Kernel Alignment Risk Estimator: Risk Prediction from Training Data

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Abstract

We study the risk (i.e. generalization error) of Kernel Ridge Regression (KRR) for a kernel K with ridge $\lambda > 0$ and i.i.d. observations. For this, we introduce two objects: the Signal Capture Threshold (SCT) and the Kernel Alignment Risk Estimator (KARE). The SCT $\vartheta_{K,\lambda}$ is a function of the data distribution: it can be used to identify the components of the data that the KRR predictor captures, and to approximate the (expected) KRR risk. This then leads to a KRR risk approximation by the KARE $\rho_{K,\lambda}$, an explicit function of the training data, agnostic of the true data distribution. We phrase the regression problem in a functional setting. The key results then follow from a finite-size analysis of the Stieltjes transform of general Wishart random matrices. Under a natural universality assumption (that the KRR moments depend asymptotically on the first two moments of the observations) we capture the mean and variance of the KRR predictor. We numerically investigate our findings on the Higgs and MNIST datasets for various classical kernels: the KARE gives an excellent approximation of the risk, thus supporting our universality assumption. Using the KARE, one can compare choices of Kernels and hyperparameters directly from the training set. The KARE thus provides a promising data-dependent procedure to select Kernels that generalize well.

1 Introduction

Kernel Ridge Regression (KRR) is a widely used statistical method to learn a function from its values on a training set [24, 26]. It is a non-parametric generalization of linear regression to infinite-dimensional feature spaces. Given a positive-definite kernel function K and (noisy) observations y^ϵ of a true function f^* at a list of points $X = x_1, \ldots, x_N$, the λ-KRR estimator $\hat{f}^\epsilon_\lambda$ of f^* is defined by

$$\hat{f}^\epsilon_\lambda(x) = \frac{1}{N} K(x, X) \left(\frac{1}{N} K(X, X) + \lambda I_N \right)^{-1} y^\epsilon,$$

where $K(x,X) = (K(x,x_i))_{i=1,..,N} \in \mathbb{R}^N$ and $K(X,X) = (K(x_i,x_j))_{i,j=1,..,N} \in \mathbb{R}^{N\times N}$.

Despite decades of intense mathematical progress, the rigorous analysis of the generalization of kernel methods remains a very active and challenging area of research. In recent years, many new

Preprint. Under review.

kernels have been introduced for both regression and classification tasks; notably, a large number of kernels have been discovered in the context of deep learning, in particular through the so-called Scattering Transform [20], and in close connection with deep neural networks [7, 15], yielding ever-improving performance for various practical tasks [1, 10, 16, 25]. Currently, theoretical tools to select the relevant kernel for a given task, i.e. to minimize the generalization error, are however lacking.

While a number of bounds for the risk of Linear Ridge Regression (LRR) or KRR [6, 28, 21] exist, most focus on the rate of convergence of the risk: these estimates typically involve constant factors which are difficult to control in practice. Recently, a number of more precise estimates have been given [19, 9, 22, 18, 5]; however, these estimates typically require a priori knowledge of the data distribution. It remains a challenge to have estimates based on the training data alone, enabling one to make informed decisions on the choices of the ridge and of the kernel.

1.1 Contributions

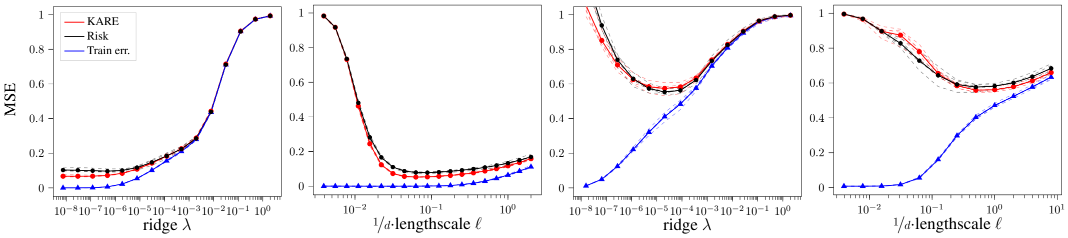
We consider a generalization of the KRR predictor $\hat{f}^{\epsilon}_{\lambda}$: one tries to reconstruct a true function f^* in a space of continuous functions $\mathcal{C}$ from noisy observations y^{ϵ} of the form $(o_1(f^*) + \epsilon e_1, \ldots, o_N(f^*) + \epsilon e_N)$, where the observations o_i are i.i.d. linear forms $\mathcal{C} \to \mathbb{R}$ sampled from a distribution π, ϵ is the level of noise, and the $e_1, \ldots, e_N$ are centered of unit variance. We work under the universality assumption that, for large N, only the first two moments of π determine the behavior of the first two moments of $\hat{f}^{\epsilon}_{\lambda}$. We obtain the following results:

1. We introduce the Signal Capture Threshold (SCT) $\vartheta(\lambda, N, K, \pi)$, which is determined by the ridge λ, the size of the training set N, the kernel K, and the observations distribution π (more precisely, the dependence on π is only through its first two moments). We give approximations for the expectation and variance of the KRR predictor in terms of the SCT.
2. Decomposing f^* along the kernel principal components of the data distribution, we observe that in expectation, the predictor $\hat{f}^{\epsilon}_{\lambda}$ captures only the signal along the principal components with eigenvalues larger than the SCT. If N increases or λ decreases, the SCT ϑ shrinks, allowing the predictor to capture more signal. At the same time, the variance of $\hat{f}^{\epsilon}_{\lambda}$ scales with the derivative $\partial_{\lambda}\vartheta$, which grows as $\lambda \to 0$, supporting the classical bias-variance tradeoff picture [13].
3. We give an explicit approximation for the expected MSE risk $R^{\epsilon}(\hat{f}^{\epsilon}_{\lambda})$ and empirical MSE risk $\hat{R}^{\epsilon}(\hat{f}^{\epsilon}_{\lambda})$ for an arbitrary continuous true function f^*. We find that, surprisingly, the expected risk and expected empirical risk are approximately related by
$$\mathbb{E}[R^{\epsilon}(\hat{f}^{\epsilon}_{\lambda})] \approx \frac{\vartheta(\lambda)^2}{\lambda^2}\mathbb{E}[\hat{R}^{\epsilon}(\hat{f}^{\epsilon}_{\lambda})].$$
4. We introduce the Kernel Alignment Risk Estimator (KARE) as the ratio ρ defined by
$$\rho(\lambda, N, y^{\epsilon}, G) = \frac{\frac{1}{N}\left(y^{\epsilon}\right)^T\left(\frac{1}{N}G + \lambda I_N\right)^{-2} y^{\epsilon}}{\left(\frac{1}{N}\mathrm{Tr}\left[\left(\frac{1}{N}G + \lambda I_N\right)^{-1}\right]\right)^2},$$
where G is the Gram matrix of K on the observations. We show that the KARE approximates the expected risk; unlike the SCT, it is agnostic of the true data distribution. This result follows from the fact that $\vartheta(\lambda) \approx 1/m_G(-\lambda)$, where m_G is the Stieltjes Transform of the Gram matrix $\frac{1}{N}G$.
5. Empirically, we find that the KARE predicts the risk on the Higgs and MNIST datasets. We see empirically that our results extend extremely well beyond the Gaussian observation setting, thus supporting our universality assumption (see Figure 1).

Our proofs (see the Appendix) rely on a finite-size analysis of generalized Wishart matrices, in particular the complex Stieltjes transform $m_G(z)$, evaluated at $z = -\lambda$, and on fixed-point arguments.

1.2 Related Works

The theoretical analysis of the risk of KRR has seen tremendous developments in the recent years. In particular, a number of upper and lower bounds for kernel risk have been obtained [6, 28, 21] in



(a) MNIST, $\ell = d$ (b) MNIST, $\lambda = 10^{-5}$ (c) Higgs, $\ell = d$ (d) Higgs, $\lambda = 10^{-4}$

Figure 1: Comparison between the KRR risk and the KARE for various choices of normalized lengthscale ℓ/d and ridge λ on the MNIST dataset (restricted to the digits 7 and 9, labeled by 1 and -1 respectively, $N = 2000$) and on the Higgs dataset (classes 'b' and 's', labeled by -1 and 1, $N = 1000$) with the RBF Kernel $K(x, x') = \exp(-\|x-x'\|_2^2/\ell)$. KRR predictor risks, and KARE curves (shown as dashed lines, 5 samples) concentrate around their respective averages (solid lines).

various settings: notably, convergence rates (i.e. without control of the constant factors) are obtained in general settings. This allows one to abstract away a number of details about the kernels (e.g. the lengthscale), which don't influence the asymptotic rates. However, this does not give access to the risk at finite data size (crucial to pick e.g. the correct lengthscale or the NTK depth [15]).

A number of recent results have given precise descriptions of the risk for ridge regression [9, 18], for random features [22, 14], and in relation to neural networks [19, 5]. These results rely on the analysis of the asymptotic spectrum of general Wishart random matrices, in particular through the Stieltjes transform [27, 3]. The limiting Stieltjes transform can be recovered from the formula for the product of freely independent matrices [12]. To extend these asymptotic results to finite-size settings, we generalize and adapt the results of [14].

While these techniques have given simple formulae for the KRR predictor expectation, approximating its variance has remained more challenging. For this reason the description of the expected risk in [19] is stated as a conjecture. In [18] only the bias component of the risk is approximated. In [9] the expected risk is given only for random true functions (in a Bayesian setting) with a specific covariance. In [5], the expected risk follows from a heuristic spectral analysis combining a PDE approximation and replica tricks. In this paper, we approximate the variance of the predictor along the principal components, giving an approximation of the risk for any continuous true function.

The SCT is related to a number of objects from previous works, such as the effective dimension of [30, 6], the companion Stieltjes transform of [9, 18], and particularly the effective ridge of [14]. The SCT can actually be viewed as a direct translation to the KRR risk setting of [14].

1.3 Outline

In Section 2, we first introduce the Kernel Ridge Regression (KRR) predictor in functional space (Section 2.1) and formulate its train error and risk for random observations (Section 2.2).

The rest of the paper is then devoted to obtaining approximations for the KRR risk. In Section 3,the Signal Capture Threshold (SCT) is introduced and used to study the mean and variance of the KRR predictor (Sections 3.1 and 3.2). An approximation of the SCT in terms of the observed data is then given (Section 3.4). In Section 4, the expected risk and the expected empirical risk are approximated in terms of the SCT and its derivative w.r.t. the ridge λ. The SCT approximation of Section 3.4, together with the estimates of Section 4.1, leads to an approximation of the KRR risk by the Kernel Alignment Risk Estimator (KARE).

2 Setup

Given a compact $\Omega \subset \mathbb{R}^d$, let $\mathcal{C}$ denote the space of continuous $f : \Omega \to \mathbb{R}$, endowed with the supremum norm $\|f\|_\infty = \sup_{x\in\Omega} |f(x)|$. In the classical regression setting, we want to reconstruct a true function $f^* \in \mathcal{C}$ from its values on a training set $x_1, \ldots, x_N$, i.e. from the noisy labels $y^\epsilon = (f^*(x_1) + \epsilon e_1, \ldots, f^*(x_N) + \epsilon e_N)^T$ for some i.i.d. centered noise $e_1, \ldots, e_N$ of unit variance and noise level $\epsilon \geq 0$.

In this paper, the observed values (without noise) of the true function f^* consist in observations $o_1, \ldots, o_N \in \mathcal{C}^*$, where $\mathcal{C}^*$ is the dual space, i.e. the space of bounded linear functionals $\mathcal{C} \to \mathbb{R}$. We thus represent the training set of N observations $o_1, \ldots, o_N$ by the *sampling operator* $\mathcal{O} : \mathcal{C} \to \mathbb{R}^N$ which maps a function $f \in \mathcal{C}$ to the vector of observations $\mathcal{O}(f) = (o_1(f), \ldots, o_N(f))^T$.

The classical setting corresponds to the case where the observations are evaluations of f^* at points $x_1, \ldots, x_N \in \Omega$, i.e. $o_i(f^*) = f^*(x_i)$ for $i = 1, \ldots, N$. In time series analysis (when $\Omega \subset \mathbb{R}$), the observations can be the averages $o_i(f^*) = \frac{1}{b_i - a_i} \int_{a_i}^{b_i} f^*(t)dt$ over time intervals $[a_i, b_i] \subset \mathbb{R}$.

2.1 Kernel Ridge Regression Predictor

The regression problem is now stated as follows: given noisy observations $y_i^\epsilon = o_i(f^*) + \epsilon e_i$ with i.i.d. centered noises $e_1, \ldots, e_N$ of unit variance, how can one reconstruct f^*?

Definition 1. *Consider a continuous positive kernel $K : \Omega \times \Omega \to \mathbb{R}$ and a ridge parameter $\lambda > 0$. The Kernel Ridge Regression (KRR) predictor with ridge λ is the function $\hat{f}_\lambda^\epsilon : \Omega \to \mathbb{R}$*

$$\hat{f}_\lambda^\epsilon = \frac{1}{N} K \mathcal{O}^T (\frac{1}{N} \mathcal{O} K \mathcal{O}^T + \lambda I_N)^{-1} y^\epsilon$$

where $\mathcal{O}^T : \mathbb{R}^N \to \mathcal{C}^*$ is the adjoint of $\mathcal{O}$ defined by $(\mathcal{O}^T y)(f) = y^T \mathcal{O}(f)$ and where we view K as a map $\mathcal{C}^* \to \mathcal{C}$ with $(K\mu)(x) = \mu(K(x, \cdot))$.

We call the $N \times N$ matrix $G = \mathcal{O} K \mathcal{O}^T$ the *Gram matrix*: in the classical setting, when the observations are $o_i = \delta_{x_i}$ (with $\delta_x(f) = f(x)$), G is the usual Gram matrix, i.e. $G_{ij} = K(x_i, x_j)$.

2.2 Training Error and Risk

We consider the least-squares error (MSE loss) of the KRR predictor, taking into account randomness of: (1) the test point, random observation o to which is added a noise ϵe (2) the training data, made of N observations o_i plus noises $\epsilon e_i \sim \nu$, where $o, o_1, \ldots, o_n \sim \pi$ and $e, e_1, \ldots, e_N$ are i.i.d. The expected risk of the KRR predictor is thus taken w.r.t. the test and training observations and their noises. Unless otherwise specified, the expectations are taken w.r.t. all these sources of randomness.

For (fixed) observations $o_1, \ldots, o_N$, the *empirical risk* or *training error* of the KRR predictor $\hat{f}_\lambda^\epsilon$ is

$$\hat{R}^\epsilon(\hat{f}_\lambda^\epsilon) = \frac{1}{N} \sum_{i=1}^{N} (o_i(\hat{f}_\lambda^\epsilon) - y_i^\epsilon)^2 = \frac{1}{N} \left\| \mathcal{O}(\hat{f}_\lambda^\epsilon) - y^\epsilon \right\|^2.$$

For a random observation o sampled from π and a noise ϵe (where $e \sim \nu$ is centered of unit variance as before), the *risk* $R^\epsilon(\hat{f}_\lambda^\epsilon)$ of the KRR predictor $\hat{f}_\lambda^\epsilon$ is defined by

$$R^\epsilon(\hat{f}_\lambda^\epsilon) = \mathbb{E}_{o \sim \pi, e \sim \nu} \left[(o(f^*) + \epsilon e - o(\hat{f}_\lambda^\epsilon))^2 \right].$$

Describing the observation variance by the bilinear form $\langle f, g \rangle_S = \mathbb{E}_{o \sim \pi} [o(f) o(g)]$ and the related semi-norm $\|f\|_S = \langle f, f \rangle_S^{1/2}$, the risk can be rewritten as $R^\epsilon(\hat{f}_\lambda^\epsilon) = \|\hat{f}_\lambda^\epsilon - f^*\|_S^2 + \epsilon^2$.

From now on, we will assume that $\langle \cdot, \cdot \rangle_S$ is a scalar product; note that in the classical setting, when o is the evaluation of f^* at a point $x \in \Omega$ with $x \sim \sigma$, the S-norm is given by $\|f\|_S^2 = \int_\Omega f(x)^2 \sigma(dx)$.

The following three operators $\mathcal{C} \to \mathcal{C}$ are central to our analysis:

Definition 2. *The KRR reconstruction operator $A_\lambda : \mathcal{C} \to \mathcal{C}$, the KRR Integral Operator $T_K : \mathcal{C} \to \mathcal{C}$, and its empirical version $T_K^N : \mathcal{C} \to \mathcal{C}$ are defined by*

$$\begin{aligned} A_\lambda &= \frac{1}{N} K \mathcal{O}^T (\frac{1}{N} \mathcal{O} K \mathcal{O}^T + \lambda I_N)^{-1} \mathcal{O}, \\ (T_K f)(x) &= \langle f, K(x, \cdot) \rangle_S = \mathbb{E}_{o \sim \pi} [o(f) o(K(x, \cdot))], \\ (T_K^N f)(x) &= \frac{1}{N} K \mathcal{O}^T \mathcal{O} f(x) = \frac{1}{N} \sum_{i=1}^{N} o_i(f) o_i(K(x, \cdot)). \end{aligned}$$

Note that in the noiseless regime (i.e. when $\epsilon = 0$), we have $\hat{f}^{\epsilon}_{\lambda}\big|_{\epsilon=0} = A_\lambda f^*$. Also note that A_λ and T^N_K are random operators, as they depend on the random observations. The operator T_K is the natural generalization to our framework of the integration operator $f \mapsto \int K(x,\cdot)f(x)\sigma(dx)$, which is defined with random observations δ_x with $x \sim \sigma$ in the classical setting.

The reconstruction and empirical integral operators are linked by $A_\lambda = T^N_K(T^N_K + \lambda I_{\mathcal{C}})^{-1}$, which follows from the identity $\left(\frac{1}{N}\mathcal{O}K\mathcal{O}^T + \lambda I_N\right)^{-1}\mathcal{O} = \mathcal{O}\left(\frac{1}{N}K\mathcal{O}^T\mathcal{O} + \lambda I_{\mathcal{C}}\right)^{-1}$. As $N \to \infty$, we have that $T^N_K \to T_K$, and it follows that

$$A_\lambda \to \tilde{A}_\lambda := T_K(T_K + \lambda I_{\mathcal{C}})^{-1}. \tag{1}$$

2.3 Eigendecomposition of the Kernel

We will assume that the kernel K can be diagonalized by a countable family of eigenfunctions $(f^{(k)})_{k\in\mathbb{N}}$ in $\mathcal{C}$ with eigenvalues $(d_k)_{k\in\mathbb{N}}$, orthonormal with respect to the scalar product $\langle\cdot,\cdot\rangle_S$, such that we have (with uniform convergence):

$$K(x,x') = \sum_{k=1}^{\infty} d_k f^{(k)}(x) f^{(k)}(x').$$

The functions $f^{(k)}$ are also eigenfunctions of T_K: we have $T_K f^{(k)} = d_k f^{(k)}$. We will also assume that $\mathrm{Tr}\left[T_K\right] = \sum_{k=1}^{\infty}\left\langle f^{(k)}, T_K(f^{(k)})\right\rangle_S = \sum_{k=1}^{\infty} d_k$ is finite. Note that in the classical setting K can be diagonalized as above (by Mercer's theorem), and $\mathrm{Tr}\left[T_K\right] = \mathbb{E}_{x\sim\sigma}\left[K(x,x)\right]$ is finite.

2.4 Gaussianity Assumption

As seen in Equation (1) above, $\tilde{A}_\lambda$ only depends on the first two moments of π (through $\langle\cdot,\cdot\rangle_S$), suggesting the following assumption, with which we will work in this paper:

Assumption A. *As far as one is concerned with the first two moments of the A_λ operator, for large but finite N, one can assume that the observations $o_1,\dots,o_N$ are Gaussian, i.e. that for any tuple of functions $(f_1,\dots,f_N)$, the vector $(o_1(f_1),\dots,o_N(f_N))$ is a Gaussian vector.*

Though our proofs use this assumption, the ideas in [19, 4] suggest a path to extend them beyond the Gaussian case, where our numerical experiments (see Figure 1) suggest that our results remain true.

3 Predictor Moments and Signal Capture Threshold

A central tool in our analysis of the KRR predictor $\hat{f}^{\epsilon}_{\lambda}$ is the Signal Capture Threshold (SCT):

Definition 3. *For $\lambda > 0$, the* Signal Capture Threshold $\vartheta(\lambda) = \vartheta(\lambda, N, K, \pi)$ *is the unique positive solution (see Section B.2 in the Appendix) to the equation:*

$$\vartheta(\lambda) = \lambda + \frac{\vartheta(\lambda)}{N}\mathrm{Tr}\left[T_K\left(T_K + \vartheta(\lambda)I_{\mathcal{C}}\right)^{-1}\right].$$

In this section, we use $\vartheta(\lambda)$ and the derivative $\partial_\lambda\vartheta(\lambda)$ for the estimation of the mean and variance of the KRR predictor $\hat{f}^{\epsilon}_{\lambda}$ upon which the Kernel Alignment Risk Estimator of Section 4 is based.

3.1 Mean predictor

The expected KRR predictor can be expressed in terms of the expected reconstruction operator A_λ

$$\mathbb{E}[\hat{f}^{\epsilon}_{\lambda}] = \mathbb{E}[\frac{1}{N}K\mathcal{O}^T(\frac{1}{N}\mathcal{O}K\mathcal{O}^T + \lambda I_N)^{-1}y^{\epsilon}] = \mathbb{E}\left[A_\lambda\right]f^*,$$

where we used the fact that $\mathbb{E}_{e_1,\dots,e_N}[y^{\epsilon}] = \mathcal{O}f^*$.

Theorem 1 (Theorem 17 in the Appendix)**.** *The expected reconstruction operator $\mathbb{E}[A_\lambda]$ is approximated by the operator $\tilde{A}_\vartheta = T_K\left(T_K + \vartheta(\lambda)I_{\mathcal{C}}\right)^{-1}$ in the sense that for all $f, g \in \mathcal{C}$,*

$$\left|\left\langle f, \left(\mathbb{E}\left[A_\lambda\right] - \tilde{A}_\vartheta\right)g\right\rangle_S\right| \leq \left(\frac{1}{N} + \boldsymbol{P}_0(\frac{\mathrm{Tr}[T_K]}{\lambda N})\right)\left|\left\langle f, \tilde{A}_\vartheta(I_{\mathcal{C}} - \tilde{A}_\vartheta)g\right\rangle_S\right|,$$

for a polynomial $\boldsymbol{P}_0$ with nonnegative coefficients and $\boldsymbol{P}_0(0) = 0$.

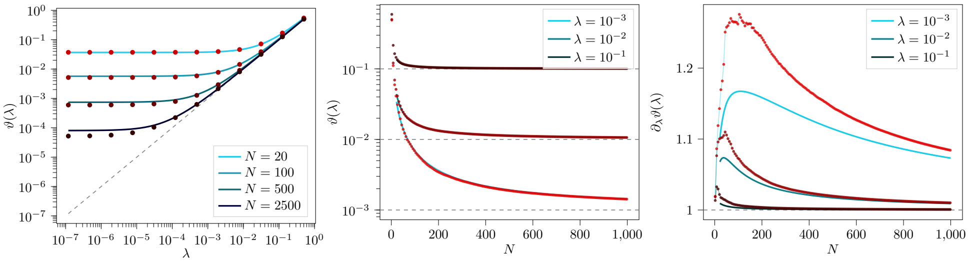


Figure 2: *Signal Capture Threshold and Derivative.* We consider the RBF Kernel on the standard d-dimensional Gaussian with $\ell = d = 20$. In blue lines, exact formulas for the SCT $\vartheta(\lambda)$ and $\partial_\lambda \vartheta(\lambda)$, computed using the eigenvalue decomposition of the integral operator T_K; in red dots, their approximation with Proposition 5.

This theorem gives the following motivation for the name SCT: if the true function f^* is an eigenfunction of T_K, i.e. $T_K f^* = \delta f^*$, then $\tilde{A}_\vartheta f^* = \frac{\delta}{\vartheta(\lambda)+\delta} f^*$ and we get:

- if $\delta \gg \vartheta(\lambda)$, then $\frac{\delta}{\vartheta(\lambda)+\delta} \approx 1$ and $\mathbb{E}\left[A_\lambda\right] f^* \approx f^*$, i.e. the function is learned on average,
- if $\delta \ll \vartheta(\lambda)$, then $\frac{\delta}{\vartheta(\lambda)+\delta} \approx 0$ and $\mathbb{E}\left[A_\lambda\right] f^* \approx 0$, i.e. the function is not learned on average.

More generally, if we decompose a true function f^* along the principal components (i.e. eigenfunctions) of T_K, the signal along the k-th principal component $f^{(k)}$ is captured whenever the corresponding eigenvalue $d_k \gg \vartheta(\lambda)$ and lost when $d_k \ll \vartheta(\lambda)$.

3.2 Variance of the predictor

We now estimate the variance of $\hat{f}^\epsilon_\lambda$ along each principal component in terms of the SCT $\vartheta(\lambda)$ and its derivative $\partial_\lambda \vartheta(\lambda)$. Along the eigenfunction $f^{(k)}$, the variance is estimated by V_k, where

$$V_k(f^*, \lambda, N, \epsilon) = \frac{\partial_\lambda \vartheta(\lambda)}{N} \left(\left\| (I_\mathcal{C} - \tilde{A}_\vartheta) f^* \right\|_S^2 + \epsilon^2 + \left\langle f^{(k)}, f^* \right\rangle_S^2 \frac{\vartheta^2(\lambda)}{(\vartheta(\lambda) + d_k)^2} \right) \frac{d_k^2}{(\vartheta(\lambda) + d_k)^2}.$$

Theorem 2 (Theorem 22 in the Appendix)**.** *There is a constant $\boldsymbol{C}_1 > 0$ and a polynomial $\boldsymbol{P}_1$ with nonnegative coefficients and with $\boldsymbol{P}_1(0) = 0$ such that*

$$\left| \mathrm{Var}\left(\left\langle f^{(k)}, \hat{f}^\epsilon_\lambda \right\rangle_S \right) - V_k \right| \leq \left(\frac{\boldsymbol{C}_1}{N} + \boldsymbol{P}_1\left(\frac{\mathrm{Tr}[T_K]}{\lambda N^{\frac{1}{2}}}\right) \right) V_k.$$

As shown in Section 4.1, understanding the variance along the principal components (rather than the covariances between the principal components) is enough to describe the risk.

