + \dots + \frac{x^{n-1}}{(n-1)!} \frac{\partial^k K}{\partial x^k}(0,y) + \frac{x^n}{n!} \frac{\partial^n K}{\partial x^n}(\eta_x,y),$$

where $0 \le \eta_x \le x$. Then the Maclaurin expansion with respect to x yields K(x,y) =

$$K(0,y) = K^{(0,0)} + \dots + \frac{y^{n-1}}{(n-1)!}K^{(0,n-1)} + y^n \frac{\partial^n K}{\partial y^n}(0,\theta_{y,1}) + xK^{(1,0)}(0,y) = xK^{(1,0)} + \dots + x\frac{y^{n-1}}{(n-1)!}K^{(1,n-1)} + \frac{xy^n}{n!} \frac{\partial^{n+1} K}{\partial x \partial y^n}(0,\theta_{y,2}) + \vdots \qquad \vdots \qquad \vdots \qquad \vdots \\ + \frac{x^{n-1}}{(n-1)!}K^{(n-1,0)}(0,y) = \frac{x^{n-1}}{(n-1)!}K^{(n-1,0)} + \dots + \frac{x^{n-1}}{(n-1)!}\frac{y^{n-1}}{(n-1)!}K^{(n-1,n-1)} + \frac{x^{n-1}y^n}{(n-1)!n!}\frac{\partial^{2n-1} K}{\partial x^{n-1}\partial y^n}(0,\theta_{y,n}) + \frac{x^n}{n!}\frac{\partial^n K}{\partial x^n}(\eta_x,y) = \frac{x^n}{n!}\frac{\partial^n K}{\partial x^n}(\eta_x,0) + \dots + \frac{x^ny^{n-1}}{n!(n-1)!}K^{(n,n-1)}(\eta_x,0) + \frac{x^ny^n}{n!n!}\frac{\partial^{2n} K}{\partial x^n\partial y^n}(\eta_x,\xi_{x,y}),$$

where we use a shorthand notation $K^{(i,j)} = K^{(i,j)}(0,0)$, and $0 \le \theta_{y,1}, \dots, \theta_{y,n} \le y$ depend only on y, and $0 \le \xi_{x,y} \le y$.

For $\varepsilon > 0$, $\varepsilon x, \varepsilon y \in \Omega$ and k = n - 1, the Maclaurin expansion can be written as

(27)
$$K(\varepsilon x, \varepsilon y) = [1, \varepsilon x, \dots, (\varepsilon x)^k] \boldsymbol{W} [1, \varepsilon y, \dots, (\varepsilon y)^k]^\mathsf{T} \\ + \varepsilon^{k+1} ([1, \varepsilon x, \dots, (\varepsilon x)^k] \boldsymbol{w}_1(y) + \boldsymbol{w}_2^\mathsf{T}(x) [1, \varepsilon y, \dots, (\varepsilon y)^k]^\mathsf{T}) + \varepsilon^{2(k+1)} w_3(x, y).$$

where \mathbf{w}_1 an \mathbf{w}_2 are bounded (and continuous) $\Omega \to \mathbb{R}^n$ vector functions depending on y and x respectively, and w_3 is a bounded (and continuous) function $\Omega \times \Omega \to \mathbb{R}^n$.

Let for $\varepsilon_0 > 0$, such that $\{\varepsilon_0 x_1, \dots, \varepsilon_0 x_n\} \subset \Omega$. From (27), the scaled kernel matrix admits for $0 < \varepsilon \le \varepsilon_0$ the expansion

(28)
$$K_{\varepsilon} = V \Delta W \Delta V^{\mathsf{T}} + \varepsilon^{k+1} (V \Delta W_{1}(\varepsilon) + W_{2}(\varepsilon) \Delta V^{\mathsf{T}}) + \varepsilon^{2(k+1)} W_{3}(\varepsilon)$$

with $W_1(\varepsilon)$, $W_2(\varepsilon)$, $W_3(\varepsilon) = \mathcal{O}(1)$, $W = W_{k,k}$, $V = V_{\leq k}$, and $\Delta = \Delta_k(\varepsilon)$ is as in (26). Let V = QR be the QR factorization. Then from Lemma 4.6, we have that

$$\Delta^{-1} Q^{\mathsf{T}} V \Delta = \widetilde{R} + \mathcal{O}(\varepsilon), \text{ where } \widetilde{R} = \operatorname{diag}(R).$$

By pre-/post-multiplying (28) by $\Delta^{-1}Q^{\mathsf{T}}$ and its transpose, we get

$$\Delta^{-1} \mathbf{Q}^{\mathsf{T}} \mathbf{K}_{\varepsilon} \mathbf{Q} \Delta^{-1} = (\widetilde{\mathbf{R}} + \mathcal{O}(\varepsilon)) \mathbf{W} (\widetilde{\mathbf{R}}^{\mathsf{T}} + \mathcal{O}(\varepsilon))
+ \varepsilon^{k+1} (\widetilde{\mathbf{R}} + \mathcal{O}(\varepsilon)) \mathbf{W}_{1}(\varepsilon) \mathbf{Q} \Delta^{-1} + \varepsilon^{k+1} \Delta^{-1} \mathbf{Q}^{\mathsf{T}} \mathbf{W}_{2}(\varepsilon) (\widetilde{\mathbf{R}}^{\mathsf{T}} + \mathcal{O}(\varepsilon))
+ (\varepsilon^{k+1} \Delta^{-1}) \mathbf{Q}^{\mathsf{T}} \mathbf{W}_{3}(\varepsilon) \mathbf{Q} (\varepsilon^{k+1} \Delta^{-1})
(29) \qquad = \widetilde{\mathbf{R}} \mathbf{W} \widetilde{\mathbf{R}}^{\mathsf{T}} + \mathcal{O}(\varepsilon).$$

where the last equality follows from $\varepsilon^{k+1} \mathbf{\Delta}^{-1} = \mathcal{O}(\varepsilon)$. Now we are ready to prove the statements of the theorem.

1. From (29) we immediately get

$$\varepsilon^{-n(n-1)} \det \mathbf{K}_{\varepsilon} = (\det \widetilde{\mathbf{R}})^2 \det \mathbf{W} + \mathcal{O}(\varepsilon) = (\det \mathbf{R})^2 \det \mathbf{W} + \mathcal{O}(\varepsilon).$$

2. We can also rewrite (29) as

(30)
$$\mathbf{Q}^{\mathsf{T}} \mathbf{K}_{\varepsilon} \mathbf{Q} = \begin{bmatrix} \mathcal{O}(1) & \mathcal{O}(\varepsilon) & \cdots & \mathcal{O}(\varepsilon^{k+1}) \\ \mathcal{O}(\varepsilon) & \mathcal{O}(\varepsilon^{2}) & \cdots & \mathcal{O}(\varepsilon^{k+2}) \\ \vdots & \vdots & & \vdots \\ \mathcal{O}(\varepsilon^{k+1}) & \mathcal{O}(\varepsilon^{k+2}) & \cdots & \mathcal{O}(\varepsilon^{2(k+1)}) \end{bmatrix},$$

whose lower right submatrices (in Matlab-like notation) have orders

$$(\boldsymbol{Q}_{:,s:n})^{\mathsf{T}} \boldsymbol{K}_{\varepsilon} \boldsymbol{Q}_{:,s:n} = \mathcal{O}(\varepsilon^{2s}),$$

which by Lemma 3.8 implies the required orders of the eigenvalues.

4.4. Proofs for the 1D finite smoothness case.

Proof of Theorem 4.4. First, we will rewrite the expansion (7) in a convenient form. We will group the elements in (10) to get

$$K_{\varepsilon} = V_{\leq 2r-2} \Delta_{2r-2}(\varepsilon) W_{\triangleright} \Delta_{2r-2}(\varepsilon) V_{\leq 2r-2}^{\mathsf{T}} + \varepsilon^{2r-1} (f_{2r-1} D_{(2r-1)} + \mathcal{O}(\varepsilon)),$$

where $W_{\blacktriangleright} \in \mathbb{R}^{(2r-1)\times(2r-1)}$ is the antitriangular matrix defined as

(31)
$$W_{\triangleright} = W_{/0} + W_{/2} + \ldots + W_{/2(r-2)},$$

where W_{s} are defined in (11). For example, in case when r=2

$$W_{\blacktriangleright} = \begin{bmatrix} f_0 & 0 & f_1 \\ 0 & -2f_1 & 0 \\ f_1 & 0 & 0 \end{bmatrix}.$$

Next, we note that W_{\triangleright} can be split as

$$oldsymbol{W}_lackbox{igspace} = egin{bmatrix} W_{r-1,r-1} & \widetilde{W}_1 \ \widetilde{W}_2 \end{bmatrix},$$

where $W_{r-1,r-1}$ is exactly the Wronskian matrix defined in (3). Therefore, since the matrices $V_{\leq 2r-2}$ and $\Delta_{2r-2}(\varepsilon)$ can be partitioned as

we get

$$\begin{aligned} & \boldsymbol{V}_{\leq 2r-2} \boldsymbol{\Delta}_{2r-2}(\varepsilon) \widetilde{\boldsymbol{W}} \boldsymbol{\Delta}_{2r-2}(\varepsilon) \boldsymbol{V}_{\leq 2r-2}^{\mathsf{T}} = \boldsymbol{V}_{\leq r-1} \boldsymbol{\Delta}_{r-1}(\varepsilon) \boldsymbol{W}_{r-1,r-1} \boldsymbol{\Delta}_{r-1}(\varepsilon) \boldsymbol{V}_{\leq r-1}^{\mathsf{T}} \\ & + \varepsilon^{r} \boldsymbol{V}_{\leq r-1} \boldsymbol{\Delta}_{r-1}(\varepsilon) \underbrace{\widetilde{\boldsymbol{W}}_{1} \boldsymbol{\Delta}_{r-2}(\varepsilon) \boldsymbol{V}_{rest}^{\mathsf{T}}}_{\boldsymbol{W}_{1}(\varepsilon)} + \varepsilon^{r} \underbrace{\boldsymbol{V}_{rest} \boldsymbol{\Delta}_{r-2}(\varepsilon) \widetilde{\boldsymbol{W}}_{2}}_{\boldsymbol{W}_{2}(\varepsilon)} \boldsymbol{\Delta}_{r-1}(\varepsilon) \boldsymbol{V}_{\leq r-1}^{\mathsf{T}}, \end{aligned}$$

³In the sum (31), $W_{/2\ell}$ are padded by zeros to $(2r-1) \times (2r-1)$ matrices.

which, after denoting $W = W_{r-1,r-1}$, $V = V_{< r-1}$, $\Delta = \Delta_{r-1}(\varepsilon)$, gives

$$\boldsymbol{K}_{\varepsilon} = \boldsymbol{V} \boldsymbol{\Delta} \boldsymbol{W} \boldsymbol{\Delta} \boldsymbol{V}^{\mathsf{T}} + \varepsilon^{r} (\boldsymbol{V} \boldsymbol{\Delta} \boldsymbol{W}_{1}(\varepsilon) + \boldsymbol{W}_{2}(\varepsilon) \boldsymbol{\Delta} \boldsymbol{V}^{\mathsf{T}}) + \varepsilon^{2r-1} (f_{2r-1} \boldsymbol{D}_{(2r-1)} + \mathcal{O}(\varepsilon)),$$

Next, we take the QR decomposition V (19) and consider a diagonal scaling matrix

$$\widetilde{\boldsymbol{\Delta}} = \begin{bmatrix} \boldsymbol{\Delta} & & \\ & \varepsilon^{r-1} \boldsymbol{I}_{n-r} \end{bmatrix} \in \mathbb{R}^{n \times n}.$$

After pre-/post-multiplying K_{ε} by $\widetilde{\Delta}^{-1}Q^{\mathsf{T}}$ and its transpose, we get

$$(32) \qquad \widetilde{\boldsymbol{\Delta}}^{-1}\boldsymbol{Q}^{\mathsf{T}}\boldsymbol{K}_{\varepsilon}\boldsymbol{Q}\widetilde{\boldsymbol{\Delta}}^{-1} = \begin{bmatrix} \boldsymbol{\Delta}^{-1}\boldsymbol{Q}_{\mathsf{thin}}^{\mathsf{T}}\boldsymbol{K}_{\varepsilon}\boldsymbol{Q}_{\mathsf{thin}}\boldsymbol{\Delta}^{-1} & \varepsilon^{1-r}\boldsymbol{\Delta}^{-1}\boldsymbol{Q}_{\mathsf{thin}}^{\mathsf{T}}\boldsymbol{K}_{\varepsilon}\boldsymbol{Q}_{\perp} \\ \varepsilon^{1-r}\boldsymbol{Q}_{\perp}^{\mathsf{T}}\boldsymbol{K}_{\varepsilon}\boldsymbol{Q}_{\mathsf{thin}}\boldsymbol{\Delta}^{-1} & \varepsilon^{2-2r}\boldsymbol{Q}_{\perp}^{\mathsf{T}}\boldsymbol{K}_{\varepsilon}\boldsymbol{Q}_{\perp} \end{bmatrix},$$

where $Q = \begin{bmatrix} Q_{\text{thin}} & Q_{\perp} \end{bmatrix}$ as in (19). For the upper-left block we get, by Lemma 4.6

$$\Delta^{-1}Q_{\mathsf{thin}}^{\mathsf{T}}K_{\varepsilon}Q_{\mathsf{thin}}\Delta^{-1} = \mathrm{diag}(R_{\mathsf{thin}})W\,\mathrm{diag}(R_{\mathsf{thin}}) + \mathcal{O}(\varepsilon).$$

