Understanding Double Descent Requires a Fine-Grained Bias-Variance Decomposition

Ben Adlam[*†] **Jeffrey Pennington**[*]
Google Brain
{adlam, jpennin}@google.com

Abstract

Classical learning theory suggests that the optimal generalization performance of a machine learning model should occur at an intermediate model complexity, with simpler models exhibiting high bias and more complex models exhibiting high variance of the predictive function. However, such a simple trade-off does not adequately describe deep learning models that simultaneously attain low bias and variance in the heavily overparameterized regime. A primary obstacle in explaining this behavior is that deep learning algorithms typically involve multiple sources of randomness whose individual contributions are not visible in the total variance. To enable fine-grained analysis, we describe an interpretable, symmetric decomposition of the variance into terms associated with the randomness from sampling, initialization, and the labels. Moreover, we compute the high-dimensional asymptotic behavior of this decomposition for random feature kernel regression, and analyze the strikingly rich phenomenology that arises. We find that the bias decreases monotonically with the network width, but the variance terms exhibit non-monotonic behavior and can diverge at the interpolation boundary, even in the absence of label noise. The divergence is caused by the *interaction* between sampling and initialization and can therefore be eliminated by marginalizing over samples (*i.e.* bagging) *or* over the initial parameters (*i.e.* ensemble learning).

1 Introduction

It is undeniable that modern neural networks (NNs) are becoming larger and more complex, with many state-of-the-art models now employing billions of trainable parameters [1–3]. While parameter count may be a crude way of quantifying complexity, there is little doubt that these models have enormous capacity, often far more than is needed to perfectly fit the training data, even if the labels are pure noise [4]. Surprisingly, these same high-capacity models generalize well when trained on real data.

These observations conflict with classical generalization theory, which contends that models of intermediate complexity should generalize best, striking a balance between the bias and the variance of their predictive functions. A paradigm for understanding the observed generalization behavior of modern methods is known as *double descent* [5], in which the test error behaves as predicted by classical theory and follows the standard U-shaped curve until the point where the training set can be fit exactly, but after this point it begins to descend again, eventually finding its global minimum in the overparameterized regime.

While double descent has been the focus of significant research, a concrete and interpretable theoretical explanation for the phenomenon has thus far been lacking. One of the challenges in developing

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such an explanation is that the full phenomenology of double descent is not evident in linear models that are easy to analyze. Indeed, for linear models the number of parameters is tied to the number of features and there is no natural way to adjust the capacity of the model without simultaneously adjusting the data distribution. In this work, we overcome this challenge by providing a precise asymptotic analysis of random feature kernel regression, which is a model rich enough to exhibit all the interesting features of double descent.

Another challenge in understanding double descent is that the classical bias-variance decomposition is *itself* insufficiently nuanced to reveal all the underlying explanatory factors. Indeed, modern learning algorithms typically involve multiple sources of randomness and isolating the variation caused by each of these sources of randomness is key to building an effective interpretation. As we will see, it is not possible to fully understand the spike in test error near the interpolation threshold without performing a truly multivariate variance decomposition.

While decomposing the variance has been proposed before, prior work has naively relied on the law of total variance, which requires specifying an ordering of conditioning that leads to some arbitrariness. Instead, we present a principled symmetric decomposition which leads to unambiguous interpretations and clear credit assignment. Decomposing the variance of a random variable in this way is related to ANOVA [6], which has been used previously in a machine learning context to find the best approximating functions (in terms of mean squared error) to a random variable with limited dependence on the inputs [7, 8] and to study quasi Monte Carlo methods for integration [9].

Finally, we remark that an improved understanding of the bias and variance of machine learning models might naturally suggest ways to improve their performance. Specifically, any prior knowledge about what sources of variance may be dominant could help inform decisions about which types of ensemble or bagging techniques to utilize.

1.1 Related Work

The idea of a trade-off between bias and variance has a long history, with theoretical and experimental support having been well established in a variety of contexts over the years. The seminal paper of Geman et al. [10] examines a number of models, ranging from kernel regression to k-nearest neighbor to neural networks, and concludes that the trade-off exists in all cases[2]. The resulting U-shaped test error curve was verified theoretically in a variety of classical settings, see *e.g.* [11].

In recent years, these conclusions have been called into question by the intriguing experimental results of [4, 12], which were later replicated in a number of settings, see *e.g.* [13], which showed that deep neural networks and kernel methods can generalize well even in the interpolation regime, implying that both the bias and the variance can decrease as the model complexity increases. A number of theoretical results have since established this behavior in certain settings, such as interpolating nearest neighbor schemes [14] and kernel regression [15, 16]. These observations have given rise to the double descent paradigm for understanding how test error depends on model complexity [5]. The influential work [17] (which actually predates [5]) established initial theoretical insights for linear networks and found empirical evidence of double descent for nonlinear networks; more evidence has followed recently in [13, 18]. Precise theoretical predictions soon confirmed this picture for linear regression in various scenarios [19–22], and recently even for kernel regression [23, 24] with random features related to neural networks.

The primary focus of these recent works has been on double descent in the total test error, or perhaps the standard bias-variance decomposition with respect to label noise [23]. A multivariate philosophy similar to ours is advanced in [25], which revisited the empirical study of the bias-variance tradeoff in neural networks from [10] and showed the variance can decrease in the overparameterized regime. However, in that work the variance is simply decomposed using the law of total variance, which, while mathematically sound, can lead to ambiguous conclusions, as we discuss in Sec. 4.

The main mathematical tools we utilize come from random matrix theory and build on the results of [26–30] for studying random matrices with nonlinear dependencies. We also rely on techniques from operator-valued free probability for computing traces of large block matrices [31]. One advantage of these tools is that they facilitate the extension of our analysis to more general settings,

[2]Interestingly, the variance of simple feed-forward neural networks was observed to eventually be a decreasing function of width, but the authors rationalized this early evidence of double descent as a quirk of the optimization.

including the case of kernel regression with respect to the Neural Tangent Kernel (NTK) [32]. To ease the exposition we have deferred the discussion of the NTK and all proofs to the Supplementary Material (SM).

While finalizing this manuscript, we became aware of several concurrent works that examine similar questions. Yang et al. [33] define the total bias and variance similarly to [25], but they do not attempt a decomposition of the variance. Their results can be derived as a special case of our fine-grained decomposition by summing the variance terms in Thm. 1. Jacot et al. [34] study the relationship between the random feature model and the nonparametric Gaussian process which it approximates. The bias-variance decomposition considered in that paper is again univariate and is with respect to the randomness in the random features (the expressions are subsequently averaged over the training data). Closest to our work is [35], which also studies a multivariate decomposition of the random feature model in the high-dimensional limit. Unlike our approach, their decomposition is not symmetric with respect to the underlying random variables, and the results depend on the chosen order of conditioning. Their particular choice, and indeed all possible choices, arise as special cases of our general result. See Sec. S8 for a detailed discussion.

1.2 Our Contributions

1. We develop a symmetric, interpretable variance decomposition suitable for modern deep learning algorithms
2. We compute this decomposition analytically for random feature kernel regression in the high-dimensional asymptotic regime
3. We prove that the bias is monotonically decreasing as the width increases and that it is finite at the interpolation threshold
4. We clarify the relationship between label noise and double descent: while the test loss can diverge at the interpolation threshold without label noise, the divergence is exacerbated by it
5. We provide a quantitative description of how both ensemble and bagging methods can eliminate double descent, since the divergence is caused by variance terms due to the interactions between sampling and initialization

2 Bias-Variance Decomposition

In this section, we trace through the evolution of several ways to analyze the bias-variance trade-off. By analyzing their shortcomings, we motivate our fine-grained analysis that follows.

2.1 Classical Bias-Variance Decomposition

The bias-variance trade-off has long served as a useful paradigm for understanding the generalization of machine learning algorithms. For a given test point $\mathbf{x}$, it decomposes the expected error as

$$\mathbb{E}\left[\hat{y}(\mathbf{x}) - y(\mathbf{x})\right]^2 = \left(\mathbb{E}\hat{y}(\mathbf{x}) - \mathbb{E}y(\mathbf{x})\right)^2 + \mathbb{V}\left[\hat{y}(\mathbf{x})\right] + \mathbb{V}[y(\mathbf{x})]\,, \tag{1}$$

and subsequently averages over the test point to obtain a decomposition of the test error in which the first term is the bias, the second term is the variance, and the third term is the irreducible noise. In classical settings, the randomness of the predictive function is usually regarded as coming from randomness in the training data, *i.e.* sampling noise. This leads to two common conventions, where the expectations in eqn. (1) are over both X and $\mathbf{y}$ or are conditional on X and only over the label noise in $\mathbf{y}$. For concreteness and to simplify the exposition, in this subsection we adopt the latter convention and make the common modelling assumption that the sampling noise is an additive term ε on the training labels but is zero on the test labels $y(\mathbf{x})$. Using $\mathbb{E}_{\mathbf{x}}$ to denote expectation over the test point, we have

$$E_{\text{test}} := \mathbb{E}_{\mathbf{x}}\mathbb{E}_{\boldsymbol{\varepsilon}}\left[\hat{y}(\mathbf{x}) - y(\mathbf{x})\right]^2 = \underbrace{\mathbb{E}_{\mathbf{x}}\left(\mathbb{E}_{\boldsymbol{\varepsilon}}[\hat{y}(\mathbf{x})] - y(\mathbf{x})\right)^2}_{\text{Bias}} + \underbrace{\mathbb{E}_{\mathbf{x}}\mathbb{V}_{\boldsymbol{\varepsilon}}\left[\hat{y}(\mathbf{x})\right]}_{\text{Variance}}\,. \tag{2}$$

We refer to eqn. (2) as the *classical bias-variance decomposition*.

2.2 Bias-Variance Decompositions for Modern Learning Methods

Modern methods for training neural networks often utilize additional sources of randomness, such as the initial parameter values, minibatch selection, *etc*., which we collectively denote by θ. One is therefore left with a choice regarding whether or not to include θ in the expectations in eqn. (1), or to simply average over θ when computing the test loss. We explore the ramifications of these different choices below.

Semi-classical Approach. In what we call the *semi-classical* approach, the additional random variables θ coming from initialization or optimization are not included in the expectations in eqn. (1); we instead average over these quantities to define

$$E_{\text{test}} := \mathbb{E}_{\mathbf{x}}\mathbb{E}_{\theta}\mathbb{E}_{\boldsymbol{\varepsilon}}[(\hat{y}(\mathbf{x}) - y(\mathbf{x}))^2|\theta] = \underbrace{\mathbb{E}_{\mathbf{x}}\mathbb{E}_{\theta}\left(\mathbb{E}_{\boldsymbol{\varepsilon}}[\hat{y}(\mathbf{x})|\theta] - y(\mathbf{x})\right)^2}_{B_{SC}} + \underbrace{\mathbb{E}_{\mathbf{x}}\mathbb{E}_{\theta}\mathbb{V}_{\boldsymbol{\varepsilon}}[\hat{y}(\mathbf{x})|\theta]}_{V_{SC}} . \tag{3}$$

In some scenarios, such as the high-dimensional setup analyzed in [23], the additional averaging over θ is unnecessary as the distributions concentrate around their mean. In those situations, the semi-classical decomposition is identical to the classical one, thus motivating this particular approach.

Multivariate Approach. In what we call the *multivariate approach*, the additional random variables θ are included in the expectations in eqn. (1), so that all random variables are on the same footing. We can then drop explicit references to θ and $\boldsymbol{\varepsilon}$ and simply write,

$$E_{\text{test}} := \mathbb{E}_{\mathbf{x}}\mathbb{E}(\hat{y}(\mathbf{x}) - y(\mathbf{x}))^2 = \underbrace{\mathbb{E}_{\mathbf{x}}\left(\mathbb{E}[\hat{y}(\mathbf{x})] - y(\mathbf{x})\right)^2}_{B} + \underbrace{\mathbb{E}_{\mathbf{x}}\mathbb{V}[\hat{y}(\mathbf{x})]}_{V} . \tag{4}$$

One advantage of this perspective is that its form is completely symmetric with respect to the underlying random variables. Another is that the predictive function $\hat{y}(\mathbf{x})$ appearing in the bias B is not conditional on any random variables. As we discuss in Sec. 4, this facilitates its interpretation as a measure of erroneous assumptions in the model.