3.3 Behavior of the SCT

The behavior of the SCT can be controlled by the following (agnostic of the exact spectrum of T_K)

Proposition 3 (Proposition 12 in the Appendix)**.** *For any $\lambda > 0$, we have*

$$\lambda < \vartheta(\lambda, N) \leq \lambda + \frac{1}{N} \mathrm{Tr}[T_K], \qquad 1 \leq \partial_\lambda \vartheta(\lambda, N) \leq \frac{1}{\lambda} \vartheta(\lambda, N),$$

moreover $\vartheta(\lambda, N)$ is decreasing as a function of N.

Remark. *As $N \to \infty$, we have $\vartheta(\lambda, N)$ decreases down to λ (see also Figure 2), in agreement with the fact that $A_\lambda \to \tilde{A}_\lambda$.*

As $\lambda \to 0$, the above upper bound for $\partial_\lambda \vartheta$ becomes useless. Still, assuming that the spectrum of K has a sufficiently fast power-law decay, we get:

Proposition 4 (Proposition 16 in the Appendix)**.** *If $d_k = \Theta(k^{-\beta})$ for some $\beta > 1$, there exist $c_0, c_1, c_2 > 0$ such that for any $\lambda > 0$*

$$\lambda + c_0 N^{-\beta} \leq \vartheta(\lambda, N) \leq \; c_2 \lambda + c_1 N^{-\beta}, \qquad 1 \leq \partial_\lambda \vartheta(\lambda, N) \leq c_2.$$

3.4 Approximation of the SCT from the training data

The SCT ϑ and its derivative $\partial_\lambda \vartheta$ are functions of λ, N, and of the spectrum of T_K. In practice, the spectrum of T_K is not known: for example, in the classical setting, one does not know the true data distribution σ. Fortunately, ϑ can be approximated by $1/m_G(-\lambda)$, where m_G is the *Stieltjes Transform* of the Gram matrix, defined by $m_G(z) = \mathrm{Tr}\left[(\frac{1}{N}G - zI_N)^{-1}\right]$. Namely, we get:

Proposition 5 (Proposition 10 in the Appendix)**.** *For any $\lambda > 0, s \in \mathbb{N}$, there is a $\boldsymbol{c}_s > 0$ such that*

$$\mathbb{E}\left[|{}^1\!/\!_{\vartheta(\lambda)} - m_G(-\lambda)|^{2s}\right] \leq \frac{\boldsymbol{c}_s(\mathrm{Tr}[T_K])^{2s}}{\lambda^{4s}N^{3s}}.$$

Remark. *Likewise, we have $\partial_\lambda \vartheta \approx \left(\partial_z m_G(z)/m_G(z)^2\right)|_{z=-\lambda}$, as shown in the Appendix.*

4 Risk Prediction with KARE

In this section, we show that the Expected Risk $\mathbb{E}[R^\epsilon(\hat{f}^\epsilon_\lambda)]$ can be approximated in terms of the training data by the Kernel Alignment Risk Estimator (KARE).

Definition 4. *The Kernel Alignment Risk Estimator (KARE) ρ is defined by*

$$\rho(\lambda, N, y^\epsilon, G) = \frac{\frac{1}{N}(y^\epsilon)^T\left(\frac{1}{N}G + \lambda I_N\right)^{-2} y^\epsilon}{\left(\frac{1}{N}\mathrm{Tr}\left[\left(\frac{1}{N}G + \lambda I_N\right)^{-1}\right]\right)^2}.$$

In the following, using Theorems 1 and 22, we give an approximation for the expected risk and expected empirical risk in terms of the SCT and the true function f^*. This yields the important relation (2) in Section 4.2, which shows that the KARE can be used to efficiently approximate the kernel risk.

4.1 Expected Risk and Expected Empirical Risk

The expected risk is approximated, in terms of the SCT and the true function f^*, by

$$\tilde{R}^\epsilon(f^*, \lambda, N, K, \pi) = \partial_\lambda \vartheta(\lambda)(\|(I_\mathcal{C} - \tilde{A}_\vartheta)f^*\|^2_S + \epsilon^2),$$

as shown by the following:

Theorem 6 (Theorem 23 in the Appendix)**.** *There exists a constant $\boldsymbol{C}_2 > 0$ and a polynomial $\boldsymbol{P}_2$ with nonnegative coefficients and with $\boldsymbol{P}_2(0) = 0$, such that we have*

$$\left|\mathbb{E}[R^\epsilon(\hat{f}^\epsilon_\lambda)] - \tilde{R}^\epsilon(f^*, \lambda, N, K, \pi)\right| \leq \left(\frac{\boldsymbol{C}_2}{N} + \boldsymbol{P}_2(\frac{\mathrm{Tr}[T_K]}{\lambda N^{\frac{1}{2}}})\right)\tilde{R}^\epsilon(f^*, \lambda, N, K, \pi).$$

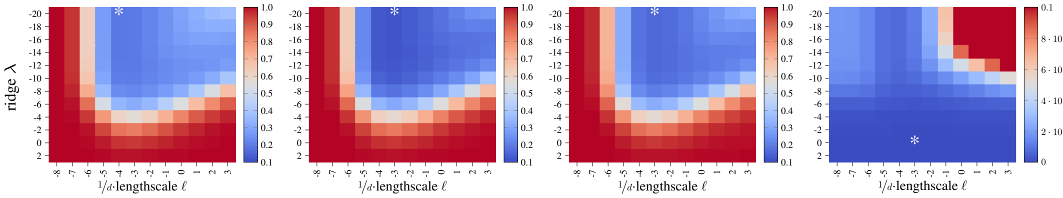
Proof. (Sketch; the full proof is given in the Appendix). From the bias-variance decomposition:

$$\mathbb{E}[R^\epsilon(\hat{f}^\epsilon_\lambda)] = R^\epsilon(\mathbb{E}[\hat{f}^\epsilon_\lambda]) + \sum_{k=1}^{\infty}\mathrm{Var}(\langle f^{(k)}, \hat{f}^\epsilon_\lambda\rangle_S).$$

By Theorem 1, and a small calculation, the bias is approximately $\|(I_\mathcal{C} - \tilde{A}_\vartheta)f^*\|^2_S + \epsilon^2$. By Theorem 22, and a calculation, the variance is approximately $(\partial_\lambda\vartheta(\lambda) - 1)(\|(I_\mathcal{C} - \tilde{A}_\vartheta)f^*\|^2_S + \epsilon^2)$. □

The approximate expected risk $\tilde{R}^\epsilon(f^*, \lambda, N, K, \pi)$ is increasing in both ϑ and $\partial_\lambda\vartheta$. As λ increases, the bias increases with ϑ, while the variance decreases with $\partial_\lambda\vartheta$: this leads to the bias-variance tradeoff. On the other hand, as a function of N, ϑ is decreasing but $\partial_\lambda\vartheta$ is generally not monotone: this can lead to so-called multiple descent curves in the risk as a function of N [17].

Remark. *For a decaying ridge $\lambda = cN^{-\gamma}$ for $0 < \gamma < \frac{1}{2}$, as $N \to \infty$, by Proposition 3, we get $\vartheta(\lambda) \to 0$ and $\partial_\lambda\vartheta(\lambda) \to 1$: this implies that $\mathbb{E}[R^\epsilon(\hat{f}^\epsilon_\lambda)] \to \epsilon^2$. Hence the KRR can learn any continuous function f^* as $N \to \infty$ (even if f^* is not in the RKHS associated with K).*



(a) Risk (b) KARE Predictions (c) Cross Val. Predictions (d) Log-likelihood Estim.

Figure 3: *Comparision of risk predictors.* We calculate the risk (i.e. test error) of $\hat{f}^\epsilon_\lambda$ on MNIST with the RBF Kernel for various values of ℓ and λ on $N = 200$ data points (same setup as Fig. 1). We mark the minimum MSE achieved with a star. We display the predictions of KARE and 4-fold cross-validation; both find the hyper-parameters minimizing the risk. We also show the (normalized) log-likehood estimator and observe that it favors large λ values. Axes are $\log_2$ scale.

Remark. *In a Bayesian setting, assuming that f^* is random with zero mean and covariance kernel Σ, the optimal choices for the KRR predictor are $K = \Sigma$ and $\lambda = {}^{\epsilon^2}/_N$ (see Section B.7 in the Appendix). When $K = \Sigma$ and $\lambda = {}^{\epsilon^2}/_N$, the formula of Theorem 6 simplifies (see Corollary in the Appendix) to*

$$\mathbb{E}\left[R^\epsilon\left(\hat{f}^\epsilon_\lambda\right)\right] \approx N\vartheta\left(\frac{\epsilon^2}{N}, \Sigma\right).$$

The empirical risk (or train error) $\hat{R}^\epsilon(\hat{f}^\epsilon_\lambda) = \lambda^2 (y^\epsilon)^T (\frac{1}{N}G + \lambda I_N)^{-2} y^\epsilon$ can be analyzed with the same theoretical tools. Its approximation in terms of the SCT is given as follows:

Theorem 7 (Theorem 24 in the Appendix)**.** *There exists a constant $\boldsymbol{C}_3 > 0$ and a polynomial $\boldsymbol{P}_3$ with nonnegative coefficients and with $\boldsymbol{P}_3(0) = 0$ such that we have*

$$\left|\mathbb{E}[\hat{R}^\epsilon(\hat{f}^\epsilon_\lambda)] - \frac{\lambda^2}{\vartheta(\lambda)^2}\tilde{R}^\epsilon(\hat{f}^\epsilon_\lambda, \lambda, N, K, \pi)\right| \leq \left(\frac{1}{N} + \boldsymbol{P}_3(\frac{\mathrm{Tr}[T_K]}{\lambda N})\right)\tilde{R}^\epsilon(f^*, \lambda, N, K, \pi).$$

4.2 KARE: Kernel Alignment Risk Estimator

While the above approximations (Theorems 6 and 7) for the expected risk and empirical risk depend on f^*, their combination yields the following relation, which is surprisingly independent of f^*:

$$\mathbb{E}\left[R^\epsilon\left(\hat{f}^\epsilon_\lambda\right)\right] \approx \frac{\vartheta^2}{\lambda^2}\mathbb{E}\left[\hat{R}^\epsilon\left(\hat{f}^\epsilon_\lambda\right)\right]. \tag{2}$$

Since ϑ can be approximated from the training set (see Proposition 5), so can the expected risk. Assuming that the risk and empirical risk concentrate around their expectations, we get the KARE:

$$R^\epsilon\left(\hat{f}^\epsilon_\lambda\right) \approx \rho(\lambda, N, y^\epsilon, G) = \frac{\frac{1}{N}\left(y^\epsilon\right)^T\left(\frac{1}{N}G + \lambda I_N\right)^{-2} y^\epsilon}{\left(\frac{1}{N}\mathrm{Tr}\left[\left(\frac{1}{N}G + \lambda I_N\right)^{-1}\right]\right)^2}.$$

Remark. *As shown in the Appendix, estimating the risk of the expected predictor $\mathbb{E}[\hat{f}^\epsilon_\lambda]$ yields:*

$$R^\epsilon(\mathbb{E}[\hat{f}^\epsilon_\lambda]) \approx \varrho(\lambda, N, y^\epsilon, G) = \frac{(y^\epsilon)^T(\frac{1}{N}G + \lambda I_N)^{-2} y^\epsilon}{\mathrm{Tr}[(\frac{1}{N}G + \lambda I_N)^{-2}]}.$$

Note that both ρ and ϱ are invariant (as is the risk) under the simultaneous rescaling $K, \lambda \rightsquigarrow \alpha K, \alpha\lambda$.

The KARE can be used to optimize the risk over the space of kernels, for instance to choose the ridge and length-scale. The most popular kernel selection techniques are (see Figure 3):

- Cross-validation: accurate estimator of the risk on a test set, but costly to optimize (the predictor must be recomputed for each kernel and differentiating it in the space of kernels is hard).
- Kernel likelihood (Chapter 5 of [23]): efficient to optimize and takes into account the ridge, but not a risk estimator; unlike the risk, not invariant under the simultaneous rescaling $K, \lambda \rightsquigarrow \alpha K, \alpha\lambda$.

- Classical kernel alignment [8]: very efficient to optimize and scale invariant, but not a risk estimator, not sensitive to small eigenvalues and inadequate to select hyperparameters such as the ridge.

The KARE combines the best features of the three above techniques:

- it can be computed efficiently on the training data, and optimized over the space of kernels;
- like the risk, it is invariant under the simultaneous rescaling $K, \lambda \rightsquigarrow \alpha K, \alpha\lambda$;
- it is sensitive to the small Gram matrix eigenvalues and to the ridge λ.

5 Conclusion

In this paper, we introduce new techniques to study the Kernel Ridge Regression (KRR) predictor and its risk. We obtain new precise estimates for the test and train error in terms of a new object, the Signal Capture Threshold (SCT), which identifies the components of a true function that are being learned by the KRR: our estimates reveal a remarkable relation, which leads one to the Kernel Alignment Risk Estimator (KARE). The KARE is a new efficient way to estimate the risk of a kernel predictor based on the training data only. Numerically, we observe that the KARE gives a very accurate prediction of the risk for Higgs and MNIST datasets for a variety of classical kernels.

Broader Impact

This work is fundamental and may be used in any research area using Kernel methods, possibly leading to indirect social impacts. However, we do not predict any direct social impact.

Acknowledgements

The authors wish to thank A. Montanari and M. Wyart for useful discussions. This work is partly supported by the ERC SG CONSTAMIS. C. Hongler acknowledges support from the Blavatnik Family Foundation, the Latsis Foundation, and the the NCCR Swissmap.

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Appendix

We organize the Appendix as follows:

1. In Section A, we present the details for the numerical results presented in the main text (and in the Appendix) and we present additional experiments and some discussions.
2. In Section B, we present the proofs of the mathematical results presented in the main text.

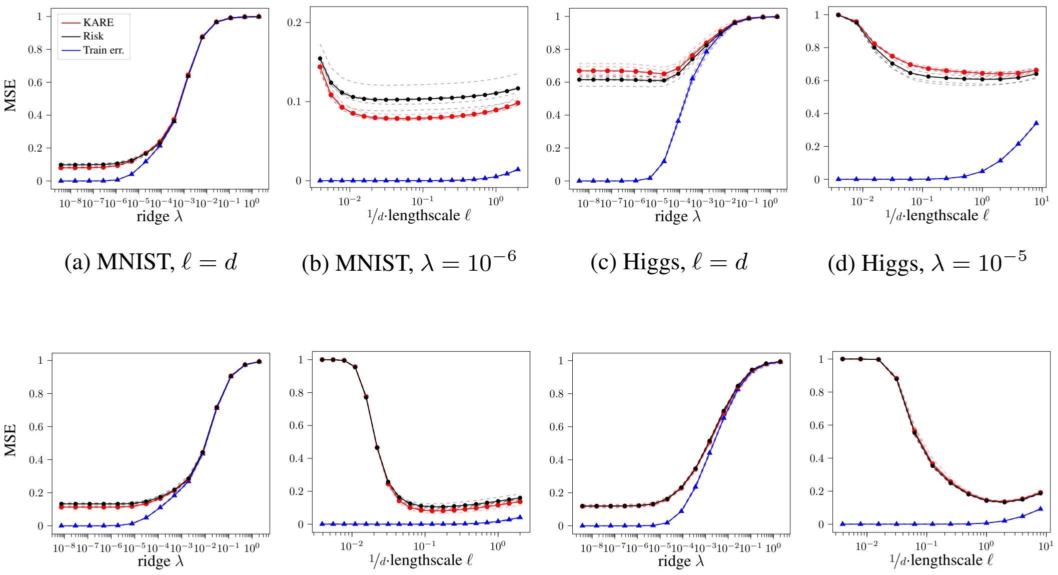
A Numerical Results

A.1 Empirical Methods

For the MNIST dataset. We sample N images of digits 7 and 9 from the MNIST training dataset (image size $d = 24 \times 24$, edge pixels cropped, all pixels rescaled down to $[0, 1]$ and recentered around the mean value) and label each of them with $+1$ and -1 labels. We perform KRR with various ridge λ on this dataset with the selected kernel k times and calculate the MSE training error, risk, and the KARE for every trial ($k = 10$ for small N and $k = 5$ for $N = 2000$). The risk is approximated using other $N_2 = 1000$ random samples of the MNIST training data.

For the Higgs Dataset. We randomly choose N samples among those that do not have any missing features marked with -999 from the Higgs training dataset. The samples have $d = 31$ features, and we normalize each feature column down to $[0, 1]$ by dividing by the maximum absolute value observed among the selected samples. We replace the categorical labels 's' and 'b' with regression values $+1$ and -1 respectively and perform KRR with various ridge λ. We repeat this procedure k times, which corresponds to sampling k different training datasets of $N = 1000$ samples to perform kernel regression, and calculate the MSE training error, the risk, and the KARE for every trial ($k = 10$ for small N and $k = 5$ for $N = 1000$). The risk is approximated using other $N_2 = 1000$ random samples of the Higgs training data.

A.2 KARE predicts risk for various Kernels



(a) MNIST, $\ell = d$ (b) MNIST, $\lambda = 10^{-6}$ (c) Higgs, $\ell = d$ (d) Higgs, $\lambda = 10^{-5}$

(e) MNIST, $\ell = d$ (f) MNIST, $\lambda = 10^{-5}$ (g) Higgs, $\ell = d$ (h) Higgs, $\lambda = 10^{-5}$

Figure 4: Comparison between the KRR risk and the KARE for various choices of normalized lengthscale ℓ/d and ridge λ on the MNIST dataset (restricted to the digits 7 and 9, labeled by 1 and -1 respectively, $N = 2000$) and on the Higgs dataset (classes 'b' and 's', labeled by -1 and 1, $N = 1000$). We present the results for the Laplacian Kernel $K(x, x') = \exp(-\|x-x'\|_2/\ell)$ (top row) and the ℓ_1-norm Kernel $K(x, x') = \exp(-\|x-x'\|_1/\ell)$ (bottom row). KRR predictor risks, and KARE curves (shown as dashed lines, 5 samples) concentrate around their respective averages (solid lines).

A.3 KRR predictor in function space

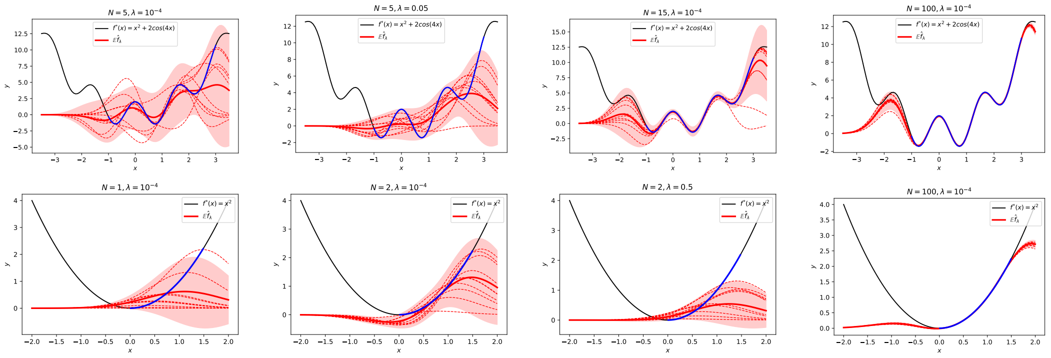
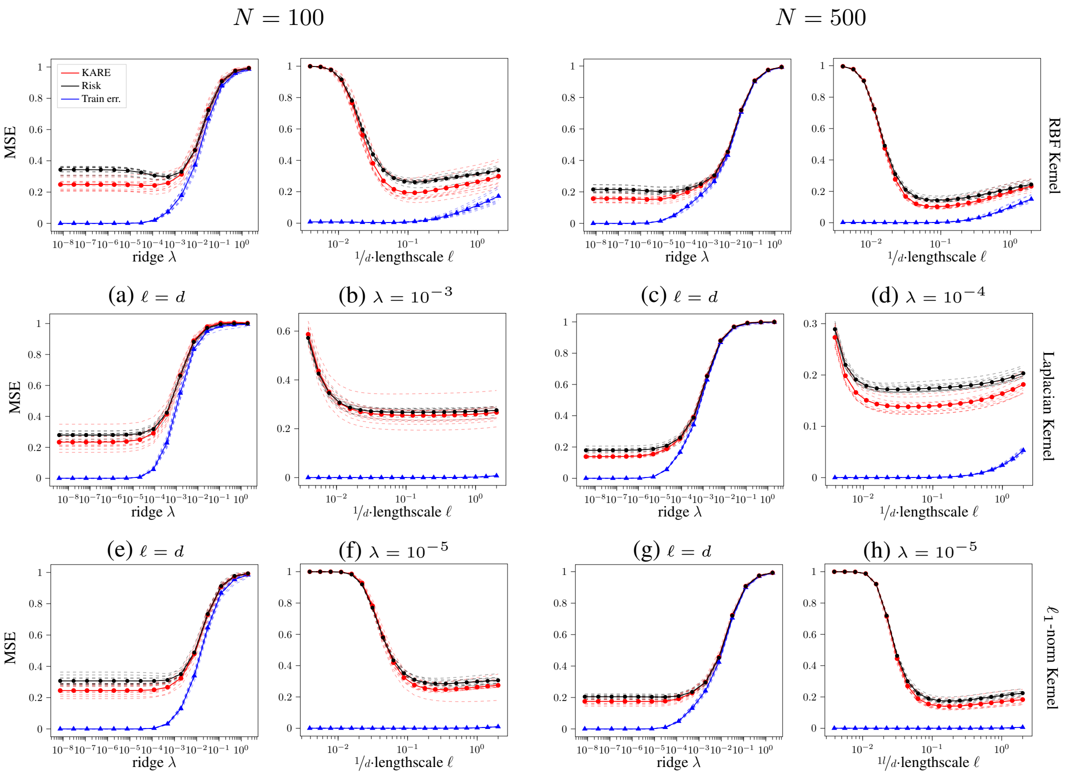


Figure 5: *KRR predictor in function space for various N and λ for the RBF Kernel K with $\ell = d = 1$.* Observations $o = \delta_x$ are sampled with uniform distribution on $x \sim U[-1, 3]$ (shown in blue) $\hat{f}_\lambda^\epsilon$ is calculated 500 times for different realizations of the training data (10 example predictors are shown in dashed lines), its mean and ± 2 standard deviation are shown in red. The true function $f^*(x) = x^2 + 2\cos(4x)$ is shown in black. *Second row.* Observations $o = \delta_x$ are sampled with uniform distribution $x \sim U[0, 1.5]$ (shown in blue) and $\hat{f}_\lambda^\epsilon$ is calculated 100 times. The true function $f^*(x) = x^2$ is shown in black.

A.4 KARE predicts risk in average for small N



(a) $\ell = d$ (b) $\lambda = 10^{-3}$ (c) $\ell = d$ (d) $\lambda = 10^{-4}$

(e) $\ell = d$ (f) $\lambda = 10^{-5}$ (g) $\ell = d$ (h) $\lambda = 10^{-5}$

(i) $\ell = d$ (j) $\lambda = 10^{-4}$ (k) $\ell = d$ (l) $\lambda = 10^{-5}$

Figure 6: *The estimation predicts the risk in average for small $N = \{100, 500\}$ on MNIST data.* In the top row, we used the RBF Kernel $K(x,z) = \exp(-\|x-z\|_2^2/\ell)$, in the second row, we used the Laplacian Kernel $K(x,z) = \exp(-\|x-z\|_2/\ell)$, and in the bottom row, we used the ℓ_1-norm Kernel $K(x,z) = \exp(-\|x-z\|_1/\ell)$ for various choices of ℓ and λ. The optimal predictor is calculated using N random samples ($N = 100$ for the plots on the left and $N = 500$ for the ones on the right) from the training data 10 times (dashed curves) and their average is plotted in the solid curves.

A.5 SCT and its behavior

In general, it is hard to compute the spectrum $(d_k)_{k\in\mathbb{N}}$ of T_K even when one has the knowledge of the true data distribution. Luckily, following an adaptation from [29, 11], we can obtain an explicit formula for d_k for centered d-dimensional Gaussian distribution with covariance matrix $\sigma^2 I_d$, and RBF Kernel $K(x,x') = \exp(-\|x-x'\|^2/\ell)$. The formula for the distinct eigenvalues λ_k is

$$\lambda_k = \left(\sqrt{\frac{1}{2A\sigma^2}}\right)^d B^k, \tag{3}$$

where $A = \frac{1}{4\sigma^2} + \frac{1}{\ell} + c$, $B = \frac{1}{A\ell}$ with $c = \frac{1}{2\sigma}\sqrt{\frac{1}{4\sigma^2} + \frac{2}{\ell}}$. Each λ_k has multiplicity

$$n_d(k) = \sum_{j=1}^{k} \binom{d}{j}\binom{k-1}{j-1} \tag{4}$$

for $k \geq 1$. In particular, we have $n_d(0) = 1, n_d(1) = \binom{d}{1}, n_d(2) = \binom{d}{2} + d, \ldots$. In general, $n_d(k)$ is the number of ways to partition k into d non-negative integers.

The true SCT is therefore approximated solving the following equation numerically

$$\vartheta = \lambda + \frac{\vartheta}{N}\sum_{i=1}^{k} \frac{n_d(k)\lambda_k}{\lambda_k + \vartheta}. \tag{5}$$

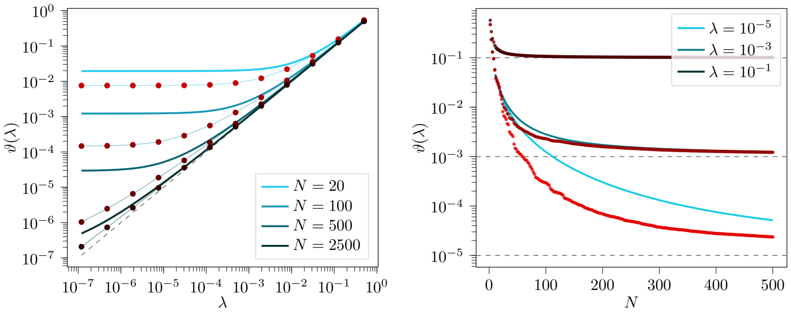


Figure 7: *Behavior of SCT as a function of* λ *and* N. True SCT is calculated on the $k = 50$ biggest distinct eigenvalues using the formula 5 for $\ell = d = 5$ and $\sigma = 1$. Red dots are the approximations obtained using Proposition 5 in the main text, i.e. $\vartheta \approx 1/\mathrm{Tr}[(\frac{1}{N}K(X,X) - \lambda I)^{-1}]$.