The lower-left block (which is a transpose of the upper-right one) becomes

$$\varepsilon^{1-r}\boldsymbol{Q}_{\perp}^{\mathsf{T}}\boldsymbol{K}_{\varepsilon}\boldsymbol{Q}_{\mathsf{thin}}\boldsymbol{\Delta}^{-1} = \varepsilon(\boldsymbol{Q}_{\perp}^{\mathsf{T}}(\boldsymbol{W}_{2}(\varepsilon)\operatorname{diag}(\boldsymbol{R}_{\mathsf{thin}}) + \varepsilon^{r-1}f_{2r-1}\boldsymbol{D}_{(2r-1)}\boldsymbol{Q}_{\mathsf{thin}}\boldsymbol{\Delta}^{-1}) + \mathcal{O}(\varepsilon)).$$

Finally, the lower right block is

$$\varepsilon^{2-2r} \boldsymbol{Q}_{\perp}^{\mathsf{T}} \boldsymbol{K}_{\varepsilon} \boldsymbol{Q}_{\perp} = \varepsilon (f_{2r-1} \boldsymbol{Q}_{\perp}^{\mathsf{T}} \boldsymbol{D}_{(2r-1)} \boldsymbol{Q}_{\perp} + \mathcal{O}(\epsilon)).$$

1. Combining the blocks in (32) gives

$$\begin{split} & \varepsilon^{-r(r-1)-2(n-r)(r-1)} \det \boldsymbol{K}_{\varepsilon} = \det(\widetilde{\boldsymbol{\Delta}}^{-1}\boldsymbol{Q}^{\mathsf{T}}\boldsymbol{K}_{\varepsilon}\boldsymbol{Q}\widetilde{\boldsymbol{\Delta}}^{-1}) = \\ & = \varepsilon^{n-r} ((\det \boldsymbol{R}_{\mathsf{thin}})^2 \det \boldsymbol{W} \det(f_{2r-1}\boldsymbol{Q}_{\perp}^{\mathsf{T}}\boldsymbol{D}_{(2r-1)}\boldsymbol{Q}_{\perp}) + \mathcal{O}(\varepsilon)), \\ & = (-1)^r \varepsilon^{n-r} \left(\det \boldsymbol{W} \det \begin{bmatrix} f_{2r-1}\mathbf{D}_{(2r-1)} & \boldsymbol{V}_{\leq r-1} \\ \boldsymbol{V}_{\leq r-1}^{\mathsf{T}} & 0 \end{bmatrix} + \mathcal{O}(\varepsilon) \right), \end{split}$$

where the last equality follows by Lemma 3.10

2. From (32) it follows that

(33)
$$\mathbf{Q}^{\mathsf{T}} \mathbf{K}_{\varepsilon} \mathbf{Q} = \begin{bmatrix} \mathcal{O}(1) & \cdots & \mathcal{O}(\varepsilon^{r-1}) & \mathcal{O}(\varepsilon^{r}) & \cdots & \mathcal{O}(\varepsilon^{r}) \\ \vdots & & \vdots & & \vdots & & \vdots \\ \mathcal{O}(\varepsilon^{r-1}) & \cdots & \mathcal{O}(\varepsilon^{2(r-1)}) & \mathcal{O}(\varepsilon^{2r-1}) & \cdots & \mathcal{O}(\varepsilon^{2r-1}) \\ \mathcal{O}(\varepsilon^{r}) & \cdots & \mathcal{O}(\varepsilon^{2r-1}) & \mathcal{O}(\varepsilon^{2r-1}) & \cdots & \mathcal{O}(\varepsilon^{2r-1}) \\ \vdots & & \vdots & & \vdots & & \vdots \\ \mathcal{O}(\varepsilon^{r}) & \cdots & \mathcal{O}(\varepsilon^{2r-1}) & \mathcal{O}(\varepsilon^{2r-1}) & \cdots & \mathcal{O}(\varepsilon^{2r-1}) \end{bmatrix},$$

thus Lemma 3.8 implies the orders of the eigenvalues, as in the proof of Theorem $4.1.\square$

Proof of Theorem 4.5. 1. Note that $K \in \mathcal{C}^{(r,r)}$, hence for $s \leq r$ we can proceed as in Theorem 4.2, taking into account the fact that the orders of the eigenvalues are given by Theorem 4.4. Therefore, (20) holds true for $1 \leq s \leq n$.

2. Now let us consider the case s > r. In this case, we have

$$\varepsilon^{-n(2r-1)+r^{2}} e_{s}(\boldsymbol{K}_{\varepsilon}) = \varepsilon^{-n(2r-1)+r^{2}} \sum_{\substack{\mathcal{Y} \subset \{1,\dots,n\}\\ |\mathcal{Y}| = s}} \det(\boldsymbol{K}_{\varepsilon,\mathcal{Y}})$$

$$= \det \boldsymbol{W}_{r-1,r-1} \sum_{|\mathcal{Y}| = s} \det(f_{2r-1} \boldsymbol{Q}_{\perp,\mathcal{Y}}^{\mathsf{T}} \boldsymbol{D}_{(2r-1),\mathcal{Y}} \boldsymbol{Q}_{\perp,\mathcal{Y}}) \det(\boldsymbol{V}_{\leq r-1,\mathcal{Y}}^{\mathsf{T}} \boldsymbol{V}_{\leq r-1,\mathcal{Y}}) + \mathcal{O}(\varepsilon)$$

$$= \det \boldsymbol{W}_{r-1,r-1} \sum_{|\mathcal{Y}| = s} [t^{r}] \left\{ \det(f_{2r-1} \boldsymbol{D}_{(2r-1),\mathcal{Y}} + t \boldsymbol{V}_{\leq r-1,\mathcal{Y}} \boldsymbol{V}_{\leq r-1,\mathcal{Y}}^{\mathsf{T}}) \right\} + \mathcal{O}(\varepsilon)$$

$$= \det \boldsymbol{W}_{r-1,r-1} [t^{r}] \left\{ e_{s}(f_{2r-1} \boldsymbol{D}_{(2r-1)} + t \boldsymbol{V}_{\leq r-1} \boldsymbol{V}_{\leq r-1}^{\mathsf{T}}) \right\} + \mathcal{O}(\varepsilon)$$

$$= \det \boldsymbol{W}_{r-1,r-1} \det(\boldsymbol{V}_{\leq r-1}^{\mathsf{T}} \boldsymbol{V}_{\leq r-1}) e_{s-r}(f_{2r-1} \boldsymbol{Q}_{\perp}^{\mathsf{T}} \boldsymbol{D}_{(2r-1)} \boldsymbol{Q}_{\perp}) + \mathcal{O}(\varepsilon),$$

where the individual steps follow from Theorem 4.4 and Lemma 3.11. Therefore, by Lemma 3.6 we get that for all $1 \le s \le n-r$

$$\widetilde{e}_s(\widetilde{\lambda}_{r+1},\ldots,\widetilde{\lambda}_n) = e_s(f_{2r-1}\boldsymbol{Q}_{\perp}^{\mathsf{T}}\mathbf{D}_{(2r-1)}\boldsymbol{Q}_{\perp}),$$

which together with Remark 3.2 completes the proof.

- 5. Multidimensional case: preliminary facts and notations. The multidimensional case requires introducing heavier notation, which we review in this section.
 - **5.1.** Multi-indices and sets. For a multi-index $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{Z}_+^d$, denote

$$\alpha! \stackrel{\text{def}}{=} \alpha_1! \cdots \alpha_d!, \qquad |\alpha| \stackrel{\text{def}}{=} \sum_{k=1}^d \alpha_k,$$

where 0! = 1 by convention. For example, |(2,1,3)| = 6 and (2,1,3)! = 12. We will frequently use the following notations

$$\mathbb{P}_k \stackrel{\text{def}}{=} \{ \boldsymbol{\alpha} \in \mathbb{Z}_+^d : |\boldsymbol{\alpha}| \leq k \}, \qquad \mathbb{H}_k \stackrel{\text{def}}{=} \{ \boldsymbol{\alpha} \in \mathbb{Z}_+^d : |\boldsymbol{\alpha}| = k \} = \mathbb{P}_k \setminus \mathbb{P}_{k-1}.$$

The cardinalities of these sets are given by the following well-known formulae:

$$\#\mathbb{P}_k = \binom{k+d}{d}, \qquad \#\mathbb{H}_k = \binom{k+d-1}{d-1} = \#\mathbb{P}_k - \#\mathbb{P}_{k-1},$$

and will be used throughout this paper.

EXAMPLE 1. For d=1, we have $\mathbb{H}_k = \{k\}$ and $\mathbb{P}_k = \{0,1,\ldots,k\}$. For d=2, an example is shown in Figure 7.



Fig. 7. Sets of multiindices, d = 2. Black dots: \mathbb{P}_2 , grey dots: \mathbb{H}_3 .

An important class of multi-index sets is the lower sets. An $\mathcal{A} \subset \mathbb{Z}_+^d$ is called a lower set [13] if for any $\alpha \in \mathcal{A}$ all "lower" multi-indices are also in the set, i.e.,

$$\alpha \in \mathcal{A}, \ \beta \leq \alpha \ \Rightarrow \ \beta \in \mathcal{A},$$

where
$$(\beta_1, \ldots, \beta_d) \leq (\alpha_1, \ldots, \alpha_d) \iff \beta_1 \leq \alpha_1, \ldots, \beta_d \leq \alpha_d$$
.

Note that all \mathbb{P}_k are lower sets.

5.2. Monomials and orderings. For a vector of variables $\mathbf{x} = \begin{bmatrix} x_1 & \cdots & x_d \end{bmatrix}^\mathsf{T}$, the monomial \mathbf{x}^{α} defined as

$$\boldsymbol{x}^{\boldsymbol{\alpha}} \stackrel{\text{def}}{=} x_1^{\alpha_1} \cdots x_d^{\alpha_d}.$$

REMARK 5.1. Note that $|\alpha|$ is the total degree of monomial x^{α} . The sets of multi-indices \mathbb{P}_k and \mathbb{H}_k therefore correspond to correspond to the sets of monomials of degree $\leq k$ and = k respectively.

$$\{z^{\alpha}: |\alpha| \le k\}, \qquad \{z^{\alpha}: |\alpha| = k\}.$$

In what follows, we assume that an ordering of multi-indices, i.e., all the elements in \mathbb{Z}_+ are linearly ordered, i.e. the relation \prec is defined for all pairs of multi-indices. For example, an ordering for d=2 is given by

$$(34)$$
 $(0,0) \prec (1,0) \prec (0,1) \prec (2,0) \prec (1,1) \prec (0,2) \prec (3,0) \prec (2,1) \prec (1,2) \prec \dots$

In this paper, the ordering will not be important, as the results will not depend on the ordering. The only requirement is that the order is graded [6, Ch.2 §2], i.e.,

$$|\alpha| < |\beta| \quad \Rightarrow \quad \alpha \prec \beta.$$

Remark 5.2. For convenience, in case $d \geq 2$, we can use an ordering satisfying

$$(1,0\ldots,0) \prec (0,1\ldots,0) \prec \cdots \prec (0,0,\ldots,1),$$

such that

$$oldsymbol{V}_1 = egin{bmatrix} oldsymbol{x}_1 & \dots & oldsymbol{x}_n \end{bmatrix}^\mathsf{T}.$$

This is not the case for graded lexicographic or reverse lexicographic [6, Ch.2 §2] orderings. Instead, a graded reflected lexicographic order [1] can be used (see (34)).

5.3. Multivariate Vandermonde matrices. Next, for an ordered set of points $\mathcal{X} = \{x_1, \dots, x_n\} \subset \mathbb{R}^d$ and set of multi-indices $\mathcal{A} = \{\alpha_1, \dots, \alpha_m\} \subset \mathbb{Z}_+^d$ ordered according to the chosen ordering, we define the multivariate Vandermonde matrix

$$oldsymbol{V}_{\mathcal{A}} = oldsymbol{V}_{\mathcal{A}}(\mathcal{X}) = [(oldsymbol{x}_i)^{oldsymbol{lpha}_j}]_{\substack{1 \leq i \leq n \ 1 \leq j \leq m}}.$$

We will introduce a special notation $V_{\leq k} \stackrel{\text{def}}{=} V_{\mathbb{P}_k}$ and $V_k \stackrel{\text{def}}{=} V_{\mathbb{H}_k}$. Since the ordering is graded, the matrix $V_{\leq k}$ can be split into blocks V_k arranged by increasing degree:

$$(35) V_{\leq k} = \begin{bmatrix} V_0 & V_1 & \cdots & V_k \end{bmatrix}.$$

It is easy to see that in the case d = 1 the definition coincides with the previous definition of the Vandermonde matrix (8).

An example of the Vandermonde matrix for d=2

$$\mathcal{X} = \{ \left[\begin{smallmatrix} y_1 \\ z_1 \end{smallmatrix} \right], \left[\begin{smallmatrix} y_2 \\ z_2 \end{smallmatrix} \right], \left[\begin{smallmatrix} y_3 \\ z_3 \end{smallmatrix} \right] \},$$

with the ordering as in (34) is given below

$$\mathbf{V}_{\leq 2} = \begin{bmatrix} 1 & y_1 & z_1 & y_1^2 & y_1 z_1 & z_1^2 \\ 1 & y_2 & z_2 & y_2^2 & y_2 z_2 & z_2^2 \\ 1 & y_3 & z_3 & y_3^2 & y_3 z_3 & z_3^2 \end{bmatrix}.$$

A special case is when the Vandermonde matrix is square, i.e., the number of monomials of degree $\leq k$ is equal to the number of points:

(36)
$$n = \binom{k+d}{k} = \#\mathbb{P}_k,$$

For example, n = k + 1 if d = 1 and $n = \frac{(k+2)(k+1)}{2}$ if d = 2.