The downside of this perspective is that the variance V no longer admits a simple interpretation since it contains contributions from multiple random variables. This problem can be remedied by further decomposing the variance.

2.2.1 Symmetric Decomposition of the Variance

To gain further insight into the structure of the total variance V and how individual random variables contribute to it, it can be useful to write V as a sum of individual terms, each with an unambiguous meaning.

One path forward is to rely on the law of total variance: $\mathbb{V}[\mathcal{Y}] = \mathbb{E}\mathbb{V}[\mathcal{Y}|\mathcal{X}] + \mathbb{V}\mathbb{E}[\mathcal{Y}|\mathcal{X}]$, where the terms represent the variance of $\mathcal{Y}$ *unexplained* and *explained* by $\mathcal{X}$ respectively. However, one is immediately confronted by the question of which source of randomness to condition on. As we discuss in Sec. 4.2, different choices yield different terms and can lead to ambiguous interpretations.

To avoid this ambiguity, we introduce a fully-symmetric decomposition, which turns out to be unique if we additionally require self-consistency under marginalization with respect to all variables.

Proposition 1. *Let $X_1, \ldots, X_K$, and Y be random variables and $\mathcal{X} := \{X_1, \ldots, X_K\}$. We define a* variance decomposition *of Y to be a multiset $\{V_1, \ldots, V_N\}$ of nonnegative real numbers such that $\mathbb{V}[Y] = \sum_i V_i$. Then there exists a unique variance decomposition $\mathcal{V} := \{V_s : s \subseteq \mathcal{X}\}$ such that $\mathcal{V}$ is invariant under permutations of $\mathcal{X}$, and such that for all $S \subseteq \mathcal{X}$ the marginal variances satisfy the subset-sum relation,*

$$\mathbb{V}\mathbb{E}[Y|X_j \textit{ for } j \in S] = \sum_{s \subseteq S} V_s . \tag{5}$$

Example 1. *Consider the case of two random variables, the parameters P and the data D. Then $\mathcal{X} = \{P, D\}$ and the decomposition satisfying Prop. 1 is given by*

$$V_P := \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|P] \tag{6}$$
$$V_D := \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|D] \tag{7}$$
$$V_{PD} := \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|P, D] - \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|P] - \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|D] . \tag{8}$$

We can interpret V_{PD} as the variance explained by the parameters and data together beyond what they explain individually.

Example 2. *Further decomposing D into randomness from sampling the inputs X and label noise ε, we can write $\mathcal{X} = \{P, X, \varepsilon\}$ and the decomposition satisfying Prop. 1 is given by,*

$$
\begin{aligned}
V_X &:= \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|X], && (9)\\
V_{\varepsilon} &:= \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|\varepsilon], && (10)\\
V_P &:= \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|P], && (11)\\
V_{X\varepsilon} &:= \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|X,\varepsilon] - \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|X] - \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|\varepsilon], && (12)\\
V_{PX} &:= \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|P,X] - \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|X] - \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|P], && (13)\\
V_{P\varepsilon} &:= \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|X,\varepsilon] - \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|\varepsilon] - \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|P], && (14)\\
V_{PX\varepsilon} &:= \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|P,X,\varepsilon] - \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|X,\varepsilon] - \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|P,X] - \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|X,\varepsilon] \\
&\quad + \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|X] + \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|\varepsilon] + \mathbb{E}_{\mathbf{x}}\mathbb{V}\mathbb{E}[\hat{y}|P]. && (15)
\end{aligned}
$$

Remark 1. *Because $V_s \geq 0$ and $V = \mathbb{V}[\hat{y}] = \sum_s V_s$, the subset-sum relation (5) yields an interpretation of V as the union of disjoint areas, forming a Venn diagram. See Fig. 1(d,e). The reader may also recognize the quantities above as those that are estimated in a three-way ANOVA.*

3 Asymptotic Variance Decomposition for Random Feature Regression

Problem setup and notation. Following prior work modeling double descent [21, 23, 24], we perform our analysis in the high-dimensional asymptotic scaling limit in which the dataset size m, feature dimensionality n_0, and hidden layer size n_1 all tend to infinity at the same rate, with $\phi := n_0/m$ and $\psi := n_0/n_1$ held constant.

We consider the task of learning an unknown function from m independent samples $(\mathbf{x}_i, y_i) \in \mathbb{R}^{n_0} \times \mathbb{R}$, $i = 1, \ldots, m$, where the datapoints are standard Gaussian, $\mathbf{x}_i \sim \mathcal{N}(0, I_{n_0})$, and the labels are generated by a linear function parameterized by $\beta \in \mathbb{R}^{n_0}$, whose entries are drawn independently from $\mathcal{N}(0,1)$. Concretely, we let

$$y(\mathbf{x}_i) = \beta^\top \mathbf{x}_i/\sqrt{n_0} + \varepsilon_i\,, \tag{16}$$

where $\varepsilon_i \sim \mathcal{N}(0, \sigma_\varepsilon^2)$ is additive label noise on the training points, yielding a signal-to-noise ratio $\mathrm{SNR} = \sigma_\varepsilon^{-2}$. Although this may seem like a simple data distribution, it turns out that, in these high-dimensional asymptotics, the much more general setting in which the labels are produced by a non-linear teacher neural network can be exactly modeled with a linear teacher of this form (see Sec. S2.1).

We consider predictive functions $\hat{y}$ defined by approximate kernel ridge regression using the random feature model[3] of [36, 37], for which the random features are given by a single-layer neural network with random weights. Specifically, we define the random features on the training set $X = [\mathbf{x}_1, \ldots, \mathbf{x}_m]$ and test point $\mathbf{x}$ to be

$$F := \sigma(W_1 X/\sqrt{n_0}) \quad \text{and} \quad f := \sigma(W_1 \mathbf{x}/\sqrt{n_0})\,, \tag{17}$$

for a weight matrix $W_1 \in \mathbb{R}^{n_1 \times n_0}$ with iid entries $[W_1]_{ij} \sim \mathcal{N}(0,1)$[4]. The kernel induced by these random features is

$$K(\mathbf{x}_1, \mathbf{x}_2) := \frac{1}{n_1}\sigma(W_1\mathbf{x}_1/\sqrt{n_0})^\top \sigma(W_1\mathbf{x}_2/\sqrt{n_0})\,, \tag{18}$$

and the model's predictions are given by

$$\hat{y}(\mathbf{x}) = Y K^{-1} K_{\mathbf{x}}\,, \tag{19}$$

where $Y := [y(\mathbf{x}_1), \ldots, y(\mathbf{x}_m)]$, $K := K(X,X) + \gamma I_m$, $K_{\mathbf{x}} := K(X, \mathbf{x})$, and γ is a ridge regularization constant. For this model, W_1 plays the role of θ from Sec. 2.2.

Altogether, the test loss can be written as

$$E_{\text{test}} = \mathbb{E}_\beta \mathbb{E}_{\mathbf{x}}(y(\mathbf{x}) - \hat{y}(\mathbf{x}))^2 = \mathbb{E}_{\mathbf{x}}(\beta^\top \mathbf{x}/\sqrt{n_0} - Y K^{-1} K_{\mathbf{x}})^2\,, \tag{20}$$

where we dropped the outer expectation over β because the distribution concentrates around its mean (see the SM).

[3] See the SM for an extension to the Neural Tangent Kernel of a single-hidden-layer neural network [32].

[4] Any non-zero variance $\sigma_{W_1}^2$ can be absorbed into a redefinition of σ.

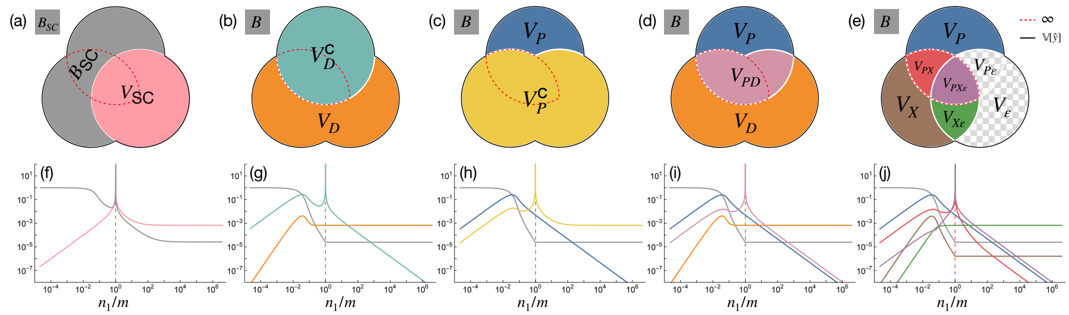

Figure 1: (a-e) The different bias-variance decompositions described in Sec. 4. (f-j) Corresponding theoretical predictions of Thm. 1 for $\gamma = 0$, $\phi = 1/16$ and $\sigma = \tanh$ with SNR $= 100$ as the model capacity varies across the interpolation threshold (dashed red). (a,f) The semi-classical decomposition of [21, 23] has a nonmonotonic and divergent bias term, conflicting with standard definitions of the bias. (b,g) The decomposition of [25] utilizing the law of total variance interprets the diverging term V_D^{c} as "variance due to optimization". (c,h) An alternative application of the law of total variance suggests the opposite, *i.e.* the diverging term V_P^{c} comes from "variance due to sampling". (d,i) A bivariate symmetric decomposition of the variance resolves this ambiguity and shows that the diverging term is actually V_{PD}, *i.e.* "the variance explained by the parameters and data together beyond what they explain individually." (e,j) A trivariate symmetric decomposition reveals that the divergence comes from two terms, V_{PX} and $V_{PX\boldsymbol{\varepsilon}}$ (outlined in dashed red), and shows that label noise exacerbates but does not cause double descent. Since $V_\varepsilon = V_{P\varepsilon} = 0$, they are not shown in (j).

3.1 Main Result: Exact Asymptotics for the Fine-Grained Variance Decomposition

Lemma 1. *Let $\eta := \mathbb{E}[\sigma(g)^2]$ and $\zeta := (\mathbb{E}[g\sigma(g)])^2$ for $g \sim \mathcal{N}(0,1)$. Then, in the high-dimensional asymptotics defined above, the traces $\tau_1(\gamma) := \frac{1}{m}\mathbb{E}\operatorname{tr}(K^{-1})$ and $\tau_2(\gamma) := \frac{1}{m}\mathbb{E}\operatorname{tr}(\frac{1}{n_0}X^\top X K^{-1})$ are given by the unique solutions to the coupled polynomial equations,*

$$\zeta\tau_1\tau_2\,(1-\gamma\tau_1) = \phi/\psi\,(\zeta\tau_1\tau_2 + \phi(\tau_2-\tau_1)) = (\tau_1-\tau_2)\,\phi\,((\eta-\zeta)\tau_1 + \zeta\tau_2)\,, \tag{21}$$

such that $\tau_1, \tau_2 \in \mathbb{C}^+$ for $\gamma \in \mathbb{C}^-$.