Note that in the Figure 2 in the main text, we limit the approximation to $k = 10$ for $d = 20$ because the multiplicity $n_d(k)$ grows polynomially with d^k.

B Proofs

Preliminary: Big-P notation

Throughout our proofs, we will frequently rely on a polynomial analogue of the big-O notation, which we call big-P:

Definition 5. *For two functions f and g (of one or several variables, defined on an arbitrary common domain $\mathcal{D}$), we write $f = \mathcal{P}(g)$ if g is nonnegative over $\mathcal{D}$ and there exists a polynomial $\mathbf{P}$ with nonnegative coefficients and $\mathbf{P}(0) = 0$ such that $|f| \leq \mathbf{P}(g)$ over $\mathcal{D}$.*

Note that the big-O notation corresponds to the case when the polynomial $\mathbf{P}$ is of degree at most one.

B.1 Objects of Interest and general strategy

The central object of our analysis is the $N \times N$ Gram matrix $\mathcal{O}K\mathcal{O}^T$, in particular the related Stieltjes transform:

$$m(z) = \frac{1}{N}\mathrm{Tr}\left[B(z)^{-1}\right]$$

where $B(z) = \frac{1}{N}\mathcal{O}K\mathcal{O}^T - zI_N$ and $z \in \mathbb{C} \setminus \mathbb{R}_+$.

From now on, we consider only $z \in \mathbb{H}_{<0} = \{z : \Re(z) < 0\}$. Note that $m(z) = \frac{1}{N}\sum_\ell \frac{1}{\lambda_\ell - z}$ where $\lambda_\ell \geq 0$ are the real eigenvalues of $\frac{1}{N}\mathcal{O}K\mathcal{O}^T$, hence $m(z)$ lies in the cone Γ spanned by 1 and $-1/z$, i.e. $\Gamma = \{a - b\frac{1}{z} | a, b \geq 0\}$. We will first show that for $z \in \mathbb{H}_{<0}$, the Stieltjes transform concentrates around the unique solution $\tilde{m}(z)$ to the equation

$$\tilde{m}(z) = -\frac{1}{z}\left(1 - \frac{1}{N}\mathrm{Tr}\left[\tilde{m}(z)T_K\left(I_\mathcal{C} + \tilde{m}(z)T_K\right)^{-1}\right]\right), \tag{6}$$

and then show that the linear map

$$A(z) = \frac{1}{N}K\mathcal{O}^T\left(\frac{1}{N}\mathcal{O}K\mathcal{O}^T - zI_N\right)^{-1}\mathcal{O} = \frac{1}{N}K\mathcal{O}^T B(z)^{-1}\mathcal{O}$$

concentrates around the map $\tilde{A}_{\vartheta(-z)} = T_K\left(T_K + \vartheta(-z)I_\mathcal{C}\right)^{-1}$, where $(T_K f)(x) = \mathbb{E}_{o\sim\pi}\left[o(K(x,\cdot))o(f)\right] = \langle K(x,\cdot), f\rangle_S$ and $\vartheta(-z) = \frac{1}{\tilde{m}(z)}$ is the Signal Capture Threshold. From Equation (6), the SCT can be also defined as the solution to the equation

$$\vartheta(-z) = -z + \frac{\vartheta(-z)}{N}\mathrm{Tr}\left[T_K\left(T_K + \vartheta(-z)I_\mathcal{C}\right)^{-1}\right]. \tag{7}$$

From now on, we denote $\vartheta(-z)$ by ϑ. Note that here, in the Appendix, we use the resolvent notation: in particular the KRR reconstruction operator A_λ is equal to $A(-\lambda)$.

B.1.1 Spectral decomposition and generalized matrix representation

Throughout this paper it is assumed that there exists an orthonormal basis of continuous functions $\left(f^{(k)}\right)_k$ for the scalar product $\langle\cdot,\cdot\rangle_S$ such that $K = \sum_{k\in\mathbb{N}} d_k f^{(k)} \otimes f^{(k)}$ and $\sum_{k\in\mathbb{N}} d_k < \infty$. For a linear map $M : \mathcal{C} \to \mathcal{C}$, we define the $(k,\ell)-$entry of M as:

$$M_{k\ell} = \left\langle f^{(k)}, Mf^{(\ell)}\right\rangle_S.$$

With this notation, the trace of a linear map M becomes $\mathrm{Tr}\,(M) = \sum_{k\in\mathbb{N}} M_{kk}$.

Similarly, using the canonical basis $(b_i)_{i=1,\dots,N}$ of $\mathbb{R}^N$, we define the entries of $\mathcal{O} : \mathcal{C} \to \mathbb{R}^N$ and $\mathcal{O}^T : \mathbb{R}^N \to \mathcal{C}^*$ by

$$\mathcal{O}_{ik} = b_i \cdot \mathcal{O}f^{(k)} = o_i(f^{(k)}), \quad \mathcal{O}^T_{ik} = \mathcal{O}^T b_k(f^{(i)}) = b_k \cdot \mathcal{O}f^{(i)} = o_k(f^{(i)}).$$

Since the observations o_i are i.i.d. Gaussians with zero mean and covariance $\mathbb{E}\left[o_i(f)o_i(g)\right] = \langle f, g\rangle_S$ and since $\left(f^{(k)}\right)_k$ is an orthonormal basis for the scalar product $\langle\cdot,\cdot\rangle_S$, the entries $\mathcal{O}_{ik}$ are i.i.d standard Gaussians.

Using the spectral decomposition of K, the entries of $\mathcal{O}K\mathcal{O}^T$ are given by:

$$\left(\mathcal{O}K\mathcal{O}^T\right)_{i,j} = \sum_{\ell} d_\ell o_i(f^{(\ell)}) o_j(f^{(\ell)}),$$

where the sum converges absolutely (thanks to the trace assumption on K) and the entries of A are then given by:

$$A_{k\ell}(z) = \frac{d_k}{N} \left(\mathcal{O}_{\cdot k}\right)^T \left(\frac{1}{N}\mathcal{O}K\mathcal{O}^T - zI_N\right)^{-1} \mathcal{O}_{\cdot \ell} \tag{8}$$

where $\mathcal{O}_{\cdot k} = \left(o_i(f^{(k)})\right)_{i=1,\dots,N}$.

B.1.2 Shermann-Morrison Formula

The Shermann-Morrison formula allows one to study how the inverse of a matrix is modified by a rank one perturbation of the matrix. The matrix $\mathcal{O}K\mathcal{O}^T$ can be seen as a perturbation of $\mathcal{O}K_{(k)}\mathcal{O}^T$ by the rank one matrix $d_k \mathcal{O}_{\cdot k}\mathcal{O}_{\cdot k}^T$, where $K_{(k)} := \sum_{\ell \neq k} d_\ell f^{(\ell)} \otimes f^{(\ell)}$. By doing so, one isolates the contribution of the k-th eigenvalue of K. Thus, one can compute $B(z)^{-1} = \left(\frac{1}{N}\mathcal{O}K\mathcal{O}^T - zI_N\right)^{-1}$ using the Shermann-Morrison formula:

$$B(z)^{-1} = B_{(k)}(z)^{-1} - \frac{1}{N}\frac{d_k}{1 + d_k g_k(z)} B_{(k)}(z)^{-1}\mathcal{O}_{\cdot k}\mathcal{O}_{\cdot k}^T B_{(k)}(z)^{-1} \tag{9}$$

where $B_{(k)}(z) = \frac{1}{N}\mathcal{O}K_{(k)}\mathcal{O}^T - zI_N$ and $g_k(z) = \frac{1}{N}\mathcal{O}_{\cdot k}^T B_{(k)}(z)^{-1}\mathcal{O}_{\cdot k}$. A crucial property is that, since $o_i\left(f^{(k)}\right)$ does not appear anymore in $\mathcal{O}K_{(k)}\mathcal{O}^T$ and, since for any $\ell \neq k$ and any i, j, we have that $o_i\left(f^{(k)}\right)$ is independent from $o_j(f^{(\ell)})$, we obtain that the matrix $B_{(k)}(z)^{-1}$ is independent of $\mathcal{O}_{\cdot k}$.

Remark. *Using the diagonalization of $B_{(k)}(z)^{-1} = U^T \operatorname{diag}\left(\frac{1}{\nu_\ell - z}\right) U$ with U orthogonal and $\nu_\ell \geq 0$, we have that $g_k(z) = \frac{1}{N}\sum_\ell \frac{\left[\sum_i U_{\ell,i} o_i(f^{(k)})\right]^2}{\nu_\ell - z}$ lies in the cone spanned by 1 and $-1/z$, in particular, $\Re(g_k) \geq 0$ on $\mathbb{H}_{<0}$.*

As a result of Equations (8) and (9), the diagonal entries of the operator $A(z) = \frac{1}{N}K\mathcal{O}^T B(z)^{-1}\mathcal{O}$ are equal to

$$A_{kk}(z) = \frac{d_k g_k(z)}{1 + d_k g_k(z)}. \tag{10}$$

Remark. *For any $z \in \mathbb{H}_{<0}$, the sum $\sum_k |A_{kk}(z)|$ is almost surely finite. Indeed, notice that*

$$\left|\frac{d_k g_k(z)}{1 + d_k g_k(z)}\right| \leq |d_k g_k(z)| \leq \frac{1}{N} d_k \left\|\mathcal{O}_{\cdot k}\right\|^2 \left\|B_{(k)}(z)^{-1}\right\|_{\mathrm{op}}.$$

For any $z \in \mathbb{H}_{<0}$, $\left\|B_{(k)}(z)^{-1}\right\|_{\mathrm{op}} \leq \frac{1}{|z|}$ and thus

$$\left|\frac{d_k g_k(z)}{1 + d_k g_k(z)}\right| \leq \frac{1}{N|z|} d_k \left\|\mathcal{O}_{\cdot k}\right\|^2.$$

Since $\mathbb{E}\left[\sum_k d_k \left\|\mathcal{O}_{\cdot k}\right\|^2\right] = N\mathrm{Tr}[T_K] < \infty$, we have that $\sum_k |A_{kk}(z)|$ is almost surely finite.

The operator A is therefore a.s. trace-class and $\mathrm{Tr}(A) = \sum_k \frac{d_k g_k(z)}{1 + d_k g_k(z)}$, where the sum is absolutely convergent.

Another important observation is that the Stieltjes transform $m(z)$ and the $g_k(z)$ are closely related.

Lemma 8. *For any $z \in \mathbb{H}_{<0}$, a.s. we have*

$$m(z) = -\frac{1}{z}\left(1 - \frac{1}{N}\sum_{k=1}^{\infty}\frac{d_k g_k(z)}{1 + d_k g_k(z)}\right). \tag{11}$$

Proof. Indeed, using the trivial relation $\mathrm{Tr}\left[B(z)B(z)^{-1}\right] = N$, expanding $B(z)$, we obtain $\mathrm{Tr}\left[\frac{1}{N}\mathcal{O}K\mathcal{O}^T B(z)^{-1}\right] - z\mathrm{Tr}\left[B(z)^{-1}\right] = N$. Since $\mathcal{O}$ is an operator from $\mathcal{C}$ to $\mathbb{R}^N$, which is a finite dimensional space, we can apply the cyclic property of the trace and obtain $\mathrm{Tr}\left[\frac{1}{N}\mathcal{O}K\mathcal{O}^T B(z)^{-1}\right] = \mathrm{Tr}\left[A(z)\right]$. Thus,

$$\mathrm{Tr}\left[A(z)\right] - z\mathrm{Tr}\left[B(z)^{-1}\right] = N.$$

Dividing both sides by N and using Equation (10), we obtain

$$1 = \frac{1}{N}\sum_{k=1}^{\infty}\frac{d_k g_k(z)}{1 + d_k g_k(z)} - zm(z),$$

hence the result. □

B.2 Concentration of the Stieltjes Transform

We will now show that $g_k(z) = \frac{1}{N}\mathcal{O}_{\cdot k}^T B_{(k)}(z)^{-1}\mathcal{O}_{\cdot k}$ is close to $\frac{1}{N}\mathrm{Tr}\left(B_{(k)}(z)^{-1}\right)$, as suggested by the fact that by Wick's formula $\mathbb{E}[g_k] = \frac{1}{N}\mathrm{Tr}\left(\mathbb{E}\left[B_{(k)}(z)^{-1}\right]\right)$. Since $B(z)$ is obtained using a rank one permutation of $B_{(k)}(z)$, $\frac{1}{N}\mathrm{Tr}\left(B_{(k)}(z)^{-1}\right)$ is close to the Stieltjes transform m. As a result, all the g_k's are close to the Stieltjes transform m: it is natural to think that for $z \in \mathbb{H}_{<0}$, both $g_k(z)$'s and $m(z)$ should concentrate around the unique solution $\tilde{m}(z)$ in the cone spanned by 1 and $-1/z$ of the equation

$$\tilde{m}(z) = -\frac{1}{z}\left(1 - \frac{1}{N}\sum_{k=1}^{\infty}\frac{d_k\tilde{m}(z)}{1 + d_k\tilde{m}(z)}\right). \tag{12}$$

Remark. *The existence and the uniqueness of the solution in the cone spanned by 1 and $-1/z$ of the equation can be argued as follows. If in Equation (12) we truncate the series and consider the sum of the first M terms, one can show that there exists a unique fixed point $\tilde{m}_M(z)$ in the region R given by intersection between the cone spanned by 1 and $-1/z$ and the cone spanned by z and $1/z$ translated by $+1$ and multiplied by $-1/z$ (see Lemma C.6 in the Supplementary Material of [14]). Since R is a compact region, we can extract a converging subsequence that solves Equation (12), the limit of which can be showed to be unique, again using the same arguments of Lemma C.6 in the Supplementary Material of [14].*

From now on we omit the z dependence and we set $m = m(z)$, $\tilde{m} = \tilde{m}(z)$ and $g_k(z) = g_k$.

B.2.1 Concentration bounds

Using Equation 11 and the definition of the fixed point $\tilde{m}$ (Equation 12), we obtain the following formula for the difference between the Stieltjes transform m and $\tilde{m}$:

$$\begin{aligned}\tilde{m} - m &= \frac{1}{z}\frac{1}{N}\sum_{k=1}^{\infty}\frac{d_k\left(\tilde{m} - g_k\right)}{(1 + d_k\tilde{m})(1 + d_k g_k)}\\ &= \frac{\tilde{m} - m}{z}\frac{1}{N}\sum_{k=1}^{\infty}\frac{d_k}{(1 + d_k\tilde{m})(1 + d_k g_k)} + \frac{1}{z}\frac{1}{N}\sum_{k=1}^{\infty}\frac{d_k\left(m - g_k\right)}{(1 + d_k\tilde{m})(1 + d_k g_k)},\end{aligned}$$

where the well-posedness of the two infinite sums of the r.h.s is granted by the fact that:

1. $\left|\frac{d_k}{(1+d_k\tilde{m})(1+d_k g_k)}\right| \leq d_k$ since $\Re\left(\tilde{m}\right), \Re(g_k)$ are positive, thus the first sum is absolutely convergent,
2. being the difference of two absolutely convergent series, the second sum is also absolutely convergent.

As a consequence, the difference $\tilde{m} - m$ can be expressed as

$$\tilde{m} - m = \frac{\frac{1}{N}\sum_{k=1}^{\infty}\frac{d_k(m - g_k)}{(1+d_k\tilde{m})(1+d_k g_k)}}{z - \frac{1}{N}\sum_{k=1}^{\infty}\frac{d_k}{(1+d_k\tilde{m})(1+d_k g_k)}}, \tag{13}$$

which allows us to show the concentration of m around $\tilde{m}$ from the concentration of g_k around m.

Regarding the concentration of the g_k's around m, we have the following result:

Lemma 9. *For any $N, s \in \mathbb{N}$ and any $z \in \mathbb{H}_{<0}$, we have*

$$\begin{aligned} \mathbb{E}\left[\left|m - g_k\right|^{2s}\right] &\leq \frac{\boldsymbol{c}_s}{|z|^{2s} N^s}, \\ \mathbb{E}\left[\left|m - m_{(k)}\right|^{2s}\right] &\leq \frac{1}{|z|^{2s} N^{2s}}. \end{aligned}$$

where $\boldsymbol{c}_s$ only depends on s.

Proof. The second inequality will be proven while proving the first one. Let $m_{(k)} = \frac{1}{N}\mathrm{Tr}\left[B_{(k)}^{-1}\right]$ where $B_{(k)}$ was defined in Section B.1.2. By convexity:

$$\mathbb{E}\left[\left|m - g_k\right|^{2s}\right] \leq 2^{2s-1}\mathbb{E}\left[\left|m - m_{(k)}\right|^{2s}\right] + 2^{2s-1}\mathbb{E}\left[\left|m_{(k)} - g_k\right|^{2s}\right]. \tag{14}$$

Bound on $\mathbb{E}[|m - m_{(k)}|^{2s}]$: We obtain the bound on the expectation by showing that a deterministic bound holds for the random variable $|m - m_{(k)}|^{2s}$. Using the Sherman-Morrison formula (Equation (9)), and using the cyclic property of the trace,

$$m = m_{(k)} - \frac{1}{N}\frac{d_k g_k'}{1 + d_k g_k}$$

since the derivative $g_k'(z)$ of $g_k(z)$ is equal to $\frac{1}{N}\mathcal{O}_{\cdot k}^T B(z)^{-2}\mathcal{O}_{\cdot k}$. As a result, we obtain $\left|m - m_{(k)}\right|^{2s} = \frac{1}{N^{2s}}\frac{d_k^{2s}\left|g_k'\right|^{2s}}{|1+d_k g_k|^{2s}}$. Using the fact that $|1 + d_k g_k| \geq |d_k g_k|$ since $\Re\left(g_k\right) \geq 0$,

$$\left|m - m_{(k)}\right|^{2s} \leq \frac{1}{N^{2s}}\frac{\left|g_k'\right|^{2s}}{\left|g_k\right|^{2s}}.$$

Notice now that

$$\left|\frac{g_k'}{g_k}\right| = \left|\frac{\mathcal{O}_{\cdot k}^T B_{(k)}(z)^{-2}\mathcal{O}_{\cdot k}}{\mathcal{O}_{\cdot k}^T B_{(k)}(z)^{-1}\mathcal{O}_{\cdot k}}\right| \leq \max_{w\in\mathbb{R}^N}\left|\frac{w^T B_{(k)}(z)^{-2} w}{w^T B_{(k)}(z)^{-1} w}\right| \leq \left\|B_{(k)}(z)^{-1}\right\|_{\mathrm{op}}.$$

The eigenvalues of $B_{(k)}(z)^{-1}$ are given by $\frac{1}{\lambda_i - z}$ where the $\lambda_i > 0$ are the eigenvalues of the symmetric matrix $\frac{1}{N}\mathcal{O}K_{(k)}\mathcal{O}^T$: $\left\|B_{(k)}(z)^{-1}\right\|_{\mathrm{op}} \leq \max_i \frac{1}{|\lambda_i - z|}$ is also bounded by $\frac{1}{|z|}$ if $z \in \mathbb{H}_{<0}$. Thus we get

$$\left|m - m_{(k)}\right|^{2s} \leq \frac{1}{|z|^{2s} N^{2s}}.$$

Bound on $\mathbb{E}[|m_{(k)} - g_k|^{2s}]$: The term $\mathbb{E}\left[\left(\left(m_{(k)} - g_k\right)\overline{\left(m_{(k)} - g_k\right)}\right)^s\right]$ is equal to

$$\mathbb{E}\left[\left(\left(\frac{1}{N}\mathrm{Tr}\left[B_{(k)}^{-1}\right] - \frac{1}{N}\mathcal{O}_{\cdot k}^T B_{(k)}^{-1}\mathcal{O}_{\cdot k}\right)\left(\frac{1}{N}\mathrm{Tr}\left[\overline{B_{(k)}^{-1}}\right] - \frac{1}{N}\mathcal{O}_{\cdot k}^T\overline{B_{(k)}^{-1}}\mathcal{O}_{\cdot k}\right)\right)^s\right].$$

Let $\boldsymbol{B} = \left(B_{(k)}, \overline{B_{(k)}}, \ldots, B_{(k)}, \overline{B_{(k)}}\right)$ and let us denote by $\boldsymbol{B}(i)$ the i^{th} element of $\boldsymbol{B}$. Using Wick's formula (Lemma 26), we have

$$\mathbb{E}\left[\left|m_{(k)} - g_k\right|^{2s}\right] = \frac{1}{N^s}\sum_{\sigma\in\mathfrak{S}_{2s}^\dagger}\frac{1}{N^{s-\boldsymbol{c}(\sigma)}}2^{2s-\boldsymbol{c}(\sigma)}\mathbb{E}\left[\prod_{c\text{ cycle of }\sigma}\frac{1}{N}\mathrm{Tr}\left[\prod_{i\in c}\boldsymbol{B}(i)\right]\right],$$

where we recall that $\mathfrak{S}_{2s}^\dagger$ is the set of permutations with no fixed points and the product over i is taken according to the order given by the cycle c and does not depend on the starting point. Using the fact that the eigenvalues of $B_{(k)}$ are of the form $1/(\lambda_i - z)$ with $\lambda_i \geq 0$,

$$\left|\frac{1}{N}\mathrm{Tr}\left[\prod_{i\in c}\boldsymbol{B}(i)\right]\right| \leq \frac{1}{|z|^{\#c}}.$$

Hence,

$$\mathbb{E}\left[\left|m_{(k)} - g_k\right|^{2s}\right] \leq \frac{1}{N^s}\frac{1}{|z|^{2s}} \sum_{\sigma \in \mathfrak{S}_{2s}^{\dagger}} \frac{2^{2s-\boldsymbol{c}(\sigma)}}{N^{s-\boldsymbol{c}(\sigma)}}.$$

Note that, since $\sigma \in \mathfrak{S}_{2s}^{\dagger}$, it has no fixed point, hence $\boldsymbol{c}(\sigma) \leq s$ and thus $K_s := \sup_N \sum_{\sigma \in \mathfrak{S}_{2s}^{\dagger}} \frac{2^{2s-\boldsymbol{c}(\sigma)}}{N^{s-\boldsymbol{c}(\sigma)}}$ is finite. This yields the inequality

$$\mathbb{E}\left[\left|m_{(k)} - g_k\right|^{2s}\right] \leq \frac{K_s}{|z|^{2s} N^s}.$$

Using the two bounds on $\mathbb{E}\left[\left|m - m_{(k)}\right|^{2s}\right]$ and $\mathbb{E}\left[\left|m_{(k)} - g_k\right|^{2s}\right]$ in Equation (14), we get

$$\mathbb{E}\left[|m - g_k|^{2s}\right] \leq \frac{\boldsymbol{c}_s}{|z|^{2s} N^s},$$

where $\boldsymbol{c}_s = 2^{2s-1}\left[1 + K_s\right]$. □

As a result, we can show the concentration of the Stieltjes transform m and of the g_k's around the fixed point $\tilde{m}$:

Proposition 10. *For any $N, s \in \mathbb{N}$, and any $z \in \mathbb{H}_{<0}$, we have*

$$\mathbb{E}\left[|\tilde{m} - m|^{2s}\right] \leq \frac{\boldsymbol{c}_s \left(\operatorname{Tr}[T_K]\right)^{2s}}{|z|^{4s} N^{3s}},$$

$$\mathbb{E}\left[|\tilde{m} - g_k|^{2s}\right] \leq \frac{2^{2s-1}\boldsymbol{c}_s \left(\operatorname{Tr}[T_K]\right)^{2s}}{|z|^{4s} N^{3s}} + \frac{2^{2s-1}\boldsymbol{c}_s}{|z|^{2s} N^s}.$$

where $\mathbf{c}_s$ is the same constant as in Lemma 9.

Proof. The second bound is a direct consequence of the first one, Lemma 9 and convexity. It remains to prove the first bound. Recall Equation (13)

$$\tilde{m} - m = \frac{\frac{1}{N}\sum_{k=1}^{\infty} \frac{d_k(m-g_k)}{(1+d_k\tilde{m})(1+d_k g_k)}}{z - \frac{1}{N}\sum_{k=1}^{\infty} \frac{d_k}{(1+d_k\tilde{m})(1+d_k g_k)}}.$$

We first bound from below the norm of the denominator using Lemma 29: since $\tilde{m}$ and g_k all lie in the cone spanned by 1 and $-1/z$ we have

$$\left| z - \frac{1}{N}\sum_{k=1}^{\infty} \frac{d_k}{(1+d_k\tilde{m})(1+d_k g_k)} \right| \geq |z|.$$

Using this bound, we can bound from below $\mathbb{E}\left[|\tilde{m} - m|^{2s}\right]$ by:

$$\frac{1}{|z|^{2s} N^{2s}} \sum_{k_1,\dots,k_{2s}=1}^{\infty} \frac{d_{k_1}\cdots d_{k_{2s}}}{|1+d_{k_1}\tilde{m}|\cdots|1+d_{k_{2s}}\tilde{m}|} \mathbb{E}\left[|m - g_{k_1}|\cdots|m - g_{k_{2s}}|\right],$$

and hence, using a generalization of Cauchy-Schwarz inequality (Lemma 28), by:

$$\frac{1}{|z|^{2s} N^{2s}} \sum_{k_1,\dots,k_{2s}=1}^{\infty} \frac{d_{k_1}\cdots d_{k_{2s}}}{|1+d_{k_1}\tilde{m}|\cdots|1+d_{k_{2s}}\tilde{m}|} \left(\mathbb{E}\left[|m - g_{k_1}|^{2s}\right]\cdots\mathbb{E}\left[|m - g_{k_{2s}}|^{2s}\right]\right)^{\frac{1}{2s}}.$$

Using the fact that $\Re(\tilde{m}) \geq 0$ and hence $|1 + d_{k_1}\tilde{m}| \geq 1$, and using Lemma 9, this gives the following upper bound:

$$\mathbb{E}\left[|m - g_k|^{2s}\right] \leq \frac{\boldsymbol{c}_s}{|z|^{4s} N^{3s}} \left(\operatorname{Tr}[T_K]\right)^{2s}.$$

□

We now give tighter bounds for $|\tilde{m} - \mathbb{E}[m]|$ and $|\tilde{m} - \mathbb{E}[g_k]|$:

Proposition 11. *For any $N \in \mathbb{N}$ and any $z \in \mathbb{H}_{<0}$, we have*

$$\begin{aligned} |\tilde{m} - \mathbb{E}[m]| &\leq \frac{\mathrm{Tr}[T_K]}{|z|^2 N^2} + \frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^2}{|z|^3 N^2} + \frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^4}{|z|^5 N^4}, \\ |\tilde{m} - \mathbb{E}[g_k]| &\leq \frac{1}{|z| N} + \frac{\mathrm{Tr}[T_K]}{|z|^2 N^2} + \frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^2}{|z|^3 N^2} + \frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^4}{|z|^5 N^4}, \end{aligned}$$

where $\boldsymbol{c}_1$ is the constant in Lemma 9.