Remark 5.3. Unlike the 1D case, even if all the points are different, the Vandermonde matrix $\mathbf{V}_{\leq k}$ is not necessarily invertible. For example, take the set of points on one of the axes

$$\mathcal{X} = \{ \begin{bmatrix} -1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \end{bmatrix} \},$$

for which the Vandermonde matrix is rank-deficient:

$$V_{\leq 1} = \begin{bmatrix} 1 & -1 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{bmatrix}.$$

This effect is well-known in approximation theory [13]. If the square Vandermonde matrix is nonsingular, then the set of points \mathcal{X} is called unisolvent. It is known [25, Prop. 4] that a general configuration of points (e.g., \mathcal{X} are drawn from an absolutely continuous probability distribution w.r.t. the Lebesgue measure), is unisolvent almost surely.

5.4. Kernels and smoothness classes. For a function $f: X \to \mathbb{R}$, $X \in \mathbb{R}^d$ and a multi-index $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_d) \in \mathbb{Z}_+^d$ we use a shorthand notation for its partial derivatives (if they exist):

$$f^{(\alpha)}(\boldsymbol{x}) = \frac{\partial f^{|\alpha|}}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}}(\boldsymbol{x})$$

It makes sense to define the smoothness classes with respect to lower sets. For a lower set $\mathcal{A} \subset \mathbb{Z}_+^d$ we define the class of functions $X \to \mathbb{R}$ which have on X all continuous derivatives $f^{(\alpha)}$, $\alpha \in \mathcal{A}$. This class is denoted by $\mathcal{C}^{\mathcal{A}}(X)$.

We will consider kernel functions $K: \Omega \times \Omega \to \mathbb{R}$ in the class $\mathcal{C}^{k,k}(\Omega) \stackrel{\text{def}}{=} \mathcal{C}^{\mathbb{P}_k \times \mathbb{P}_k}(\Omega)$, i.e., which has all partial derivatives up to order k for \boldsymbol{x} and \boldsymbol{y} separately.

Next, assume that we are given a kernel $K \in \mathcal{C}^{\mathcal{A} \times \mathcal{B}}(\Omega)$ for lower sets \mathcal{A} and \mathcal{B} . We will define the Wronskian matrix for this function as

(37)
$$W_{\mathcal{A},\mathcal{B}} = \left[\frac{K^{(\alpha,\beta)}(\mathbf{0},\mathbf{0})}{\alpha!\beta!} \right]_{\alpha\in\mathcal{A},\beta\in\mathcal{B}},$$

where the rows and columns are indexed by multi-indices in \mathcal{A} and \mathcal{B} , according to the chosen ordering.

As a special case, we will denote $W_{k,k} = W_{\mathbb{P}_k,\mathbb{P}_k}$. For example, for d = 2 and k = 2 (Example in Figure 7), and ordering (34) we have $W_{2,2} =$

$$\begin{bmatrix} K^{((0,0),(0,0))} & K^{((0,0),(1,0))} & K^{((0,0),(0,1))} & \frac{K^{((0,0),(2,0))}}{2} & K^{((0,0),(1,1))} & \frac{K^{((0,0),(0,2))}}{2} \\ K^{((1,0),(0,0))} & K^{((1,0),(1,0))} & K^{((1,0),(0,1))} & \frac{K^{((1,0),(2,0))}}{2} & K^{((1,0),(1,1))} & \frac{K^{((1,0),(0,2))}}{2} \\ K^{((0,1),(0,0))} & K^{((0,1),(1,0))} & K^{((0,1),(0,1))} & \frac{K^{((0,1),(0,1))}}{2} & K^{((0,1),(1,1))} & \frac{K^{((0,1),(0,2))}}{2} \\ \frac{K^{((2,0),(0,0))}}{2} & \frac{K^{((2,0),(1,0))}}{2} & \frac{K^{((2,0),(0,1))}}{2} & \frac{K^{((2,0),(2,0))}}{2} & K^{((2,0),(1,1))} & \frac{K^{((2,0),(0,2))}}{2} \\ K^{((1,1),(0,0))} & K^{((1,1),(1,0))} & K^{((1,1),(0,1))} & \frac{K^{((1,1),(2,0))}}{2} & K^{((1,1),(1,1))} & \frac{K^{((1,1),(0,2))}}{2} \\ \frac{K^{((0,2),(0,0))}}{2} & \frac{K^{((0,2),(1,0))}}{2} & \frac{K^{((0,2),(0,1))}}{2} & \frac{K^{((0,2),(1,1))}}{2} & \frac{K^{((0,2),(1,1))}}{2} & \frac{K^{((0,2),(0,2))}}{4} \end{bmatrix}$$

where we omit the arguments of $K^{(\alpha,\beta)}$. We will also need block-antidiagonal matrices $\mathbf{W}_{/s} \in \mathbb{R}^{\#\mathbb{P}_s \times \mathbb{P}_s}$ defined as follows

(38)
$$\mathbf{W}_{/s} = \begin{bmatrix} & \mathbf{W}_{\mathbb{H}_0, \mathbb{H}_s} \\ & \ddots & \\ \mathbf{W}_{\mathbb{H}_s, \mathbb{H}_0} & & \end{bmatrix},$$

where $W_{\mathcal{A},\mathcal{B}}$ are blocks of the Wronskian matrix defined in (37). For example

$$\boldsymbol{W}_{/0} = \begin{bmatrix} W_{0,0} \end{bmatrix}, \quad \boldsymbol{W}_{/1} = \begin{bmatrix} & \boldsymbol{W}_{\mathbb{H}_0,\mathbb{H}_1} \\ \boldsymbol{W}_{\mathbb{H}_1,\mathbb{H}_0} & \end{bmatrix},$$

and in general $W_{/s}$ contains the main block antidiagonal of $W_{s,s}$.

5.5. Taylor expansions. The standard Taylor expansion in the multivariate case is as follows [36, §8.4.4]. Let $f \in \mathcal{C}^{k+1}(\Omega)$, where Ω is a neigbourhood of the point $\boldsymbol{x} \in \mathbb{R}^d$ and $\boldsymbol{h} \in \mathbb{R}^d$ such that

$$[\boldsymbol{x}, \boldsymbol{h}] \stackrel{\text{def}}{=} [x_1, x_1 + h_1] \times \cdots \times [x_d, x_d + h_d] \in \Omega.$$

Without abuse of notation we say that [x, x - h] = [x - h, h].

Then the following Taylor expansion with remainder in Lagrange form holds:

(39)
$$f(\boldsymbol{x} + \boldsymbol{h}) = \sum_{\boldsymbol{\alpha} \in \mathbb{P}_k} \frac{\boldsymbol{h}^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!} f^{(\boldsymbol{\alpha})}(\boldsymbol{x}) + \sum_{\boldsymbol{\beta} \in \mathbb{H}_{k+1}} \frac{\boldsymbol{h}^{\boldsymbol{\beta}}}{\boldsymbol{\beta}!} f^{(\boldsymbol{\beta})}(\boldsymbol{x} + \boldsymbol{\theta}\boldsymbol{h}),$$

for some $\theta \in [0,1]$. Note that for d=1 we retrieve the classic Taylor expansion. A more general Taylor expansion has remainder in the Peano form, and requires smoothness of order one less, i.e., if $f \in \mathcal{C}^k(\Omega)$, we have:

(40)
$$f(\boldsymbol{x} + \boldsymbol{h}) = \sum_{\boldsymbol{\alpha} \in \mathbb{P}_k} \frac{\boldsymbol{h}^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!} f^{(\boldsymbol{\alpha})}(\boldsymbol{x}) + o(\|\boldsymbol{h}\|_2^k).$$

We will also need a bivariate version. For a "bivariate" (the arguments are split into two groups) function $f: \Omega \times \Omega \to \mathbb{R}$ such that $f \in \mathcal{C}^{\mathbb{P}_{k_1+1} \times \mathbb{P}_{k_2+1}}(\Omega \times \Omega)$, where Ω is an open neighborhood of $(\mathbf{0}, \mathbf{0})$. Again, for simplicity we consider the Maclaurin expansion. Now take (x, y) such that $[\mathbf{0}, x] \times [\mathbf{0}, y] \subset \Omega$.

Then we can apply the same steps as in the proof of Theorem 4.1 and get

$$\begin{split} f(\boldsymbol{x}, \boldsymbol{y}) &= \sum_{\boldsymbol{\alpha} \in \mathbb{P}_{k_1}, \boldsymbol{\beta} \in \mathbb{P}_{k_2}} \frac{\boldsymbol{x}^{\boldsymbol{\alpha}} \boldsymbol{y}^{\boldsymbol{\beta}}}{\boldsymbol{\alpha}! \boldsymbol{\beta}!} f^{(\boldsymbol{\alpha}, \boldsymbol{\beta})}(\boldsymbol{0}, \boldsymbol{0}) + \sum_{\boldsymbol{\alpha} \in \mathbb{P}_{k_1}, \boldsymbol{\beta} \in \mathbb{H}_{k_2 + 1}} \frac{\boldsymbol{x}^{\boldsymbol{\alpha}} \boldsymbol{y}^{\boldsymbol{\beta}}}{\boldsymbol{\alpha}! \boldsymbol{\beta}!} f^{(\boldsymbol{\alpha}, \boldsymbol{\beta})}(\boldsymbol{0}, \boldsymbol{\theta}_{\boldsymbol{y}} \boldsymbol{y}) \\ &+ \sum_{\boldsymbol{\alpha} \in \mathbb{H}_{k_1 + 1}, \boldsymbol{\beta} \in \mathbb{P}_{k_2}} \frac{\boldsymbol{x}^{\boldsymbol{\alpha}} \boldsymbol{y}^{\boldsymbol{\beta}}}{\boldsymbol{\alpha}! \boldsymbol{\beta}!} f^{(\boldsymbol{\alpha}, \boldsymbol{\beta})}(\boldsymbol{\theta}_{\boldsymbol{x}, \boldsymbol{\beta}} \boldsymbol{x}, \boldsymbol{0}) + \sum_{\boldsymbol{\alpha} \in \mathbb{H}_{k_1 + 1}, \boldsymbol{\beta} \in \mathbb{H}_{k_2 + 1}} \frac{\boldsymbol{x}^{\boldsymbol{\alpha}} \boldsymbol{y}^{\boldsymbol{\beta}}}{\boldsymbol{\alpha}! \boldsymbol{\beta}!} f^{(\boldsymbol{\alpha}, \boldsymbol{\beta})}(\boldsymbol{\xi}_{\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\beta}}, \boldsymbol{\theta}_{\boldsymbol{y}} \boldsymbol{y}), \end{split}$$

where $\{\eta_{x,\beta}\}_{\beta\in\mathbb{P}_{k_2}}\subset[0,1]$ depend on $\boldsymbol{x},\theta_{\boldsymbol{y}}\in[0,1]$ depend on $\boldsymbol{y},$ and $\{\xi_{x,y,\beta}\}_{\beta\in\mathbb{H}_{k_2+1}}\subset[0,1]$ depends on both \boldsymbol{x} and \boldsymbol{y} .

5.6. Distance matrices and RBF expansions. Next, we consider the RBF kernel $K(\boldsymbol{x}, \boldsymbol{y}) = f(\|\boldsymbol{x} - \boldsymbol{y}\|_2)$ with order of smoothness r. In this case, the expansion (7) is still valid, but the distance matrices are now defined as:

$$\mathbf{D}_{(k)} = \left[\left\| oldsymbol{x}_i - oldsymbol{x}_j
ight\|_2^k
ight]_{i,j}.$$

For even k, as in the univariate case, we will need an expansion in the form similar to (10). In the univariate case we obtained the formula via a binomial expansion (9), an approach which does not work in the multivariate case. We need to derive this expansion directly from Taylor's formula. Let $K \in \mathcal{C}^{2r-2}$ (not necessarily an RBF). Then the Taylor expansion in Peano's form (40) yields an expansion in ε

$$K(\boldsymbol{x},\boldsymbol{y}) = \sum_{k=0}^{2r-2} \varepsilon^k \sum_{\substack{\boldsymbol{\alpha},\boldsymbol{\beta} \in \mathbb{P}_k \\ |\boldsymbol{\alpha}| + |\boldsymbol{\beta}| = k}} \frac{\boldsymbol{x}^{\boldsymbol{\alpha}} \boldsymbol{y}^{\boldsymbol{\beta}}}{\boldsymbol{\alpha}! \boldsymbol{\beta}!} K^{(\boldsymbol{\alpha},\boldsymbol{\beta})}(\boldsymbol{0},\boldsymbol{0}) + o(\varepsilon^{2r-2}).$$

which in matrix form can be written as

(41)
$$\mathbf{K}_{\varepsilon} = \sum_{k=0}^{2r-2} \varepsilon^{k} \mathbf{V}_{\leq k} \mathbf{W}_{k} \mathbf{V}_{\leq k}^{\mathsf{T}} + o(\varepsilon^{2r-2}).$$

For an RBF kernel, the two expansions (41) and (7) coincide, therefore the distance matrices of even order $D_{(2\ell)}$ have a compact expression as:

$$f_{2\ell} \boldsymbol{D}_{(2\ell)} = \boldsymbol{V}_{\leq 2\ell} \boldsymbol{W}_{\geq 2\ell} \boldsymbol{V}_{\leq 2\ell}^{\mathsf{T}},$$

and moreover the expansion of K_{ε} given in (10) is also valid in the multivariate case.

REMARK 5.4. For k odd, the matrices $\mathbf{D}_{(k)}$ in the multivariate case also have the conditional positive-definiteness property (as in Lemma 2.1), except that the number of points should be $n > \#\mathbb{P}_{r-1}$.