Theorem 1. *Let τ_1 and τ_2 be defined as in Lemma 1, and use the prime symbol to denote their derivatives with respect to γ. Then, as $\Im(\gamma) \to 0^-$, the asymptotic bias and variance terms of eqns.* (9)-(15) *are given by*

$$\begin{aligned}
B &= \tau_2^2/\tau_1^2 & V_{PX} &= -\tau_2'/\tau_1^2 - B - V_P - V_X\\
V_P &= \tau_2'/\tau_1' - B & V_{P\boldsymbol{\varepsilon}} &= 0\\
V_X &= \phi B(\tau_1-\tau_2)^2/(\tau_1^2 - \phi(\tau_1-\tau_2)^2) & V_{X\boldsymbol{\varepsilon}} &= \sigma_{\boldsymbol{\varepsilon}}^2 V_X/B\\
V_{\boldsymbol{\varepsilon}} &= 0 & V_{PX\boldsymbol{\varepsilon}} &= \sigma_{\boldsymbol{\varepsilon}}^2(-\tau_1'/\tau_1^2 - 1) - V_{X\boldsymbol{\varepsilon}}\,.
\end{aligned} \tag{22}$$

Corollary 1. *In the ridgeless setting, the bias B is a non-increasing function of the overparameterization ratio $n_1/m = \phi/\psi$. Furthermore, at the interpolation boundary $\psi = \phi$, V_{PX} and $V_{PX\boldsymbol{\varepsilon}}$ are divergent while the remaining terms are bounded.*

4 Fine-Grained Analysis of Double Descent

The fine-grained variance decomposition given in Thm. 1 provides a powerful tool for understanding the origins of double descent. In this section, we use this tool to reinterpret several counterintuitive observations made in prior work and to provide a clear and unambiguous characterization of the source of double descent.

4.1 Semi-classical Approach: The Bias Diverges

In [21, 23], double descent in random feature kernel regression was analyzed through the lens of the semi-classical bias-variance decomposition introduced in eqn. (3). In our setting,

$$E_{\text{test}} = B_{SC} + V_{SC}\,, \tag{23}$$

where,

$$B_{SC} = \mathbb{E}_{\mathbf{x}}\mathbb{E}_{PX}\left(\mathbb{E}_{\boldsymbol{\varepsilon}}[\hat{y}(\mathbf{x})|P,X] - y(\mathbf{x})\right)^2 , \quad \text{and} \quad V_{SC} = \mathbb{E}_{\mathbf{x}}\mathbb{E}_{PX}[\mathbb{V}_{\boldsymbol{\varepsilon}}[\hat{y}|P,X]|\mathbf{x}] . \tag{24}$$

To gain further insight into this decomposition, we can express B_{SC} and V_{SC} in terms of the variables in Thm. 1:

$$B_{SC} = B + V_P + V_X + V_{PX} , \quad \text{and} \quad V_{SC} = V_{\boldsymbol{\varepsilon}} + V_{P\boldsymbol{\varepsilon}} + V_{X\boldsymbol{\varepsilon}} + V_{PX\boldsymbol{\varepsilon}} . \tag{25}$$

Using the correspondence between the variance terms and areas mentioned in Remark 1, we illustrate this decomposition in Fig. 1(a). The figure shows that B_{SC} is partially comprised of variance terms. Thm. 1 allows us to exactly characterize how B_{SC} and V_{SC} depend on the capacity of the model, with results shown in Fig. 1(f). As in [23], we observe that the bias B_{SC} and variance V_{SC} exhibit nonmonotonic behavior with respect to the model size and both diverge at the interpolation threshold.

Because $V_{\boldsymbol{\varepsilon}} = V_{P\boldsymbol{\varepsilon}} = 0$ and $V_{X\boldsymbol{\varepsilon}}$ and $V_{PX\boldsymbol{\varepsilon}}$ both vanish in the noiseless setting, the semi-classical decomposition has the nice property that $V_{SC} = 0$ when there is no label noise. However, it is hard to reconcile the nonmonotonicity of the bias with its desired interpretation as a measure of the erroneous assumptions in the model as the latter are expected to decrease as the model increases in capacity. For this reason, we believe the multivariate approach outlined in Sec. 2.2 provides a more interpretable basis for understanding double descent.

4.2 Multivariate Approach

The Law of Total Variance: Ambiguous Conclusions. Neal *et al.* [25] adopt the multivariate approach of Sec. 2.2 and decompose the test loss in terms of two sources of randomness, the optimization/initial parameters P and data sampling D. The total variance is additionally decomposed according to the law of total variance:

$$V = \underbrace{\mathbb{E}_{\mathbf{x}}\mathbb{V}_D[\mathbb{E}_P[\hat{y}|D]|\mathbf{x}]}_{V_D} + \underbrace{\mathbb{E}_{\mathbf{x}}\mathbb{E}_D[\mathbb{V}_P[\hat{y}|D]|\mathbf{x}]}_{V_D^{\mathsf{c}}} , \tag{26}$$

where Neal *et al.* [25] suggests an interpretation for the two terms as "variance due to sampling" and "variance due to optimization," respectively. While the expressions in eqn. (26) are themselves unambiguous, we will see that attributing such an interpretation to them can be somewhat misleading.

Some simple algebra allows us to express V_D^{c} in terms of the terms in Thm. 1 as

$$V_D^{\mathsf{c}} = V_P + V_{PX} + V_{P\boldsymbol{\varepsilon}} + V_{PX\boldsymbol{\varepsilon}} . \tag{27}$$

Because eqn. (27) contains V_{PX} and $V_{PX\boldsymbol{\varepsilon}}$, Corollary 1 implies that V_D^{c} diverges at the interpolation threshold, and indeed we observe that in Fig. 1(g). From the above interpretation of the meaning of V_D^{c}, we might therefore conclude that the "variance due to optimization" is the source of double descent.

On the other hand, we could have equally well decided to decompose the variance by conditioning on P instead of D, yielding,

$$V = \underbrace{\mathbb{E}_{\mathbf{x}}\mathbb{V}_P[\mathbb{E}_D[\hat{y}|P]|\mathbf{x}]}_{V_P} + \underbrace{\mathbb{E}_{\mathbf{x}}\mathbb{E}_P[\mathbb{V}_D[\hat{y}|P]|\mathbf{x}]}_{V_P^{\mathsf{c}}} . \tag{28}$$

The corresponding interpretations of these terms would then be "variance due to optimization" and "variance due to sampling," respectively. As above, it is straightforward to express V_P^{c} as,

$$V_P^{\mathsf{c}} = V_X + V_{PX} + V_{X\boldsymbol{\varepsilon}} + V_{PX\boldsymbol{\varepsilon}} . \tag{29}$$

In this case, Corollary 1 implies that V_P^{c} diverges at the interpolation threshold, as Fig. 1(h) confirms. In this case, we might therefore conclude that the "variance due to sampling" is the source of double descent.

The above analysis reveals conflicting explanations for the source double descent, depending on which source of randomness is conditioned on when applying the law of total variance. We believe this ambiguity is undesirable and provides further motivation for the symmetric variance decomposition in Prop. 1.

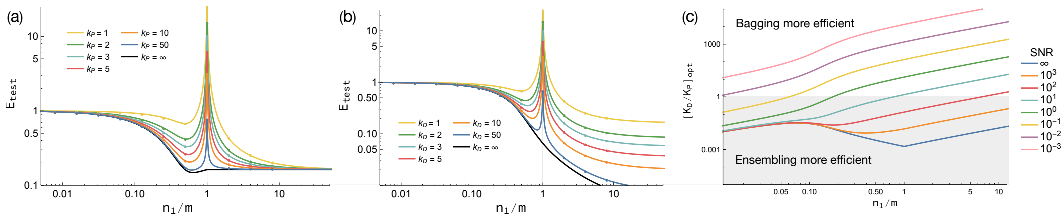

Figure 2: Comparison of (a) ensembles and (b) bagging. Solid lines are theoretical predictions and dots are simulation results. In (a,b) we set $\gamma = 10^{-6}$, $n_0 = 2^{13}$, $m = 2^{14}$, $\sigma = \tanh$, and SNR $= 5$. Note that as either k_P or k_D increase, the peak around the interpolation threshold decreases. In (c), we plot the optimal ratio $[k_D/k_P]_{\text{optimal}}$ (35) as a function of n_1/m for different SNRs. The shaded area, $[k_D/k_P]_{\text{optimal}} < 1$, is where averaging over the parameters reduces variance more efficiently. As expected, for large width, bagging is much more efficient.

Bivariate Symmetric Decomposition: V_{PD} is the Source of Divergence. In the previous two-variable setting, the symmetric decomposition can be written as (see Example 1),

$$V = V_P + V_D + V_{PD}\,. \tag{30}$$

See Fig. 1(d) for an illustration of this decomposition. This figure shows that V_{PD} inhabits the ambiguous overlap region that was responsible for the inconsistent interpretations arising from a naive application of the law of total variance. From the theoretical results shown in Fig. 1(i), it is clear that neither the variance explained by the parameters, V_P, nor the variance explained by the data, V_D, can be responsible for double descent; instead it must be V_{PD} that is causing the divergence. Recalling the definition of V_{PD} in Ex. 1, we conclude that the divergence at the interpolation boundary is caused by "the variance explained by the parameters and training data together beyond what they explain individually."

One implication of this interpretation is that if we had a way of removing *either* the variance from the parameters *or* the variance from the data, then the divergence would be eliminated. We examine this phenomenon from the perspective of ensemble and bagging methods in Sec. 5 and confirm empirically that this is indeed the case. See Fig. 2.

Trivariate Symmetric Decomposition: Divergence Persists in Absence of Label Noise. Returning to the full model from Sec. 3 with three sources of randomness, we know from Thm. 1 that

$$V = V_P + V_X + V_{PX} + V_{X\boldsymbol{\varepsilon}} + V_{PX\boldsymbol{\varepsilon}}\,, \tag{31}$$

while the other two variance terms $V_{\boldsymbol{\varepsilon}}$ and $V_{P\boldsymbol{\varepsilon}}$ vanish. The seven variance terms are illustrated in Fig. 1(e). The dependence of the five non-zero terms on the model's capacity is plotted in Fig. 1(j). We find that V_{PX} and $V_{PX\boldsymbol{\varepsilon}}$ both diverge at the interpolation threshold while the other terms remain finite. This result helps explain recent empirical results that have found that label noise amplifies the double descent phenomena [13]: because V_{PX} itself diverges, there is double descent even without label noise, but because $V_{PX\boldsymbol{\varepsilon}}$ also diverges, label noise can exacerbate the effect.

5 Ensemble Learning

The understanding we have developed for the sources of variance enables explicit prediction of the effectiveness of ensemble and bagging techniques. We consider averaging the predictive functions of several independently initialized base learners as well as bagging the predictions from models with independent samples of training data. Specifically, we consider k_P independent samples of the parameters, P_i, and k_D independent samples of the training data, X_j and ε_j. Then our predictive function on a test point $\mathbf{x}$ is

$$\hat{y}^*(\mathbf{x}) := \frac{1}{k_P k_D}\sum_{i,j}\hat{y}_{ij}(\mathbf{x})\,, \tag{32}$$

where the indicies of $\hat{y}$ indicate the specific sample of parameters and training data used to construct the predictor. A simple calculation gives the variance decomposition of $\hat{y}^*$ as

$$V_P^* = \frac{V_P}{k_P},\; V_X^* = \frac{V_X}{k_D},\; V_\varepsilon^* = \frac{V_\varepsilon}{k_D},\; V_{X\varepsilon}^* = \frac{V_{X\varepsilon}}{k_D}, \tag{33}$$

$$V^*_{P\varepsilon} = \frac{V_{P\varepsilon}}{k_P k_D},\ V^*_{PX} = \frac{V_{PX}}{k_P k_D},\ \text{and}\ V^*_{PX\varepsilon} = \frac{V_{PX\varepsilon}}{k_P k_D}\,, \tag{34}$$

while the bias remains the same. We illustrate these results empirically in Fig. 2 and show that ensembles of base learners and bagging are both able to independently reduce the divergence around the interpolation threshold, as they reduce the divergent terms V_{PX} and $V_{PX\varepsilon}$.