Proof. **First bound:** Following similar ideas to the one which provided Equation (13), notice that

$$\begin{aligned} \tilde{m} - m &= \frac{1}{z}\frac{1}{N}\sum_{k=1}^{\infty} \frac{d_k\left(\tilde{m} - g_k\right)}{(1 + d_k\tilde{m})(1 + d_k g_k)} \\ &= \frac{1}{z}\frac{1}{N}\sum_{k=1}^{\infty} \frac{d_k\left(\tilde{m} - g_k\right)}{(1 + d_k\tilde{m})^2} + \frac{1}{z}\frac{1}{N}\sum_{k=1}^{\infty} \frac{d_k^2\left(\tilde{m} - g_k\right)^2}{(1 + d_k\tilde{m})^2(1 + d_k g_k)} \\ &= \frac{\tilde{m} - m}{z}\frac{1}{N}\sum_{k=1}^{\infty} \frac{d_k}{(1 + d_k\tilde{m})^2} + \frac{1}{z}\frac{1}{N}\sum_{k=1}^{\infty} \frac{d_k\left(m - g_k\right)}{(1 + d_k\tilde{m})^2} + \frac{1}{z}\frac{1}{N}\sum_{k=1}^{\infty} \frac{d_k^2\left(\tilde{m} - g_k\right)^2}{(1 + d_k\tilde{m})^2(1 + d_k g_k)}, \end{aligned}$$

hence the new identity:

$$\tilde{m} - m = \frac{\frac{1}{N}\sum_{k=1}^{\infty} \frac{d_k(m - g_k)}{(1 + d_k\tilde{m})^2} + \frac{1}{N}\sum_{k=1}^{\infty} \frac{d_k^2(\tilde{m} - g_k)^2}{(1 + d_k\tilde{m})^2(1 + d_k g_k)}}{z - \frac{1}{N}\sum_{k=1}^{\infty} \frac{d_k}{(1 + d_k\tilde{m})^2}}.$$

Again, using Lemma 29, the norm of the denominator is bounded from below by $|z|$. From Lemma 26, $\mathbb{E}[g_k] = \mathbb{E}\left[m_{(k)}\right]$, and thus from Lemma 9, $|\mathbb{E}[m - g_k]| \leq \mathbb{E}\left[\left|m - m_{(k)}\right|\right] \leq \frac{1}{|z| N}$. Furthermore, from Proposition 10, $\mathbb{E}\left[\left|g_k - \tilde{m}\right|^2\right] \leq \frac{2\boldsymbol{c}_1 (\mathrm{Tr}[T_K])^2}{|z|^4 N^3} + \frac{2\boldsymbol{c}_1}{|z|^2 N}$. Thus, the expectation of the numerator is bounded by

$$\frac{1}{|z| N^2}\sum_{k=1}^{\infty} \frac{d_k}{\left|1 + d_k\tilde{m}\right|^2} + \left(\frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^2}{|z|^4 N^4} + \frac{2\boldsymbol{c}_1}{|z|^2 N^2}\right)\sum_{k=1}^{\infty} \frac{d_k^2}{\left|1 + d_k\tilde{m}\right|^2}.$$

Hence, using again the inequality $|1 + d_k\tilde{m}| \geq 1$, it is bounded by

$$\frac{\mathrm{Tr}[T_K]}{|z| N^2} + \frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^2}{|z|^2 N^2} + \frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^4}{|z|^4 N^4}.$$

This allows us to conclude that

$$|\tilde{m} - \mathbb{E}[m]| \leq \frac{\mathrm{Tr}[T_K]}{|z|^2 N^2} + \frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^2}{|z|^3 N^2} + \frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^4}{|z|^5 N^4}.$$

Second bound: Since $\mathbb{E}[g_k] = \mathbb{E}\left[m_{(k)}\right]$, one has

$$|\tilde{m} - \mathbb{E}[g_k]| \leq \left|\tilde{m} - \tilde{m}_{(k)}\right| + \left|\tilde{m}_{(k)} - \mathbb{E}\left[m_{(k)}\right]\right|,$$

where $\tilde{m}_{(k)}$ is the unique solution in the cone spanned by 1 and $-1/z$ to the equation

$$\tilde{m}_{(k)} = -\frac{1}{z}\left(1 - \frac{1}{N}\sum_{m \neq k}^{\infty} \frac{d_m \tilde{m}_{(k)}}{1 + d_m \tilde{m}_{(k)}}\right).$$

From Lemma 30, $\left|\tilde{m} - \tilde{m}_{(k)}\right| \leq \frac{1}{|z| N}$. The second term $\left|\tilde{m}_{(k)} - \mathbb{E}\left[m_{(k)}\right]\right|$ is bounded by applying the first bound of this proposition to the Stieltjes transform $m_{(k)}$. As a result, we obtain

$$|\tilde{m} - \mathbb{E}[g_k]| \leq \frac{1}{|z| N} + \frac{\mathrm{Tr}[T_K]}{|z|^2 N^2} + \frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^2}{|z|^3 N^2} + \frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^4}{|z|^5 N^4}.$$

□

B.3 Properties of the effective dimension and SCT

B.3.1 General properties

We begin with general properties on the Signal Capture Threshold ϑ (which depends on λ, N and on the eigenvalues d_k of T_K), valid for any kernel K.

Proposition 12. *For any $\lambda > 0$, we have*

$$\lambda < \vartheta(\lambda, N) \leq \lambda + \frac{1}{N}\mathrm{Tr}[T_K], \qquad 1 \leq \partial_\lambda \vartheta(\lambda, N) \leq \frac{1}{\lambda}\vartheta(\lambda, N),$$

moreover $\vartheta(\lambda, N)$ is decreasing as a function of N and $\partial_\lambda\vartheta(\lambda, N)$ is decreasing as a function of λ.

Proof. Let $\lambda > 0$.

1. Recall that $\vartheta(\lambda)$ is the unique positive real number such that

$$\vartheta(\lambda) = \lambda + \frac{\vartheta(\lambda)}{N}\mathrm{Tr}\left[T_K\left(T_K + \vartheta(\lambda)I_{\mathcal{C}}\right)^{-1}\right].$$

   Since T_K is a positive operator, $\mathrm{Tr}\left[T_K\left(T_K + \vartheta(\lambda)I_{\mathcal{C}}\right)^{-1}\right] \geq 0$ and thus $\vartheta(\lambda) \geq \lambda$. Moreover, $T_K + \vartheta(\lambda)I_{\mathcal{C}} \geq \vartheta(\lambda)I_{\mathcal{C}}$, thus

$$T_K\left(T_K + \vartheta(\lambda)I_{\mathcal{C}}\right)^{-1} \leq \frac{T_K}{\vartheta(\lambda)}$$

   and thus $\vartheta(\lambda) \leq \lambda + \frac{1}{N}\mathrm{Tr}\left[T_K\right]$, which gives the desired inequality.

2. Differentiating Equation (7), the derivative $\partial_\lambda\vartheta(\lambda)$ is given by:

$$\partial_\lambda\vartheta(\lambda) = \frac{1}{\left(1 - \frac{1}{N}\mathrm{Tr}\left[\left(T_K\left(T_K + \vartheta(\lambda)I_{\mathcal{C}}\right)^{-1}\right)^2\right]\right)}. \tag{15}$$

   Using the fact that $T_K\left(T_K + \vartheta(\lambda)I_{\mathcal{C}}\right)^{-1} \leq I_{\mathcal{C}}$, one has

$$\left(T_K\left(T_K + \vartheta(\lambda)I_{\mathcal{C}}\right)^{-1}\right)^2 \leq T_K\left(T_K + \vartheta(\lambda)I_{\mathcal{C}}\right)^{-1},$$

   thus $0 \leq \frac{1}{N}\mathrm{Tr}\left[\left(T_K\left(T_K + \vartheta(\lambda)I_{\mathcal{C}}\right)^{-1}\right)^2\right] \leq \frac{1}{N}\mathrm{Tr}\left[T_K\left(T_K + \vartheta(\lambda)I_{\mathcal{C}}\right)^{-1}\right]$. Using Equation (7), $\frac{1}{N}\mathrm{Tr}\left[T_K\left(T_K + \vartheta(\lambda)I_{\mathcal{C}}\right)^{-1}\right] = 1 - \frac{\lambda}{\vartheta(\lambda)}$. This yields

$$0 \leq \frac{\lambda}{\vartheta(\lambda)} \leq 1 - \frac{1}{N}\mathrm{Tr}\left[\left(T_K\left(T_K + \vartheta(\lambda)I_{\mathcal{C}}\right)^{-1}\right)^2\right] \leq 1.$$

   Inverting this inequality yields the desired inequalities.

3. In order to study the variation of $\vartheta(\lambda, N)$ as a function of N, we take the derivatives of Equation (7) w.r.t λ and N, and notice that

$$\partial_N\vartheta(\lambda, N) = \frac{1}{N}(\lambda - \vartheta)\partial_\lambda\vartheta(\lambda, N).$$

   In particular, since $\vartheta > \lambda$ and $\partial_\lambda\vartheta \geq 1$, we get that $\partial_N\vartheta(\lambda, N) < 0$ hence $\vartheta(\lambda, N)$ is decreasing as a function of N.

4. Finally, we conclude by noting that since $\partial_\lambda\vartheta(\lambda, N) > 0$, $\vartheta(\lambda, N)$ is an increasing function of λ and thus, from the Equation (15) we have that $\partial_\lambda\vartheta(\lambda, N)$ is decreasing as a function of ϑ and thus as a function of λ.

□

B.3.2 Bounds under polynomial decay hypothesis

In this subsection only, we assume that $d_k = \Theta(k^{-\beta})$ with $\beta > 1$, i.e, there exist c_ℓ and c_h positive such that for any $k \geq 1$, $c_\ell k^{-\beta} \leq d_k \leq c_h k^{-\beta}$. We first study the asymptotic behavior of $\vartheta(0, N)$ and $\partial_\lambda \vartheta(0, N)$ as N goes to infinity, then using these results, we investigate the asymptotic behavior of $\vartheta(\lambda, N)$ and $\partial_\lambda \vartheta(\lambda, N)$ as N goes to infinity.

For any $t \in \mathbb{R}^+$, let $\mathcal{N}(t)$ denote the t-effective dimension [30, 6] defined by

$$\mathcal{N}(t) := \sum_{k=1}^{\infty} \frac{d_k}{t + d_k}.$$

For any $\lambda > 0$, the SCT is the unique solution of $\vartheta\left(\lambda, N\right) = \lambda + \frac{\vartheta(\lambda, N)}{N} \mathcal{N}(\vartheta(\lambda, N))$. In particular, $\vartheta(0, N)$ is the unique solution of $\mathcal{N}(\vartheta(0, N)) = N$.

Since $\mathcal{N}(t)$ is decreasing from ∞ to 0, in order to study the asymptotic behavior of $\vartheta(0, N)$ as N goes to infinity, one has to understand the rate of explosion of $\mathcal{N}(t)$ as t goes to zero.

Lemma 13. *If $d_k = \Theta(k^{-\beta})$ with $\beta > 1$, then $\mathcal{N}(t) = \Theta(t^{-\frac{1}{\beta}})$ when $t \to 0$.*

Proof. For any $m \in \mathbb{R}_+$, $\mathcal{N}(t) = \sum_{k \leq m} \frac{d_k}{t + d_k} + \sum_{k>m}^{\infty} \frac{d_k}{t + d_k} \leq m + t^{-1} \sum_{k>m} d_k$. Then there exists $c, d > 0$ such that $\sum_{k>m} d_k \leq c \sum_{k>m} k^{-\beta} \leq d m^{1-\beta}$. Thus $\mathcal{N}(t)$ is bounded by $m + d t^{-1} m^{1-\beta}$ for any m. Taking $m = t^{-1} m^{1-\beta}$, i.e. $m = t^{-\frac{1}{\beta}}$, one gets that $\mathcal{N}(t) \leq C t^{-\frac{1}{\beta}}$.

For the lower bound, notice that $\mathcal{N}(t) \geq \sum_{k | d_k \geq t} \frac{d_k}{t + d_k} \geq \frac{1}{2} \# \left\{k \mid d_k \geq t\right\}$. Using the fact that there exists $c_\ell > 0$ such that $d_k \geq c_\ell k^{-\beta}$, $\# \left\{k \mid d_k \geq t\right\} \geq \# \left\{k \mid c_\ell k^{-\beta} \geq t\right\} = \left\lfloor \left({}^{t}/{}_{c_\ell}\right)^{-\frac{1}{\beta}} \right\rfloor$. This yields the lower bound on $\mathcal{N}(t)$. □

Lemma 14. *If $d_k = \Theta(k^{-\beta})$ with $\beta > 1$, then $\vartheta(0, N) = \Theta\left(N^{-\beta}\right)$.*

Proof. From the previous lemma, there exist $b_\ell, b_h > 0$ such that $b_\ell \vartheta(0, N)^{-\frac{1}{\beta}} \leq \mathcal{N}(\vartheta(0, N)) \leq b_h \vartheta(0, N)^{-\frac{1}{\beta}}$. From the definition of $\vartheta(0, N)$, $\mathcal{N}(\vartheta(0, N)) = N$, thus we get $\left({}^{N}/{}_{b_\ell}\right)^{-\beta} \leq \vartheta(0, N) \leq \left({}^{N}/{}_{b_h}\right)^{-\beta}$. □

With no assumption on the spectrum of T_K, the upper bound for the derivative of the SCT $\partial_\lambda \vartheta$ obtained in Proposition 3, becomes useless in the ridgeless limit $\lambda \to 0$. Yet, with the assumption of power-law decay of the eigenvalues of T_K we can refine the bound with a meaningful one. In order to obtain this we first prove a technical lemma.

Lemma 15. *If $d_k = \Theta(k^{-\beta})$ with $\beta > 1$, then $\sup_N \partial_\lambda \vartheta(0, N) < \infty$.*

Proof. The derivative of the SCT with respect to λ at $\lambda = 0$ is given by:

$$\partial_\lambda \vartheta(0, N) = \frac{N}{\vartheta(0, N) \sum_{k=1}^{\infty} \frac{d_k}{(\vartheta(0,N) + d_k)^2}}.$$

Set $\alpha > 1$, then for all $d_k \in [\alpha^{-1} t, \alpha t]$, we have that $\frac{d_k}{(t+d_k)^2} \geq \frac{\alpha t}{(t + \alpha t)^2} = \frac{\alpha}{(1+\alpha)^2} \frac{1}{t}$. Thus,

$$t \sum_{k=1}^{\infty} \frac{d_k}{(t + d_k)^2} \geq t \sum_{\alpha^{-1} t < d_k < \alpha t} \frac{d_k}{(t + d_k)^2} \geq \frac{\alpha}{(1 + \alpha)^2} \# \{k \mid \alpha^{-1} t < d_k < \alpha t\}.$$

It follows that

$$\partial_\lambda \vartheta(0, N) \leq N \frac{(1 + \alpha)^2}{\alpha} \frac{1}{\# \{k \mid \alpha^{-1} \vartheta(0, N) < d_k < \alpha \vartheta(0, N)\}}$$

Now, using Lemma 14, we are going to find a value of α such that $\# \{k \mid \alpha^{-1} \vartheta(0, N) < d_k < \alpha \vartheta(0, N)\} \geq cN$ for some universal constant c: this will conclude the proof.

By using the assumption that there exist $c_\ell, c_h > 0$ such that $c_\ell k^{-\beta} \leq d_k \leq c_h k^{-\beta}$, in Lemma 14 we saw that there exist $c'_\ell, c'_h > 0$ such that $c'_\ell N^{-\beta} \leq \vartheta(0, N) \leq c'_h N^{-\beta}$. For sake of simplicity, let us assume that the ratios $\frac{c_\ell}{c'_\ell}$ and $\frac{c_h}{c'_h}$ are not integer. Hence we have

$$\begin{aligned}
\#\{k \mid \alpha^{-1}\vartheta(0,N) \leq d_k \leq \alpha\vartheta(0,N)\} &\geq \# \left\{ k \mid \frac{1}{\alpha c_\ell}\vartheta(0,N) \leq k^{-\beta} \leq \frac{\alpha}{c_h}\vartheta(0,N) \right\} \\
&\geq \# \left\{ k \mid \frac{1}{\alpha c_\ell} c'_h N^{-\beta} \leq k^{-\beta} \leq \frac{\alpha}{c_h} c'_\ell N^{-\beta} \right\} \\
&= \left(\left\lfloor \left(\frac{\alpha c_\ell}{c'_h} \right)^{\frac{1}{\beta}} \right\rfloor - \left\lfloor \left(\frac{c_h}{\alpha c'_\ell} \right)^{\frac{1}{\beta}} \right\rfloor \right) N
\end{aligned}$$

For one of the two values $\alpha \in \{\frac{c_h}{c_\ell}, \alpha = \frac{c'_h}{c'_\ell}\}$, we have a meaningful (positive) bound:

$$\# \left\{ k \mid \alpha^{-1}\vartheta(0,N) \leq d_k \leq \alpha\vartheta(0,N) \right\} \geq \left| \left\lfloor \left(\frac{c_h}{c'_h} \right)^{\frac{1}{\beta}} \right\rfloor - \left\lfloor \left(\frac{c_\ell}{c'_\ell} \right)^{\frac{1}{\beta}} \right\rfloor \right| N.$$

This allows us to conclude. □

Proposition 16. *If there exist $\beta > 1$ and $c_\ell, c_h > 0$ s.t. for any $k \in \mathbb{N}$, $c_\ell k^{-\beta} \leq d_k \leq c_h k^{-\beta}$, then for any integer N,*

1. *$\lambda + a_\ell N^{-\beta} \leq \vartheta(\lambda, N) \leq c\lambda + a_h N^{-\beta}$,*
2. *$1 \leq \partial_\lambda \vartheta(\lambda, N) \leq c$,*

where $a_\ell, a_h \geq 0$ and $c \geq 1$ depend only on c_ℓ, c_h, β.

Proof. We start by proving the inequalities for the derivative of the SCT $\partial_\lambda \vartheta(\lambda, N)$. The left side of the inequality has already been proven in Proposition 3. For the right side, from Proposition 3, the derivative $\partial_\lambda \vartheta(\lambda, N)$ is decreasing in λ. In particular, by Lemma 15, $\partial_\lambda \vartheta(\lambda, N) \leq \sup_N \partial_\lambda \vartheta(0, N) < \infty$. Thus, the right side holds with $c := \sup_N \partial_\lambda \vartheta(0, N)$.

The inequality for the SCT $\vartheta(\lambda, N)$ is then obtained by integrating the second inequality and by using the initial value condition $a_\ell N^{-\beta} \leq \vartheta(0, N) \leq a_h N^{-\beta}$ provided by Lemma 14. □

B.4 The Operator $A(z)$

We have now the tools to describe the moments of the operator $A(z)$ which allow us to describe the moments of the predictor $\hat{f}_\lambda$.

B.4.1 Expectation

Writing $\tilde{A}_{\vartheta(-z)} = T_K \left(T_K + \vartheta(-z) I_{\mathcal{C}}\right)^{-1}$ and for any diagonalizable operator A writing $|A|$ for the operator with the same eigenfunctions but with eigenvalues replaced by their absolute values, we have:

Theorem 17. *For any $z \in \mathbb{H}_{<0}$, for any $f, g \in \mathcal{C}$, we have*

$$\left| \left\langle f, \left(\mathbb{E}\left[A(z)\right] - \tilde{A}_{\vartheta(-z)} \right) g \right\rangle_S \right| \leq \left| \left\langle f, |\tilde{A}_{\vartheta(-z)}| |I_{\mathcal{C}} - \tilde{A}_{\vartheta(-z)}| g \right\rangle_S \right| \left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[K]}{|z| N} \right) \right) \quad (16)$$

using the big-P notation of Definition 5.

Remark. *Note that in particular since the polynomial implicitly embedded in $\mathcal{P}$ vanishes at 0, the right hand side tends to 0 as $N \to \infty$.*

Proof. As before, let $(f^{(k)})_{k \in \mathbb{N}}$ be the orthonormal basis of $\mathcal{C}$ defined above and $A_{k\ell}(z) = \langle f^{(k)}, A(z) f^{(\ell)} \rangle_S$. Using a symmetry argument, we first show that for any $\ell \neq k$, $\mathbb{E}\left[A_{\ell k}(z)\right] = 0$: this implies that $\mathbb{E}\left[A(z)\right]$ and $\tilde{A}_{\vartheta(-z)}$ have the same eigenfunctions $f^{(k)}$. Thus, to conclude the proof, we only need to prove Equation 16 for $f = g = f^{(k)}$.

- **Off-Diagonal terms:** By a symmetry argument, we show that the off-diagonal terms are null. Consider the map $s_k : \mathcal{C} \to \mathcal{C}$ defined by $s_k : f \mapsto f - 2\left\langle f, f^{(k)} \right\rangle_S f^{(k)}$, and note that $s_k(f^{(m)}) = f^{(m)}$ if $m \neq k$ and $s_k(f^{(k)}) = -f^{(k)}$. The map s_k is a symmetry for the observations, i.e. for any observations $o_1, \dots, o_N$, and any functions $f_1, \dots, f_N$, the vector $(o_i(s_k(f_i))_{i=1,\dots,N}$ and $(o_i(f_i))_{i=1,\dots,N}$ have the same law. Thus, the sampling operator $\mathcal{O}$ and the operator $\mathcal{O}s_k$ have the same law, hence so do $A(z)$ and $A^{s_k}(z)$, where

$$A^{s_k}(z) := \frac{1}{N} K s_k^T \mathcal{O}^T \left(\frac{1}{N}\mathcal{O} s_k K s_k^T \mathcal{O}^T - zI_N\right)^{-1} \mathcal{O} s_k.$$

Note that $Ks_k^T = s_k K$ and since $s_k^2 = \mathrm{Id}$, $s_k K s_k^T = K$. This implies that $A^{s_k}(z) = s_k A(z) s_k$. For any $\ell \neq k$, $A^{s_k}_{\ell k}(z) = -A_{\ell k}(z)$, hence $\mathbb{E}[A_{\ell k}(z)] = 0$.

- **Diagonal terms:** Using Equation 10, we have

$$\begin{aligned} A_{kk}(z) = \frac{d_k g_k}{1 + d_k g_k} &= \frac{d_k \tilde{m}}{1 + d_k \tilde{m}} + \frac{d_k (g_k - \tilde{m})}{(1 + d_k \tilde{m})\,(1 + d_k g_k)} \\ &= \frac{d_k \tilde{m}}{1 + d_k \tilde{m}} + \frac{d_k (g_k - \tilde{m})}{(1 + d_k \tilde{m})^2} - \frac{d_k^2 (g_k - \tilde{m})^2}{(1 + d_k \tilde{m})^2\,(1 + d_k g_k)}. \end{aligned}$$

From this, using the fact that $\Re(g_k) > 0$, we obtain

$$\left|\mathbb{E}\left[A_{kk}(z)\right] - \frac{d_k \tilde{m}}{1 + d_k \tilde{m}}\right| \leq \frac{d_k \left|\mathbb{E}\left[g_k\right] - \tilde{m}\right|}{\left|1 + d_k \tilde{m}\right|^2} + \frac{d_k^2 \mathbb{E}\left[\left|g_k - \tilde{m}\right|^2\right]}{\left|1 + d_k \tilde{m}\right|^2}.$$

Using Proposition 11, we can bound the first fraction by

$$\begin{aligned} \frac{d_k \left|\mathbb{E}\left[g_k\right] - \tilde{m}\right|}{\left|1 + d_k \tilde{m}\right|^2} &\leq \frac{d_k}{\left|1 + d_k \tilde{m}\right|^2} \left(\frac{1}{|z|\,N} + \frac{\mathrm{Tr}[T_K]}{|z|^2 N^2} + \frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^2}{|z|^3 N^2} + \frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^4}{|z|^5 N^4}\right) \\ &\leq \frac{d_k |\vartheta(-z)|^2}{|\vartheta(-z) + d_k|^2} \left(\frac{1}{|z|\,N} + \frac{\mathrm{Tr}[T_K]}{|z|^2 N} + \frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^2}{|z|^3 N^2} + \frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^4}{|z|^5 N^4}\right) \\ &\leq \frac{d_k}{|\vartheta(-z) + d_k|} \left|1 - \frac{d_k}{\vartheta(-z) + d_k}\right| \left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|\,N}\right)\right), \end{aligned}$$

by substituting $\vartheta(-z) = \frac{1}{\tilde{m}(z)}$, using the bound $|\vartheta(-z)| \leq |z| + \frac{\mathrm{Tr}[T_K]}{N}$ (see Proposition 3).