6. Results in the multivariate case.

6.1. Determinants in the smooth case. For a degree k, we will introduce a notation for the sum of all total degrees of monomials in \mathcal{P}_k

$$M=M(k,d)\stackrel{\mathrm{def}}{=} \sum_{\boldsymbol{\alpha}\in\mathbb{P}_k} |\boldsymbol{\alpha}|, \quad \text{such that } \prod_{\boldsymbol{\alpha}\in\mathbb{P}_k} \varepsilon^{|\boldsymbol{\alpha}|}=\varepsilon^{M(k,d)},$$

which is given by 4

$$M(k,d) = d\binom{k+d}{d+1}.$$

Theorem 6.1. Assume that the kernel is in $C^{(k+1,k+1)}$ and also

$$\#\mathbb{P}_{k-1} < n \le \#\mathbb{P}_k$$
.

1. If $n = \#\mathbb{P}_k$, then

$$\det \mathbf{K}_{\varepsilon} = \varepsilon^{2M} (\det \mathbf{W}_{k,k} (\det (\mathbf{V}_{\leq k}))^2 + \mathcal{O}(\varepsilon)).$$

2. If $n < \#\mathbb{P}_k$, for $\ell = \#\mathbb{P}_k - n$, we have

$$\det \boldsymbol{K}_{\varepsilon} = \varepsilon^{2(M-k\ell)} (\det(\boldsymbol{Y}\boldsymbol{W}_{k,k}\boldsymbol{Y}^{\mathsf{T}}) \det(\boldsymbol{V}_{\leq k-1}^{\mathsf{T}}\boldsymbol{V}_{\leq k-1}) + \mathcal{O}(\varepsilon)),$$

where $\mathbf{Y} \in \mathbb{R}^{n \times \#\mathbb{P}_k}$ is defined as

$$oldsymbol{Y} = egin{bmatrix} oldsymbol{I}_{\#\mathbb{P}_{k-1}} & & \ oldsymbol{Q}_{oldsymbol{\perp}}^{\intercal} oldsymbol{V}_k \end{bmatrix},$$

 $^{^4 \}mathrm{See}$ [22, eq. (3.19)–(3.20)], where M(k,d) is given in a slightly different form.

 V_k is the Vandermonde matrix (35) for monomials of degree k, and $Q_{\perp} \in \mathbb{R}^{n \times \ell}$ comes from the full QR decomposition of $V = V_{\leq k-1}$ (see (19)).

3. If, in addition, K_{ε} is positive semidefinite, the eigenvalues split in k+1 groups

(42)
$$\underbrace{\widetilde{\lambda}_{0,0}}_{\mathcal{O}(1)}, \underbrace{\{\widetilde{\lambda}_{1,j}\}_{j=1}^{d}}_{\mathcal{O}(\varepsilon^{2})}, \dots, \underbrace{\{\widetilde{\lambda}_{s,j}\}_{j=1}^{\#\mathbb{H}_{s}}}_{\mathcal{O}(\varepsilon^{2s})}, \dots, \underbrace{\{\widetilde{\lambda}_{k,j}\}_{j=1}^{\#\mathbb{H}_{k}-\ell}}_{\mathcal{O}(\varepsilon^{2k})}.$$

The proof of Theorem 6.1 is postponed to Subsection 6.3.

From Theorem 6.1, we can also get a result on eigenvalues.

THEOREM 6.2. Let $K \in \mathcal{C}^{(k+1,k+1)}(\Omega)$ be the kernel function, such that K_{ε} is symmetric positive semidefinite and analytic in ε in a neighbourhood of 0. Then we the eigenvalues in the groups have the form

$$\lambda_{s,j} = \varepsilon^{2s} (\widetilde{\lambda}_{s,j} + \mathcal{O}(\varepsilon)),$$

where $\widetilde{\lambda}_{0,0} = nK^{(0,0)}$ and other main terms are given as follows. 1. For $1 \leq s < k$, if $\det \mathbf{W}_{s-1,s-1} \neq 0$ and $\mathbf{V}_{\leq s-1}$ is full rank, then

(43)
$$\widetilde{\lambda}_{s,1} \cdots \widetilde{\lambda}_{s,\#\mathbb{H}_s} = \frac{\det(\boldsymbol{V}_{\leq s}^{\mathsf{T}} \boldsymbol{V}_{\leq s}) \det(\boldsymbol{W}_{s,s})}{\det(\boldsymbol{V}_{\leq s-1}^{\mathsf{T}} \boldsymbol{V}_{\leq s-1}) \det(\boldsymbol{W}_{s-1,s-1})}.$$

2. Consider the partition of the ${m Q}$ matrix in the full QR factorization of ${m V}_{\le k-1}$

$$(44) Q = \begin{bmatrix} Q_0 & Q_1 & \dots & Q_k \end{bmatrix}$$

with $Q_s \in \mathbb{R}^{n \times \#\mathbb{H}_s}$, $0 \le s < k$, and $Q_k \in \mathbb{R}^{n \times (\#\mathbb{H}_k - \ell)}$.

Then for any $1 \leq s \leq k$, if $\det \mathbf{W}_{s-1,s-1} \neq 0$ and $\mathbf{V}_{\leq s-1}$ is full rank, the main terms $\widetilde{\lambda}_{s,1},\ldots,\widetilde{\lambda}_{s,\#\mathbb{H}_s}$ (or $\widetilde{\lambda}_{k,1},\ldots,\widetilde{\lambda}_{k,\#\mathbb{H}_k-\ell}$ if s=k) are the eigenvalues of

(45)
$$\boldsymbol{Q}_{s}^{\mathsf{T}}\boldsymbol{V}_{s}(\boldsymbol{W}_{\lrcorner}-\boldsymbol{W}_{\llcorner}\boldsymbol{W}_{s-1,s-1}^{-1}\boldsymbol{W}_{\urcorner})\boldsymbol{V}_{s}^{\mathsf{T}}\boldsymbol{Q}_{s},$$

where

$$\boldsymbol{W}_{s,s} = \begin{bmatrix} \boldsymbol{W}_{s-1,s-1} & \boldsymbol{W}_{\urcorner} \\ \boldsymbol{W}_{ \sqcup} & \boldsymbol{W}_{ \sqcup} \end{bmatrix} = \begin{bmatrix} \boldsymbol{W}_{s-1,s-1} & \boldsymbol{W}_{ \urcorner,s} \\ \boldsymbol{W}_{ \sqcup,s} & \boldsymbol{W}_{ \sqcup,s} \end{bmatrix},$$

is the partition of the Wronskian.

The proof of Theorem 6.2 is postponed to Subsection 6.4.

6.2. Finite smoothness case. We prove an analogue of Theorem 4.4 for RBF kernels (which is a generalization of Theorem 4.4).

THEOREM 6.3. For small ε and an RBF kernel (5) with order of smoothness r: 1. the determinant of \mathbf{K}_{ε} in the case $n = \#\mathbb{P}_{r-1} + N$ given in (1) has the expansion

$$\det(\boldsymbol{K}_{\varepsilon}) = \varepsilon^{2M(r\text{-}1,d) + (2r\text{-}1)N} \left(\widetilde{k} + \mathcal{O}(\varepsilon) \right),$$

where \widetilde{k} has exactly the same expression as in (23) or (24) (with $V_{\leq r}$ and $D_{(2r-1)}$ replaced with their multivariate counterparts).

2. In the positive semidefinite case, the eigenvalues are split into r+1 groups

$$\underbrace{\widetilde{\lambda}_{0,0}}_{\mathcal{O}(1)}, \underbrace{\{\widetilde{\lambda}_{1,j}\}_{j=1}^d}_{\mathcal{O}(\varepsilon^2)}, \dots, \underbrace{\{\widetilde{\lambda}_{r-1,j}\}_{j=1}^{\#\mathbb{H}_r - 1}}_{\mathcal{O}(\varepsilon^{2(r-1)})}, \dots, \underbrace{\{\widetilde{\lambda}_{k,j}\}_{j=1}^N}_{\mathcal{O}(\varepsilon^{2r-1})}.$$

3. In the analytic in ε case, the main terms for the first r groups are the same as in Theorem 6.2. For the last group, if $\det \mathbf{W}_{r-1,r-1} \neq 0$ and $\mathbf{V}_{\leq r-1}$ is full rank, the main terms are the eigenvalues of

$$f_{2r-1}(\boldsymbol{Q}_{\perp}^{\mathsf{T}}\mathbf{D}_{(2r-1)}\boldsymbol{Q}_{\perp}).$$

where Q_{\perp} comes from the full QR factorization (19) of $V_{\leq r-1}$.

The proof of Theorem 6.3, is postponed to Subsection 6.4.

6.3. Determinants in the smooth case. Before proving Theorem 6.1, we again need a technical lemma, which is an analogue of (4.6).

Lemma 6.4. Let R be an upper-block-triangular matrix

$$oldsymbol{R} = egin{bmatrix} oldsymbol{R}_{1,1} & oldsymbol{R}_{1,k} & \cdots & oldsymbol{R}_{1,k+1} \ 0 & \ddots & & dots \ dots & \ddots & \ddots & oldsymbol{R}_{k,k+1} \ 0 & \cdots & 0 & oldsymbol{R}_{k+1,k+1} \end{bmatrix},$$

where the blocks $\mathbf{R}_{i,j} \in \mathbb{R}^{M_i \times N_j}$ are not necessarily square. Then it holds that

$$\begin{bmatrix} I_{M_1} & & & & & \\ & \varepsilon^{\text{-}1}I_{M_2} & & & & \\ & & \ddots & & & \\ & & & \varepsilon^{\text{-}k}I_{M_{k+1}} \end{bmatrix} \boldsymbol{R} \begin{bmatrix} I_{N_1} & & & & \\ & \varepsilon I_{N_2} & & & \\ & & \ddots & & \\ & & & \varepsilon^k I_{N_{k+1}} \end{bmatrix} = \text{blkdiag}(\boldsymbol{R}) + \mathcal{O}(\varepsilon),$$

where $diag(\mathbf{R})$ is just the block-diagonal part of \mathbf{R} :

$$ext{blkdiag}(oldsymbol{R}) = egin{bmatrix} oldsymbol{R}_{1,1} & & & & & & \\ & \ddots & & & & & \\ & & oldsymbol{R}_{k+1,k+1} \end{bmatrix}$$

Proof. The proof is analogous to that of Lemma 4.6

Proof of Theorem 6.1. First, we fix a degree-compatible ordering of multi-indices

$$\mathbb{P}_k = \{ \boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_{\#\mathbb{P}_k} \},$$

and denote the $\#\mathbb{P}_k \times \#\mathbb{P}_k$ matrix (note that $\#\mathbb{P}_k = n + \ell$)

(46)
$$\Delta = \Delta_k(\varepsilon) \stackrel{\text{def}}{=} \begin{bmatrix} \varepsilon^{|\alpha_1|} & & & \\ & \ddots & & \\ & & \varepsilon^{|\alpha_{\#\mathbb{P}_k}|} \end{bmatrix} = \begin{bmatrix} 1 & & & & \\ & \varepsilon I_{\#\mathbb{H}_1} & & & \\ & & \ddots & & \\ & & & \varepsilon^k I_{\#\mathbb{H}_k} \end{bmatrix},$$

and by D_n the principal $n \times n$ submatrix of Δ . Note that their determinants are

(47)
$$\det(\mathbf{\Delta}) = \varepsilon^{M(k,d)} \text{ and } \det(\mathbf{D}_n) = \varepsilon^{M(k,d)-\ell k}.$$

From the bi-multivariate Taylor expansion we get:

$$K(\varepsilon \boldsymbol{x}, \varepsilon \boldsymbol{y}) = [(\varepsilon \boldsymbol{x})^{\alpha_1}, \dots, (\varepsilon \boldsymbol{x})^{\alpha_{n+\ell}}] \boldsymbol{W}[(\varepsilon \boldsymbol{y})^{\alpha_1}, \dots, (\varepsilon \boldsymbol{y})^{\alpha_{n+\ell}}]^{\mathsf{T}}$$

$$(48) + \varepsilon^{k+1} [(\varepsilon \boldsymbol{x})^{\alpha_1}, \dots, (\varepsilon \boldsymbol{x})^{\alpha_{n+\ell}}] \boldsymbol{w}_1(\boldsymbol{y}, \varepsilon) + \varepsilon^{k+1} \boldsymbol{w}_2(\boldsymbol{y}, \varepsilon)^{\mathsf{T}} [(\varepsilon \boldsymbol{y})^{\alpha_1}, \dots, (\varepsilon \boldsymbol{y})^{\alpha_{n+\ell}}]^{\mathsf{T}}$$

$$+ \varepsilon^{2(k+1)} \boldsymbol{w}_3(\boldsymbol{x}, \boldsymbol{y}, \varepsilon),$$

where w_1 an w_2 are bounded (and continuous) $\Omega \to \mathbb{R}^n$ vector functions depending on y and x respectively, and w_3 is a bounded (and continuous) function $\Omega \times \Omega \to \mathbb{R}^{k+1}$.

Let for $\varepsilon_0 > 0$, such that $\{\varepsilon_0 \boldsymbol{x}_1, \dots, \varepsilon_0 \boldsymbol{x}_n\} \in \Omega$ for all i. From (48), the scaled kernel matrix admits for $0 < \varepsilon \le \varepsilon_0$ the expansion

(49)
$$K_{\varepsilon} = V_{\leq k} \Delta W \Delta V_{\leq k}^{\mathsf{T}} + \varepsilon^{n} (V_{\leq k} \Delta W_{1}(\varepsilon) + W_{2}(\varepsilon) \Delta V_{\leq k}^{\mathsf{T}}) + \varepsilon^{2n} W_{3}(\varepsilon),$$

where $W_1(\varepsilon)$, $W_2(\varepsilon)$, $W_3(\varepsilon) = \mathcal{O}(1)$, $W = W_{k,k}$, $V = V_{\leq k}$.