As the computation of eqn. (32) requires evaluating $k_P k_D$ base learners, it is natural to try to characterize the optimal combination of ensembles and bagging given a fixed computational budget. We find the optimal ratio is given as

$$[k_D/k_P]_{\text{optimal}} = (V_X + V_\varepsilon + V_{X\varepsilon})/V_P\,. \tag{35}$$

See Fig. 2, which shows that, for the kernel regression problem studied here, ensembles are typically more efficient at small width and bagging is more efficient at large width.

6 Conclusion

We analyzed the bias and variance trade-off in the modern setting, where the difference to the classical picture of under- and overfitting is marked. We argued that understanding the behavior of the bias and variance in learning algorithms that depend on large sources of randomness requires rethinking the classical definitions to encompass these sources.

We presented a bias-variance decomposition that is suitable for these settings, and showed how it can help attribute components of the loss to their causes, while avoiding counterintuitive or ambiguous conclusions. For random feature kernel regression, we gave exact predictions for all of the terms in the decomposition and proved that the bias is monotonically decreasing and identified the source of divergence at the interpolation threshold to be the interaction between the noise from sampling and initialization. We showed that while label noise does not cause the divergence, it can exacerbate the effect. Finally, we made exact predictions for ensemble learning and bagging and provided the computationally optimal strategy to combine them.

Broader Impact

While it is hard to envision all future applications of this research, the authors do not believe this theoretical work will raise any ethical concerns or will generate any adverse future societal consequences.

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References

[1] Alec Radford, Jeffrey Wu, Rewon Child, David Luan, Dario Amodei, and Ilya Sutskever. Language models are unsupervised multitask learners. *OpenAI Blog*, 1(8):9, 2019.

[2] Daniel Adiwardana, Minh-Thang Luong, David R So, Jamie Hall, Noah Fiedel, Romal Thoppilan, Zi Yang, Apoorv Kulshreshtha, Gaurav Nemade, Yifeng Lu, et al. Towards a human-like open-domain chatbot. *arXiv preprint arXiv:2001.09977*, 2020.

[3] Noam Shazeer, Azalia Mirhoseini, Krzysztof Maziarz, Andy Davis, Quoc Le, Geoffrey Hinton, and Jeff Dean. Outrageously large neural networks: The sparsely-gated mixture-of-experts layer. *arXiv preprint arXiv:1701.06538*, 2017.

[4] Chiyuan Zhang, Samy Bengio, Moritz Hardt, Benjamin Recht, and Oriol Vinyals. Understanding deep learning requires rethinking generalization. *arXiv preprint arXiv:1611.03530*, 2016.

[5] Mikhail Belkin, Daniel Hsu, Siyuan Ma, and Soumik Mandal. Reconciling modern machine-learning practice and the classical bias–variance trade-off. *Proceedings of the National Academy of Sciences*, 116(32):15849–15854, 2019.

[6] Bradley Efron and Charles Stein. The jackknife estimate of variance. *The Annals of Statistics*, pages 586–596, 1981.

[7] Charles J Stone. The use of polynomial splines and their tensor products in multivariate function estimation. *The Annals of Statistics*, pages 118–171, 1994.

[8] Jianhua Z Huang et al. Projection estimation in multiple regression with application to functional anova models. *The annals of statistics*, 26(1):242–272, 1998.

[9] Art B Owen. The dimension distribution and quadrature test functions. *Statistica Sinica*, pages 1–17, 2003.

[10] Stuart Geman, Elie Bienenstock, and René Doursat. Neural networks and the bias/variance dilemma. *Neural computation*, 4(1):1–58, 1992.

[11] Vladimir N Vapnik. An overview of statistical learning theory. *IEEE transactions on neural networks*, 10(5):988–999, 1999.

[12] Mikhail Belkin, Siyuan Ma, and Soumik Mandal. To understand deep learning we need to understand kernel learning. *arXiv preprint arXiv:1802.01396*, 2018.

[13] Preetum Nakkiran, Gal Kaplun, Yamini Bansal, Tristan Yang, Boaz Barak, and Ilya Sutskever. Deep double descent: Where bigger models and more data hurt. *arXiv preprint arXiv:1912.02292*, 2019.

[14] Mikhail Belkin, Daniel J Hsu, and Partha Mitra. Overfitting or perfect fitting? risk bounds for classification and regression rules that interpolate. In *Advances in neural information processing systems*, pages 2300–2311, 2018.

[15] Mikhail Belkin, Alexander Rakhlin, and Alexandre B Tsybakov. Does data interpolation contradict statistical optimality? *arXiv preprint arXiv:1806.09471*, 2018.

[16] Tengyuan Liang and Alexander Rakhlin. Just interpolate: Kernel "ridgeless" regression can generalize. *arXiv preprint arXiv:1808.00387*, 2018.

[17] Madhu S Advani and Andrew M Saxe. High-dimensional dynamics of generalization error in neural networks. *arXiv preprint arXiv:1710.03667*, 2017.

[18] Mario Geiger, Arthur Jacot, Stefano Spigler, Franck Gabriel, Levent Sagun, Stéphane d'Ascoli, Giulio Biroli, Clément Hongler, and Matthieu Wyart. Scaling description of generalization with number of parameters in deep learning. *arXiv preprint arXiv:1901.01608*, 2019.

[19] Dmitry Kobak, Jonathan Lomond, and Benoit Sanchez. Optimal ridge penalty for real-world high-dimensional data can be zero or negative due to the implicit ridge regularization. *arXiv preprint arXiv:1805.10939*, 2018.

[20] Mikhail Belkin, Daniel Hsu, and Ji Xu. Two models of double descent for weak features. *arXiv preprint arXiv:1903.07571*, 2019.

[21] Trevor Hastie, Andrea Montanari, Saharon Rosset, and Ryan J Tibshirani. Surprises in high-dimensional ridgeless least squares interpolation. *arXiv preprint arXiv:1903.08560*, 2019.

[22] Partha P Mitra. Understanding overfitting peaks in generalization error: Analytical risk curves for l_2 and l_1 penalized interpolation. *arXiv preprint arXiv:1906.03667*, 2019.

[23] Song Mei and Andrea Montanari. The generalization error of random features regression: Precise asymptotics and double descent curve. *arXiv preprint arXiv:1908.05355*, 2019.

[24] Ben Adlam and Jeffrey Pennington. The neural tangent kernel in high dimensions: Triple descent and a multi-scale theory of generalization. In *Proceedings of the 37th International Conference on Machine Learning (ICML 2020)*, 2020.

[25] Brady Neal, Sarthak Mittal, Aristide Baratin, Vinayak Tantia, Matthew Scicluna, Simon Lacoste-Julien, and Ioannis Mitliagkas. A modern take on the bias-variance tradeoff in neural networks. *arXiv preprint arXiv:1810.08591*, 2018.

[26] Jeffrey Pennington and Pratik Worah. Nonlinear random matrix theory for deep learning. In *Advances in Neural Information Processing Systems*, pages 2637–2646, 2017.

[27] Jeffrey Pennington and Pratik Worah. The spectrum of the fisher information matrix of a single-hidden-layer neural network. In *Advances in Neural Information Processing Systems*, pages 5410–5419, 2018.

[28] Ben Adlam, Jake Levinson, and Jeffrey Pennington. A random matrix perspective on mixtures of nonlinearities for deep learning. *arXiv preprint arXiv:1912.00827*, 2019.

[29] Cosme Louart, Zhenyu Liao, Romain Couillet, et al. A random matrix approach to neural networks. *The Annals of Applied Probability*, 28(2):1190–1248, 2018.

[30] S Péché et al. A note on the pennington-worah distribution. *Electronic Communications in Probability*, 24, 2019.

[31] Reza Rashidi Far, Tamer Oraby, Wlodzimierz Bryc, and Roland Speicher. Spectra of large block matrices. *arXiv preprint cs/0610045*, 2006.

[32] Arthur Jacot, Franck Gabriel, and Clément Hongler. Neural tangent kernel: Convergence and generalization in neural networks. In *Advances in neural information processing systems*, pages 8571–8580, 2018.

[33] Zitong Yang, Yaodong Yu, Chong You, Jacob Steinhardt, and Yi Ma. Rethinking bias-variance trade-off for generalization of neural networks. *arXiv preprint arXiv:2002.11328*, 2020.

[34] Arthur Jacot, Berfin Şimşek, Francesco Spadaro, Clément Hongler, and Franck Gabriel. Implicit regularization of random feature models. *arXiv preprint arXiv:2002.08404*, 2020.

[35] Stéphane d'Ascoli, Maria Refinetti, Giulio Biroli, and Florent Krzakala. Double trouble in double descent: Bias and variance (s) in the lazy regime. *arXiv preprint arXiv:2003.01054*, 2020.

[36] Radford M Neal. Priors for infinite networks. In *Bayesian Learning for Neural Networks*, pages 29–53. Springer, 1996.

[37] Ali Rahimi and Benjamin Recht. Random features for large-scale kernel machines. In *Advances in neural information processing systems*, pages 1177–1184, 2008.

[38] Behrooz Ghorbani, Song Mei, Theodor Misiakiewicz, and Andrea Montanari. Linearized two-layers neural networks in high dimension. *arXiv preprint arXiv:1904.12191*, 2019.

[39] J William Helton, Tobias Mai, and Roland Speicher. Applications of realizations (aka linearizations) to free probability. *Journal of Functional Analysis*, 274(1):1–79, 2018.

[40] James A Mingo and Roland Speicher. *Free probability and random matrices*, volume 35. Springer, 2017.

[41] Laszlo Erdos. The matrix dyson equation and its applications for random matrices. *arXiv preprint arXiv:1903.10060*, 2019.

S1 Symmetric variance decomposition

The purpose of this section is to prove Prop. 1 and derive eqns. (33)-(35). The strategy is to use the subset-sum relationship, eqn. (5), as a definition, derive explicit formulae for the variance terms, then prove all terms are nonnegative. In the statistics literature this approach is referred to as functional ANOVA [6–9], but we present a derivation here as it may be unfamiliar to members of the machine learning community.

Motivation. The law of total variance for two random variables X and Y is

$$\mathbb{V}[Y] = \mathbb{E}\mathbb{V}[Y|X] + \mathbb{V}\mathbb{E}[Y|X], \tag{S1}$$

where the two terms represents the variance of Y that is unexplained and explained by X respectively. Since the variance must be nonnegative it is possible to interpret it as an area. In Fig. S1a, the total variance is represented by the square, which is in turn broken up into the explained variance (red circle) and unexplained variance (area outside of the circle).

It is possible to extend this idea to several variables. An observation that is key to the interpretation is

$$\mathbb{V}\mathbb{E}[Y|X_1] + \mathbb{V}\mathbb{E}[Y|X_2] \leq \mathbb{V}\mathbb{E}[Y|X_1, X_2], \tag{S2}$$

i.e. the "variance explained" is a superadditive function. So the decomposition for two variables could be written as

$$\mathbb{V}[Y] = \mathbb{V}\mathbb{E}[Y|X_1] + \mathbb{V}\mathbb{E}[Y|X_2] + (\mathbb{V}\mathbb{E}[Y|X_1, X_2] - \mathbb{V}\mathbb{E}[Y|X_1] - \mathbb{V}\mathbb{E}[Y|X_2]) + \mathbb{E}\mathbb{V}[Y|X_1, X_2], \tag{S3}$$

with the terms interpreted as the variance explained by X_1, the variance explained by X_2, the additional variance explained by X_1 and X_2 together, and the variance left unexplained by X_1 and X_2. Note that the terms are all guaranteed to be positive by eqn. (S2). See Fig S1b.

Several variables. Generalizing, let $\mathbf{X} := (X_1, \ldots, X_k)$ be a collection of random variables. Consider a Venn diagram of k circles, and denote the disjoint areas using $V_{\mathbf{i}}$ for a vector $\mathbf{i} \in \{0, 1\}^k$, where i_j indicates whether the area is inside the jth circle (see Fig S1). We make use of the natural partial ordering on $\{0, 1\}^k$, *i.e.* $\mathbf{i} \leq \mathbf{j}$ if and only if $i_l \leq j_l$ for all l. Note the ordering indicates the subset relation if the vectors are thought of as indicator vectors. We also use the notation $\mathbf{e}_j$ for the standard basis vectors, and define the vectors $\mathbf{X}_{\mathbf{i}} := (X_j : i_j = 1)$.