Using Proposition 10, the inequality $d_k^2 \leq d_k \mathrm{Tr}[T_K]$ and similar arguments as above, we can bound the second fraction by

$$\begin{aligned} \frac{d_k^2 \mathbb{E}\left[\left|g_k - \tilde{m}\right|^2\right]}{\left|1 + d_k \tilde{m}\right|^2} &\leq \frac{d_k^2}{\left|1 + d_k \tilde{m}\right|^2} \left(\frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^2}{|z|^4 N^3} + \frac{2\boldsymbol{c}_1}{|z|^2 N}\right) \\ &\leq \frac{d_k |\vartheta(-z)|^2}{|\vartheta(-z) + d_k|^2} \left(\frac{2\boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^3}{|z|^4 N^3} + \frac{2\boldsymbol{c}_1 \mathrm{Tr}[T_K]}{|z|^2 N}\right) \\ &\leq \frac{d_k}{|\vartheta(-z) + d_k|} \left|1 - \frac{d_k}{\vartheta(-z) + d_k}\right| \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|\,N}\right) \end{aligned}$$

Finally, putting everything together, we get:

$$\left|\mathbb{E}\left[A_{kk}(z)\right] - \frac{d_k \tilde{m}}{1 + d_k \tilde{m}}\right| \leq \frac{d_k}{|\vartheta(-z) + d_k|} \left|1 - \frac{d_k}{\vartheta(-z) + d_k}\right| \left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|\,N}\right)\right) \tag{17}$$

□

B.4.2 Variance

To study the variance of $A(z)$ we will need to apply the Shermann-Morrison formula twice, to isolate the contribution of the two eigenfunctions $f^{(k)}$ and $f^{(\ell)}$. Similarly to above, we set $K_{(k\ell)} =$

$\sum_{n\notin\{k,\ell\}} d_n f^{(n)} \otimes f^{(n)}$ and we define

$$B_{(k\ell)}(z) = \frac{1}{N}\mathcal{O}K_{(k\ell)}\mathcal{O}^T - zI_N, \qquad m_{(k\ell)}(z) = \frac{1}{N}\mathrm{Tr}\left[B_{(k\ell)}(z)^{-1}\right].$$

Note that the concentration results of Section B.2 apply to $m_{(k\ell)}$: it concentrates around $\tilde{m}_{(k\ell)}$, the unique solution, in the cone spanned by 1 and $-1/z$, to the equation

$$\tilde{m}_{(k\ell)} = -\frac{1}{z}\left(1 - \frac{\tilde{m}_{(k\ell)}}{N}\mathrm{Tr}\left[T_{K_{(k\ell)}}\left(T_{K_{(k\ell)}} + \tilde{m}_{(k\ell)}I_{\mathcal{C}}\right)^{-1}\right]\right).$$

In order to compute the off-diagonal entry $A_{k\ell}(z) = \frac{1}{N}d_k\mathcal{O}_{.k}^T B(z)^{-1}\mathcal{O}_{.\ell}$, we use the Shermann-Morrison formula twice: when applied to $B(z) = B_{(k)}(z) + \frac{d_k}{N}\mathcal{O}_{.k}\mathcal{O}_{.k}^T$ we get

$$B(z)^{-1} = B_{(k)}(z)^{-1} - \frac{d_k}{N}\frac{B_{(k)}(z)^{-1}\mathcal{O}_{.k}\mathcal{O}_{.k}^T B_{(k)}(z)^{-1}}{1 + \frac{d_k}{N}\mathcal{O}_{.k}^T B_{(k)}(z)^{-1}\mathcal{O}_{.k}};$$

thus, recalling that $g_{(k)} = \frac{1}{N}\mathcal{O}_{.,k}^T B_{(k)}(z)^{-1}\mathcal{O}_{.,k}$, we have

$$A_{k\ell}(z) = \frac{d_k}{1 + d_k g_k}\frac{1}{N}\mathcal{O}_{.k}^T B_{(k)}(z)^{-1}\mathcal{O}_{.\ell}.$$

We then apply the Shermann-Morrison formula to $B_{(k)}(z) = B_{(k\ell)}(z) + \frac{d_\ell}{N}\mathcal{O}_{.\ell}\mathcal{O}_{.\ell}^T$ and obtain

$$B_{(k)}(z)^{-1} = B_{(k\ell)}(z)^{-1} - \frac{d_\ell}{N}\frac{B_{(k\ell)}(z)^{-1}\mathcal{O}_{.\ell}\mathcal{O}_{.\ell}^T B_{(k\ell)}(z)^{-1}}{1 + \frac{d_\ell}{N}\mathcal{O}_{.\ell}^T B_{(k\ell)}(z)^{-1}\mathcal{O}_{.\ell}}.$$

Thus, we obtain the following formula for the off-diagonal entry:

$$A_{k\ell}(z) = \frac{d_k}{1 + d_k g_k}\frac{h_{k\ell}}{1 + d_\ell h_\ell} \tag{18}$$

where $h_\ell = \frac{1}{N}\left(\mathcal{O}_{.\ell}\right)^T B_{(k\ell)}^{-1}(z)\mathcal{O}_{.\ell}$ and $h_{k\ell} = \frac{1}{N}\left(\mathcal{O}_{.k}\right)^T B_{(k\ell)}^{-1}(z)\mathcal{O}_{.\ell}$.

We can apply the results of Section B.2 showing the concentration of g_k around $\tilde{m}_{(k)}$: h_ℓ concentrates around $\tilde{m}_{(k)}$ which itself is close to $\tilde{m}$:

Lemma 18. *For $z \in \mathbb{H}_{<0}$, and $s \in \mathbb{N}$, we have*

$$\mathbb{E}\left[\left|h_\ell - \tilde{m}\right|^{2s}\right] \leq \frac{\boldsymbol{a}_s\left(\mathrm{Tr}[T_K]\right)^{2s}}{|z|^{4s}N^{3s}} + \frac{\boldsymbol{b}_s}{|z|^{2s}N^s},$$

where $\boldsymbol{a}_s, \boldsymbol{b}_s$ only depend on s.

Proof. By convexity, for $k \neq \ell$,

$$\begin{aligned}\mathbb{E}\left[\left|h_\ell - \tilde{m}\right|^{2s}\right] &\leq 2^{2s-1}\mathbb{E}\left[\left|h_\ell - \tilde{m}_{(k)}\right|^{2s}\right] + 2^{2s-1}\left|\tilde{m}_{(k)} - \tilde{m}\right|^{2s} \\ &\leq 2^{2s-1}\left(\frac{2^{2s-1}\boldsymbol{c}_s\left(\mathrm{Tr}[T_K]\right)^{2s}}{|z|^{4s}N^{3s}} + \frac{2^{2s-1}\boldsymbol{c}_s}{|z|^{2s}N^s}\right) + \frac{2^{2s-1}}{|z|^{2s}N^{2s}}\end{aligned}$$

where for the first term, we applied Proposition 10 to the matrix $B_{(k)}$ instead of B and the second term is bounded by $\left|\tilde{m}_{(k)} - \tilde{m}\right| \leq \frac{1}{|z|N}$ by Lemma 30. Finally, letting $\boldsymbol{a}_s = 4^{2s-1}\boldsymbol{c}_s$ and $\boldsymbol{b}_s = 4^{2s-1}\boldsymbol{c}_s + 2^{2s-1}$, we obtain the result. □

The scalar $h_{k\ell}$ on the other hand has 0 expectation and, using Wick's formula (Lemma 26), its variance $\mathbb{E}\left[h_{k\ell}^2\right]$ is equal to $\frac{1}{N^2}\mathbb{E}[\mathrm{Tr}[B_{(k\ell)}^{-2}]] = \frac{1}{N}\mathbb{E}\left[\partial_z m_{(k\ell)}(z)\right]$. Since $\mathbb{E}\left[m_{(k\ell)}(z)\right]$ is close to $\tilde{m}(z)$, from Lemma 27, its derivative, and hence the variance of $h_{k\ell}$, is close to $\frac{1}{N}\partial_z\tilde{m}$:

Lemma 19. *For $z \in \mathbb{H}_{<0}$, we have:*

$$\left|\mathbb{E}\left[m_{(k\ell)}(z)\right] - \tilde{m}(z)\right| \leq \frac{\mathrm{Tr}[T_K]}{|z|^2 N^2} + \frac{2\boldsymbol{c}_1\left(\mathrm{Tr}[T_K]\right)^2}{|z|^3 N^2} + \frac{2\boldsymbol{c}_1\left(\mathrm{Tr}[T_K]\right)^4}{|z|^5 N^4} + \frac{2}{|z|N},$$

where $\boldsymbol{c}_1$ is as in Proposition 11.

Proof. We use Proposition 11 and Lemma 30 twice to obtain

$$\begin{aligned}\left|\mathbb{E}\left[m_{(k\ell)}(z)\right]-\tilde{m}(z)\right| &\leq \left|\mathbb{E}\left[m_{(k\ell)}(z)\right]-\tilde{m}_{(k\ell)}(z)\right|+\left|\tilde{m}_{(k\ell)}(z)-\tilde{m}_{(k)}(z)\right|+\left|\tilde{m}_{(k)}(z)-\tilde{m}(z)\right| \\ &\leq \frac{\mathrm{Tr}[T_K]}{|z|^2 N^2}+\frac{2\boldsymbol{c}_1\left(\mathrm{Tr}[T_K]\right)^2}{|z|^3 N^2}+\frac{2\boldsymbol{c}_1\left(\mathrm{Tr}[T_K]\right)^4}{|z|^5 N^4}+\frac{2}{|z|N},\end{aligned}$$

which yields the desired result. □

To approximate the variance $\mathrm{Var}\left(\left\langle f^{(k)}, A_\lambda f^*\right\rangle_S\right)$ of the coordinate of the noiseless predictor, we need the following results regarding the covariance of the entries of $A(z)$.

Proposition 20. *For $z \in \mathbb{H}_{<0}$, any $k, \ell \in \mathbb{N}$, we have*

$$\left|\mathrm{Var}\left(A_{kk}(z)\right)-\frac{2}{N}\frac{d_k^2 \partial_z \tilde{m}}{\left(1+d_k\tilde{m}\right)^4}\right| \leq \frac{1}{N}\frac{d_k^2|\partial_z\tilde{m}|}{|1+d_k\tilde{m}|^4}\left(\frac{1}{N}+\frac{|z|}{-\Re(z)}\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N^{\frac{1}{2}}}\right)\right)$$

$$\left|\mathrm{Var}\left(A_{k\ell}(z)\right)-\frac{1}{N}\frac{d_k^2 \partial_z \tilde{m}}{\left(1+d_k\tilde{m}\right)^2\left(1+d_\ell\tilde{m}\right)^2}\right| \leq \frac{1}{N}\frac{d_k^2|\partial_z\tilde{m}|}{|1+d_k\tilde{m}|^2|1+d_\ell\tilde{m}|^2}\frac{|z|}{-\Re(z)}\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N^{\frac{1}{2}}}\right)$$

$$\left|\mathrm{Cov}\left(A_{k\ell}(z), A_{\ell k}(z)\right)-\frac{1}{N}\frac{d_k d_\ell \partial_z \tilde{m}}{\left(1+d_k\tilde{m}\right)^2\left(1+d_\ell\tilde{m}\right)^2}\right| \leq \frac{1}{N}\frac{d_k d_\ell|\partial_z\tilde{m}|}{|1+d_k\tilde{m}|^2|1+d_\ell\tilde{m}|^2}\frac{|z|}{-\Re(z)}\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N^{\frac{1}{2}}}\right)$$

where we use the big-P notation of Definition 5. Whenever a value in the quadruple (k, h, n, ℓ) appears an odd number of times, we have

$$\mathrm{Cov}\left(A_{kh}(z), A_{n\ell}(z)\right)=0.$$

Proof. Let s_k be the symmetry map in the proof of Theorem 17: the matrices $A(z)$ and $A^{s_k}(z)$ have the same law. Since $A_{\ell n}^{s_k}(z)=-A_{\ell n}(z)$ whenever exactly one of ℓ, n is equal to k, we have for h, n, ℓ distinct from k:

$$\mathrm{Cov}\left(A_{kh}(z), A_{n\ell}(z)\right)=\mathrm{Cov}\left(A_{kh}^{s_k}(z), A_{n\ell}^{s_k}(z)\right)=\mathrm{Cov}\left(-A_{kh}(z), A_{n\ell}(z)\right)$$

which implies that $\mathrm{Cov}\left(A_{kh}(z), A_{n\ell}(z)\right)=0$ when h, n, ℓ are distinct from k. More generally, it is easy to see that $\mathrm{Cov}\left(A_{kh}(z), A_{n\ell}(z)\right)=0$ whenever a value in the quadruple (k, h, n, ℓ) appears an odd number of times.

Approximation of $\mathrm{Var}\left(A_{kk}(z)\right)$**:** Since $\mathbb{E}[A_{kk}(z)] \approx \frac{d_k\tilde{m}}{1+d_k\tilde{m}}$ (Theorem 17), we decompose the variance of $A_{kk}(z)$ as follows:

$$\mathrm{Var}\left(A_{kk}\right)=\mathbb{E}\left[\left(A_{kk}-\frac{d_k\tilde{m}}{1+d_k\tilde{m}}\right)^2\right]-\left[\mathbb{E}\left[A_{kk}\right]-\frac{d_k\tilde{m}}{1+d_k\tilde{m}}\right]^2.$$

This gives us an approximation $\mathrm{Var}\left(A_{kk}\right) \approx \mathbb{E}\left[\left(A_{kk}-\frac{d_k\tilde{m}}{1+d_k\tilde{m}}\right)^2\right]$ since the term $\left|\mathbb{E}\left[A_{kk}\right]-\frac{d_k\tilde{m}}{1+d_k\tilde{m}}\right|^2$, by using Theorem 17, we get the following bound :

$$\begin{aligned}\left|\mathbb{E}\left[A_{kk}\right]-\frac{d_k\tilde{m}}{1+d_k\tilde{m}}\right|^2 &\leq \left|\frac{d_k\tilde{m}}{(1+d_k\tilde{m})^2}\left(\frac{1}{N}+\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N}\right)\right)\right|^2 \\ &= \frac{1}{N}\frac{d_k^2|\tilde{m}|^2}{|1+d_k\tilde{m}|^4}\left(\frac{1}{N}+2\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N}\right)+N\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N}\right)^2\right)\end{aligned}$$

Since $\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N}\right)=\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N^{1/2}}\right)$ and $N\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N}\right)^2=\mathcal{P}\left(\frac{(\mathrm{Tr}[T_K])^2}{|z|^2N}\right)$, we can bound $\left|\mathbb{E}\left[A_{kk}\right]-\frac{d_k\tilde{m}}{1+d_k\tilde{m}}\right|^2$ by

$$\frac{1}{N}\frac{d_k^2|\tilde{m}|^2}{|1+d_k\tilde{m}|^4}\left(\frac{1}{N}+\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N^{\frac{1}{2}}}\right)\right).$$

Using Formula (10) for the diagonal entries of A, we have:

$$\left(A_{kk} - \frac{d_k\tilde{m}}{1+d_k\tilde{m}}\right)^2 = \frac{d_k^2\left[g_k - \tilde{m}\right]^2}{(1+d_kg_k)^2(1+d_k\tilde{m})^2}.$$

which can be also expressed as:

$$\left(\frac{d_k\left[g_k - \tilde{m}\right]}{(1+d_kg_k)(1+d_k\tilde{m})}\right)^2 = \left(\frac{d_k\left[g_k - \tilde{m}\right]}{(1+d_k\tilde{m})(1+d_k\tilde{m})} - \frac{d_k^2\left[g_k - \tilde{m}\right]^2}{(1+d_kg_k)(1+d_k\tilde{m})^2}\right)^2.$$

This yields

$$\begin{aligned}\mathbb{E}\left[\left(A_{kk} - \frac{d_k\tilde{m}}{1+d_k\tilde{m}}\right)^2\right] &- \mathbb{E}\left[\left(\frac{d_k\left[g_k - \tilde{m}\right]}{(1+d_k\tilde{m})^2}\right)^2\right] \\ &= -\mathbb{E}\left[\frac{d_k^2\left[g_k - \tilde{m}\right]^2}{(1+d_kg_k)(1+d_k\tilde{m})^2}\left(\frac{2d_k\left[g_k - \tilde{m}\right]}{(1+d_k\tilde{m})(1+d_k\tilde{m})} - \frac{d_k^2\left[g_k - \tilde{m}\right]^2}{(1+d_kg_k)(1+d_k\tilde{m})^2}\right)\right].\end{aligned}$$

Using Proposition 10, the absolute value of the r.h.s. can now be bounded by

$$\begin{aligned}\frac{d_k^3\left(2\mathbb{E}\left[\left|g_k - \tilde{m}\right|^3\right] + d_k\mathbb{E}\left[\left|g_k - \tilde{m}\right|^4\right]\right)}{\left|1+d_k\tilde{m}\right|^4} \leq & \frac{d_k^3}{|1+d_k\tilde{m}|^4}2\left(\frac{2^3\boldsymbol{c}_2\left(\mathrm{Tr}[T_K]\right)^4}{|z|^8 N^6} + \frac{2^3\boldsymbol{c}_2}{|z|^4 N^2}\right)^{\frac{3}{4}} \\ & + \frac{d_k^4}{|1+d_k\tilde{m}|^4}\left(\frac{2^3\boldsymbol{c}_2\left(\mathrm{Tr}[T_K]\right)^4}{|z|^8 N^6} + \frac{2^3\boldsymbol{c}_2}{|z|^4 N^2}\right) \\ \leq & \frac{2}{N}\frac{d_k^2|\tilde{m}|^2}{|1+d_k\tilde{m}|^4}\frac{\mathrm{Tr}[T_K]}{|\tilde{m}|^2}\left(\frac{2^{\frac{9}{4}}\boldsymbol{c}_2^{\frac{3}{4}}\left(\mathrm{Tr}[T_K]\right)^3}{|z|^6 N^{\frac{7}{2}}} + \frac{2^{\frac{9}{4}}\boldsymbol{c}_2^{\frac{3}{4}}}{|z|^3 N^{\frac{1}{2}}}\right) \\ & + \frac{1}{N}\frac{d_k^2|\tilde{m}|^2}{|1+d_k\tilde{m}|^4}\frac{\left(\mathrm{Tr}[T_K]\right)^2}{|\tilde{m}|^2}\left(\frac{2^3\boldsymbol{c}_2\left(\mathrm{Tr}[T_K]\right)^4}{|z|^8N^5} + \frac{2^3\boldsymbol{c}_2}{|z|^4N}\right),\end{aligned}$$

using the inequality $(a+b)^{\frac{3}{4}} \leq a^{\frac{3}{4}} + b^{\frac{3}{4}}$ and the fact that $d_k \leq \mathrm{Tr}[T_K]$. From Proposition 3, we have $\frac{1}{\tilde{m}^2} \leq \left(|z| + \frac{\mathrm{Tr}[T_K]}{N}\right)^2$, so that

$$\left|\mathbb{E}\left[\left(A_{kk} - \frac{d_k\tilde{m}}{1+d_k\tilde{m}}\right)^2\right] - \mathbb{E}\left[\left(\frac{d_k\left[g_k - \tilde{m}\right]}{(1+d_k\tilde{m})^2}\right)^2\right]\right| \leq \frac{1}{N}\frac{d_k^2|\tilde{m}|^2}{|1+d_k\tilde{m}|^4}\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N^{\frac{1}{2}}}\right).$$

This yields the approximation $\mathrm{Var}\left(A_{kk}\right) \approx \frac{d_k^2\mathbb{E}\left[(g_k - \tilde{m})^2\right]}{(1+d_k\tilde{m})^4}$.

Using Wick's formula (Lemma 26),

$$\mathbb{E}\left[\left(g_k - \tilde{m}\right)^2\right] = \mathbb{E}\left[\left(m_{(k)} - \tilde{m}\right)^2\right] + \frac{2}{N}\mathbb{E}[\partial_z m_{(k)}(z)],$$

hence we get:

$$\frac{d_k^2\mathbb{E}\left[\left(g_k - \tilde{m}\right)^2\right]}{(1+d_k\tilde{m})^4} = \frac{\frac{2}{N}d_k^2\partial_z\mathbb{E}[m_{(k)}(z)]}{(1+d_k\tilde{m})^4} + \frac{d_k^2\mathbb{E}\left[\left(m_{(k)} - \tilde{m}\right)^2\right]}{(1+d_k\tilde{m})^4}.$$

Using Proposition 10,

$$\begin{aligned}\frac{d_k^2\mathbb{E}\left[\left|m_{(k)} - \tilde{m}\right|^2\right]}{|1+d_k\tilde{m}|^4} &\leq \frac{d_k^2}{|1+d_k\tilde{m}|^4}\left|\frac{\boldsymbol{c}_1(\mathrm{Tr}[T_K])^2}{|z|^4N^3}\right| \\ &\leq \frac{1}{N}\frac{d_k^2|\tilde{m}|^2}{|1+d_k\tilde{m}|^4}\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N}\right),\end{aligned}$$

hence the approximation $\mathrm{Var}\left(A_{kk}\right) \approx \frac{\frac{2}{N}d_k^2\partial_z\mathbb{E}[m_{(k)}(z)]}{(1+d_k\tilde{m})^4}$.

At last, by using the approximation $\mathbb{E}[\partial_z m_{(k)}(z)] = \mathbb{E}[\partial_z g_k(z)] \approx \partial_z \tilde{m}(z)$ (Proposition 11 and Lemma 27), we obtain

$$\begin{aligned}
&\left| \frac{\frac{2}{N} d_k^2 \partial_z \mathbb{E}[m_{(k)}(z)]}{(1+d_k\tilde{m})^4} - \frac{\frac{2}{N} d_k^2 \partial_z \tilde{m}(z)}{(1+d_k\tilde{m}(z))^4} \right| \\
&\leq \frac{2}{N} \frac{d_k^2}{|1+d_k\tilde{m}|^4} \frac{2}{-\Re(z)} \left(\frac{2^2 \mathrm{Tr}[T_K]}{|z|^2 N^2} + \frac{2^4 \boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^2}{|z|^3 N^2} + \frac{2^6 \boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^4}{|z|^5 N^4} + \frac{2^2}{|z| N} \right) \\
&\leq \frac{2}{N} \frac{d_k^2 |\tilde{m}|^2}{|1+d_k\tilde{m}|^4} \frac{2|z|}{-\Re(z)} \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N} \right).
\end{aligned}$$

Hence we get the approximation $\mathrm{Var}\left(A_{kk}\right) \approx \frac{\frac{2}{N} d_k^2 \partial_z \tilde{m}(z)}{(1+d_k\tilde{m}(z))^4}$, more precisely $\left|\mathrm{Var}\left(A_{kk}\right) - \frac{\frac{2}{N} d_k^2 \partial_z \tilde{m}(z)}{(1+d_k\tilde{m}(z))^4}\right|$ is bounded by

$$\frac{2}{N} \frac{d_k^2 |\tilde{m}|^2}{|1+d_k\tilde{m}|^4} \left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z| N^{\frac{1}{2}}} \right) + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N} \right) + \frac{|z|}{-\Re(z)} \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N} \right) \right).$$

Putting everything together, we get

$$\left| \mathrm{Var}\left(A_{kk}\right) - \frac{\frac{2}{N} d_k^2 \partial_z \tilde{m}(z)}{(1+d_k\tilde{m}(z))^4} \right| \leq \frac{2}{N} \frac{d_k^2 |\tilde{m}|^2}{|1+d_k\tilde{m}|^4} \left(\frac{1}{N} + \frac{|z|}{-\Re(z)} \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z| N^{\frac{1}{2}}} \right) \right).$$

Since $\partial_z \vartheta = \frac{\partial_z \tilde{m}}{\tilde{m}^2}$, from Proposition 3 we have $|\partial_\lambda \vartheta(\lambda)| \geq 1$, i.e. $|\tilde{m}|^2 \leq |\partial_\lambda \tilde{m}|$ and thus we conclude.

Approximation of $\mathrm{Cov}\left(A_{k\ell}(z), A_{\ell k}(z)\right)$**:** Note that $A_{k\ell}(z) = \frac{d_k}{N} \mathcal{O}_{.k}^T B(z)^{-1} \mathcal{O}_{.\ell}$, hence, since $B(z)$ is symmetric,

$$A_{k\ell}(z) = \frac{d_k}{d_\ell} A_{\ell k}(z).$$

In particular, we have $\mathrm{Cov}\left(A_{k\ell}(z), A_{\ell k}(z)\right) = \frac{d_\ell}{d_k} \mathrm{Var}\left(A_{k\ell}(z)\right)$. Hence the approximation of $\mathrm{Cov}\left(A_{k\ell}(z), A_{\ell k}(z)\right)$ follows from the one of $\mathrm{Var}\left(A_{k\ell}(z)\right)$.