Next, we take the full QR decomposition of $V = V_{\leq k-1}$, V = QR partitioned as in (19), so that $R_{\mathsf{thin}} \in \mathbb{R}^{\#\mathbb{P}_{k-1} \times \#\mathbb{P}_{k-1}}$ and $Q_{\perp} \in \mathbb{R}^{n \times (n-\#\mathbb{P}_{k-1})}$. We note that

$$oldsymbol{Q}^\mathsf{T} oldsymbol{V}_{\leq k} = egin{bmatrix} oldsymbol{R}_\mathsf{thin} & oldsymbol{Q}_\mathsf{thin}^\mathsf{T} oldsymbol{V}_k \ oldsymbol{O} & oldsymbol{Q}_\perp^\mathsf{T} oldsymbol{V}_k \end{bmatrix},$$

and by Lemma 6.4 we have

$$\boldsymbol{D}_n^{-1}\boldsymbol{Q}^\mathsf{T}\boldsymbol{V}_{\leq k}\boldsymbol{\Delta} = \underbrace{\begin{bmatrix} \mathrm{blkdiag}\,\boldsymbol{R}_\mathsf{thin} & \\ & \boldsymbol{Q}_\perp^\mathsf{T}\boldsymbol{V}_k \end{bmatrix}}_{\widetilde{\boldsymbol{\mathcal{B}}}} + \mathcal{O}(\varepsilon).$$

Next, we pre/post multiply (49) by $D_n^{-1}Q^{\mathsf{T}}$ and its transpose, we get (as in (29)),

(50)
$$D_n^{-1} Q^{\mathsf{T}} K_{\varepsilon} Q \Delta_n^{-1} = \widetilde{R} W \widetilde{R}^{\mathsf{T}} + \mathcal{O}(\varepsilon).$$

Finally, we prove the statements of the theorem.

1. From (47) we have that

$$\varepsilon^{-2(M(k,d)-\ell k)} \det \mathbf{K}_{\varepsilon} = \det(\widetilde{\mathbf{R}} \mathbf{W} \widetilde{\mathbf{R}}^{\mathsf{T}}).$$

Thus, if $n = \#\mathbb{P}_k$, then we have

$$\det(\widetilde{\boldsymbol{R}}\boldsymbol{W}\widetilde{\boldsymbol{R}}^\mathsf{T}) = (\det(\widetilde{\boldsymbol{R}}))^2 \det(\boldsymbol{W}) = (\det(\boldsymbol{V}_{\leq k})^2 \det(\boldsymbol{W}),$$

where the last equality follows from the fact that

$$\det(\widetilde{\boldsymbol{R}}) = \det(\operatorname{blkdiag} \boldsymbol{R}_{\mathsf{thin}}) \det(\boldsymbol{Q}_{\perp}^{\mathsf{T}} \boldsymbol{V}_k) = \det(\boldsymbol{Q}^{\mathsf{T}} \boldsymbol{V}_{< k}) = \det(\boldsymbol{V}_{< k}),$$

because $Q^{\mathsf{T}}V_{\leq k}$ is block-triangular.

2. For $n < \#\mathbb{P}_k$, we note that

hence

$$\det(\widetilde{\boldsymbol{R}}\boldsymbol{W}\widetilde{\boldsymbol{R}}^\mathsf{T}) = (\det(\boldsymbol{R}_\mathsf{thin}))^2 \det(\boldsymbol{Y}\boldsymbol{W}\boldsymbol{Y}^\mathsf{T}) = \det(\boldsymbol{V}_{\leq k\text{-}1}^\mathsf{T}\boldsymbol{V}_{\leq k\text{-}1}) \det(\boldsymbol{Y}\boldsymbol{W}\boldsymbol{Y}^\mathsf{T}).$$

3. Finally, as in the proof of Theorem 4.1, (50) implies that the matrix $\mathbf{Q}^{\mathsf{T}} \mathbf{K}_{\varepsilon} \mathbf{Q}$ has the form similar to (30), but where the orders are block-wise; this, together with Theorem 3.3 completes the proof.

6.4. Individual eigenvalues and finite smoothness.

Proof of Theorem 6.2. Choose a subset \mathcal{Y} of \mathcal{X} of size m, $\#\mathbb{P}_{s-1} < m \leq \#\mathbb{P}_s$, $s \leq k$. Then we have that

$$\boldsymbol{K}_{\varepsilon,\mathcal{Y}} = \varepsilon^{2(M-s(\#\mathbb{P}_s-m))}(\det(\boldsymbol{Y}\boldsymbol{W}_{s,s}\boldsymbol{Y}^\mathsf{T})\det(\boldsymbol{V}_{\leq s-1,\mathcal{Y}}^\mathsf{T}\boldsymbol{V}_{\leq s-1,\mathcal{Y}}) + \mathcal{O}(\varepsilon)),$$

and

$$oldsymbol{Y} = egin{bmatrix} oldsymbol{I}_{\#\mathbb{P}_{s-1}} & \ R_{s,\mathcal{Y}} \end{bmatrix},$$

where $\mathbf{R}_{s,\mathcal{Y}} = \mathbf{Q}_{2,\mathcal{Y}}^{\mathsf{T}} \mathbf{V}_s$. In particular

$$\begin{split} \det(\boldsymbol{Y}\boldsymbol{W}_{s,s}\boldsymbol{Y}^\mathsf{T}) &= \det \begin{bmatrix} \boldsymbol{W}_{s-1,s-1} & \boldsymbol{W}^\mathsf{T}\boldsymbol{R}_{s,\mathcal{Y}}^\mathsf{T} \\ \boldsymbol{R}_{s,\mathcal{Y}}\boldsymbol{W}_\mathsf{L} & \boldsymbol{R}_{s,\mathcal{Y}}\boldsymbol{W}_\mathsf{L}\boldsymbol{R}_{s,\mathcal{Y}}^\mathsf{T} \end{bmatrix} \\ &= \det \boldsymbol{W}_{s-1,s-1}\det(\boldsymbol{R}_{s,\mathcal{Y}}\boldsymbol{W}_\mathsf{L}\boldsymbol{R}_{s,\mathcal{Y}}^\mathsf{T} - \boldsymbol{R}_{s,\mathcal{Y}}\boldsymbol{W}_\mathsf{L}\boldsymbol{W}_{s-1,s-1}^{-1}\boldsymbol{W}^\mathsf{T}\boldsymbol{R}_{s,\mathcal{Y}}^\mathsf{T}) \\ &= \det \boldsymbol{W}_{s-1,s-1}\det(\boldsymbol{Q}_{\mathsf{L},\mathcal{Y}}(\boldsymbol{V}_s(\boldsymbol{W}_\mathsf{L} - \boldsymbol{W}_\mathsf{L}\boldsymbol{W}_{s-1,s-1}^{-1}\boldsymbol{W}^\mathsf{T})\boldsymbol{V}_s^\mathsf{T})\boldsymbol{Q}_{\mathsf{L},\mathcal{Y}}^\mathsf{T}) \end{split}$$

hence by Lemma 3.10

and therefore

$$\begin{aligned} &\det(\boldsymbol{Y}\boldsymbol{W}_{s,s}\boldsymbol{Y}^\mathsf{T})\det(\boldsymbol{V}_{\leq s-1,\mathcal{Y}}^\mathsf{T}\boldsymbol{V}_{\leq s-1,\mathcal{Y}}) \\ &= \det \boldsymbol{W}_{s-1,s-1}[\gamma^{\#\mathbb{P}_{s-1}}] \left\{ \det(\boldsymbol{V}_{s,\mathcal{Y}}(\boldsymbol{W}_{\lrcorner} - \boldsymbol{W}_{\llcorner}\boldsymbol{W}_{s-1,s-1}^{-1}\boldsymbol{W}_{\urcorner})\boldsymbol{V}_{s,\mathcal{Y}}^\mathsf{T} + \gamma \boldsymbol{V}_{\leq s-1,\mathcal{Y}}\boldsymbol{V}_{\leq s-1,\mathcal{Y}}^\mathsf{T}) \right\} \blacksquare \end{aligned}$$

$$\begin{split} \widetilde{e}_{m} &= \det \boldsymbol{W}_{s-1,s-1}[\gamma^{\#\mathbb{P}_{s-1}}] \left\{ e_{m}(\boldsymbol{V}_{s}(\boldsymbol{W}_{J} - \boldsymbol{W}_{L}\boldsymbol{W}_{s-1,s-1}^{-1}\boldsymbol{W}_{\neg})\boldsymbol{V}_{s}^{\mathsf{T}} + \gamma \boldsymbol{V}_{\leq s-1}\boldsymbol{V}_{\leq s-1}^{\mathsf{T}}) \right\} \\ &= \det \boldsymbol{W}_{s-1,s-1} \det(\boldsymbol{V}_{\leq s-1}^{\mathsf{T}}\boldsymbol{V}_{\leq s-1}) e_{m-\#\mathbb{P}_{s-1}}(\boldsymbol{Q}_{s:k}^{\mathsf{T}}\boldsymbol{V}_{s}(\boldsymbol{W}_{J} - \boldsymbol{W}_{L}\boldsymbol{W}_{s-1,s-1}^{-1}\boldsymbol{W}_{\neg})\boldsymbol{V}_{s}^{\mathsf{T}}\boldsymbol{Q}_{s:k}) \\ &= \det \boldsymbol{W}_{s-1,s-1} \det(\boldsymbol{V}_{\leq s-1}^{\mathsf{T}}\boldsymbol{V}_{\leq s-1}) e_{m-\#\mathbb{P}_{s-1}}(\boldsymbol{Q}_{s}^{\mathsf{T}}\boldsymbol{V}_{s}(\boldsymbol{W}_{J} - \boldsymbol{W}_{L}\boldsymbol{W}_{s-1,s-1}^{-1}\boldsymbol{W}_{\neg})\boldsymbol{V}_{s}^{\mathsf{T}}\boldsymbol{Q}_{s}), \end{split}$$

where $Q_{s:k} = [Q_s \cdots Q_k]$, the last but one equality follows from Lemma 3.10, and the last equality follows from the fact that only the top block of $Q_{s:k}^{\mathsf{T}} V_s$ is nonzero.

Proof of Theorem 6.3. 1. The proof repeats that of Theorem 4.4 with the following minor modifications (in order to take into account the multivariate case):

• the matrix $W_{\triangleright} \in \mathbb{R}^{\#\mathbb{P}_{2r-2} \times \#\mathbb{P}_{2r-2}}$ is defined as

$$W_{\blacktriangleright,\alpha,\beta} = \begin{cases} \frac{K^{(\alpha,\beta)}(0,0)}{\alpha!\beta!}, & |\alpha| + |\beta| \le 2r, \\ 0, & |\alpha| + |\beta| > 2r; \end{cases}$$

i.e., in the sum (31) the matrices $W_{/s}$ are defined according to (38).

- the matrix $\Delta_k(\varepsilon)$ is defined in (46), and Lemma 6.4 is used instead of Lemma 4.6;
- the extended diagonal scaling matrix is

$$\widetilde{\boldsymbol{\Delta}} = \begin{bmatrix} \boldsymbol{\Delta}_{r-1} & & \\ & \varepsilon^{r-1} \boldsymbol{I}_N \end{bmatrix} \in \mathbb{R}^{n \times n},$$

where $N = n - \#\mathbb{P}_{r-1}$.

• the last displayed formula in the proof of Theorem 4.4 becomes

$$\begin{split} \varepsilon^{-2M(r-1,d)-2N(r-1)} \det \boldsymbol{K}_{\varepsilon} &= \det(\widetilde{\boldsymbol{\Delta}}^{-1}\boldsymbol{Q}^{\mathsf{T}}\boldsymbol{K}_{\varepsilon}\boldsymbol{Q}\widetilde{\boldsymbol{\Delta}}^{-1}) \\ &= \varepsilon^{N}((\det \boldsymbol{R}_{\mathsf{thin}})^{2} \det \boldsymbol{W} \det(f_{2r-1}\boldsymbol{Q}_{\perp}^{\mathsf{T}}\boldsymbol{D}_{(2r-1)}\boldsymbol{Q}_{\perp}) + \mathcal{O}(\varepsilon)), \end{split}$$

- 2. Again, as in the proof of Theorem 4.4, the matrix $Q^{\mathsf{T}}K_{\varepsilon}Q$ has the form (33) (block-wise), hence the order follow from Theorem 3.3.
- 3. The proof of this statement repeats the proof of Theorem 4.5 without changes. \square

7. Perturbation theory: a summary for selfadjoint operators. This section contains a summary of facts from [18, Ch. II] to deal with analytic perturbations.

Formally, and in keeping with the notation used in [18], we assume that we are given an operator-valued function depending on ε such that

(51)
$$T(\varepsilon) = T^{(0)} + \varepsilon T^{(1)} + \varepsilon^2 T^{(2)} + \cdots,$$

where we assume that the matrices $T_k \in \mathbb{C}^{n \times n}$ are self-adjoint. In a neighborhood of $0, 0 \in \mathcal{D}_0 \subset \mathbb{C}$, $T(\varepsilon)$ has $s \leq n$ semi-simple eigenvalues genericaly (i.e., except a finite number of exceptional points). For simplicity of presentation⁵, we assume that s = n, which is the case if there exist $\varepsilon_1 \in \mathcal{D}_0$ having all distinct eigenvalues. The interesting case (considered in this paper) is when $\varepsilon = 0$ is an exceptional point, i.e. $T(0) = T^{(0)}$ has multiple eigenvalues (for example, if it is a low-rank matrix, with a multiple eigenvalue 0).

7.1. Perturbation of eigenvalues and group eigenprojectors. Since all matrices are self-adjoint, by [18, Theorem 1.10, Ch. II] (see Theorem 3.9), the eigenvalues $\lambda_1(\varepsilon), \ldots, \lambda_n(\varepsilon)$ and the rank-one projectors on the corresponding eigenspaces $P_1(\varepsilon), \ldots, P_n(\varepsilon)$ are holomorphic functions of ε in a neighborhood of $0, 0 \in \mathcal{D} \subset \mathbb{C}$.