For simplicity, assume $Y \in \sigma(\mathbf{X})$, so that $\mathbb{E}[f(Y)|\mathbf{X}] = f(Y)$ for any measurable function f and all the variance of Y is explained by $\mathbf{X}$, *i.e.*

$$\mathbb{V}\mathbb{E}[Y|\mathbf{X}] = \mathbb{V}[Y] \tag{S4}$$

or $V_{\mathbf{0}} = 0$. In fact, let us write $Y = h(\mathbf{X})$. We make this assumption without loss of generality as one can otherwise consider $X_{k+1} := Y - \mathbb{E}(Y|\mathbf{X})$, *i.e.* the orthogonal complement of Y under projection onto the sigma algebra generated by $\mathbf{X}$.

Consistent with the $k = 1$ case, we define

$$V_{\mathbf{e}_j} = \mathbb{V}\mathbb{E}[Y|X_j], \tag{S5}$$

or more generally

$$\sum_{\mathbf{i}:\mathbf{i}\leq\mathbf{j}} V_{\mathbf{i}} = \mathbb{V}\mathbb{E}[Y|\mathbf{X}_{\mathbf{j}}]. \tag{S6}$$

Eqn. (S6) is exactly the subset-sum relationship in (5).

Lemma S1. *Eqn.* (S6) *is sufficient to define* $V_{\mathbf{i}}$ *for all* $\mathbf{i}$.

Proof. This lemma follows directly from the fact that (S6) defines 2^k equations in terms of 2^k unknowns, $V_{\mathbf{i}}$. However, we may get a more explicit solution for each $V_{\mathbf{i}}$: We proceed by induction on $|\mathbf{i}| := \sum_j i_j$. The special case of eqn. (S6), eqn. (S5), proves the base case, $|\mathbf{i}| = 1$. Assume we have defined $V_{\mathbf{i}}$ for all $|\mathbf{i}| \leq m$. Then for $\mathbf{i}$ such that $|\mathbf{i}| = m + 1$, using eqn. (S6) we may write

$$V_{\mathbf{i}} + \sum_{\mathbf{j}:\mathbf{j}\leq\mathbf{i},\mathbf{j}\neq\mathbf{i}} V_{\mathbf{j}} = \mathbb{V}\mathbb{E}[Y|\mathbf{X}_{\mathbf{i}}]. \tag{S7}$$

Noting that $|\mathbf{j}| \leq m$ if $\mathbf{j} \leq \mathbf{i}$ and $\mathbf{j} \neq \mathbf{i}$ completes the proof. □

Calculating Variances To calculate the variances terms used above for our model, we use a coupling: we introduce a copy of the underlying random variables $\mathbf{X}$ and take expectations under different independence assumptions on $\mathbf{X}$ and its copy. The simplest illustration of this idea is to express the variance of a random variable Y using an iid copy of Y, denoted Y', then define $\tilde{Y} := BY + (1-B)Y'$ for $B \sim \text{Bern}(1/2)$ independent of Y and Y'. We have

$$\mathbb{V}[Y] = \mathbb{E}[Y^2] - \mathbb{E}[Y]^2 = \mathbb{E}[YY] - \mathbb{E}[YY'] = \mathbb{E}[Y\tilde{Y}|B=1] - \mathbb{E}[Y\tilde{Y}|B=0]. \tag{S8}$$

This idea extends naturally to our setting. Recall $Y = h(\mathbf{X})$, then let $\tilde{\mathbf{X}} := (B_1X_1 + (1-B_1)X_1', \ldots, B_kX_k + (1-B_k)X_k')$ for $\mathbf{X}'$ an iid copy of $\mathbf{X}$ and $B_i \sim \text{Bern}(1/2)$ iid. Define

$$H_{\mathbf{i}} := \mathbb{E}\left[h(\mathbf{X})h(\tilde{\mathbf{X}})|\mathbf{B} = \mathbf{i}\right]. \tag{S9}$$

Thus, $\mathbb{V}\mathbb{E}[Y|\mathbf{X_i}] = H_{\mathbf{i}} - H_{\mathbf{0}}$ and $\mathbb{E}\mathbb{V}[Y|\mathbf{X_i}] = H_{\mathbf{1}} - H_{\mathbf{i}}$.

Theorem S1. *Using H, we have the following formula for the areas. Let $|\mathbf{i}| > 0$, then*

$$V_{\mathbf{i}} := \sum_{l=0}^{|\mathbf{i}|} \sum_{\mathbf{j}:\mathbf{j}\le\mathbf{i},|\mathbf{j}|=l} (-1)^{|\mathbf{i}|-l} H_{\mathbf{j}}. \tag{S10}$$

Proof. We again use induction on $|\mathbf{i}|$. The formula clearly holds for $|\mathbf{i}| = 1$. Then using the induction hypothesis and eqn. (S7), we see

$$\begin{aligned} V_{\mathbf{i}} &= H_{\mathbf{i}} - H_{\mathbf{0}} - \sum_{\mathbf{j}:\mathbf{j}\le\mathbf{i},\mathbf{j}\ne\mathbf{i}} \sum_{l=0}^{|\mathbf{j}|} \sum_{\mathbf{k}:\mathbf{k}\le\mathbf{j},|\mathbf{k}|=l} (-1)^{|\mathbf{j}|-l} H_{\mathbf{k}} \qquad \text{(S11)} \\ &= \sum_{l=0}^{|\mathbf{i}|} \sum_{\mathbf{j}:\mathbf{j}\le\mathbf{i},|\mathbf{j}|=l} (-1)^{|\mathbf{i}|-l} H_{\mathbf{j}}. \end{aligned}$$

□

Lemma S2. *The function H is partially ordered, that is*

$$H_{\mathbf{i}} \le H_{\mathbf{j}}, \tag{S12}$$

if and only if $i_k \le j_k$ for all $k \in \{1, \ldots, k\}$.

Proof. Define $Z := \mathbb{E}[Y|X_{\mathbf{i}}]$, then

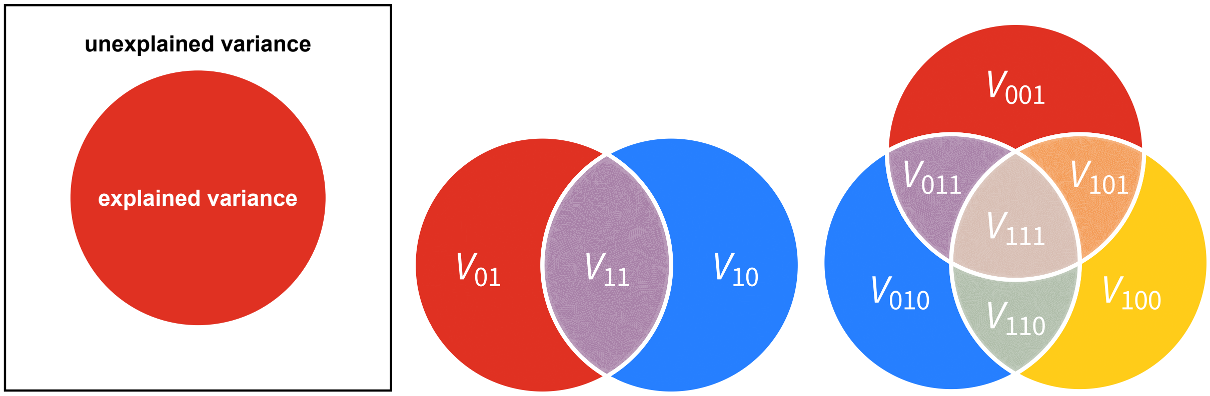
$$H_{\mathbf{i}} - H_{\mathbf{j}} = \mathbb{E}\left[Z^2 - \mathbb{E}[Z|X_{\mathbf{j}}]^2\right] \ge \mathbb{E}\left[Z^2 - \mathbb{E}[Z^2|X_{\mathbf{j}}]\right] = 0. \tag{S13}$$

□

Theorem S2. *The areas $V_{\mathbf{i}}$ are nonnegative.*

Proof. The idea is similar to the proof of Lemma S2, and indeed this generalize the result. First we prove eqn. (S2) to illustrate the idea with simple notation. We see

$$\begin{aligned} &\mathbb{V}\mathbb{E}[Y|X_1, X_2] - \mathbb{V}\mathbb{E}[Y|X_1] - \mathbb{V}\mathbb{E}[Y|X_2] \qquad \text{(S14)} \\ &\quad = H_{11} + H_{00} - H_{01} - H_{10} \\ &\quad = \frac{1}{4}\mathbb{E}\left(h(X_1, X_2) + h(\tilde{X}_1, \tilde{X}_2) - h(\tilde{X}_1, X_2) - h(X_1, \tilde{X}_2)\right)^2 \\ &\quad \ge 0. \end{aligned}$$



(a) $k = 1$ (b) $k = 2$ (c) $k = 3$

Figure S1: In (a) the two disjoint areas represent $\mathbb{VE}[Y|X]$, the variance of Y explained by X, and $\mathbb{EV}[Y|X]$, the variance of Y unexplained by X. For simplicity, we assume that in (b) and (c) there is no variance that is not explained by $\mathbf{X}$, so that the area outside of the circles is zero.

For the general case, fix $\mathbf{i}$ and define

$$\bar{h}(\mathbf{X}_\mathbf{i}) := \mathbb{E}_{\mathbf{X}_{\mathbf{1}-\mathbf{i}}}[h(\mathbf{X})|\mathbf{X}_\mathbf{i}], \tag{S15}$$

that is, marginalize over all X_j such that $i_j = 0$. Then note for $\mathbf{j} \leq \mathbf{i}$ that

$$H_\mathbf{j} = \mathbb{E}h(\mathbf{X}_\mathbf{j}, \mathbf{X}_{\mathbf{i}-\mathbf{j}}, \mathbf{X}_{\mathbf{1}-\mathbf{i}})h(\mathbf{X}_\mathbf{j}, \tilde{\mathbf{X}}_{\mathbf{i}-\mathbf{j}}, \tilde{\mathbf{X}}_{\mathbf{1}-\mathbf{i}}) = \mathbb{E}\bar{h}(\mathbf{X}_\mathbf{j}, \mathbf{X}_{\mathbf{i}-\mathbf{j}})\bar{h}(\mathbf{X}_\mathbf{j}, \tilde{\mathbf{X}}_{\mathbf{i}-\mathbf{j}}). \tag{S16}$$

Now using Theorem S1, we see

$$\begin{aligned} V_\mathbf{i} &= \sum_{l=0}^{|\mathbf{i}|} \sum_{\mathbf{j}:\mathbf{j}\leq\mathbf{i},|\mathbf{j}|=l} (-1)^{|\mathbf{i}|-l}\mathbb{E}\bar{h}(\mathbf{X}_\mathbf{j}, \mathbf{X}_{\mathbf{i}-\mathbf{j}})\bar{h}(\mathbf{X}_\mathbf{j}, \tilde{\mathbf{X}}_{\mathbf{i}-\mathbf{j}}) \\ &= \frac{1}{2^{|\mathbf{i}|}}\mathbb{E}\left(\sum_{\mathbf{j}:\mathbf{j}\leq\mathbf{i}} \bar{h}(\mathbf{X}_\mathbf{j}, \tilde{\mathbf{X}}_{\mathbf{i}-\mathbf{j}})\right)^2 \\ &\geq 0. \end{aligned} \tag{S17}$$

$\square$

Examples for $k = 2$ and $k = 3$ used in the main text. See Fig S1b. For $k = 2$, we have:

$$\begin{aligned} V_{01} &= H_{10} - H_{00} \\ V_{10} &= H_{01} - H_{00} \\ V_{11} &= H_{11} - H_{01} - H_{10} + H_{00}. \end{aligned}$$

See Fig S1c. For $k = 3$, we have:

$$\begin{aligned}
V_{001} &= H_{001} - H_{000} \\
V_{010} &= H_{010} - H_{000} \\
V_{100} &= H_{100} - H_{000} \\
V_{011} &= H_{011} - H_{001} - H_{010} + H_{000} \\
V_{101} &= H_{101} - H_{001} - H_{100} + H_{000} \\
V_{110} &= H_{110} - H_{010} - H_{100} + H_{000} \\
V_{111} &= H_{111} - H_{011} - H_{101} - H_{110} + H_{001} + H_{010} + H_{100} - H_{000}.
\end{aligned} \tag{S18}$$

Ensemble and bagging formulas. To obtain these results, we first calculate the $H_{\mathbf{i}}$ terms associated with the averaged predictor. Specifically, define $P := \{P_1, \ldots, P_{k_P}\}$, $X := \{X_1, \ldots, X_{k_D}\}$, $\varepsilon := \{\varepsilon_1, \ldots, \varepsilon_{k_D}\}$, and

$$Y := \frac{1}{k_P k_D} \sum_{i,j} \hat{y}_{ij}(\mathbf{x}) \,, \tag{S19}$$

where the indices denote iid samples. We consider the variance decomposition of Y with respect to P, X, and ε. Note, we could instead use the notation

$$Y = \hat{y}(P, X, \varepsilon) = \frac{1}{k_P k_D} \sum_{i=1}^{k_P} \sum_{j=1}^{k_D} \hat{y}(P_i, X_j, \varepsilon_j), \tag{S20}$$

to make explicit the dependence on each of the random variables.