Approximation of $\mathrm{Var}\left(A_{k\ell}(z)\right)$**:** We have seen in Theorem 17 that $\mathbb{E}\left(A_{k\ell}(z)\right) = 0$: we need to bound $\mathbb{E}\left(A_{k\ell}(z)^2\right)$. Using Equation (18):

$$\mathbb{E}\left[A_{k\ell}(z)^2\right] = \mathbb{E}\left[\left(\frac{d_k}{1+d_k g_k} \frac{h_{k\ell}}{1+d_\ell h_\ell} \right)^2 \right],$$

where we recall that $h_\ell = \frac{1}{N} \mathcal{O}_{.,\ell}^T B_{(k\ell)}(z)^{-1} \mathcal{O}_{.,\ell}$ and $h_{k\ell} = \frac{1}{N} \mathcal{O}_{.,k}^T B_{(k\ell)}(z)^{-1} \mathcal{O}_{.,\ell}$. Since

$$\frac{d_k}{1+d_k g_k} \frac{h_{k\ell}}{1+d_\ell h_\ell} = \frac{d_k}{1+d_k\tilde{m}} \frac{h_{k\ell}}{1+d_\ell\tilde{m}} - d_k h_{k\ell} \left(\frac{d_k \left(g_k - \tilde{m}\right)\left(1+d_\ell h_\ell\right) + d_\ell \left(1+d_k\tilde{m}\right)\left(h_\ell - \tilde{m}\right)}{\left(1+d_k\tilde{m}\right)\left(1+d_\ell\tilde{m}\right)\left(1+d_k g_k\right)\left(1+d_\ell h_\ell\right)} \right), \tag{19}$$

using Lemma 21 below, we get the approximation $\mathbb{E}\left[A_{k\ell}(z)^2\right] \approx \mathbb{E}\left[\frac{d_k^2 h_{k\ell}^2}{(1+d_k\tilde{m})^2(1+d_\ell\tilde{m})^2}\right]$. Using Wick's formula (Lemma 26 below):

$$\mathbb{E}\left[h_{k\ell}^2\right] = \frac{1}{N} \partial_z \mathbb{E}\left[m_{(k\ell)}(z)\right].$$

Hence the approximation $\mathbb{E}\left[A_{k\ell}(z)^2\right] \approx \frac{\frac{1}{N} d_k^2 \partial_z \mathbb{E}\left[m_{(k\ell)}(z)\right]}{(1+d_k\tilde{m})^2(1+d_\ell\tilde{m})^2}$. At last, by using the approximation $\mathbb{E}[\partial_z m_{(kl)}(z)] \approx \partial_z \tilde{m}(z)$ (Lemma 19 above and the technical complex analysis Lemma 27 below), we can bound the difference $\left| \frac{\frac{1}{N} d_k^2 \partial_z \mathbb{E}\left[m_{(k\ell)}(z)\right]}{(1+d_k\tilde{m})^2(1+d_\ell\tilde{m})^2} - \frac{\frac{1}{N} d_k^2 \partial_z \tilde{m}(z)}{(1+d_k\tilde{m})^2(1+d_\ell\tilde{m})^2} \right|$ by

$$\begin{aligned}
&\frac{1}{N} \frac{d_k^2}{|1+d_k\tilde{m}|^2 |1+d_\ell\tilde{m}|^2} \frac{2}{-\Re(z)} \left(\frac{2^2 \mathrm{Tr}[T_K]}{|z|^2 N^2} + \frac{2^4 \boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^2}{|z|^3 N^2} + \frac{2^6 \boldsymbol{c}_1 \left(\mathrm{Tr}[T_K]\right)^4}{|z|^5 N^4} + \frac{2^2}{|z| N} \right) \\
&\leq \frac{1}{N} \frac{d_k^2 |\tilde{m}|^2}{|1+d_k\tilde{m}|^2 |1+d_\ell\tilde{m}|^2} \frac{2|z|}{-\Re(z)} \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N} \right)
\end{aligned}$$

Finally, we can bound the error $\left|\mathbb{E}\left[\left(A_{k\ell}(z)\right)^2\right]-\frac{1}{N}\frac{d_k^2\partial_z\tilde{m}}{(1+d_k\tilde{m})^2(1+d_\ell\tilde{m})^2}\right|$ by

$$\begin{aligned}
&\frac{1}{N}\frac{d_k^2|\partial_z\tilde{m}|}{|1+d_k\tilde{m}|^2|1+d_\ell\tilde{m}|^2}\left(\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N^{\frac{1}{2}}}\right)+\frac{2|z|}{-\Re(z)}\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N^{\frac{1}{2}}}\right)\right)\\
&\le\frac{1}{N}\frac{d_k^2|\partial_z\tilde{m}|}{|1+d_k\tilde{m}|^2|1+d_\ell\tilde{m}|^2}\frac{|z|}{-\Re(z)}\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N^{\frac{1}{2}}}\right).
\end{aligned}$$

□

Lemma 21. *Using the same notation as in the proof of Proposition 20,*

$$\epsilon_{k\ell}=\mathbb{E}\left[A_{k\ell}(z)^2\right]-\frac{d_k^2h_{k\ell}^2}{(1+d_k\tilde{m})^2(1+d_\ell\tilde{m})^2}$$

is bounded by:

$$|\epsilon_{k\ell}|\le\frac{1}{N}\frac{d_k^2\partial_\lambda\tilde{m}}{|1+d_\ell\tilde{m}|^2|1+d_k\tilde{m}|^2}\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N^{\frac{1}{2}}}\right)$$

Proof. Using Equation 19, by setting $c=2\frac{1}{1+d_k\tilde{m}}\frac{1}{1+d_\ell\tilde{m}}$, $X_1=d_kh_{k\ell}$, and

$$X_2=\frac{d_k\left(g_k-\tilde{m}\right)}{\left(1+d_k\tilde{m}\right)\left(1+d_\ell\tilde{m}\right)\left(1+d_kg_k\right)}+\frac{d_\ell\left(h_\ell-\tilde{m}\right)}{\left(1+d_\ell\tilde{m}\right)\left(1+d_kg_k\right)\left(1+d_\ell h_\ell\right)},$$

we have that $\epsilon_{k\ell}$ is equal to:

$$\epsilon_{k\ell}=\mathbb{E}\left[-X_1^2X_2(c-X_2)\right]$$

we can thus control $\epsilon_{k\ell}$ with the following bound

$$\begin{aligned}
|\epsilon_{k\ell}|&\le c\mathbb{E}\left[|X_1|^2|X_2|\right]+\mathbb{E}\left[|X_1|^2|X_2|^2\right]\\
&\le\mathbb{E}\left[|X_1|^4\right]^{\frac{1}{2}}\left(c\mathbb{E}\left[|X_2|^2\right]^{\frac{1}{2}}+\mathbb{E}\left[|X_2|^4\right]^{\frac{1}{2}}\right).
\end{aligned}$$

- Bound on $\mathbb{E}[|X_1|^4]$: using the same argument as for $\mathbb{E}\left[|m_{(k)}-g_k|^{2s}\right]$ and Wick's formula (Lemma 26), there exists a constant $\boldsymbol{a}$ such that

$$\mathbb{E}\left[|X_1|^4\right]^{\frac{1}{2}}=\mathbb{E}\left[|d_kh_{k\ell}|^4\right]^{\frac{1}{2}}=d_k^2\mathbb{E}\left[|h_{k\ell}|^4\right]^{\frac{1}{2}}\le\frac{\boldsymbol{a}d_k^2}{|z|^2N}$$

- Bound on $\mathbb{E}[|X_2|^{2s}]$: in order to bound $\mathbb{E}[|X_2|^{2s}]$ we decompose X_2 as $X_2=Y_1+Y_2+Y_3$ where

$$\begin{aligned}
Y_1&=\frac{d_k\left(g_k-\tilde{m}\right)}{\left(1+d_k\tilde{m}\right)\left(1+d_\ell\tilde{m}\right)\left(1+d_kg_k\right)},\\
Y_2&=\frac{d_\ell\left(h_\ell-\tilde{m}\right)}{\left(1+d_\ell\tilde{m}\right)\left(1+d_k\tilde{m}\right)\left(1+d_\ell h_\ell\right)},\\
Y_3&=\frac{d_\ell d_k\left(h_\ell-\tilde{m}\right)\left(\tilde{m}-g_k\right)}{\left(1+d_\ell\tilde{m}\right)\left(1+d_k\tilde{m}\right)\left(1+d_kg_k\right)\left(1+d_\ell h_\ell\right)},
\end{aligned}$$

so that by Minkowski inequality,

$$\mathbb{E}\left[|X_2|^{2s}\right]^{\frac{1}{2s}}\le\mathbb{E}\left[|Y_1|^{2s}\right]^{\frac{1}{2s}}+\mathbb{E}\left[|Y_2|^{2s}\right]^{\frac{1}{2s}}+\mathbb{E}\left[|Y_3|^{2s}\right]^{\frac{1}{2s}},$$

We can bound the terms in the r.h.s. of the above by applying Proposition 10 and Lemma 18:

– Bound on $\mathbb{E}[|Y_1|^{2s}]$:

$$\mathbb{E}\left[|Y_1|^{2s}\right]^{\frac{1}{2s}}\le\frac{d_k}{|1+d_\ell\tilde{m}||1+d_k\tilde{m}|}\mathbb{E}\left[|\left(g_k-\tilde{m}\right)|^{2s}\right]^{\frac{1}{2s}}\le\frac{d_k}{|1+d_\ell\tilde{m}||1+d_k\tilde{m}|}\left[\frac{2^{2s-1}\boldsymbol{c}_s(\mathrm{Tr}[T_K])^{2s}}{|z|^{4s}N^{3s}}+\frac{2^{2s-1}\boldsymbol{c}_s}{|z|^{2s}N^s}\right]^{\frac{1}{2s}}$$

- Bound on $\mathbb{E}[|Y_2|^{2s}]$:

$$\mathbb{E}\left[|Y_2|^{2s}\right]^{\frac{1}{2s}} \leq \frac{d_\ell}{|1+d_\ell\tilde{m}|\,|1+d_k\tilde{m}|}\mathbb{E}\left[|\left(h_\ell-\tilde{m}\right)|^{2s}\right]^{\frac{1}{2s}} \leq \frac{d_k}{|1+d_\ell\tilde{m}|\,|1+d_k\tilde{m}|}\left[\frac{\boldsymbol{a}_s(\mathrm{Tr}[T_K])^{2s}}{|z|^{4s}N^{3s}}+\frac{\boldsymbol{b}_s}{|z|^{2s}N^s}\right]^{\frac{1}{2s}}$$

- Bound on $\mathbb{E}\left[|Y_3|^{2s}\right]^{\frac{1}{2s}}$:

$$\begin{aligned}
\mathbb{E}\left[|Y_3|^{2s}\right]^{\frac{1}{2s}} &\leq \frac{d_\ell d_k}{|1+d_\ell\tilde{m}|\,|1+d_k\tilde{m}|}\mathbb{E}\left[|(h_\ell-\tilde{m})|^{2s}\,|(\tilde{m}-g_k)|^{2s}\right]^{\frac{1}{2s}}\\
&\leq \frac{d_\ell d_k}{|1+d_\ell\tilde{m}|\,|1+d_k\tilde{m}|}\mathbb{E}\left[|(h_\ell-\tilde{m})|^{4s}\right]^{\frac{1}{4s}}\mathbb{E}\left[|(\tilde{m}-g_k)|^{4s}\right]^{\frac{1}{4s}}\\
&\leq \frac{d_\ell d_k}{|1+d_\ell\tilde{m}|\,|1+d_k\tilde{m}|}\left[\frac{\boldsymbol{a}_{2s}(\mathrm{Tr}[T_K])^{4s}}{|z|^{8s}N^{6s}}+\frac{\boldsymbol{b}_{2s}}{|z|^{4s}N^{2s}}\right]^{\frac{1}{4s}}\left[\frac{2^{4s-1}\boldsymbol{c}_{2s}(\mathrm{Tr}[T_K])^{4s}}{|z|^{8s}N^{6s}}+\frac{2^{4s-1}\boldsymbol{c}_{2s}}{|z|^{4s}N^{2s}}\right]^{\frac{1}{4s}}
\end{aligned}$$

Let $\boldsymbol{r}_s=\max\{2^{2s-1}\boldsymbol{c}_s,\boldsymbol{a}_s\}$ and $\boldsymbol{t}_s=\max\{2^{2s-1}\boldsymbol{c}_s,\boldsymbol{b}_s\}$; then putting the pieces together we have

$$\mathbb{E}\left[|X_2|^{2s}\right]^{\frac{1}{2s}} \leq \frac{d_\ell+d_k}{|1+d_\ell\tilde{m}|\,|1+d_k\tilde{m}|}\left[\frac{\boldsymbol{r}_s(\mathrm{Tr}[T_K])^{2s}}{|z|^{4s}N^{3s}}+\frac{\boldsymbol{t}_s}{|z|^{2s}N^s}\right]^{\frac{1}{2s}}+\frac{d_\ell d_k}{|1+d_\ell\tilde{m}|\,|1+d_k\tilde{m}|}\left[\frac{\boldsymbol{r}_{2s}(\mathrm{Tr}[T_K])^{4s}}{|z|^{8s}N^{6s}}+\frac{\boldsymbol{t}_{2s}}{|z|^{4s}N^{2s}}\right]^{\frac{1}{2s}}$$

and thus

$$\mathbb{E}\left[|X_2|^{2}\right]^{\frac{1}{2}} \leq \frac{d_\ell+d_k}{|1+d_\ell\tilde{m}|\,|1+d_k\tilde{m}|}\left[\frac{\boldsymbol{r}_1^{1/2}(\mathrm{Tr}[T_K])}{|z|^2N^{3/2}}+\frac{\boldsymbol{t}_1^{1/2}}{|z|\sqrt{N}}\right]+\frac{d_\ell d_k}{|1+d_\ell\tilde{m}|\,|1+d_k\tilde{m}|}\left[\frac{\boldsymbol{r}_2^{1/2}(\mathrm{Tr}[T_K])^2}{|z|^4N^3}+\frac{\boldsymbol{t}_2^{1/2}}{|z|^2N^1}\right]$$

$$\mathbb{E}\left[|X_4|^{4}\right]^{\frac{1}{2}} \leq \frac{2(d_\ell+d_k)^2}{|1+d_\ell\tilde{m}|^2\,|1+d_k\tilde{m}|^2}\left[\frac{\boldsymbol{r}_2^{1/2}(\mathrm{Tr}[T_K])^2}{|z|^4N^3}+\frac{\boldsymbol{t}_2^{1/2}}{|z|^2N}\right]+\frac{2d_\ell^2d_k^2}{|1+d_\ell\tilde{m}|^2\,|1+d_k\tilde{m}|^2}\left[\frac{\boldsymbol{r}_4^{1/2}(\mathrm{Tr}[T_K])^4}{|z|^8N^6}+\frac{\boldsymbol{t}_4^{1/2}}{|z|^4N^2}\right]$$

And finally, putting all the pieces together, we have

$$\begin{aligned}
|\epsilon_{k\ell}| &\leq \mathbb{E}\left[|X_1|^4\right]^{\frac{1}{2}}\left(c\mathbb{E}\left[|X_2|^2\right]^{\frac{1}{2}}+\mathbb{E}\left[|X_2|^4\right]^{\frac{1}{2}}\right)\\
&\leq \frac{\boldsymbol{a}d_k^2}{|z|^2N}\frac{2(d_\ell+d_k)}{|1+d_\ell\tilde{m}|^2\,|1+d_k\tilde{m}|^2}\left[\frac{\boldsymbol{r}_1^{1/2}(\mathrm{Tr}[T_K])}{|z|^2N^{3/2}}+\frac{\boldsymbol{t}_1^{1/2}}{|z|\sqrt{N}}\right]\\
&\quad+\frac{\boldsymbol{a}d_k^2}{|z|^2N}\frac{2(d_\ell+d_k)^2+2d_\ell d_k}{|1+d_\ell\tilde{m}|^2\,|1+d_k\tilde{m}|^2}\left[\frac{\boldsymbol{r}_2^{1/2}(\mathrm{Tr}[T_K])^2}{|z|^4N^3}+\frac{\boldsymbol{t}_2^{1/2}}{|z|^2N}\right]\\
&\quad+\frac{\boldsymbol{a}d_k^2}{|z|^2N}\frac{2d_\ell^2d_k^2}{|1+d_\ell\tilde{m}|^2\,|1+d_k\tilde{m}|^2}\left[\frac{\boldsymbol{r}_4^{1/2}(\mathrm{Tr}[T_K])^4}{|z|^8N^6}+\frac{\boldsymbol{t}_4^{1/2}}{|z|^4N^2}\right].
\end{aligned}$$

Using the fact that $|\partial_z\tilde{m}|\leq|\tilde{m}|^2$ and Proposition 3, we get:

$$\frac{1}{|z|^2}\leq\frac{|\partial_z\tilde{m}|}{|z|^2|\tilde{m}|^2}\leq|\partial_z\tilde{m}|\left(1+2\frac{\mathrm{Tr}[T_K]}{|z|N}+\frac{(\mathrm{Tr}[T_K])^2}{|z|^2N^2}\right),$$

we conclude saying that

$$|\epsilon_{k\ell}|\leq\frac{1}{N}\frac{d_k^2\partial_z\tilde{m}}{|1+d_\ell\tilde{m}|^2\,|1+d_k\tilde{m}|^2}\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|z|N^{\frac{1}{2}}}\right).$$

□

Remark. *Since $\tilde{m}(z)=\frac{1}{\vartheta(-z)}$, the derivative $\partial_z\tilde{m}(z)$ can also be expressed in terms of the SCT: $\partial_z\tilde{m}(z)=\partial_z\vartheta(-z)\frac{1}{\vartheta(-z)^2}$, hence the previous approximations can also be written as:*

$$\mathrm{Var}\left(A_{kk}(z)\right)\approx\frac{2}{N}\frac{d_k^2\vartheta(-z)^2\partial_z\vartheta(-z)}{(\vartheta(-z)+d_k)^4}\qquad\mathrm{Var}\left(A_{k\ell}(z)\right)\approx\frac{1}{N}\frac{d_k^2\vartheta(-z)^2\partial_z\vartheta(-z)}{(\vartheta(-z)+d_k)^2(\vartheta(-z)+d_\ell)^2}.$$

We can now describe the variance of the predictor. The variance of the predictor along the eigenfunction $f^{(k)}$ is estimated by V_k, where

$$V_k(f^*, \lambda, N, \epsilon) = \frac{\partial_\lambda \vartheta(\lambda)}{N} \left(\left\| (I_{\mathcal{C}} - \tilde{A}_\vartheta) f^* \right\|_S^2 + \epsilon^2 + \left\langle f^{(k)}, f^* \right\rangle_S^2 \frac{\vartheta^2(\lambda)}{(\vartheta(\lambda) + d_k)^2} \right) \frac{d_k^2}{(\vartheta(\lambda) + d_k)^2}.$$

Theorem 22. *There is a constant $\boldsymbol{C}_1 > 0$ such that, with the notation of Definition 5, we have*

$$\left| \mathrm{Var}\left(\left\langle f^{(k)}, \hat{f}_\lambda^\epsilon \right\rangle_S \right) - V_k(f^*, \lambda, N, \epsilon) \right| \leq \left(\frac{\boldsymbol{C}_1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N^{\frac{1}{2}}} \right) \right) V_k(f^*, \lambda, N, \epsilon).$$

Proof. Using the law of total variance, we decompose the variance with respect to the observations $\mathcal{O}$ and the vector of noise $E = (e_1, \ldots, e_N)^T$

$$\begin{aligned} \mathrm{Var}\left(\left\langle f^{(k)}, \hat{f}_\lambda^\epsilon \right\rangle_S \right) &= \mathrm{Var}_{\mathcal{O}}\left(\left\langle f^{(k)}, \mathbb{E}_E\left[\hat{f}_\lambda^\epsilon \right] \right\rangle_S \right) + \epsilon^2 \mathbb{E}_{\mathcal{O}}\left[\mathrm{Var}_E\left(\frac{d_k}{N} (\mathcal{O}_{\cdot k})^T \left(\frac{1}{N} \mathcal{O} K \mathcal{O}^T + \lambda I_N \right)^{-1} E \right) \right] \\ &= \mathrm{Var}_{\mathcal{O}}\left(\left\langle f^{(k)}, A(-\lambda) f^* \right\rangle_S \right) + \epsilon^2 \mathbb{E}_{\mathcal{O}}\left[\frac{d_k}{N} \partial_\lambda A_{kk}(-\lambda) \right]. \end{aligned}$$

Since the randomness is now only on A through $\mathcal{O}$, from now on, we will lighten the notation by sometimes omitting the $\mathcal{O}$ dependence in the expectations.

We first show how the approximation $V_k(f^*, \lambda, N, \epsilon)$ appears, and then establish the bounds which allow one to study the quality of this approximation.

Approximations: Decomposing the true function along the principal components $f^* = \sum_{k=1}^\infty b_k f^{(k)}$ with $b_k = \left\langle f^{(k)}, f^* \right\rangle_S$, we have

$$\mathrm{Var}(\langle f^{(k)}, A(-\lambda) f^* \rangle_S) = \sum_\ell b_\ell^2 \mathrm{Var}\left(A_{k\ell}(-\lambda) \right).$$

From Proposition 20 and the remark after, we have two different approximations for $\mathrm{Var}\left(A_{k\ell}(-\lambda) \right)$. For any $\ell \neq k$, we have

$$\mathrm{Var}\left(A_{kk}(-\lambda) \right) \approx \frac{2}{N} \frac{d_k^2 \vartheta(\lambda)^2 \partial_\lambda \vartheta(\lambda)}{(\vartheta(\lambda) + d_k)^4}, \qquad \mathrm{Var}\left(A_{k\ell}(-\lambda) \right) \approx \frac{1}{N} \frac{d_k^2 \vartheta(\lambda)^2 \partial_\lambda \vartheta(\lambda)}{(\vartheta(\lambda) + d_k)^2 (\vartheta(\lambda) + d_\ell)^2}.$$

Hence

$$\begin{aligned} \mathrm{Var}(\langle f^{(k)}, A_\lambda f^* \rangle_S) &\approx \frac{b_k^2}{N} \frac{d_k^2 \vartheta(\lambda)^2 \partial_\lambda \vartheta(\lambda)}{(\vartheta(\lambda) + d_k)^4} + \sum_\ell \frac{b_\ell^2}{N} \frac{d_k^2 \vartheta(\lambda)^2 \partial_\lambda \vartheta(\lambda)}{(\vartheta(\lambda) + d_k)^2 (\vartheta(\lambda) + d_\ell)^2} \\ &= \frac{\partial_\lambda \vartheta(\lambda)}{N} \left(\left\langle f^{(k)}, f^* \right\rangle_S^2 \frac{\vartheta^2(\lambda)}{(\vartheta(\lambda) + d_k)^2} + \sum_\ell b_\ell^2 \frac{\vartheta(\lambda)^2}{(\vartheta(\lambda) + d_\ell)^2} \right) \frac{d_k^2}{(\vartheta(\lambda) + d_k)^2}. \end{aligned}$$

Since $\sum_\ell b_\ell^2 \frac{\vartheta(\lambda)^2}{(\vartheta(\lambda) + d_\ell)^2} = \| (I_{\mathcal{C}} - \tilde{A}_\vartheta) f^* \|_S^2$, this provides the approximation:

$$\mathrm{Var}(\langle f^{(k)}, A_\lambda f^* \rangle_S) \approx \frac{\partial_\lambda \vartheta(\lambda)}{N} \left(\| (I_{\mathcal{C}} - \tilde{A}_\vartheta) f^* \|_S^2 + \langle f^{(k)}, f^* \rangle_S^2 \frac{\vartheta^2(\lambda)}{(\vartheta(\lambda) + d_k)^2} \right) \frac{d_k^2}{(\vartheta(\lambda) + d_k)^2}. \tag{20}$$

Now, using Lemma 27 and Theorem 17:

$$\epsilon^2 \mathbb{E}_{\mathcal{O}}\left[\frac{d_k}{N} \partial_\lambda A_{kk}(-\lambda) \right] \approx \epsilon^2 \frac{\partial_\lambda \vartheta(\lambda)}{N} \frac{d_k^2}{(\vartheta(\lambda) + d_k)^2}. \tag{21}$$

Combining Equations 20 and 21, we obtain the approximation

$$\mathrm{Var}(\langle f^{(k)}, \hat{f}_\lambda^\epsilon \rangle_S) \approx V_k(f^*, \lambda, N, \epsilon).$$

Now, we explain how to quantify the quality of the approximations, and thus how to get the bound stated in the theorem. Recall that we decomposed $\mathrm{Var}(\langle f^{(k)}, \hat{f}^{\epsilon}_{\lambda}\rangle_S)$ into two terms using the law of total variance.

First term: We have seen that:

$$\mathrm{Var}\left(\left\langle f^{(k)}, A_\lambda f^* \right\rangle_S\right) = b_k^2 \mathrm{Var}\left(A_{kk}(-\lambda)\right) + \sum_{\ell \neq k} b_\ell^2 \mathrm{Var}\left(A_{k\ell}(-\lambda)\right).$$

By Proposition 20, we have

$$\begin{aligned}\left| b_k^2 \mathrm{Var}\left(A_{kk}(-\lambda)\right) - 2 b_k^2 \frac{\partial_\lambda \vartheta(\lambda)}{N} \frac{\vartheta(\lambda)^2 d_k^2}{(\vartheta(\lambda) + d_k)^4} \right| &= b_k^2 \left| \mathrm{Var}\left(A_{kk}(-\lambda)\right) - \frac{2}{N} \frac{d_k^2 \partial_\lambda \tilde{m}}{(1 + d_k \tilde{m})^4} \right| \\ &\leq b_k^2 \frac{|\partial_\lambda \vartheta(\lambda)|}{N} \frac{|\vartheta(\lambda)|^2 d_k^2}{|\vartheta(\lambda) + d_k|^4} \left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N^{\frac{1}{2}}} \right) \right)\end{aligned}$$

and

$$\left| b_\ell^2 \mathrm{Var}\left(A_{k\ell}(-\lambda)\right) - \frac{1}{N} b_\ell^2 \frac{d_k^2 \partial_\lambda \tilde{m}}{(1 + d_k \tilde{m})^2 (1 + d_\ell \tilde{m})^2} \right| \leq b_\ell^2 \frac{1}{N} \frac{d_k^2 \left|\vartheta(\lambda)\right|^2 \left|\partial_\lambda \vartheta(\lambda)\right|}{\left|\vartheta(\lambda) + d_k\right|^2 \left|\vartheta(\lambda) + d_\ell\right|^2} \mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{\lambda N^{\frac{1}{2}}} \right).$$

Thus we have

$$\begin{aligned}&\left| \sum_\ell b_\ell^2 \mathrm{Var}\left(A_{k\ell}(-\lambda)\right) - \frac{\partial_\lambda \vartheta(\lambda)}{N} \frac{d_k^2}{(\vartheta(\lambda) + d_k)^2} \left(2 b_k^2 \frac{\vartheta(\lambda)^2}{(\vartheta(\lambda) + d_k)^2} + \sum_{\ell \neq k} b_\ell^2 \frac{\vartheta(\lambda)^2}{(\vartheta(\lambda) + d_\ell)^2} \right) \right| \\ &\leq b_k^2 \left| \mathrm{Var}\left(A_{kk}(-\lambda)\right) - \frac{2}{N} \frac{d_k^2 \partial_\lambda \tilde{m}}{(1 + d_k \tilde{m})^4} \right| + \sum_{\ell \neq k} b_\ell^2 \left| \mathrm{Var}\left(A_{k\ell}(-\lambda)\right) - \frac{1}{N} \frac{d_k^2 \partial_\lambda \tilde{m}}{(1 + d_k \tilde{m})^2 (1 + d_\ell \tilde{m})^2} \right| \\ &\leq b_k^2 \frac{1}{N} \frac{d_k^2 \left|\vartheta(\lambda)\right|^2 \left|\partial_\lambda \vartheta(\lambda)\right|}{\left|\vartheta(\lambda) + d_k\right|^4} \left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N^{\frac{1}{2}}} \right) \right) + \sum_{\ell \neq k} b_\ell^2 \frac{1}{N} \frac{d_k^2 \left|\vartheta(\lambda)\right|^2 \left|\partial_\lambda \vartheta(\lambda)\right|}{\left|\vartheta(\lambda) + d_k\right|^2 \left|\vartheta(\lambda) + d_\ell\right|^2} \mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{\lambda N^{\frac{1}{2}}} \right) \\ &\leq \frac{\left|\partial_\lambda \vartheta(\lambda)\right|}{N} \frac{d_k^2}{\left|\vartheta(\lambda) + d_k\right|^2} \sum_\ell b_\ell^2 \frac{|\vartheta(\lambda)|^2}{|\vartheta(\lambda) + d_\ell|^2} \left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{\lambda N^{\frac{1}{2}}} \right) \right) \\ &\leq \frac{\left|\partial_\lambda \vartheta(\lambda)\right|}{N} \frac{d_k^2}{\left|\vartheta(\lambda) + d_k\right|^2} \left\| \left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)} \right) f^* \right\|_S^2 \left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{\lambda N^{\frac{1}{2}}} \right) \right).\end{aligned}$$