Remark 7.1. If the matrix $T^{(0)}$ has d multiple eigenvalues $\{\mu_k\}_{k=1}^d$ with multiplicities m_1, \ldots, m_d , i.e., after proper reordering, at $\varepsilon = 0$

$$(\lambda_1(0),\ldots,\lambda_n(0)) = (\underbrace{\mu_1,\ldots,\mu_1}_{m_1 \text{ times}},\underbrace{\mu_2,\ldots,\mu_2}_{m_2 \text{ times}},\ldots,\underbrace{\mu_d,\ldots,\mu_d}_{m_d \text{ times}})$$

then the projectors on the invariant subspaces associated to μ_1, \ldots, μ_s are sums of the corresponding rank-one projectors on the eigenspaces:

$$\begin{aligned} & \boldsymbol{P}_{\mu,1} = \boldsymbol{P}_{1}(0) + \ldots + \boldsymbol{P}_{m_{1}}(0) \\ & \boldsymbol{P}_{\mu,2} = \boldsymbol{P}_{m_{1}+1}(0) + \ldots + \boldsymbol{P}_{m_{1}+m_{2}}(0) \\ & \vdots \\ & \boldsymbol{P}_{\mu,d} = \boldsymbol{P}_{m_{1}+\cdots+m_{d-1}+1}(0) + \ldots + \boldsymbol{P}_{n}(0) \end{aligned}$$

In this paper, our aim is to obtain a limiting eigenstructure at $\varepsilon = 0$. In case of multiple eigenvalues, this information cannot be retrieved from the spectral decomposition of $T^{(0)}$ alone (we can only retrieve the group projectors $P_{\mu,j}$ from the spectral decomposition of $T^{(0)}$). In what follows, we look in details at perturbation expansions in order to find individual $P_k(0)$.

As shown in [18, Ch. II], we can consider perturbations of a possibly multiple eigenvalue. Let λ be an eigenvalue of $T^{(0)}$ of multiplicity m, and P is the corresponding orthogonal projector on the m-dimensional eigenspace. The projector on the perturbed m-dimensional invariant subspace is an analytic matrix-valued function

$$P(\varepsilon) = \sum_{k=0}^{\infty} \varepsilon^k P^{(k)},$$

 $^{^5\}mathrm{We}$ can also consider the general case if needed.

with the coefficients given by

$$m{P}^{(0)} = m{P}, \quad m{P}^{(1)} = -m{P}m{T}^{(1)}m{S} - m{S}m{T}^{(1)}m{P},$$

(52)
$$\boldsymbol{P}^{(k)} = -\sum_{p=1}^{k} (-1)^{p} \sum_{\substack{\nu_{1}+\dots+\nu_{p}=k\\k_{1}+\dots+k_{p+1}=p\\\nu_{j}\geq 1, k_{j}\geq 0}} \boldsymbol{S}^{(k_{1})} \boldsymbol{T}^{(\nu_{1})} \boldsymbol{S}^{(k_{2})} \cdots \boldsymbol{S}^{(k_{p})} \boldsymbol{T}^{(\nu_{p})} \boldsymbol{S}^{(k_{p+1})},$$

where
$$\mathbf{S} = (\mathbf{T} - \lambda \mathbf{I})^{\dagger}$$
, $\mathbf{S}^{(0)} = -\mathbf{P}$ and $\mathbf{S}^{(k)} = \mathbf{S}^{k}$.

7.2. Reduction and splitting the groups. In order to find the individual projectors of the eigenspaces corresponding to a multiple λ , and the expansion of the corresponding eigenvalues, the following reduction (or splitting) procedure [18, Ch. II, §2.3] can be applied, which localises the operator to the m-dimensional subspace corresponding to the perturbations of λ .

We first define the eigennilpotent matrix $D(\varepsilon)$ as

$$\boldsymbol{D}(\varepsilon) = (\boldsymbol{T}(\varepsilon) - \lambda \boldsymbol{I})\boldsymbol{P}(\varepsilon) = \boldsymbol{P}(\varepsilon)(\boldsymbol{T}(\varepsilon) - \lambda \boldsymbol{I}) = \boldsymbol{P}(\varepsilon)(\boldsymbol{T}(\varepsilon) - \lambda \boldsymbol{I})\boldsymbol{P}(\varepsilon),$$

which from [18, Ch. II, §2.2] has an expansion

$$D(\varepsilon) = 0 + \sum_{k=1}^{\infty} \varepsilon^k \widetilde{T}^{(k)},$$

where the expressions for $\widetilde{T}^{(k)}$ are as follows:

$$\widetilde{T}^{(1)} = PT^{(1)}P,$$

$$\widetilde{T}^{(2)} = PT^{(2)}P - PT^{(1)}PT^{(1)}S - PT^{(1)}ST^{(1)}P - ST^{(1)}PT^{(1)}P.$$

$$\vdots$$

(53)
$$\widetilde{\boldsymbol{T}}^{(k)} = -\sum_{p=1}^{k} (-1)^p \sum_{\substack{\nu_1 + \dots + \nu_p = k \\ k_1 + \dots + k_{p+1} = p-1 \\ \nu_j \ge 1, k_j \ge 0}} \boldsymbol{S}^{(k_1)} \boldsymbol{T}^{(\nu_1)} \boldsymbol{S}^{(k_2)} \cdots \boldsymbol{S}^{(k_p)} \boldsymbol{T}^{(\nu_p)} \boldsymbol{S}^{(k_{p+1})}.$$

Remark 7.2. Note that the matrices $\widetilde{T}^{(k)}$ are selfadjoint, which follows from the fact that for real ε the matrices $T(\varepsilon)$ and $P(\varepsilon)$ (and hence $D(\varepsilon)$) are selfadjoint.

Next, we define the matrix $\widetilde{T}(\varepsilon)$ as

$$\widetilde{T}(\varepsilon) = \frac{1}{\varepsilon} D(\varepsilon) = \sum_{k=0}^{\infty} \varepsilon^k \widetilde{T}^{(k+1)},$$

such that $\widetilde{\boldsymbol{T}}(0) = \widetilde{\boldsymbol{T}}^{(1)}$. Note that by Remark 7.2, all the matrices $\widetilde{\boldsymbol{T}}^{(k+1)}$ are self-adjoint and all the eigenvalues of $\widetilde{\boldsymbol{T}}^{(1)}(\varepsilon)$ are holomorphic functions of ε . The idea of the reduction process is to apply the perturbation theory to the matrix $\widetilde{\boldsymbol{T}}^{(1)}(\varepsilon)$.

Let $T^{(1)}$ have s eigenvalues $\lambda_1, \ldots, \lambda_s$ with multiplicities

$$\ell_1 + \ldots + \ell_s = m,$$

where we take into account only the m eigenvalues⁶ in the subspace spanned by $P(\varepsilon)$. Then $\widetilde{\lambda}_1, \ldots, \widetilde{\lambda}_s$ determine the splitting of λ in the following way.

Lemma 7.3 (A summary of [18, Ch. II, §2.3]). Let

$$\underbrace{\widetilde{\lambda}_{1,1}(\varepsilon),\ldots,\widetilde{\lambda}_{1,\ell_1}(\varepsilon)}_{pert.\ of\ \widetilde{\lambda}_1},\ldots,\underbrace{\widetilde{\lambda}_{s,1}(\varepsilon),\ldots,\widetilde{\lambda}_{s,\ell_s}(\varepsilon)}_{pert.\ of\ \widetilde{\lambda}_s},$$

be the holomorphic functions for the perturbations of the eigenvalues $\widetilde{\lambda}_1, \ldots, \widetilde{\lambda}_s$ of $\widetilde{T}(\varepsilon)$. Then the holomorphic functions corresponding to perturbations of the eigenvalue λ of the original operator $T(\varepsilon)$ are given by

$$\{\lambda_1(\varepsilon),\ldots,\lambda_m(\varepsilon)\} = \bigcup_{k=1}^s \{\lambda + \varepsilon \widetilde{\lambda}_{k,1}(\varepsilon),\ldots,\lambda + \varepsilon \widetilde{\lambda}_{k,\ell_k}(\varepsilon)\}.$$

Moreover, the expansions $\widetilde{P}_{k,j}(\varepsilon)$ of the projectors on the eigenspaces of $\widetilde{T}(\varepsilon)$ (corresponding to $\widetilde{\lambda}_{k,j}(\varepsilon)$) give the expansions of the projectors on the eigenspaces of $T(\varepsilon)$ corresponding to $\lambda_1(\varepsilon), \ldots, \lambda_m(\varepsilon)$.

Lemma 7.3 can be applied recursively: for each individual eigenvalue $\widetilde{\lambda}_k$ (of multiplicity $\ell_k > 1$) we can consider the corresponding reduced operator

$$\overset{2}{T}(arepsilon) = rac{1}{arepsilon}\widetilde{m{P}}_{k}(arepsilon)(\widetilde{m{T}}^{(1)}(arepsilon) - m{I})\widetilde{m{P}}_{k}(arepsilon),$$

where $\widetilde{P}_k(\varepsilon)$ is the perturbation of the total projection on the ℓ_k -dimensional eigenspace corresponding to $\widetilde{\lambda}_k$ (which can be computed as in the previous subsection). Depending on the eigenvalues of the main term of the reduced operator, either the splitting will occur again, or there will be no splitting; in any case, after a finite number of steps, all the individual eigenvalues will be split into simple (multiplicity 1) eigenvalues⁷.

The next subsections will give a specialization of the splitting process for the case of the kernel matrices.

8. Results on eigenvectors.

8.1. Summary of results. This section summarizes results on limiting eigenvectors for kernel matrices. We are interested in finding the limiting rank-one projectors from Theorem 3.9 i.e.,

$$P_k = \lim_{\varepsilon \to 0} P_k(\varepsilon) = P_k(0),$$

where the last equality follows from analyticity of $P_k(\varepsilon)$ at 0. In what follows, instead of limiting eigenprojectors P_k we will talk about limiting eigenvectors p_k (i.e., $P_k = p_k p_k^{\mathsf{T}}$), although the latter are defined only up to the change of sign.

In the univariate case, limiting eigenvectors are given by the following theorem.

THEOREM 8.1. Let $K \in \mathbb{C}^{2n}(\Omega \times \Omega)$ be the kernel and \mathcal{X} be the set of distinct points, such that $K_{\varepsilon}(\mathcal{X})$ is analytic in ε and positive semidefinite, and such that the Wronskian matrix $W_{n-2,n-2}$ is nonsingular. Then the limiting eigenvectors as $\varepsilon \to 0$ are the columns of the Q matrix of the QR decomposition of $V_{\leq n-1}$.

⁶Other n-m eigenvalues are 0.

⁷This follows from our assumption that the eigenvalues are simple generically.

Theorem 8.1 is in fact, a special case of the following theorem for the multivariate case (thus the proof of Theorem 8.1 will not be given).

THEOREM 8.2. Let \mathcal{X} be a set of n points, and $K \in \mathbb{C}^{2(k+1)}(\Omega \times \Omega)$, such that k and n are as in Theorem 6.1. Assume that the following conditions are satisfied:

- the Wronskian matrix $W_{k-1,k-1}$ is positive definite;
- the Vandermonde matrix $V_{\leq k-1}$ is nonsingular.

Let Q be the matrix from the full QR decomposition of $V_{\leq k-1}$ partitioned into blocks Q_s as in (44). Then the subspace spanned by the limiting eigenvectors corresponding to the $\mathcal{O}(\varepsilon^{2s})$ group of eigenvalues in (42) is

- is spanned by the columns of Q_s , if s < k or s = k and $n = \#\mathbb{P}_k$;
- is a subspace of the column span of Q_k if s = k and $n < \#\mathbb{P}_k$.

The proof of Theorem 8.2 is postponed to Subsection 8.2. We also formulate the following conjecture, which we validated numerically.

Conjecture 1. For the $\mathcal{O}(\varepsilon^{2s})$ group, the limiting eigenvectors are columns of

$$Q_sU_s$$
,

where U_s contains in its columns a system⁸ of eigenvectors of the matrix from (45)

$$oldsymbol{Q}_s^{\mathsf{T}} oldsymbol{V}_s (oldsymbol{W}_{ extsf{J}} - oldsymbol{W}_{ extsf{W}}^{-1} oldsymbol{W}_{ extsf{S}-1.s-1} oldsymbol{W}_{ extsf{J}}) oldsymbol{V}_s^{\mathsf{T}} oldsymbol{Q}_s.$$

Next, we assume that the kernel is RBF, i.e., $K(x, y) = f(||x - y||_2)$, with order of smoothness r (see (5)). Then the following result on eigenvectors holds.

THEOREM 8.3. Let the RBF kernel be as in (4.5). Then for s < r, the subspace spanned by the limiting eigenvectors corresponding to the $\mathcal{O}(\varepsilon^{2s})$ group of eigenvalues, is as in Theorem 8.2. For the last group of $\mathcal{O}(\varepsilon^{2r-1})$ eigenvalues, the eigenvectors are given by columns of

$$Q_{\perp}U$$

where the columns of U are eigenvectors of $Q_{\perp}^{\mathsf{T}} D_{(2r-1)} Q_{\perp}$, and the matrix Q_{\perp} comes from the full QR factorization (19) of $V_{\leq r-1}$ (as in Theorem 4.5).

We conjecture that in the finite smoothness as well the individual eigenvectors for the $\mathcal{O}(\varepsilon^{2s})$ group can be obtained as in Conjecture 1.