Clearly, $\mathbb{E}\hat{y}(P, X, \varepsilon) = \hat{y}(P_1, X_1, \varepsilon_1)$, so the predictors have the same bias. Now, we calculate the Hs using superscripts to denote the ensemble and bagging sizes. First,

$$H_{000}^{k_P k_D} = \mathbb{E}\hat{y}(P, X, \varepsilon)\hat{y}(\tilde{P}, \tilde{X}, \tilde{\varepsilon}) = H_{000}^{11} \,. \tag{S21}$$

Next, we see

$$\begin{aligned}
H_{100}^{k_P k_D} &= \mathbb{E}\hat{y}(P, X, \varepsilon)\hat{y}(P, \tilde{X}, \tilde{\varepsilon}) \\
&= \frac{1}{k_P^2 k_D^2} \sum_{i=1}^{k_P} \sum_{j=1}^{k_D} \sum_{i'=1}^{k_P} \sum_{j'=1}^{k_D} \mathbb{E}\hat{y}(P_i, X_j, \varepsilon_j)\hat{y}(P_{i'}, \tilde{X}_{j'}, \tilde{\varepsilon}_{j'}) \\
&= \frac{1}{k_P^2 k_D^2} \sum_{i,j,j'} \mathbb{E}\hat{y}(P_i, X_j, \varepsilon_j)\hat{y}(P_i, \tilde{X}_{j'}, \tilde{\varepsilon}_{j'}) + \frac{1}{k_P^2 k_D^2} \sum_{i \neq i'} \sum_{j,j'} \mathbb{E}\hat{y}(P_i, X_j, \varepsilon_j)\mathbb{E}\hat{y}(P_{i'}, \tilde{X}_{j'}, \tilde{\varepsilon}_{j'}) \\
&= \frac{H_{100}^{11} - H_{000}^{11}}{k_P} + H_{000}^{11} \,.
\end{aligned} \tag{S22}$$

Similarly, to above we find

$$H_{010}^{k_P k_D} = \frac{H_{010}^{11} - H_{000}^{11}}{k_D} + H_{000}^{11} \,, \tag{S23}$$

$$H_{001}^{k_P k_D} = \frac{H_{001}^{11} - H_{000}^{11}}{k_D} + H_{000}^{11} \,, \tag{S24}$$

and

$$H_{011}^{k_P k_D} = \frac{H_{011}^{11} - H_{000}^{11}}{k_D} + H_{000}^{11} \,. \tag{S25}$$

The other terms are more complex, but the idea is the same. We find

$$
\begin{aligned}
H_{110}^{k_P k_D} &= \frac{1}{k_P^2 k_D^2} \sum_{i=1}^{k_P} \sum_{j=1}^{k_D} \sum_{i'=1}^{k_P} \sum_{j'=1}^{k_D} \mathbb{E}\hat{y}(P_i, X_j, \varepsilon_j)\hat{y}(P_{i'}, X_{j'}, \tilde{\varepsilon}_{j'}) \\
&= \frac{1}{k_P^2 k_D^2} \sum_i \sum_j \mathbb{E}\hat{y}(P_i, X_j, \varepsilon_j)\hat{y}(P_i, X_j, \tilde{\varepsilon}_j) + \frac{1}{k_P^2 k_D^2} \sum_{i\neq i'} \sum_j \mathbb{E}\hat{y}(P_i, X_j, \varepsilon_j)\hat{y}(P_{i'}, X_j, \tilde{\varepsilon}_j) && \text{(S26)} \\
&\quad + \frac{1}{k_P^2 k_D^2} \sum_i \sum_{j\neq j'} \mathbb{E}\hat{y}(P_i, X_j, \varepsilon_j)\hat{y}(P_i, X_{j'}, \tilde{\varepsilon}_{j'}) + \frac{1}{k_P^2 k_D^2} \sum_{i\neq i'} \sum_{j\neq j'} \mathbb{E}\hat{y}(P_i, X_j, \varepsilon_j)\hat{y}(P_{i'}, X_{j'}, \tilde{\varepsilon}_{j'}) && \text{(S27)} \\
&= \frac{H_{110}^{11} - H_{010}^{11} - H_{100}^{11} + H_{000}^{11}}{k_D k_P} + \frac{H_{010}^{11} - H_{000}^{11}}{k_P} + \frac{H_{100}^{11} - H_{000}^{11}}{k_D} + H_{000}^{11}\,. && \text{(S28)}
\end{aligned}
$$

Similarly, we have

$$
H_{101}^{k_P k_D} = \frac{H_{101}^{11} - H_{001}^{11} - H_{100}^{11} + H_{000}^{11}}{k_D k_P} + \frac{H_{001}^{11} - H_{000}^{11}}{k_P} + \frac{H_{100}^{11} - H_{000}^{11}}{k_D} + H_{000}^{11} \tag{S29}
$$

and

$$
H_{111}^{k_P k_D} = \frac{H_{111}^{11} - H_{011}^{11} - H_{100}^{11} + H_{000}^{11}}{k_D k_P} + \frac{H_{011}^{11} - H_{000}^{11}}{k_P} + \frac{H_{100}^{11} - H_{000}^{11}}{k_D} + H_{000}^{11}. \tag{S30}
$$

Finally, substituting the expressions for the Hs into eqn. (S18) and simplifying completes the derivation.

To find the optimal ratio, we write the test error as

$$
B + \frac{V_P}{k_P} + \frac{V_X}{k_D} + \frac{V_\varepsilon}{k_D} + \frac{V_{X\varepsilon}}{k_D} + \frac{V_{PX}}{k_P k_D} + \frac{V_{P\varepsilon}}{k_P k_D} + \frac{V_{PX\varepsilon}}{k_P k_D} \tag{S31}
$$

and substitute $k_D = K/k_P$, where K is a fixed constant. Then differentiating eqn. (S31) with respect to k_P and solving for the stationary point yields eqn. (35).

S2 Model Definitions for the Full Neural Tangent Kernel

For clarity of presentation, in the main text we focused on a linear teacher and a simple unstructured random feature model. This model can also be viewed as a degeneration of the Neural Tangent Kernel (NTK) of a single-hidden-layer neural network under which the first-layer weights are held at their randomly-initialized values and only the second-layer weights are optimized. Our analysis and results actually extend to the full NTK, where all weights are optimized, and to a wide nonlinear teacher neural network. The results in the main text are special cases of the more general results we present here.

S2.1 Data distribution

Following [24], we consider the task of learning an unknown function from m independent samples $(\mathbf{x}_i, y_i) \in \mathbb{R}^{n_0} \times \mathbb{R}$, $i \le m$, where the datapoints are standard Gaussian, $\mathbf{x}_i \sim \mathcal{N}(0, I_{n_0})$, and the labels are generated by a wide[5] single-hidden-layer neural network:

$$
y_i | \mathbf{x}_i, \Omega, \omega \sim \omega\sigma_{\mathrm{T}}(\Omega\mathbf{x}_i/\sqrt{n_0})/\sqrt{n_{\mathrm{T}}} + \varepsilon_i\,. \tag{S32}
$$

The teacher's activation function σ_{T} is applied coordinate-wise, and its parameters $\Omega \in \mathbb{R}^{n_{\mathrm{T}} \times n_0}$ and $\omega \in \mathbb{R}^{1\times n_{\mathrm{T}}}$ are matrices whose entries are independently sampled once for all data from $\mathcal{N}(0,1)$. We also allow for independent label noise, $\varepsilon_i \sim \mathcal{N}(0, \sigma_\varepsilon^2)$. In this case, the test loss for a predictive function $\hat{y}$ becomes,

$$
\mathbb{E}(\omega\sigma_{\mathrm{T}}(\Omega\mathbf{x}/\sqrt{n_0})/\sqrt{n_{\mathrm{T}}} + \varepsilon - \hat{y}(\mathbf{x}))^2\,. \tag{S33}
$$

[5] We assume the width $n_{\mathrm{T}} \to \infty$, but the rate is not important.

Recall that in our high-dimensional asymptotics the limiting ratios $n_0/m \to \phi$ and $n_0/n_1 \to \psi$ are constant. As we will discuss in Sec. S3, in this regime only linear functions of the data can be learned, a finding that is consistent with observations made in [38, 23]. When the teacher width $n_{\mathrm{T}} \to \infty$, a precise decomposition of the teacher emerges that neatly captures its learning and unlearnable components. Specifically, if we define,

$$\zeta_{\mathrm{T}} := (\mathbb{E}\sigma_{\mathrm{T}}'(g))^2 \,, \quad \text{and} \quad \eta_{\mathrm{T}} := \mathbb{E}\sigma_{\mathrm{T}}(g)^2 \,, \tag{S34}$$

then there is an equivalent linear teacher plus noise with signal-to-noise ratio given by,

$$\mathrm{SNR} = \zeta_{\mathrm{T}} / \left(\eta_{\mathrm{T}} - \zeta_{\mathrm{T}} + \sigma_{\boldsymbol{\varepsilon}}^2\right) \,. \tag{S35}$$

We often make this equivalence to a linear teacher explicit by setting $\sigma_{\mathrm{T}}(x) = x$ (which implies $\eta_{\mathrm{T}} = \zeta_{\mathrm{T}} = 1$) and explicitly adding label noise $\sigma_\varepsilon^2 = 1/\mathrm{SNR}$. This procedure also removes the noise from the test label, but since this noise merely contributes an additive shift to the test loss, removing it does not change any of our conclusions.

S2.2 NTK Regression

We consider predictive functions $\hat{y}$ defined by approximate (*i.e.* random feature) kernel ridge regression using the NTK of a single-hidden-layer neural network of width n_1 with entry-wise activation function σ, defined by,

$$N_0(\mathbf{x}) = W_2 \sigma(W_1 \mathbf{x}/\sqrt{n_0})/\sqrt{n_1} \,, \tag{S36}$$

for initial $n_1 \times n_0$ and $1 \times n_1$ weight matrices with iid entries $[W_1]_{ij} \sim \mathcal{N}(0,1)$[6] and $[W_2]_i \sim \mathcal{N}(0, \sigma_{W_2}^2)$.