We deduce:

$$\begin{aligned}&\left| \mathrm{Var}_{\mathcal{O}}\left(\left\langle f^{(k)}, A_\lambda f^* \right\rangle_S\right) - \frac{\partial_\lambda \vartheta(\lambda)}{N} \left(\left\| \left(I_{\mathcal{C}} - \tilde{A}_\lambda \right) f^* \right\|_S^2 + \left\langle f^{(k)}, f^* \right\rangle_S^2 \frac{\vartheta(\lambda)^2}{(\vartheta(\lambda) + d_k)^2} \right) \frac{d_k^2}{(\vartheta(\lambda) + d_k)^2} \right| \\ &\leq \frac{\partial_\lambda \vartheta(\lambda)}{N} \left(\left\| \left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)} \right) f^* \right\|_S^2 \right) \frac{d_k^2}{(\vartheta(\lambda) + d_k)^2} \left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{\lambda N^{\frac{1}{2}}} \right) \right) \\ &\leq \frac{\partial_\lambda \vartheta(\lambda)}{N} \left(\left\| \left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)} \right) f^* \right\|_S^2 + \left\langle f^{(k)}, f^* \right\rangle_S^2 \frac{\vartheta(\lambda)^2}{(\vartheta(\lambda) + d_k)^2} \right) \frac{d_k^2}{(\vartheta(\lambda) + d_k)^2} \left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{\lambda N^{\frac{1}{2}}} \right) \right).\end{aligned}$$

Second term: To approximate, we apply Cauchy's inequality to Equation (17) of Theorem 17:

$$\begin{aligned}\left| \mathbb{E}\left[\partial_z A_{kk}(z)\right] - \partial_z \vartheta(-z) \frac{d_k}{(\vartheta(-z) + d_k)^2} \right| &\leq \frac{2}{-\Re(z)} \sup_{|w - z| = -\frac{1}{2}\Re(z)} \left| \mathbb{E}[A_{kk}(w)] - \frac{d_k}{\vartheta(-w) + d_k} \right| \\ &\leq \frac{2}{-\Re(z)} \sup_{|w - z| = -\frac{1}{2}\Re(z)} \frac{d_k \left|\vartheta(-w)\right|}{\left|\vartheta(-w) + d_k\right|^2} \left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{|w|\, N} \right) \right).\end{aligned}$$

By choosing $z = -\lambda$, in the region $\{w \in \mathbb{C} \mid |w + \lambda| = \frac{\lambda}{2}\}$ the polynomial $\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{|w|N}\right)$ is uniformly bounded by $\mathcal{P}\left(\frac{2\mathrm{Tr}[T_K]}{\lambda N}\right)$ and $\frac{d_k|\vartheta(-w)|}{|\vartheta(-w)+d_k|^2} \leq \frac{d_k|\vartheta(\lambda)|}{|\vartheta(\lambda)+d_k|^2}$. Thus we get

$$\begin{aligned}\left|\mathbb{E}\left[\partial_\lambda A_{kk}(-\lambda)\right] - \partial_\lambda\vartheta(\lambda)\frac{d_k}{(\vartheta(\lambda)+d_k)^2}\right| &\leq 2\frac{d_k}{|\vartheta(\lambda)+d_k|^2}\frac{\vartheta(\lambda)}{\lambda}\left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{\lambda N}\right)\right)\\ &\leq 2\frac{d_k}{|\vartheta(\lambda)+d_k|^2}\left(1 + \frac{\mathrm{Tr}[T_K]}{\lambda N}\right)\left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{\lambda N}\right)\right)\\ &\leq \frac{d_k}{|\vartheta(\lambda)+d_k|^2}\left(\frac{2}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{\lambda N}\right)\right).\end{aligned}$$

By using the fact that $1 \leq |\partial_\lambda\vartheta(\lambda)|$ (see Proposition 3), we have that

$$\left|\frac{d_k}{N}\mathbb{E}\left[\partial_\lambda A_{kk}(-\lambda)\right] - \frac{\partial_\lambda\vartheta(\lambda)}{N}\frac{d_k^2}{(\vartheta(\lambda)+d_k)^2}\right| \leq \frac{|\partial_\lambda\vartheta(\lambda)|}{N}\frac{d_k^2}{|\vartheta(\lambda)+d_k|^2}\left(\frac{2}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{|z|\,N}\right)\right).$$

Finally, by putting the bounds for the two terms together we have

$$\begin{aligned}&\left|\mathrm{Var}\left(\left\langle f^{(k)}, \hat{f}_\lambda^\epsilon\right\rangle_S\right) - \frac{\partial_\lambda\vartheta(\lambda)}{N}\frac{d_k^2}{(\vartheta(\lambda)+d_k)^2}\left(2b_k^2\frac{\vartheta(\lambda)^2}{(\vartheta(\lambda)+d_k)^2} + \sum_{\ell\neq k} b_\ell^2\frac{\vartheta(\lambda)^2}{(\vartheta(\lambda)+d_\ell)^2} + \epsilon^2\right)\right|\\ &\leq \left|\mathrm{Var}\left(\left\langle f^{(k)}, A_\lambda f^*\right\rangle_S\right) - \frac{\partial_\lambda\vartheta(\lambda)}{N}\frac{d_k^2}{(\vartheta(\lambda)+d_k)^2}\left(2b_k^2\frac{\vartheta(\lambda)^2}{(\vartheta(\lambda)+d_k)^2} + \sum_{\ell\neq k} b_\ell^2\frac{\vartheta(\lambda)^2}{(\vartheta(\lambda)+d_\ell)^2}\right)\right|\\ &\qquad\qquad + \epsilon^2\frac{d_k}{N}\left|\partial_\lambda\mathbb{E}[A_{kk}(-\lambda)] - \partial_\lambda\vartheta(\lambda)\frac{d_k}{(\vartheta(\lambda)+d_k)^2}\right|\\ &\leq \frac{\partial_\lambda\vartheta(\lambda)}{N}\left(\left\|\left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}\right)f^*\right\|_S^2 + \epsilon^2\right)\frac{d_k^2}{(\vartheta(\lambda)+d_k)^2}\left(\frac{2}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{\lambda N^{\frac{1}{2}}}\right)\right).\end{aligned}$$

This concludes the proof. □

B.5 Expected Risk

We now have all the tools required to describe the expected risk and empirical risk. In particular, we now show that the distance between the expected risk $\mathbb{E}[R^\epsilon(\hat{f}_\lambda^\epsilon)]$ and

$$\tilde{R}^\epsilon(f^*, \lambda) = \partial_\lambda\vartheta(\lambda)(\|(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)})f^*\|_S^2 + \epsilon^2)$$

is relatively small:

Theorem 23. *We have*

$$\left|\mathbb{E}\left[R^\epsilon\left(\hat{f}_\lambda^\epsilon\right)\right] - \tilde{R}^\epsilon\left(f^*, \lambda\right)\right| \leq \tilde{R}^\epsilon\left(f^*, \lambda\right)\left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{\lambda N^{\frac{1}{2}}}\right)\right).$$

Proof. The expected risk can be written as $\mathbb{E}[R^\epsilon(\hat{f}_\lambda^\epsilon)] = \mathbb{E}[\|\hat{f}_\lambda^\epsilon - f^*\|_S^2] + \epsilon^2 = \sum_k \mathbb{E}[(a_k - b_k)^2] + \epsilon^2$, where $a_k = \langle f^{(k)}, \hat{f}_\lambda^\epsilon\rangle_S$ and $b_k = \langle f^{(k)}, f^*\rangle_S$. Hence, using the classical bias-variance decomposition for each summand, we get that the expected risk is equal to:

$$\mathbb{E}[R^\epsilon(\hat{f}_\lambda^\epsilon)] = R^\epsilon(\mathbb{E}[\hat{f}_\lambda^\epsilon]) + \sum_{k=1}^{\infty}\mathrm{Var}(\langle f^{(k)}, \hat{f}_\lambda^\epsilon\rangle_S).$$

Similarly to the proof of Theorem 22, we explain how the approximation of the expected arises, then we establish the bounds which allow one to study the quality of this approximation.

Approximations: The bias term $R^\epsilon(\mathbb{E}[\hat{f}_\lambda^\epsilon])$ is equal to $\|\mathbb{E}[\hat{f}_\lambda^\epsilon] - f^*\|_S^2 + \epsilon^2 = \|(I_{\mathcal{C}} - \mathbb{E}[A_\lambda])f^*\|_S^2 + \epsilon^2$. Using Theorem 17, one gets the approximation of the bias term:

$$R^\epsilon(\mathbb{E}[\hat{f}_\lambda^\epsilon]) \approx \|(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)})f^*\|_S^2 + \epsilon^2.$$

As for the variance term $\sum_{k=1}^{\infty} \mathrm{Var}(\langle f^{(k)}, \hat{f}_{\lambda}^{\epsilon}\rangle_S)$, we use Theorem 22.

$$\sum_{k=1}^{\infty} \mathrm{Var}(\langle f^{(k)}, \hat{f}_{\lambda}^{\epsilon}\rangle_S) \approx \sum_{k=1}^{\infty} V_k(f^*, \lambda, N, \epsilon),$$

where

$$V_k(f^*, \lambda, N, \epsilon) = \frac{\partial_\lambda \vartheta(\lambda)}{N} \left(\left\| (I_{\mathcal{C}} - \tilde{A}_\vartheta) f^* \right\|_S^2 + \epsilon^2 + \left\langle f^{(k)}, f^* \right\rangle_S^2 \frac{\vartheta^2(\lambda)}{(\vartheta(\lambda) + d_k)^2} \right) \frac{d_k^2}{(\vartheta(\lambda) + d_k)^2}.$$

Thus the variance term is approximately equal to:

$$(\|(I_{\mathcal{C}} - \tilde{A}_\vartheta) f^*\|_S^2 + \epsilon^2) \frac{\partial_\lambda \vartheta(\lambda)}{N} \sum_{k=1}^{\infty} \frac{d_k^2}{(\vartheta(\lambda) + d_k)^2} + \frac{\partial_\lambda \vartheta(\lambda)}{N} \sum_{k=1}^{\infty} \langle f^{(k)}, f^* \rangle_S^2 \frac{\vartheta^2(\lambda) d_k^2}{(\vartheta(\lambda) + d_k)^4}.$$

Noting that from Equation 15, we have $(\partial_\lambda \vartheta(\lambda) - 1) = \frac{\partial_\lambda \vartheta(\lambda)}{N} \sum_{k=1}^{\infty} \frac{d_k^2}{(\vartheta(\lambda)+d_k)^2}$, we get:

$$\sum_{k=1}^{\infty} \mathrm{Var}(\langle f^{(k)}, \hat{f}_{\lambda}^{\epsilon}\rangle_S) \approx (\partial_\lambda \vartheta(\lambda) - 1)(\|(I_{\mathcal{C}} - \tilde{A}_\vartheta) f^*\|_S^2 + \epsilon^2) + \frac{\partial_\lambda \vartheta(\lambda)}{N} \sum_{k=1}^{\infty} \langle f^{(k)}, f^* \rangle_S^2 \frac{\vartheta^2(\lambda) d_k^2}{(\vartheta(\lambda) + d_k)^4}.$$

The second term in the r.h.s. is a residual term: using the fact that $\frac{d_k^2}{(\vartheta(\lambda)+d_k)^2} \leq 1$, this term is bounded by $\frac{\partial_\lambda \vartheta(\lambda)}{N} \|(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}) f^*\|_S^2$.

Hence, we get the following approximation of the variance term:

$$\sum_{k=1}^{\infty} \mathrm{Var}(\langle f^{(k)}, \hat{f}_{\lambda}^{\epsilon}\rangle_S) \approx (\partial_\lambda \vartheta(\lambda) - 1)(\|(I_{\mathcal{C}} - \tilde{A}_\vartheta) f^*\|_S^2 + \epsilon^2).$$

Putting the approximations of the bias and variance terms together, we obtain:

$$\mathbb{E}\left[R^\epsilon \left(\hat{f}_\lambda^\epsilon \right) \right] \approx \tilde{R}^\epsilon (f^*, \lambda).$$

Now, we explain how to quantify the quality of the approximations, and thus how to get the bound stated in the theorem. Recall that, using the bias-variance decomposition, we split the expected risk into two terms, the bias term and the variance term. We show now that:

$$\left| R^\epsilon(\mathbb{E}_{\mathcal{O},E}[\hat{f}_\lambda^\epsilon]) - \left(\|(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}) f^*\|_S^2 + \epsilon^2 \right) \right| \leq \|(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}) f^*\|_S^2 \left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}\,[T_K]}{\lambda N} \right) \right)$$

and

$$\left| \sum_{k=1}^{\infty} \mathrm{Var}(\langle f^{(k)}, \hat{f}_{\lambda}^{\epsilon}\rangle_S) - (\partial_\lambda \vartheta(\lambda) - 1) \left(\|(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}) f^*\|_S^2 + \epsilon^2 \right) \right| \leq$$

$$\partial_\lambda \vartheta(\lambda) \left(\|(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}) f^*\|_S^2 + \epsilon^2 \right) \left(\frac{2}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}\,[T_K]}{\lambda N^{\frac{1}{2}}} \right) \right).$$

Combining the two inequations, and using the fact that $1 \leq \partial_\lambda \vartheta(\lambda)$, we then get the desired inequality.

Bias term: Since $|\tilde{A}_{\vartheta(\lambda),kk}| \leq 1$, Equation (17) of Theorem 17 implies that

$$\left| \tilde{A}_{\vartheta(\lambda),kk} - \mathbb{E}\left[A_{kk}(-\lambda) \right] \right| \leq |1 - \tilde{A}_{\vartheta(\lambda),kk}| \left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N} \right) \right).$$

We then get

$$1 - \mathbb{E}\left[A_{\lambda,kk} \right] \leq 1 - \tilde{A}_{\lambda,kk} + \frac{c}{\lambda^2 N} \left(1 - \tilde{A}_{\lambda,kk} \right) \tilde{A}_{\lambda,kk} \leq \left(1 - \tilde{A}_{\lambda,kk} \right) \left(1 + \frac{c}{\lambda^2 N} \right).$$

We decompose the true function f^* into $f^* = \sum_{k=1}^{\infty} b_k f^{(k)}$ for $b_k = \left\langle f^*, f^{(k)} \right\rangle_S$, and obtain

$$\begin{aligned}
\left| R^{\epsilon}\left(\mathbb{E}_{\mathcal{O},E}\left[\hat{f}_{\lambda}^{\epsilon}\right]\right) - \left(\left\|\left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}\right) f^*\right\|_S^2 + \epsilon^2\right)\right| &= \left| \left\|\left(I_{\mathcal{C}} - \mathbb{E}\left[A_{\lambda}\right]\right) f^*\right\|_S^2 - \left\|\left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}\right) f^*\right\|_S^2 \right| \\
&= \left| \sum_{k=1}^{\infty} b_k^2 \left(\left(1 - \mathbb{E}\left[A_{\lambda,kk}\right]\right)^2 - \left(1 - \tilde{A}_{\vartheta(\lambda),kk}\right)^2 \right) \right| \\
&\leq \sum_{k=1}^{\infty} b_k^2 \left| \tilde{A}_{\vartheta(\lambda),kk} - \mathbb{E}\left[A_{\lambda,kk}\right] \right| \left| 2 - \tilde{A}_{\vartheta(\lambda),kk} - \mathbb{E}\left[A_{\vartheta(\lambda),kk}\right] \right| .
\end{aligned}$$

By the triangular inequality, we get that

$$\left| 2 - \tilde{A}_{\vartheta(\lambda),kk} - \mathbb{E}\left[A_{\vartheta(\lambda),kk}\right] \right| \leq \left| 1 - \tilde{A}_{\vartheta(\lambda),kk} \right| \left(2 + \left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N} \right) \right) \right)$$

and thus

$$\begin{aligned}
&\left| R^{\epsilon}\left(\mathbb{E}_{\mathcal{O},E}\left[\hat{f}_{\lambda}^{\epsilon}\right]\right) - \left(\left\|\left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}\right) f^*\right\|_S^2 + \epsilon^2\right)\right| \\
&\leq \sum_{k=1}^{\infty} b_k^2 \left| 1 - \tilde{A}_{\vartheta(\lambda),kk} \right|^2 \left(2 + \frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N} \right) \right) \left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N} \right) \right) \\
&\leq \sum_{k=1}^{\infty} b_k^2 \left| 1 - \tilde{A}_{\vartheta(\lambda),kk} \right|^2 \left(\frac{\boldsymbol{C}_2}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N} \right) \right) .
\end{aligned}$$

Variance term: For the second term, recall that $(\partial_{\lambda}\vartheta(\lambda) - 1) = \frac{\partial_{\lambda}\vartheta(\lambda)}{N} \sum_{k=1}^{\infty} \frac{d_k^2}{(\vartheta(\lambda)+d_k)^2}$, and that

$$\begin{aligned}
&\left| \sum_{k=1}^{\infty} \mathrm{Var}\left(\left\langle f^{(k)}, \hat{f}_{\lambda}^{\epsilon} \right\rangle_S \right) - (\partial_{\lambda}\vartheta(\lambda) - 1) \left(\left\|\left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}\right) f^*\right\|_S^2 + \epsilon^2 \right) \right| \\
&\leq \sum_{k=1}^{\infty} \left| \mathrm{Var}_{\mathcal{O}}\left(\left\langle f^{(k)}, A(-\lambda) f^* \right\rangle_S \right) - \frac{\partial_{\lambda}\vartheta(\lambda)}{N} \left(\left\|\left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}\right) f^*\right\|_S^2 + \epsilon^2 + \left\langle f^{(k)}, f^* \right\rangle_S^2 \frac{\vartheta(\lambda)^2}{(\vartheta(\lambda) + d_k)^2} \right) \frac{d_k^2}{(\vartheta(\lambda) + d_k)^2} \right| \\
&+ \sum_{k=1}^{\infty} \frac{\partial_{\lambda}\vartheta(\lambda)}{N} \left\langle f^{(k)}, f^* \right\rangle_S^2 \frac{\vartheta(\lambda)^2 d_k^2}{(\vartheta(\lambda) + d_k)^4} .
\end{aligned}$$

Using Theorem 22, we can control the terms in the first series: there is a constant $\boldsymbol{C}_1 > 0$ such that

$$\begin{aligned}
&\sum_{k=1}^{\infty} \left| \mathrm{Var}_{\mathcal{O}}\left(\left\langle f^{(k)}, A(-\lambda) f^* \right\rangle_S \right) - \frac{\partial_{\lambda}\vartheta(\lambda)}{N} \left(\left\|\left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}\right) f^*\right\|_S^2 + \epsilon^2 + \left\langle f^{(k)}, f^* \right\rangle_S^2 \frac{\vartheta(\lambda)^2}{(\vartheta(\lambda) + d_k)^2} \right) \frac{d_k^2}{(\vartheta(\lambda) + d_k)^2} \right| \\
&\leq \left(\frac{\boldsymbol{C}_1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N^{\frac{1}{2}}} \right) \right) \frac{\partial_{\lambda}\vartheta(\lambda)}{N} \sum_{k=1}^{\infty} \left(\left\|(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}) f^*\right\|_S^2 + \epsilon^2 + \left\langle f^{(k)}, f^* \right\rangle_S^2 \frac{\vartheta^2(\lambda)}{(\vartheta(\lambda) + d_k)^2} \right) \frac{d_k^2}{(\vartheta(\lambda) + d_k)^2} \\
&\leq \left(\frac{\boldsymbol{C}_1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N^{\frac{1}{2}}} \right) \right) \frac{\partial_{\lambda}\vartheta(\lambda)}{N} \left(\left\|\left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}\right) \tilde{A}_{\vartheta(\lambda)} f^*\right\|_S^2 + \left(\left\|(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}) f^*\right\|_S^2 + \epsilon^2 \right) \sum_{k=1}^{\infty} \frac{d_k^2}{(\vartheta(\lambda) + d_k)^2} \right) \\
&\leq \left(\frac{\boldsymbol{C}_1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N^{\frac{1}{2}}} \right) \right) \left(\frac{\partial_{\lambda}\vartheta(\lambda)}{N} \left\|\left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}\right) \tilde{A}_{\vartheta(\lambda)} f^*\right\|_S^2 + (\partial_{\lambda}\vartheta(\lambda) - 1) \left(\left\|(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}) f^*\right\|_S^2 + \epsilon^2 \right) \right) \\
&\leq \left(\frac{\boldsymbol{C}_1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N^{\frac{1}{2}}} \right) \right) \left(\frac{\partial_{\lambda}\vartheta(\lambda)}{N} \left\|\left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}\right) f^*\right\|_S^2 + (\partial_{\lambda}\vartheta(\lambda) - 1) \left(\left\|(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}) f^*\right\|_S^2 + \epsilon^2 \right) \right) ,
\end{aligned}$$

whereas for the second series, as explained already above, we have

$$\sum_{k=1}^{\infty} \frac{\partial_{\lambda}\vartheta(\lambda)}{N} \left\langle f^{(k)}, f^* \right\rangle_S^2 \frac{\vartheta(\lambda)^2 d_k^2}{(\vartheta(\lambda) + d_k)^4} = \frac{\partial_{\lambda}\vartheta(\lambda)}{N} \left\|\left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}\right) \tilde{A}_{\vartheta(\lambda)} f^*\right\|_S^2 \leq \frac{\partial_{\lambda}\vartheta(\lambda)}{N} \left\|\left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}\right) f^*\right\|_S^2 .$$

Finally, putting the pieces together, we conclude. □

B.6 Expected Empirical Risk

The expected empirical risk can be approximated as follows:

Theorem 24. *We have*

$$\left| \mathbb{E}\left[\hat{R}^{\epsilon}\left(\hat{f}^{\epsilon}_{\lambda,E}\right)\right] - \frac{\lambda^2}{\vartheta(\lambda)^2}\tilde{R}^{\epsilon}\left(f^*,\lambda\right)\right| \leq \tilde{R}^{\epsilon}\left(f^*,\lambda\right)\mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{\lambda N}\right).$$

Proof. A small computation allows one to show that:

$$\hat{R}^{\epsilon}\left(\hat{f}^{\epsilon}_{\lambda,E}\right) = \frac{\lambda^2}{N}\left(y^{\epsilon}\right)^T\left(\frac{1}{N}G+\lambda I_N\right)^{-2} y^{\epsilon}.$$

Using the definition of y^{ϵ} and the fact that the noise on the labels is centered and independent from the observations, this yields:

$$\begin{aligned}\mathbb{E}\left[\hat{R}^{\epsilon}\left(\hat{f}^{\epsilon}_{\lambda,E}\right)\right] &= \frac{\lambda^2}{N}f^*\mathbb{E}\left[\mathcal{O}^T\left(\frac{1}{N}G+\lambda I_N\right)^{-2}\mathcal{O}\right]f^* + \lambda^2\epsilon^2\mathbb{E}\left[\frac{1}{N}\mathrm{Tr}\left(\frac{1}{N}G+\lambda I_N\right)^{-2}\right] \\ &= \lambda^2\sum_{k=1}^{N}\langle f^{(k)}, f^*\rangle_S^2\frac{\mathbb{E}\left[\partial_\lambda A_{kk}(-\lambda)\right]}{d_k} + \lambda^2\epsilon^2\mathbb{E}\left[\partial_z m(-\lambda)\right].\end{aligned}$$

Similarly to the proof of Theorem 22, we explain how the approximation of the expected empirical risk appears, then we establish the bounds which allow one to study the quality of this approximation.

Approximations: Using Equation 21, $\mathbb{E}\left[\partial_\lambda A_{kk}(-\lambda)\right] \approx \partial_\lambda\vartheta(\lambda)\frac{d_k}{(\vartheta(\lambda)+d_k)^2}$ hence

$$\begin{aligned}\lambda^2\sum_{k=1}^{N}\langle f^{(k)}, f^*\rangle_S^2\frac{\mathbb{E}\left[\partial_\lambda A_{kk}(-\lambda)\right]}{d_k} &\approx \frac{\partial_\lambda\vartheta(\lambda)\lambda^2}{\vartheta(\lambda)^2}\sum_{k=1}^{N}\langle f^{(k)}, f^*\rangle_S^2\frac{\vartheta(\lambda)^2}{(\vartheta(\lambda)+d_k)^2} \\ &= \frac{\partial_\lambda\vartheta(\lambda)\lambda^2}{\vartheta(\lambda)^2}\|(I_{\mathcal{C}}-\tilde{A}_{\vartheta(\lambda)})f^*\|_S^2.\end{aligned}$$

The second term can be approximated using Proposition 11 and Lemma 27: this yields

$$\mathbb{E}\left[\partial_\lambda m(-\lambda)\right] \approx \partial_\lambda\tilde{m}(-\lambda) = \frac{\partial_\lambda\vartheta(\lambda)}{\vartheta(\lambda)^2}.$$

Hence, putting the two approximations together, the expected empirical risk is approximated by:

$$\mathbb{E}\left[\hat{R}^{\epsilon}\left(\hat{f}^{\epsilon}_{\lambda,E}\right)\right] \approx \frac{\partial_\lambda\vartheta(\lambda)\lambda^2}{\vartheta(\lambda)^2}\left(\|(I_{\mathcal{C}}-\tilde{A}_{\vartheta(\lambda)})f^*\|_S^2+\epsilon^2\right) = \frac{\lambda^2}{\vartheta(\lambda)^2}R^{\epsilon}(f^*,\lambda).$$

Now, we explain how to quantify the quality of the approximations, and thus how to get the bound stated in the theorem. Recall that, we split the expected empirical risk into two terms.