8.2. Proofs for results on eigenvectors.

8.2.1. Block staircase matrices. We first need some facts about block staircase matrices. Let $\mathbf{n} = (n_0, \dots, n_s) \in \mathbb{N}^{s+1}$ such that

$$n = n_0 + \cdots + n_s$$

and consider the following block partition of a matrix $\mathbf{A} \in \mathbb{C}^{m \times m}$

$$oldsymbol{A} = egin{bmatrix} oldsymbol{A}^{(0,0)} & \cdots & oldsymbol{A}^{(0,s)} \ dots & & dots \ oldsymbol{A}^{(s,0)} & \cdots & oldsymbol{A}^{(s,s)} \end{bmatrix}$$

where the blocks are of size $A^{(k,l)} \in \mathbb{C}^{n \times n}$. Assuming that the partition is fixed, we define the classes \mathcal{S}_p of "staircase" matrices

$$\{\mathbf{0}\} = \mathbb{S}_{-1} \subset \mathbb{S}_0 \subset \mathbb{S}_1 \subset \mathbb{S}_2 \subset \cdots \subset \mathbb{S}_{2s-1} = \mathbb{S}_{2s} = \mathbb{S}_{2s+1} = \cdots = \mathbb{C}^{n \times n},$$

⁸There is a usual issue of ambiguous definition of U_s if the matrix has repeating eigenvalues.

such that the matrices in S_p have nonzero blocks only up to the s-th antidiagonal

$$S_p = \{ \boldsymbol{A} \in \mathbb{C}^{m \times n} \mid \boldsymbol{A}^{(k,l)} = 0 \text{ for all } k + l > p \}.$$

In Fig. 8, we illustrate the classes for s = 2:

$$S_0 = \left\{ \begin{array}{|c|c|} \\ \\ \end{array} \right\}, \ S_1 = \left\{ \begin{array}{|c|c|} \\ \\ \end{array} \right\}, \ S_3 = \left\{ \begin{array}{|c|c|} \\ \\ \end{array} \right\}, \ S_4 = \left\{ \begin{array}{|c|c|} \\ \\ \end{array} \right\}.$$

Fig. 8. Classes of staircase matrices. White color stands for zero blocks.

The following obvious property will be useful.

Lemma 8.4. 1. $\mathbf{A} \in \mathbb{S}_p, \mathbf{B} \in \mathbb{S}_q \Rightarrow \mathbf{A}\mathbf{B} \in \mathbb{S}_{p+q}$.

- 2. For any upper triangular \mathbf{R} , it follows that $\mathbf{R}\mathbf{A}\mathbf{R}^{\mathsf{T}} \in \mathbb{S}_{p}$.
- 3. For any $\mathbf{A} \in \mathbb{S}_p$ and block-diagonal matrix $\mathbf{\Lambda}$ it holds that $\mathbf{\Lambda}\mathbf{A}, \mathbf{A}\mathbf{\Lambda} \in \mathbb{S}_p$.

Proof. The proof follows from straighforward verification.

8.2.2. Proof of Theorem 8.2. This theorem concerns the behaviour of eigenvectors in the infinitely smooth case.

Proof. From the ordinary Taylor expansion (40) and the corresponding expansion of the kernel matrix (41), we have that

$$\boldsymbol{K}_{\varepsilon} = \boldsymbol{V}_{0} \boldsymbol{W}_{0,0} \boldsymbol{V}_{0}^{\mathsf{T}} + \varepsilon \boldsymbol{V}_{\leq 1} \boldsymbol{W}_{/1} \boldsymbol{V}_{<1}^{\mathsf{T}} + \dots + \varepsilon^{2k} \boldsymbol{V}_{\leq 2k} \boldsymbol{W}_{/2k} \boldsymbol{V}_{<2k}^{\mathsf{T}} + \mathcal{O}(\varepsilon^{2k+1}),$$

where $W_{/s}$ is defined in (38). Next, we will take $Q \in \mathbb{R}^{n \times n}$, from the full QR decomposition of $V_{\leq 2k}$, and we will consider the transformed matrix

$$\boldsymbol{T}(\varepsilon) = \boldsymbol{Q}^\mathsf{T} \boldsymbol{K}_\varepsilon \boldsymbol{Q} = \boldsymbol{T}_0 + \varepsilon \boldsymbol{T}_1 + \ldots + \varepsilon^{2k} \boldsymbol{T}_{2k} + \mathcal{O}(\varepsilon^{2k+1}), \quad \boldsymbol{T}_s = \boldsymbol{Q}^\mathsf{T} \boldsymbol{V}_{\leq s} \boldsymbol{W}_{\text{\tiny /} s} \boldsymbol{V}_{\leq s}^\mathsf{T} \boldsymbol{Q}$$

Due to the fact that $W_{/s}$ is block antidiagonal, $Q^{\mathsf{T}}V_{\leq s}$ is upper triangular and by Lemma 8.4, we have that T_s is block staircase, i.e. $T_{/s} \in \mathcal{S}_s$.

We will proceed by series of Kato's reductions, according to Lemma 7.3. At each order of ε , a multiple eigenvalue 0 is split into a group of nonzero eigenvalues and the eigenvalue 0 of smaller multiplicity (see an example of the splitting process in (2)).

Formally, we will consider a sequence of reduced operators $\overset{\circ}{T}(\varepsilon) = T(\varepsilon)$

$$\overset{\text{s+1}\sim}{T}(\varepsilon) = \frac{1}{\varepsilon} \boldsymbol{P_s}(\varepsilon) \overset{\text{s}\sim}{T}(\varepsilon),$$

where $P_k(\varepsilon)$ is the projector onto the perturbation of the nullspace of $\overset{\circ}{T}(0)$ (i.e., the invariant subspace associated with the eigenvalue 0). Its power series expansion

$$\overset{\mathrm{s}}{\boldsymbol{T}}(\varepsilon) = \sum_{j=s}^{\infty} \varepsilon^{j-s} \cdot \overset{\mathrm{s}}{\boldsymbol{T}}_{j}$$

can be computed according to (53). For each operator we will be interested only in

the first 2k - s terms, as summarized below,

since we are interested only in the terms

$$oldsymbol{T}_0, \widetilde{oldsymbol{T}}_1, \widetilde{oldsymbol{T}}_2, \ldots, \widetilde{oldsymbol{T}}_{2k}, \ldots, \widetilde{oldsymbol{T}}_{2k},$$

whose eigenvectors give limiting eigenvectors for the original operator $T(\varepsilon)$.

Next, we will look in detail at the form of coefficients of the reduced operators. The projector on the image space of \mathbf{T}_0 is $\mathbf{\Pi}_0 = \mathbf{e}_0 \mathbf{e}_0^\mathsf{T}$ (where $\mathbf{e}_0 = (1, 0, \dots, 0)^\mathsf{T}$), and the projector on the nullspace is

$$P_0 = \begin{bmatrix} 0 & & \\ & I_{n-1} \end{bmatrix},$$

and the matrix $\mathbf{S} = \mathbf{S}_0$ in (52), By examining the terms in (52), we have that the coefficients of the reduced operators preserve the staircase class, i.e. $\widetilde{T}_s \in \mathcal{S}_s$. This can be seen by verifying that if $\mathbf{A}_s \in \mathcal{S}_s$ and $\mathbf{S}^{(j)}$ are diagonal, then the sums

(54)
$$\mathbf{S}^{(k_1)} \mathbf{A}^{(\nu_1)} \mathbf{S}^{(k_2)} \cdots \mathbf{S}^{(k_p)} \mathbf{A}^{(\nu_p)} \mathbf{S}^{(k_{p+1})} \in \mathcal{S}_s.$$

if $\nu_1 + \cdots + \nu_p = s$.

Next, we note that since $T_1 \in S_1$, then we have

$$\widetilde{\boldsymbol{T}}_1 = \boldsymbol{P}_0 \boldsymbol{T}_1 \boldsymbol{P}_0 = 0,$$

hence we have that $P_1 = I$ and $S_1 = 0$, hence the second step of reduction does not change the matrices, i.e. $\widetilde{T}_s = \widetilde{T}_s$. Finally, we note that since $T_2 \in \mathcal{S}_2$, the matrix $\widetilde{T}_2 = \widetilde{T}_2$, hence it contains only one nonzero block of size $d \times d$, i.e.,

$$\widetilde{T}_2 = egin{bmatrix} 0_{1 imes 1} & & & & \\ & *_{d imes d} & & & \end{bmatrix}$$

Therefore, the leading terms of the d eigenvalues in the $\mathcal{O}(\varepsilon^2)$ block are the eigenvalues of \tilde{T}_2 . Since we know that these leading terms are non-zero by Theorem 6.1, the limiting projector Π_2 for this block of eigenvalues and the projector on the eigenspace for the 0 eigenvalue are given by

$$oldsymbol{\Pi}_2 = egin{bmatrix} 0_{1 imes 1} & & & & & \\ & & oldsymbol{I}_d & & & & \\ & & 0_{n-d-1} \end{bmatrix}, \quad oldsymbol{P}_2 = egin{bmatrix} 0_{(d+1) imes (d+1)} & & & & \\ & & oldsymbol{I}_{n-d-1} \end{bmatrix}.$$

Proceeding by induction, at the step of reduction $2s-2 \to 2s-1$ the staircase order of the matrices is preserved due to (54), and block diagonality of P_{2s-1} and T_{2s-2} . Since the reduction step $2s-1 \to 2s$ that does not change anything we get

(55)
$$P_{2s} = \begin{bmatrix} 0_{(\#\mathbb{P}_s) \times (\#\mathbb{P}_s)} & \\ I_{(n-\#\mathbb{P}_s) \times (n-\#\mathbb{P}_s)} \end{bmatrix},$$

such that

(56)
$$T_{2s} = \begin{bmatrix} 0_{(\#\mathbb{P}_s) \times (\#\mathbb{P}_s)} \\ *_{(\#\mathbb{H}_{s+1}) \times (\#\mathbb{H}_{s+1})} \\ 0_{(n-\#\mathbb{P}_{s+1}) \times (n-\#\mathbb{P}_{s+1})} \end{bmatrix},$$

for s < k and

$$\overset{^{2\mathbf{k}}\widetilde{\boldsymbol{T}}_{2k}}{\boldsymbol{T}_{2k}} = \begin{bmatrix} 0_{(\#\mathbb{P}_{k-1})\times(\#\mathbb{P}_{k-1})} & \\ & * \end{bmatrix},$$

which completes the proof.

8.2.3. Proof of Theorem 8.3. This theorem concerns the behavior of eigenvectors in the finite-smoothness case. The proof proceeds much like the infinitely-smooth case, but the reduction process is interrupted early.

Proof. Here we assume that the kernel is RBF, i.e. it is given by $K(\boldsymbol{x}, \boldsymbol{y}) = f(\|\boldsymbol{x} - \boldsymbol{y}\|)$, having smoothness of order r. Therefore, the kernel matrix has an expansion with only even powers of ε until 2r - 2

$$\boldsymbol{K}_{\varepsilon} = \sum_{j=0}^{r-1} \varepsilon^{2j} \boldsymbol{V}_{\leq 2j} \boldsymbol{W}_{/2j} \boldsymbol{V}_{\leq 2j}^{\mathsf{T}} + \varepsilon^{2r-1} f_{2r-1} \boldsymbol{D}_{(2r-1)} + \mathcal{O}(\varepsilon^{2r}),$$

because the odd block diagonals $W_{/2j-1}$, j < r vanish.

As in the proof of Theorem 8.2, we look at the transformed matrix

$$T(\varepsilon) = Q^{\mathsf{T}} K_{\varepsilon} Q = T_0 + \varepsilon T_1 + \ldots + \varepsilon^{2r-1} T_{2r-1} + \mathcal{O}(\varepsilon^{2r}),$$

where Q is the matrix of the full QR decomposition of V_{2r-2}

$$T_s = \begin{cases} \boldsymbol{Q}^\mathsf{T} \boldsymbol{V}_{\leq s} \boldsymbol{W}_{/s} \boldsymbol{V}_{\leq s}^\mathsf{T} \boldsymbol{Q}, & s \text{ even, } s < 2r - 1, \\ 0, & s \text{ odd, } s < 2r - 1, \\ f_{2r-1} \boldsymbol{Q}^\mathsf{T} \boldsymbol{D}_{(2r-1)} \boldsymbol{Q}, & s = 2r - 1, \end{cases}$$

and we will perform the reduction until the step 2r-1:

the reduction until the step $s \leq 2r - 2$ is completely analogous to the proof of Theorem 8.2 with P_{2s} and T_{2s} as in (55) and (56) respectively.

The last reduction step is different, as we obtain T_{2r-1} which is not equal to zero. In order to obtain the form of that last step, we remark the following: at the first step of the reduction the matrices T_{2j-1} defined by (53), are the sums of the terms running over multi-indices

$$\nu_1 + \dots + \nu_p = 2j - 1,$$

where at least one of ν_{ℓ} should be odd and all $\nu_{\ell} \leq 2j-1$. Therefore, we have $\widetilde{T}_{2j-1} = 0$ if j < r and $\widetilde{T}_{2r-1} = PT_{2r-1}P$. Proceeding by induction, we get that

$$\overset{\circ}{T}_{2j-1} = \begin{cases} 0, & j < r \text{ and } s < 2r - 1, \\ f_{2r-1} P_{2r-2} T_{2r-1} P_{2r-2}, & j = r \text{ and } s = 2r - 1, \end{cases}$$

where P_{2r-2} is defined in (55).

Thus we have that the limiting eigenvectors of $QT_{\varepsilon}Q^{\mathsf{T}}$ are the limiting eigenvectors (corresponding to non-zero eigenvalues) of the matrix

$$oldsymbol{Q}_{oldsymbol{\perp}} oldsymbol{Q}_{oldsymbol{\perp}}^{\mathsf{T}} oldsymbol{D}_{(2r-1)} oldsymbol{Q}_{oldsymbol{\perp}}^{\mathsf{T}},$$

where $Q = \begin{bmatrix} Q_{\mathsf{thin}} & Q_{\perp} \end{bmatrix}$ is the splitting of Q such that $Q_{\perp} \in \mathbb{R}^{n \times (n - \# \mathbb{P}_{r-1})}$.