The NTK can be considered a kernel K that is approximated by random features corresponding to the Jacobian J of the network's output with respect to its parameters, *i.e.* $K(\mathbf{x}_1, \mathbf{x}_2) = J(\mathbf{x}_1) J(\mathbf{x}_2)^\top$. The Jacobian itself naturally decomposes into the Jacobian with respect to W_1 and W_2, *i.e.* $J(\mathbf{x}) = [\partial N_0(\mathbf{x})/\partial W_1, \partial N_0(\mathbf{x})/\partial W_2] = [J_1(\mathbf{x}), J_2(\mathbf{x})]$. Therefore the kernel K also decomposes this way, and we can write.

$$K(\mathbf{x}_1, \mathbf{x}_2) = \; J_1(\mathbf{x}_1) J_1(\mathbf{x}_2)^\top + J_2(\mathbf{x}_1) J_2(\mathbf{x}_2)^\top =: \; K_1(\mathbf{x}_1, \mathbf{x}_2) + K_2(\mathbf{x}_1, \mathbf{x}_2). \tag{S37}$$

As the width of the network becomes very large (compared to all other relevant scales in the system), the approximate NTK converges to a constant kernel determined by the network's initial parameters and describes the trajectory of the network's output under gradient descent.[7] In this work, we focus on the predictive function defined by the solution to this kernel regression problem,

$$\hat{y}(\mathbf{x}) := N_0(\mathbf{x}) + (Y - N_0(X)) K^{-1} K_{\mathbf{x}} \tag{S38}$$

for $K := K(X, X) + \gamma I_m$, $K_{\mathbf{x}} := K(X, \mathbf{x})$, and γ is a ridge regularization constant. A simple calculation yields the per-layer constituent kernels,

$$K_1(\mathbf{x}_1, \mathbf{x}_2) = \frac{X^\top X}{n_0} \odot \frac{(F')^\top \operatorname{diag}(W_2)^2 F'}{n_1} \quad \text{and} \tag{S39}$$

$$K_2(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{n_1} F^\top F \,, \tag{S40}$$

where we have introduced the abbreviations $F := \sigma(W_1 X/\sqrt{n_0})$ and $F' := \sigma'(W_1 X/\sqrt{n_0})$. Notice that when $\sigma_{W_2}^2 \to 0$, $K = K_2$, *i.e.* the NTK degenerates into the standard random features kernel of the main text.

[6] Any non-zero $\sigma_{W_1}^2$ can be absorbed into a redefinition of σ.

[7] If the width is not asymptotically larger than the dataset size, the kernel system may not accurately describe the late-time predictions of the neural network.

Centering The predictive function (S38) contains an offset $N_0(\mathbf{x})$ which would typically be set to zero in standard random feature kernel regression because it simply increases the variance of test predictions. Removing this variance component has an analogous operation in neural network training: either the function value at initialization can be subtracted throughout training, or a symmetrization trick can be used in which two copies of the neural network are initialized identically, and their normalized difference $N \equiv \left(N^{(a)} - N^{(b)}\right)/\sqrt{2}$ is trained with gradient descent. Either method preserves the kernel K while enforcing $N_0 \equiv 0$. We call this procedure *centering*, and present results with and without it.

Finally, we note that ridge regularization in the kernel perspective corresponds to using L2 regularization of the neural network's weights toward their initial values.

S2.3 Exact Asymptotics for the Fine-Grained Variance Decomposition of the NTK

Here we state a generalization of the results from Sec. 3.1 to the NTK. As discussed above, the results for random feature kernel regression follow by setting $\sigma_{W_2} = 0$. The proofs are presented in the subsequent sections.

High-dimensional asymptotics. We consider the limiting behavior of tracial expressions as the dimensions in our model diverge to infinity as their ratios are held fixed according to ϕ and ψ. The tracial expressions are random variables that converge in probability to deterministic constants, which are specified as the solution to a coupled equation defined below.

Lemma S3. *Let $g \sim \mathcal{N}(0,1)$ and define,*

$$\zeta := (\mathbb{E}\sigma'(g))^2\,, \quad \eta := \mathbb{E}\sigma(g)^2\,, \quad \textit{and} \quad \eta' := \mathbb{E}\sigma'(g)^2\,. \tag{S41}$$

Then, in the high-dimensional asymptotics defined above, the limits of the traces $\tau_1(\gamma) = \frac{1}{m}\mathbb{E}\,\mathrm{tr}(K^{-1})$ and $\tau_2(\gamma) = \frac{1}{m}\mathbb{E}\,\mathrm{tr}(\frac{1}{n_0}X^\top X K^{-1})$ converge in probability to the unique solutions to the coupled polynomial equations,

$$0 = \phi\left(\zeta\tau_2\tau_1 + \phi(\tau_2 - \tau_1)\right) + \zeta\tau_1\tau_2\psi\left(\gamma\tau_1 - 1\right) + \zeta\tau_1\tau_2\sigma_{W_2}^2\left(\zeta\left(\tau_2 - \tau_1\right)\psi + \tau_1\psi\eta' + \phi\right) \tag{S42}$$

$$0 = \zeta\tau_1^2\tau_2\left(\eta' - \eta\right)\sigma_{W_2}^2 + \zeta\tau_1\tau_2\left(\gamma\tau_1 - 1\right) - \left(\tau_2 - \tau_1\right)\phi\left(\zeta\left(\tau_2 - \tau_1\right) + \eta\tau_1\right)\,. \tag{S43}$$

such that $\tau_1, \tau_2 \in \mathbb{C}^+$ for $\gamma \in \mathbb{C}^+$.

Corollary S1. *Lemma 1 follows from Lemma S3 by setting $\sigma_{W_2} = 0$.*

Theorem S3. *Let τ_1 and τ_2 be defined as in Lemma S3. Then the asymptotic bias and variance terms of eqns.* (9)-(15) *for the NTK are given by,*

$$\begin{aligned}
B &= \tau_2^2/\tau_1^2 & V_{PX} &= -\tau_2'/\tau_1^2 - B - V_P - V_X + \nu T_2/(\gamma\tau_1)^2 \\
V_P &= \tau_2'/\tau_1' - B - \nu T_2/\tau_1' & V_{P\boldsymbol{\varepsilon}} &= 0 \\
V_X &= \phi B(\tau_1 - \tau_2)^2/(\tau_1^2 - \phi(\tau_1 - \tau_2)^2) & V_{X\boldsymbol{\varepsilon}} &= \sigma_{\boldsymbol{\varepsilon}}^2 V_X/B \\
V_{\boldsymbol{\varepsilon}} &= 0 & V_{PX\boldsymbol{\varepsilon}} &= \sigma_{\boldsymbol{\varepsilon}}^2(-\tau_1'/\tau_1^2 - 1) - V_{X\boldsymbol{\varepsilon}}\,,
\end{aligned} \tag{S44}$$

where

$$T_2 := \sigma_{W_2}^2\gamma^2\left(\tau_1 + (\sigma_{W_2}^2(\eta' - \zeta) + \gamma)\tau_1' + \sigma_{W_2}^2\zeta\tau_2'\right)\,, \tag{S45}$$

τ_i' is the derivative of τ_i with respect to γ, and $\nu = 0$ with centering and $\nu = 1$ without it.

Corollary S2. *Theorem 1 follows from Theorem S3 by setting $\sigma_{W_2} = 0$.*

S2.4 Discussion of Results for the NTK

We briefly highlight some results for the full version of Theorem S3 that are distinct from the special case Theorem 1. Note that since the model in eqn. (S38) corresponds to the full NTK, the model has $n_1(n_0+1)$ parameters. Thus $n_1 = m$ does not occur at the interpolation threshold but instead represents a significantly overparameterized model. Previous work has found nonmonotonic behavior in the test loss for the model in eqn. (S38) at both the interpolation threshold and when $n_1 = m$ [24].

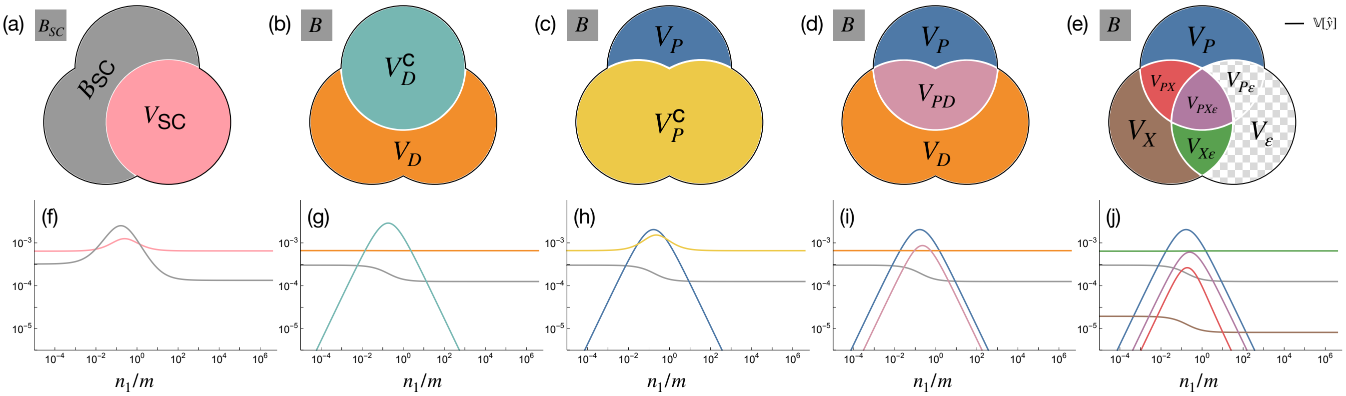


Figure S2: We replicate Fig. 1 from the main text but using the NTK. As before we set $\gamma = 0$, $\phi = 1/16$ and $\sigma = \tanh$ with SNR $= 100$, and we use centering. Recall that the number of trainable parameters for the NTK is $n_1(n_0 + 1)$, so $n_1 = m$ no longer corresponds to the interpolation threshold but represents very overparameterized models. Despite this we still find nonmonotonic behavior in many of the variance terms. Specifically, V_P, V_{PX}, and $V_{PX\varepsilon}$ are all nonmonotonic and have a peak slightly before $n_1 = m$. In the semi-classical decomposition (a), these nonmonotonicities would again cause the bias to be nonmonotonic. Similar ambiguities to the random feature case occur for the NTK in (b) and (c). (d) shows the two variable decomposition and (e) the three variable decomposition. As in Fig. 1 the terms V_ε and $V_{P\varepsilon}$ are zero.

Since $n_1 = m$ is far beyond the interpolation threshold, this second occurrence of nonmonotonicity is qualitatively different than double descent behavior. Our variance decomposition sheds light on the source of this second occurrence of nonmonotonic behavior (see Fig. S2).

We find that none of the variance terms are divergent, but the sources of the nonmonotonicity are V_P, V_{PX}, and $V_{PX\varepsilon}$. Curiously, bagging this predictive function for a large number of dataset samples would remove all other sources of variance except V_P. This would have the effect of highlighting the nonmonotonicity in the total variance.

S3 Gaussian Equivalents

Here we review the analysis from [24] for computing the test loss in our high-dimensional asymptotic limit. In the next sections, we extend this procedure to compute the constituent bias and variance terms.