First term: We have already seen in Theorem 22 that by applying Lemma 27 to Equation (17) of Theorem 17 we get

$$\left|\mathbb{E}\left[\partial_z A_{kk}(-\lambda)\right] - \partial_\lambda\vartheta(\lambda)\frac{d_k}{(\vartheta(\lambda)+d_k)^2}\right| \leq \frac{d_k}{|\vartheta(\lambda)+d_k|^2}\left(\frac{2}{N}+\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N}\right)\right)$$

and thus

$$\begin{aligned}&\left|\lambda^2\sum_{k=1}^N \left\langle f^{(k)}, f^*\right\rangle_S^2 \frac{\mathbb{E}\left[\partial_\lambda A_{kk}(-\lambda)\right]}{d_k} - \frac{\partial_\lambda\vartheta(\lambda)\lambda^2}{\vartheta(\lambda)^2}\left\|\left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}\right)f^*\right\|_S^2\right|\\
&\leq \lambda^2\sum_{k=1}^N \left\langle f^{(k)}, f^*\right\rangle_S^2 \left|\frac{\mathbb{E}\left[\partial_\lambda A_{kk}(-\lambda)\right]}{d_k} - \frac{\partial_\lambda\vartheta(\lambda)}{\vartheta(\lambda)^2}\frac{\vartheta(\lambda)^2}{(\vartheta(\lambda)+d_k)^2}\right|\\
&\leq \lambda^2\sum_{k=1}^N \left\langle f^{(k)}, f^*\right\rangle_S^2 \frac{1}{\left|\vartheta(\lambda)+d_k\right|^2}\left(\frac{2}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N}\right)\right)\\
&= \frac{\lambda^2}{\vartheta(\lambda)^2}\left\|\left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}\right)f^*\right\|_S^2\left(\frac{2}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N}\right)\right)\\
&\leq \frac{\partial_\lambda\vartheta(\lambda)\lambda^2}{\vartheta(\lambda)^2}\left\|\left(I_{\mathcal{C}} - \tilde{A}_{\vartheta(\lambda)}\right)f^*\right\|_S^2\left(\frac{2}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N}\right)\right).\end{aligned}$$

Second Term: Using Proposition 11 and Lemma 27:

$$\left|\mathbb{E}\left[\partial_z m(z)\right] - \partial_z\tilde{m}(z)\right| \leq \frac{|z|}{-\Re(z)}\left(\frac{2^3\mathrm{Tr}\left[T_K\right]}{|z|^3 N^2} + \frac{2^4\boldsymbol{c}_1\left(\mathrm{Tr}\left[T_K\right]\right)^2}{|z|^4 N^2} + \frac{2^6\boldsymbol{c}_1\left(\mathrm{Tr}\left[T_K\right]\right)^4}{|z|^6 N^4}\right).$$

Thus, since $\partial_\lambda\tilde{m}(-\lambda) = \frac{\partial_\lambda\vartheta(\lambda)}{\vartheta(\lambda)^2}$,

$$\left|\lambda^2\epsilon^2\mathbb{E}\left[\partial_\lambda m(-\lambda)\right] - \frac{\lambda^2\epsilon^2}{\vartheta(\lambda)^2}\partial_\lambda\vartheta(\lambda)\right| \leq \epsilon^2\mathcal{P}\left(\frac{\mathrm{Tr}[T_K]}{\lambda N}\right).$$

□

B.7 Bayesian Setting

In this section, we consider the following Bayesian setting: let the true function f^* be random with zero mean and covariance kernel $\Sigma(x,y) = \mathbb{E}_{f^*}[f^*(x)f^*(y)]$. We will first show that in this setting the KRR predictor with kernel $K = \Sigma$ and ridge $\lambda = \frac{\epsilon^2}{N}$ is optimal amongst all predictors which depend linearly on the noisy labels y^ϵ. Second, given a kernel K and a ridge λ, we provide a simple formula for the expected risk.

Let us consider predictors $\hat{f}$ that depend linearly on the labels y^ϵ, i.e. for all x, there is a $M_x \in \mathbb{R}^N$ such that $\hat{f}(x) = M_x^T y^\epsilon$. Clearly, the KRR predictor belongs to this family of predictors. The pointwise expected squared error can be expressed for any such predictors in terms of the Gram matrix $\mathcal{O}\Sigma\mathcal{O}^T + \epsilon^2 I_N$ and the vector $\mathcal{O}\Sigma(\cdot,x)$

$$\mathbb{E}[(M_x^T y^\epsilon - f^*(x))^2] = M_x^T(\mathcal{O}\Sigma\mathcal{O}^T + \epsilon^2 I_N)M_x - 2M_x^T\mathcal{O}\Sigma(\cdot,x) + \Sigma(x,x).$$

Differentiating w.r.t. M_x, we obtain that the above error is minimized when

$$M_x = \Sigma(x,\cdot)\mathcal{O}^T(\mathcal{O}\Sigma\mathcal{O}^T + \epsilon^2 I_N)^{-1}.$$

In other terms, in this Bayesian setting, the KRR predictor with kernel $K = \Sigma$ and ridge $\lambda = \frac{\epsilon^2}{N}$ minimizes the expected squared error at all points x.

Using Theorem 6, we obtain the following approximation of the expected risk for a general kernel K and ridge λ:

Corollary 25. *For a random true function of zero mean and covariance kernel Σ the expected risk is approximated by*

$$B(\lambda,K;\epsilon^2,\Sigma) = N\vartheta(\lambda,K) + N\partial_\lambda\vartheta(\lambda,K)(\frac{\epsilon^2}{N} - \lambda) + \partial_\tau\vartheta(\lambda,K+\tau(\Sigma-K))\big|_{\tau=0},$$

in the sense that

$$\left|\mathbb{E}[R^\epsilon(\hat{f}_\lambda^\epsilon)] - B(\lambda,K;\epsilon^2,\Sigma)\right| \leq B(\lambda,K;\epsilon^2,\Sigma)\left(\frac{1}{N} + \mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{|z|\,N^{\frac{1}{2}}}\right)\right).$$

Proof. Denoting by $\mathbb{E}$ the expectation taken with respect to the data points and the noise, and by $\mathbb{E}_{f^*}$ the expectation taken with respect to the random true function f^*, from Theorem 6 we obtain

$$\begin{aligned}\left|\mathbb{E}_{f^*}\left[\mathbb{E}\left[R^\epsilon\left(\hat{f}^\epsilon_\lambda\right)\right]\right]-\mathbb{E}_{f^*}\left[\tilde{R}^\epsilon\left(f^*,\lambda\right)\right]\right| &\le \mathbb{E}_{f^*}\left[\left|\mathbb{E}\left[R^\epsilon\left(\hat{f}^\epsilon_\lambda\right)\right]-\tilde{R}^\epsilon\left(f^*,\lambda\right)\right|\right]\\ &\le \mathbb{E}_{f^*}\left[\tilde{R}^\epsilon\left(f^*,\lambda\right)\right]\left(\frac{1}{N}+\mathcal{P}\left(\frac{\mathrm{Tr}\left[T_K\right]}{|z|\,N^{\frac{1}{2}}}\right)\right)\end{aligned}$$

it therefore suffices to show that $\mathbb{E}_{f^*}\left[\tilde{R}^\epsilon\left(f^*,\lambda\right)\right]=B(\lambda,K;\epsilon^2,\Sigma)$.

$$\begin{aligned}\mathbb{E}_{f^*}[\tilde{R}^\epsilon(f^*,\lambda,N)] &= \partial_\lambda\vartheta(\lambda)\left(\mathbb{E}_{f^*}\left[\|(I_{\mathcal{C}}-\tilde{A}_\vartheta)f^*\|_S^2\right]+\epsilon^2\right)\\ &= \partial_\lambda\vartheta(\lambda,K)\left(\mathrm{Tr}\left[T_\Sigma(I_{\mathcal{C}}-\tilde{A}_\vartheta)^2\right]+\epsilon^2\right)\\ &= \partial_\lambda\vartheta(\lambda,K)\left(\vartheta^2\mathrm{Tr}\left[T_K(T_K+\vartheta(\lambda,K)I_{\mathcal{C}})^{-2}\right]+\epsilon^2\right)\\ &+ \partial_\lambda\vartheta(\lambda,K)\mathrm{Tr}\left[(T_\Sigma-T_K)(I_{\mathcal{C}}-\tilde{A}_\vartheta)^2\right].\end{aligned}$$

This formula can be further simplified. First note that differentiating both sides of Equation 7 w.r.t. to λ, we obtain that

$$\frac{\vartheta^2}{N}\mathrm{Tr}\left[T_K(T_K+\vartheta(\lambda,K)I_{\mathcal{C}})^{-2}\right]=\frac{\vartheta}{\partial_\lambda\vartheta}-\lambda.$$

Secondly, differentiating both sides of Equation 7, we obtain, writing $K(\tau)=K+\tau(\Sigma-K)$

$$\begin{aligned}\partial_\tau\vartheta(\lambda,K(\tau)) &= \frac{\partial_\tau\vartheta}{N}\mathrm{Tr}\left[\tilde{A}_\vartheta\right]+\frac{\vartheta}{N}\mathrm{Tr}\left[\partial_\tau\tilde{A}_\vartheta\right]\\ &= \frac{\partial_\tau\vartheta}{N}\mathrm{Tr}\left[T_K(T_K+\vartheta I_{\mathcal{C}})^{-1}\right]+\frac{\vartheta^2}{N}\mathrm{Tr}\left[(T_K+\vartheta I_{\mathcal{C}})^{-1}T_{(\Sigma-K)}(T_K+\vartheta I_{\mathcal{C}})^{-1}\right]\\ &- \frac{\partial_\tau\vartheta\vartheta}{N}\mathrm{Tr}\left[T_K(T_K+\vartheta I_{\mathcal{C}})^{-2}\right]\\ &= \frac{\partial_\tau\vartheta}{N}\mathrm{Tr}\left[T_K(T_K+\vartheta I_{\mathcal{C}})^{-1}-\vartheta T_K(T_K+\vartheta I_{\mathcal{C}})^{-2}\right]+\frac{\vartheta^2}{N}\mathrm{Tr}\left[T_{(\Sigma-K)}(T_K+\vartheta I_{\mathcal{C}})^{-2}\right]\\ &= \frac{\partial_\tau\vartheta}{N}\mathrm{Tr}\left[T_K^2(T_K+\vartheta I_{\mathcal{C}})^{-2}\right]+\frac{\vartheta^2}{N}\mathrm{Tr}\left[T_{(\Sigma-K)}(T_K+\vartheta I_{\mathcal{C}})^{-2}\right]\\ &= \partial_\tau\vartheta-\frac{\partial_\tau\vartheta}{\partial_\lambda\vartheta}+\frac{\vartheta^2}{N}\mathrm{Tr}\left[T_{(\Sigma-K)}(T_K+\vartheta I_{\mathcal{C}})^{-2}\right],\end{aligned}$$

where we used the fact that $\frac{1}{N}\mathrm{Tr}\left[T_K^2(T_K+\vartheta I_{\mathcal{C}})^{-2}\right]=1-1/\partial_\lambda\vartheta$. This implies that

$$\begin{aligned}\partial_\tau\vartheta &= \partial_\lambda\vartheta\frac{\vartheta^2}{N}\mathrm{Tr}\left[T_{(\Sigma-K)}(T_K+\vartheta I_{\mathcal{C}})^{-2}\right]\\ &= \partial_\lambda\vartheta(\lambda,K)\mathrm{Tr}\left[(T_\Sigma-T_K)(I_{\mathcal{C}}-\tilde{A}_\vartheta)^2\right].\end{aligned}$$

Putting everything together, we obtain that

$$\mathbb{E}_{f^*}[\tilde{R}^\epsilon(f^*,\lambda,N)]=N\vartheta(\lambda,K)+N\partial_\lambda\vartheta(\lambda,K)(\frac{\epsilon^2}{N}-\lambda)+\partial_\tau\vartheta(\lambda,K+\tau(\Sigma-K))\big|_{\tau=0}.$$

□

B.8 Technical Lemmas

B.8.1 Matricial observations and Wick formula

For any family $\boldsymbol{A}=\left(A^{(1)},\ldots,A^{(k)}\right)$ of k square matrices of same size, any permutation $\sigma\in\mathfrak{S}_k$, we define:

$$\sigma\left(\boldsymbol{A}\right)=\prod_{c\text{ cycle of }\sigma}\mathrm{Tr}\left[\prod_{i\in c}A^{(i)}\right],$$

where the product inside the trace is taken following the order given by the cycle and, by the cyclic property, does not depend on the starting point (see [12]). For example if $k = 4$ and σ is the product of transpositions $(1, 3)(2, 4)$,

$$\sigma(\boldsymbol{A}) = \mathrm{Tr}(A^{(1)}A^{(3)})\mathrm{Tr}(A^{(2)}A^{(4)}).$$

The number of cycles of σ is denoted by $\mathrm{c}(\sigma)$. The set of permutations without fixed points, i.e. such that $\sigma(i) \neq i$ for any $i \in [1, \dots, k]$ is denoted by $\mathfrak{S}_k^\dagger$ and the set of permutations with cycles of even size is denoted by $\mathfrak{S}_k^{\mathrm{even}}$.

The following lemma, which is reminiscent of Lemma 4.5 in [2] and which is a rephrasing of Lemma C.3 of [14], is a consequence of Wick's formula for Gaussian random variables and is key to study the g_k and $h_{k,\ell}$.

Lemma 26. *If $\boldsymbol{A} = \left(A^{(1)}, \dots, A^{(k)}\right)$ is a family of k square symmetric random matrices of size P independent from a standard Gaussian vector w of size P, we have*

$$\mathbb{E}\left[\prod_{i=1}^{k} w^T A^{(i)} w\right] = \sum_{\sigma\in\mathfrak{S}_k} 2^{k-\mathrm{c}(\sigma)}\mathbb{E}\left[\sigma(\boldsymbol{A})\right], \tag{22}$$

and,

$$\mathbb{E}\left[\prod_{i=1}^{k}\left(w^T A^{(i)} w - \mathrm{Tr}\left(A^{(i)}\right)\right)\right] = \sum_{\sigma\in\mathfrak{S}_k^\dagger} 2^{k-\mathrm{c}(\sigma)}\mathbb{E}\left[\sigma(\boldsymbol{A})\right]. \tag{23}$$

Furthermore, if w and v are independent Gaussian vectors of size P and independent from $\boldsymbol{A}$, then

$$\mathbb{E}\left[\prod_{i=1}^{k} w^T A^{(i)} v\right] = \sum_{\sigma\in\mathfrak{S}_k^{\mathrm{even}}} \mathbb{E}\left[\sigma(\boldsymbol{A})\right]. \tag{24}$$

Proof. The only differences with Lemma C.3 of [14] are in the r.h.s. and the combinatorial sets used to express the left side. We only prove Equation (22); Equations (23) and (24) can be proven similarly. Let $\boldsymbol{P}_2(2k)$ be the set of pair partitions of $\{1, \dots, 2k\}$ and let $p \in \boldsymbol{P}_2(2k)$. Let $p[\boldsymbol{A}] = \sum_{\substack{p\le\mathrm{Ker}(i_1,\dots,i_{2k}) \\ i_1,\dots,i_{2k}\in\{1,\dots,P\}}} \mathbb{E}\left[A^{(1)}_{i_1i_2}\dots A^{(k)}_{i_{2k-1}i_{2k}}\right]$ where $\le$ is the coarsed order (i.e. $p \le q$ if q is coarser than p) and where for any $i_1, \dots, i_{2k}$ in $1, ..., P$, $\mathrm{Ker}(i_1, \dots, i_{2k})$ is the partition of $\{1, \dots, 2k\}$ such that two elements u and v in $\{1, ..., 2k\}$ are in the same block (i.e. pair) of $\mathrm{Ker}(i_1, \dots, i_{2k})$ if and only if $i_u = i_v$. By Wick's formula, we have

$$\mathbb{E}\left[\prod_{i=1}^{k} w^T A^{(i)} w\right] = \sum_{p\in\boldsymbol{P}_2(2k)} p[\boldsymbol{A}];$$

therefore, it is sufficient to prove that

$$\sum_{p\in\boldsymbol{P}_2(2k)} p[\boldsymbol{A}] = \sum_{\sigma\in\mathfrak{S}_k} 2^{k-\mathrm{c}(\sigma)}\sigma(\boldsymbol{A}),$$

Let Po be the set of polygons on $\{1, \dots, k\}$, i.e. the set of collections of non-crossing loops (disjoint unoriented cycles) which cover $\{1, \dots, k\}$. Consider the two maps $F : \boldsymbol{P}_2(2k) \to \mathrm{Po}$ and $G : \mathfrak{S}_k \mapsto \mathrm{Po}$ obtained by forgetting the underlying structure: for any partition $p \in \boldsymbol{P}_2(2k)$, $F(p)$ is the collection of edges (ℓ, m) (viewed as collection of non-crossing loops) such that there exists $u \in \{2\ell - 1, 2\ell\}$ and $v \in \{2m - 1, 2m\}$ with $\{u, v\} \in p$; for any permutation $\sigma \in \mathfrak{S}_k$, $G(\sigma)$ is the set of its loops (unoriented cycles).

One can check that for any $\pi \in \mathrm{Po}$,

$$\#\left\{p \in \boldsymbol{P}_2(2k) \mid F(p) = \pi\right\} = 2^{k-\mathrm{c}_{\le 2}(\pi)}, \quad \#\left\{\sigma \in \mathfrak{S}_k \mid G(\sigma) = \pi\right\} = 2^{\mathrm{c}(\pi)-\mathrm{c}_{\le 2}(\pi)},$$

where $\mathrm{c}(\pi)$, resp. $\mathrm{c}_{\le 2}(\pi)$, is the number of unoriented cycles, resp. unoriented cycles of size smaller than or equal to 2, of π. Note that $\mathrm{c}(\pi)$, resp. $\mathrm{c}_{\le 2}(\pi)$ are also the number of cycles, resp.

cycles of size smaller than or equal to 2 of any σ such that $G(\sigma) = \pi$. Notice also that, since the matrices are symmetric, for any $p, p' \in \boldsymbol{P}_2(2k)$ and any $\sigma \in \mathfrak{S}_k$, if $F(p) = F(p') = G(\sigma)$, then $p\,[\boldsymbol{A}] = p'\,[\boldsymbol{A}] = \sigma\,[\boldsymbol{A}]$. Hence:

$$\sum_{p \in \boldsymbol{P}_2(2k)} p\,[\boldsymbol{A}] = \sum_{p \in \boldsymbol{P}_2(2k)} \sum_{\pi = F(p)} p\,[\boldsymbol{A}] = \sum_{\pi \in \mathrm{Po}} \sum_{p : F(p) = \pi} \pi\,[\boldsymbol{A}] = \sum_{\pi \in \mathrm{Po}} 2^{k - \mathrm{c}_{\leq 2}(\pi)} \pi\,[\boldsymbol{A}]$$

hence

$$\sum_{p \in \boldsymbol{P}_2(2k)} p\,[\boldsymbol{A}] = \sum_{\pi \in \mathrm{Po}} 2^{k - \mathrm{c}_{\leq 2}(\pi)} \frac{1}{2^{\mathrm{c}(\pi) - \mathrm{c}_{\leq 2}(\pi)}} \sum_{\sigma : G(\sigma) = \pi} \pi\,[\boldsymbol{A}] = \sum_{\sigma \in \mathfrak{S}_k} 2^{k - \mathrm{c}(\pi)} \sigma\,[\boldsymbol{A}]\,,$$

as required. □

B.8.2 Bound on derivatives

Given a bound on a holomorphic function, one can obtain a bound on its derivative.

Lemma 27. *Let $f, g : \mathbb{H}_{<0} \to \mathbb{C}$ be two holomorphic functions such that for any $z \in \mathbb{H}_{<0}$,*

$$|f(z) - g(z)| \leq F(|\,z\,|),$$

where $F : \mathbb{R}^+ \to \mathbb{R}$ is a decreasing function, then for any $z \in \mathbb{H}_{<0}$:

$$|\partial_z f(z) - \partial_z g(z)| \leq \frac{2}{-\Re(z)} F\left(\frac{|\,z\,|}{2}\right),$$

Proof. This is a consequence of Cauchy's inequality: for any $r < -\Re(z)$ (so that the circle of center z and radius r lies inside $\mathbb{H}_{<0}$),

$$|\partial_z f(z) - \partial_z g(z)| \leq \frac{1}{r} \sup_{|w - z| = r} |f(w) - g(w)| \leq \frac{1}{r} \sup_{|w - z| = r} F(|\,w\,|).$$

The inequality follows by considering $r = -\frac{1}{2}\Re(z)$ and using the fact that F is decreasing. □

B.8.3 Generalized Cauchy-Schwarz inequality

Another result that we will use is the following generalization of the Cauchy-Schwarz inequality, which is a consequence of Hölder's inequality.

Lemma 28. *For complex random variables $a_1, ..., a_s$, we have*

$$\mathbb{E}\left[|a_1 \cdots a_s|\right] \leq \sqrt[s]{\mathbb{E}\left[|a_1|^s\right] \cdots \mathbb{E}\left[|a_s|^s\right]}.$$

Proof. The proof is done using an induction argument. The initialization, i.e. when $s = 1$, is trivial.

For the induction step, assume that the result is true for s terms and let us prove it for $s + 1$ terms. By Hölder's inequality applied for $p = s + 1$ and $q = \frac{s+1}{s}$, we obtain:

$$\begin{aligned} \mathbb{E}\left[|a_0 a_1 \cdots a_s|\right] &\leq \left(\mathbb{E}\left[|a_0|^{s+1}\right]\right)^{\frac{1}{s+1}} \left(\mathbb{E}\left[|a_1 \cdots a_s|^{\frac{s+1}{s}}\right]\right)^{\frac{s}{s+1}} \\ &\leq \left(\mathbb{E}\left[|a_0|^{s+1}\right]\right)^{\frac{1}{s+1}} \left(\mathbb{E}\left[|a_1|^{s+1}\right] \cdots \mathbb{E}\left[|a_s|^{s+1}\right]\right)^{\frac{1}{s+1}}, \end{aligned}$$

where the second inequality is obtained by the induction hypothesis. □

B.8.4 Control on fixed points

Lemma 29. *Let $z \in \mathbb{H}_{<0}$, let $(a_k)_k$ and $(b_k)_k$ be sequences of complex numbers in the cone spanned by 1 and $-1/z$ and let $(d_k)_k$ be positive numbers. Then*

$$\left| z - \sum_{k=1}^{\infty} \frac{d_k}{(1 + a_k)(1 + b_k)} \right| \geq |z|\,.$$

Proof. For any complex numbers z_1 and z_2, let Γ_{z_1,z_2} be the cone spanned by z_1 and z_2, i.e. $\Gamma_{z_1,z_2} = \{w \in \mathbb{C} \ : w = az_1 + bz_2 \text{for } a, b \geq 0\}$. Since $a_k, b_k \in \Gamma_{1,-{}^{1}/_{z}}$, ${}^{1}/_{1+a_k}$ and ${}^{1}/_{1+b_k}$ are in $\Gamma_{1,-z}$. All the summands $\frac{d_k}{(1+a_k)(1+b_k)}$ lie in Γ_{1,z^2}, hence so does $\sum_{k=1}^{\infty} \frac{d_k}{(1+a_k)(1+b_k)}$. Since $\Re(z) < 0$, the closest point to z in this cone is 0 and this yields the lower bound:

$$\left| z - \sum_{k=1}^{\infty} \frac{d_k}{(1+a_k)(1+b_k)} \right| \geq |z| \,,$$

hence the result. □

Recall that $\tilde{m}(z)$, resp. $\tilde{m}_{(k)}(z)$, is the unique fixed point of the function $\psi(x) := -\frac{1}{z}\left(1 - \frac{1}{N}\sum_{\ell=1}^{\infty} \frac{d_\ell x}{1+d_\ell x}\right)$, resp. $\psi_{(k)}(x) := -\frac{1}{z}\left(1 - \frac{1}{N}\sum_{\ell\neq k} \frac{d_\ell x}{1+d_\ell x}\right)$, inside the cone spanned by 1 and $-{}^{1}/_{z}$. We have the following control on the distance between $\tilde{m}(z)$ and $\tilde{m}_{(k)}(z)$.

Lemma 30. *For any $z \in \mathbb{H}_{<0}$,*

$$\left|\tilde{m}_{(k)}(z) - \tilde{m}(z)\right| \leq \frac{1}{|z|\, N}.$$

Proof. Let $z \in \mathbb{H}_{<0}$, $\tilde{m} = \tilde{m}(z)$ and $\tilde{m}_{(k)} = \tilde{m}_{(k)}(z)$. We have:

$$\begin{aligned} \tilde{m}_{(k)} - \tilde{m} &= -\frac{1}{z}\left(-\frac{1}{N}\sum_{\ell\neq k} \frac{d_\ell \tilde{m}_{(k)}}{1+d_\ell \tilde{m}_{(k)}} + \frac{1}{N}\sum_{m} \frac{d_\ell \tilde{m}}{1+d_\ell \tilde{m}}\right) \\ &= -\frac{1}{z}\left(\frac{1}{N}\sum_{\ell\neq k}^{\infty} \frac{d_\ell}{\left(1+d_\ell \tilde{m}_{(k)}\right)(1+d_\ell \tilde{m})}(\tilde{m} - \tilde{m}_{(k)}) + \frac{1}{N}\frac{d_k \tilde{m}}{1+d_k \tilde{m}}\right) \end{aligned}$$

which allows us to express the difference $\tilde{m}_{(k)} - \tilde{m}$ as

$$\tilde{m}_{(k)} - \tilde{m} = \frac{\frac{1}{N}\frac{d_k \tilde{m}}{1+d_k \tilde{m}}}{\left(\frac{1}{N}\sum_{\ell\neq k}^{\infty} \frac{d_\ell}{\left(1+d_\ell \tilde{m}_{(k)}\right)(1+d_\ell \tilde{m})} - z\right)}.$$

Since $\tilde{m}_{(k)}$ and $\tilde{m}$ lie in the cone spanned by 1 and $-\frac{1}{z}$, from Lemma 29, we have the lower bound on the norm of the denominator:

$$\left| \frac{1}{N}\sum_{\ell\neq k}^{\infty} \frac{d_\ell}{\left(1+d_\ell \tilde{m}_{(k)}\right)(1+d_\ell \tilde{m})} - z \right| \geq \mid z \mid .$$

Since $\Re(\tilde{m}) \geq 0$, $|1 + d_k \tilde{m}| \geq |d_k \tilde{m}|$ and hence $\left|\frac{1}{N}\frac{d_k \tilde{m}}{1+d_k \tilde{m}}\right| \leq \frac{1}{N}$. This yields the inequality $\left|\tilde{m}_{(k)}(z) - \tilde{m}(z)\right| \leq \frac{1}{N|z|}$. □