9. Discussion. We have shown that kernel matrices become tractable in the flat limit, and exhibit deep ties to orthogonal polynomials. We would like to add some remarks and highlight some open problems.

First, we expect our analysis to generalise in a mostly straightforward manner to the "continuous" case, i.e., to kernel integral operators. This should make it possible to examine a double asymptotic, in which $n \to \infty$ as $\varepsilon \to 0$. One could then leverage recent results on the asymptotics of orthogonal polynomials, for instance [19].

Second, our results may be used empirically to create preconditioners for kernel matrices. There is already a vast literature on approximate kernel methods, including in the flat limit (e.g., [11, 20]), and future work should examine how effective polynomial preconditioners are compared to other available methods.

Third, many interesting problems (e.g., spectral clustering [32]) involve not the kernel matrix itself but some rescaled variant. We expect that multiplicative perturbation theory could be brought to bear here [29].

Finally, while multivariate polynomials are relatively well-understood objects, our analysis also shows that in the finite smoothness case, a central role is played by a different class of objects: namely, multivariate polynomials are replaced by the eigenvectors of distance matrices of an odd power. To our knowledge, very little has been proved about such objects but some literature from statistical physics [4] points to a link to "Anderson localization". Anderson localization is a well-known phenomenon in physics whereby eigenvectors of certain operators are localised, in the sense of having fast decay over space. This typically does not hold for orthogonal polynomials, which tend rather to be localised in frequency. Thus, we conjecture that eigenvectors of completely smooth kernels are localised in frequency, contrary to eigenvectors of finitely smooth kernels, which (at low energies) are localised in space. The results in [4] are enough to show that this holds for the exponential kernel in d=1, but extending this to d>1 and higher regularity orders is a fascinating and probably non-trivial problem.

Appendix A. Proofs for saddle point matrices.

Proof of Lemma 3.10. We note that $(\det \mathbf{R}_{\mathsf{thin}})^2 = \det(\mathbf{V}^\mathsf{T}\mathbf{V})$ and

Before proving Lemma 3.11, we need a technical lemma first.

LEMMA A.1. For $G \in \mathbb{R}^{r \times r}$ and $M = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in \mathbb{R}^{n \times n}$, $A \in \mathbb{R}^{r \times r}$ it holds that

$$\begin{bmatrix} t^r \end{bmatrix} \left\{ \det \left(oldsymbol{M} + t \begin{pmatrix} oldsymbol{G} & 0 \\ 0 & 0 \end{pmatrix} \right)
ight\} = \det oldsymbol{G} \det oldsymbol{D}$$

Proof. From [3, Theorem 1], we have that⁹

$$\frac{1}{r!}\frac{d^r}{dt^r}\det\left(\boldsymbol{M}+t\begin{pmatrix}\boldsymbol{G}&0\\0&0\end{pmatrix}\right)=\det\begin{pmatrix}\boldsymbol{G}&\boldsymbol{B}\\0&\boldsymbol{D}\end{pmatrix}=\det\boldsymbol{G}\det\boldsymbol{D}.$$

Proof of Lemma 3.11. Due to invariance under similarity transformations of the elementary polynomials, we get

$$\begin{split} &[t^r]\left\{e_k(\boldsymbol{A}+t\boldsymbol{V}\boldsymbol{V}^{\mathsf{T}})\right\} = [t^r]\left\{e_k(\boldsymbol{Q}^{\mathsf{T}}(\boldsymbol{A}+t\boldsymbol{V}\boldsymbol{V}^{\mathsf{T}})\boldsymbol{Q})\right\} \\ &= [t^r]\left\{e_k\left(\underbrace{\begin{bmatrix}\boldsymbol{Q}_{\mathsf{thin}}^{\mathsf{T}}\boldsymbol{A}\boldsymbol{Q}_{\mathsf{thin}} + t\boldsymbol{R}_{\mathsf{thin}}\boldsymbol{R}_{\mathsf{thin}}^{\mathsf{T}} & \boldsymbol{Q}_{\mathsf{thin}}^{\mathsf{T}}\boldsymbol{A}\boldsymbol{Q}_{\perp}}{\boldsymbol{Q}_{\perp}^{\mathsf{T}}\boldsymbol{A}\boldsymbol{Q}_{\perp}}\right]\right)\right\} \\ &= \sum_{\substack{|\mathcal{J}|=k\\\mathcal{J}\subseteq\{1,\ldots,n\}}} [t^r]\left\{\det\left(\boldsymbol{B}_{\mathcal{J},\mathcal{J}}(t)\right)\right\} = \sum_{\substack{|\mathcal{J}|=k\\\{1,\ldots,r\}\subseteq\mathcal{J}\subseteq\{1,\ldots,n\}}} [t^r]\left\{\det\left(\boldsymbol{B}_{\mathcal{J},\mathcal{J}}(t)\right)\right\}, \end{split}$$

where the last equality follows from the fact that the polynomial $\det (\boldsymbol{B}_{\mathcal{J},\mathcal{J}}(t))$ has degree that is equal to the cardinality of the intersection $\mathcal{J} \cap \{1,\ldots,r\}$. Any such \mathcal{J} can be written as $\{1,\ldots,r\} \cup \mathcal{J}'$, where $\mathcal{J}' \subseteq \{r+1,\ldots,n\}$. Applying lemma A.1 to each term individually, we get

$$\left[t^r\right]\left\{\det\left(\boldsymbol{B}_{\mathcal{I},\mathcal{I}}(t)\right)\right\} = \det(\boldsymbol{R}_{\mathsf{thin}}\boldsymbol{R}_{\mathsf{thin}}^{\mathsf{T}})\det\left((\boldsymbol{Q}_{\perp}^{\mathsf{T}}\boldsymbol{A}\boldsymbol{Q}_{\perp})_{\mathcal{I}',\mathcal{I}'}\right),$$

thus, summing over all $\mathcal{J}' \subseteq \{r+1,\ldots,n\}$ yields

$$\det(\boldsymbol{R}_{\mathsf{thin}}\boldsymbol{R}_{\mathsf{thin}}^{\mathsf{T}}) \sum_{\substack{\mathcal{J}' \subseteq \{r+1,\dots,n\}\\|\mathcal{J}'|=k-r}} \det\left((\boldsymbol{Q}_{\perp}^{\mathsf{T}}\boldsymbol{A}\boldsymbol{Q}_{\perp})_{\mathcal{J}',\mathcal{J}'}\right) = \det(\boldsymbol{R}_{\mathsf{thin}}^{\mathsf{T}}\boldsymbol{R}_{\mathsf{thin}}^{\mathsf{T}}) e_{k-r}(\boldsymbol{Q}_{\perp}^{\mathsf{T}}\boldsymbol{A}\boldsymbol{Q}_{\perp}).$$

Acknowledgments. The authors would like to acknowledge Pierre Comon for his help at the beginning of this project, and Cosme Louart and Malik Tiomoko for their help in improving the presentation of the results.

⁹Note that in the sum in [3, eq. (7)] only one term is nonzero.

REFERENCES

- [1] OEIS orderings wiki page. https://oeis.org/wiki/Orderings. Accessed: 2019-09-25.
- [2] M. Benzi and V. Simoncini, On the eigenvalues of a class of saddle point matrices, Numerische Mathematik, 103 (2006), pp. 173–196.
- [3] R. Bhatia and T. Jain, Higher order derivatives and perturbation bounds for determinants, Linear Algebra and its Applications, 431 (2009), pp. 2102–2108, https://doi.org/https://doi.org/10.1016/j.laa.2009.07.003.
- [4] E. BOGOMOLNY, O. BOHIGAS, AND C. SCHMIT, Spectral properties of distance matrices, Journal of Physics A: Mathematical and General, 36 (2003), p. 3595.
- [5] R. COUILLET, F. BENAYCH-GEORGES, ET AL., Kernel spectral clustering of large dimensional data, Electronic Journal of Statistics, 10 (2016), pp. 1393–1454.
- [6] D. Cox, J. LITTLE, AND D. O'SHEA, Ideals, Varieties and Algorithms: An Introduction to Computational Algebraic Geometry and Commutative Algebra, Springer, 2nd ed., 1997.
- [7] T. A. DRISCOLL AND B. FORNBERG, Interpolation in the limit of increasingly flat radial basis functions, Computers & Mathematics with Applications, 43 (2002), pp. 413–422.
- [8] N. El Karoui, The spectrum of kernel random matrices, The Annals of Statistics, 38 (2010), pp. 1–50.
- [9] G. E. FASSHAUER, Meshfree approximation methods with MATLAB, vol. 6, World Scientific, 2007.
- [10] B. FORNBERG, E. LARSSON, AND N. FLYER, Realistic eigenvalue bounds for galerkin mass matrix, IMA Journal on Numerical Analysis, 7 (1987), pp. 449–457.
- [11] B. FORNBERG, E. LARSSON, AND N. FLYER, Stable computations with Gaussian radial basis functions, SIAM Journal on Scientific Computing, 33 (2011), pp. 869–892.
- [12] D. GARREAU, W. JITKRITTUM, AND M. KANAGAWA, Large sample analysis of the median heuristic, arXiv preprint arXiv:1707.07269, (2017).
- [13] M. GASCA AND T. SAUER, Polynomial interpolation in several variables, Advances in Computational Mathematics, 12 (2000), p. 377.
- [14] U. GRENANDER AND G. SZEGÖ, Toeplitz Forms and their Applications, Chelsea, New York, 1984.
- [15] R. A. HORN AND C. R. JOHNSON, Matrix Analysis, Cambridge University Press, 1990.
- [16] I. IPSEN AND R. REHMAN, Perturbation bounds for determinants and characteristic polynomials, SIAM Journal on Matrix Analysis and Applications, 30 (2008), pp. 762–776, https://doi. org/10.1137/070704770.
- [17] T. Jain, Derivatives for antisymmetric tensor powers and perturbation bounds, Linear Algebra and its Applications, 435 (2011), pp. 1111 – 1121, https://doi.org/https://doi.org/10.1016/ j.laa.2011.02.026, http://www.sciencedirect.com/science/article/pii/S0024379511001467.
- [18] T. KATO, Perturbation theory for linear operators, Springer-Verlag, 2nd corrected ed., 1995.
- [19] A. Kroó and D. Lubinsky, Christoffel functions and universality in the bulk for multivariate orthogonal polynomials, Canadian Journal of Mathematics, 65 (2013), pp. 600–620.
- [20] S. LE BORNE, Factorization, symmetrization, and truncated transformation of radial basis function-ga stabilized gaussian radial basis functions, SIAM Journal on Matrix Analysis and Applications, 40 (2019), pp. 517–541.
- [21] Y. J. LEE AND C. A. MICCHELLI, On collocation matrices for interpolation and approximation, Journal of Approximation Theory, 174 (2013), pp. 148–181, https://doi.org/https://doi. org/10.1016/j.jat.2013.06.007.
- [22] Y. J. LEE, C. A. MICCHELLI, AND J. YOON, A study on multivariate interpolation by increasingly flat kernel functions, Journal of Mathematical Analysis and Applications, 427 (2015), pp. 74–87.
- [23] C. A. MICCHELLI, Interpolation of scattered data: Distance matrices and conditionally positive definite functions, Constructive Approximation, 2 (1986), pp. 11–22.
 [24] M. MIRANDA AND P. TILLI, Asymptotic spectra of Hermitian block Toeplitz matrices and
- [24] M. MIRANDA AND P. TILLI, Asymptotic spectra of Hermitian block Toeplitz matrices and preconditioning results, SIAM Journal on Matrix Analysis and Applications, 21 (2000), pp. 867–881.
- [25] T. Sauer, Polynomial interpolation in several variables: lattices, differences, and ideals, 12 (2006), pp. 191–230.
- [26] R. Schaback and H. Wendland, Kernel techniques: from machine learning to meshless methods, Acta numerica, 15 (2006), pp. 543-639.
- [27] B. Schölkopf, A. J. Smola, F. Bach, et al., Learning with kernels: support vector machines, regularization, optimization, and beyond, MIT press, 2002.
- [28] G. Song, J. Riddle, G. E. Fasshauer, and F. J. Hickernell, Multivariate interpolation with increasingly flat radial basis functions of finite smoothness, Advances in Computational

- Mathematics, 36 (2012), pp. 485-501.
- [29] F. Sosa and J. Moro, First order asymptotic expansions for eigenvalues of multiplicatively perturbed matrices, SIAM Journal on Matrix Analysis and Applications, 37 (2016), pp. 1478–1504.
- [30] M. L. Stein, Interpolation of Spatial Data: Some Theory for Kriging, Springer, 1999.
 [31] E. E. Tyrtyshnikov, A unifying approach to some old and new theorems on distribution and clustering, Linear Algebra and its Applications, 232 (1996), pp. 1–43, https://doi.org/https: //doi.org/10.1016/0024-3795(94)00025-5.
- [32] U. VON LUXBURG, M. BELKIN, AND O. BOUSQUET, Consistency of spectral clustering, The Annals of Statistics, (2008), pp. 555–586.
- [33] R. WANG, Y. LI, AND E. DARVE, On the numerical rank of radial basis function kernels in high dimensions, SIAM Journal on Matrix Analysis and Applications, 39 (2018), pp. 1810–1835.
- [34] A. J. Wathen and S. Zhu, On spectral distribution of kernel matrices related to radial basis functions, Numerical Algorithms, 70 (2015), pp. 709–726, https://doi.org/10.1007/ s11075-015-9970-0.
- [35] C. K. WILLIAMS AND C. E. RASMUSSEN, Gaussian processes for machine learning, vol. 2, MIT press Cambridge, MA, 2006.
- [36] V. A. ZORICH, Mathematical Analysis I, Springer, 2004.