As a first step, we exploit some simplifications that happen in our asymptotic limit that allow us to make the following replacements without changing any of the variance terms or the bias:

$$K_1 \to \sigma_{W_2}^2(\eta' - \zeta)I_m + \frac{\sigma_{W_2}^2\zeta}{n_0}X^\top X \tag{S46}$$

$$F \to \sqrt{\frac{\zeta}{n_0}}W_1X + \sqrt{\eta - \zeta}\,\Theta_F \tag{S47}$$

$$Y \to \sqrt{\frac{\zeta_{\mathrm{T}}}{n_{\mathrm{T}}n_0}}\omega\Omega X + \sqrt{\frac{\eta_{\mathrm{T}} - \zeta_{\mathrm{T}}}{n_{\mathrm{T}}}}\omega\Theta_Y + \mathcal{E} \tag{S48}$$

$$f \to \sqrt{\frac{\zeta}{n_0}}W_1\mathbf{x} + \sqrt{\eta - \zeta}\,\theta_f \tag{S49}$$

$$y \to \sqrt{\frac{\zeta_{\mathrm{T}}}{n_{\mathrm{T}}n_0}}\omega\Omega\mathbf{x} + \sqrt{\frac{\eta_{\mathrm{T}} - \zeta_{\mathrm{T}}}{n_{\mathrm{T}}}}\omega\theta_y\,. \tag{S50}$$

where $f := \sigma(W_1\mathbf{x}/\sqrt{n_0})$ is the random feature representation of the test point $\mathbf{x}$ and $y := \omega\sigma_{\mathrm{T}}(\Omega\mathbf{x}/\sqrt{n_0})/\sqrt{n_{\mathrm{T}}}$ is its label. The new objects Θ_F, Θ_Y, θ_f, and θ_y are matrices of the appropriate shapes with iid standard Gaussian entries. The constants η', η, and ζ (see eq. (S41)), as well as η_{T} and ζ_{T} (see eqn. (S34)) are chosen so that the mixed moments up to second order are the same for the original and linearized versions.

To give some intuition on these substitutions, many of the statistics of random matrices are universal, that is, their limiting behavior as the matrix gets larger is insensitive to the detailed properties of their entries' distributions. Considerable work has gone into demonstrating universality for an increasingly large class of random matrices and a growing number of detailed statistics. In our case, the test loss is a global measurement of several random matrices. This perspective gives some intuition for why we are able to replace many of the intractable terms in the expressions we analyze with tractable terms, which only need to match quite superficial properties of the distributions to ensure the limiting test loss is the same.

In Secs. S4 and S5, we use this replacement strategy in two distinct situations. The first is for terms of the form

$$\mathrm{tr}(AB) = \sum_{ij} A_{ij} B_{ji}, \tag{S51}$$

for deterministic A and random B. Under assumptions on A and B, standard concentration inequalities can be used to describe the limiting behavior of sums like eqn. (S51). In our setting, one finds that this behavior only depends on the the low-order moments of B. By matching these low-order moments with Gaussian random variables, we can replace B with a Gaussian random matrix with the same limiting behavior. Note, often A is not actually deterministic, we are simply conditioning on it and only considering the randomness in B. The approach is suitable for determining the average behavior of eqn. (S51) when we have control over the (weak) correlations in the entries of A and B. Linearizing the matrices A and B in this setting is just a convenient bookkeeping device for performing these computations.

When one of the matrices in eqn. (S51) is inverted, the situation is more complex, and indeed this is the case for the kernel matrix K in expressions for the training and test loss. As in [24], to apply the linear pencil algorithm [39, 40], we must first replace the kernels in all expressions with linearized versions (using eqns. (S46)-(S50)), yielding a rational expression of the i.i.d. Gaussian matrices, X, W_1, *etc.*

It should be expected that a linearized version of F will lead to the same asymptotic statistics due to some very general results on the limiting behavior of expressions of the form,

$$\mathrm{tr}\left(A\frac{1}{B - zI}\right), \tag{S52}$$

where A is symmetric and $z \in \mathbb{C}^+$. The resolvent matrix $(B - z)^{-1}$ is intimately related to the spectral properties of B. Recently, isotropic results for quite general A have been developed for matrices with correlated entries, which show that under certain assumptions the limiting behavior of eqn. (S52) depends only on the low-order moments of B. Specifically, the limiting behavior of eqn. (S52) is described by the matrix Dyson equation in many cases. For a summary of these results and related topics see e.g. [41].

Finding Gaussian equivalents for A and B in expressions like eqns. (S51) and (S52) is relatively simple in our case. We encounter terms for which the matrix B depends on some other random matrix C through a coordinate-wise nonlinear function $f(C)$. For such cases, Taylor expanding the function f is the key tool to finding these equivalents (see e.g. [28] for more details on this type of approach).

S4 Exact asymptotics for the training loss

S4.1 Decomposition of terms

The model's predictions on the training set, $\hat{y}(X)$, take a simple form,

$$\hat{y}(X) = N_0(X) + (Y - N_0(X))K^{-1}K(X, X) \tag{S53}$$

$$= Y - \gamma(Y - N_0(X))K^{-1}\,. \tag{S54}$$

The training loss can be written as,

$$E_{\text{train}} = \frac{1}{m}\mathbb{E}_{(X,Y)}\operatorname{tr}\left((Y - \hat{y}(X))(Y - \hat{y}(X))^\top\right) \tag{S55}$$

$$= \frac{\gamma^2}{m}\mathbb{E}_{(X,\varepsilon)}\operatorname{tr}\left((Y - N_0(X))^\top(Y - N_0(X))K^{-2}\right) \tag{S56}$$

$$= T_1 + \nu T_2 \tag{S57}$$

where $\nu = 0$ with centering and $\nu = 1$ without it and,

$$T_1 := \frac{\gamma^2}{m}\mathbb{E}_\varepsilon \operatorname{tr}(Y^\top Y K^{-2}) \tag{S58}$$

$$T_2 := \frac{\gamma^2}{m}\operatorname{tr}(N_0(X)^\top N_0(X) K^{-2})\,. \tag{S59}$$

We have suppressed the terms linear in N_0 since they vanish owing to the linear dependence on the symmetric random variable W_2. The Neural Tangent Kernel $K = K(X, X) + \gamma I_m$ and is given by,

$$K = \sigma_{W_2}^2\left[(\eta' - \zeta)I_m + \frac{\zeta X^\top X}{n_0}\right] + \frac{F^\top F}{n_1} + \gamma I_m\,. \tag{S60}$$

Note that $N_0(X)^\top N_0(X) = \sigma_{W_2}^2/n_1 F^T F$, so eqn. (S60) gives,

$$N_0(X)^\top N_0(X) = \sigma_{W_2}^2 K - \sigma_{W_2}^2\left[\sigma_{W_2}^2\big(\eta' - \zeta\big) + \gamma I_m\right] - \sigma_{W_2}^4\frac{\zeta X^\top X}{n_0}\,. \tag{S61}$$

Next we recall the substitution (S48) (as mentioned above, without loss of generality we special to the case of a linear teacher),

$$Y \to \sqrt{\frac{1}{n_{\mathrm{T}} n_0}}\omega\Omega X + \mathcal{E}\,, \tag{S62}$$

and consider the leading order behavior with respect to the random variables ω, Ω, and W_2 using eqn. (S51) to find

$$Y^\top Y = \frac{1}{n_0}X^\top X + \sigma_\varepsilon^2 I_m\,. \tag{S63}$$

Putting these pieces together, we can write for $\tau_1 = \tau_1(\gamma)$ and $\tau_2 = \tau_2(\gamma)$,

$$T_1 = -\gamma^2(\sigma_\varepsilon^2\tau_1' + \tau_2') \tag{S64}$$

$$T_2 = \sigma_{W_2}^2\gamma^2\left(\tau_1 + (\sigma_{W_2}^2(\eta' - \zeta) + \gamma)\tau_1' + \sigma_{W_2}^2\zeta\tau_2'\right)\,, \tag{S65}$$

where,

$$\tau_1 = \frac{1}{m}\operatorname{tr}(K^{-1})\,, \quad \text{and} \quad \tau_2 = \frac{1}{m}\operatorname{tr}(\frac{1}{n_0}X^\top X K^{-1})\,. \tag{S66}$$

Self-consistent equations for τ_1 and τ_2 can be computed using the resolvent method, as was done in [28] for the case of $\sigma_{W_2} = 0$. In order to pave the way for the analysis of the test error, we instead demonstrate how to compute these traces using operator-valued free probability.

Remark 2. *In the remainder of this section, and in Sec. S5, we assume at times that σ is non-linear (so that $\eta' > \zeta$ and $\eta > \zeta$) and/or $\gamma > 0$ in order that certain denominator factors are non-zero. The linear and/or ridgeless cases can be obtained by limits of our general results, or through special cases of the pertinent intermediate formulas.*

S4.2 Linear pencils

To begin, we construct linear pencils for τ_1 and τ_2. Specifically, straightforward block-matrix inversion confirms that

$$\tau_1 = \mathrm{tr}([Q_T^{-1}]_{1,1}) \quad \text{and} \quad \tau_2 = \mathrm{tr}([Q_T^{-1}]_{2,4})\,, \tag{S67}$$

where,

$$Q_T = \begin{pmatrix} I_m\left(\gamma + \sigma_{W_2}^2\left(\eta' - \zeta\right)\right) & \frac{\zeta X^\top \sigma_{W_2}^2}{n_0} & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} \\ -X & I_{n_0} & 0 & 0 \\ -\sqrt{\eta-\zeta}\Theta_F & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & I_{n_1} & 0 \\ 0 & 0 & \frac{\sqrt{\zeta}\psi W_1^\top}{\sqrt{n_0}\phi} & -\frac{\sqrt{\zeta}\psi I_{n_0}}{\sqrt{n_0}\phi} \end{pmatrix}. \tag{S68}$$

The matrix Q_T is not self-adjoint, but a self-adjoint representation can be obtained from it by doubling the dimensionality. In particular, letting

$$\bar{Q}_T = \begin{pmatrix} 0 & Q_T^\top \\ Q_T & 0 \end{pmatrix}, \tag{S69}$$

we have,

$$\tau_1 = \mathrm{tr}([\bar{Q}_T^{-1}]_{1,5})\,, \quad \text{and} \quad \mathrm{tr}([\bar{Q}_T^{-1}]_{2,8})\,. \tag{S70}$$

Observe that $\bar{Q}_T$ is a self-adjoint matrix whose blocks are either constants or proportional to one of $\{X, X^\top, W_1, W_1^\top, \Theta_F, \Theta_F^\top\}$; let us denote the constant terms as Z. As such, we can directly utilize the results of [31, 40] to compute the necessary traces.

S4.3 Operator-valued Stieltjes transform

The traces can be extracted from the operator-valued Stieltjes transform $G : M_d(\mathbb{C})^+ \to M_d(\mathbb{C})^+$, which is a solution of the equation,

$$ZG = I_d + \eta(G)G\,, \tag{S71}$$

where d is the number of blocks, $\eta : M_d(\mathbb{C}) \to M_d(\mathbb{C})$ defined by

$$[\eta(D)]_{ij} = \sum_{kl} \sigma(i,k;l,j)\alpha_k D_{kl}\,, \tag{S72}$$

where α_k is dimensionality of the kth block and $\sigma(i,k;l,k)$ denotes the covariance between the entries of the blocks ij block of $\bar{Q}$ and entries of the kl block of $\bar{Q}$. Eqn. (S71) may admit many solutions, but there is a unique solution such that Im$G \succ 0$ for Im$Z \succ 0$.

The constants Z, the entries of σ, and therefore the equations (S72) are manifest by inspection of the block matrix representation for $\bar{Q}_T$. Although the matrix representation of the equations is too large to reproduce here, we can nevertheless extract the equations satisfied by each entry of G.

The equations satisfied by the operator-valued Stieltjes transform G of $\bar{Q}_T$ induce the following structure on G,

$$G = \begin{pmatrix} 0 & G_{12} \\ G_{12}^\top & 0 \end{pmatrix}, \tag{S73}$$

where,

$$G_{12} = \begin{pmatrix} \tau_1 & 0 & 0 & 0 \\ 0 & g_3 & 0 & \tau_2 \\ 0 & 0 & g_4 & 0 \\ 0 & g_6 & 0 & g_5 \end{pmatrix} \tag{S74}$$

and the independent entry-wise component functions g_i, τ_1 and τ_2 satisfy the following system of polynomial equations,

$$0 = \sqrt{\zeta}g_6\psi - \zeta g_3 g_4 \sqrt{n_0} \tag{S75}$$

$$0 = \sqrt{\zeta}\psi\big(\tau_2 - g_3\tau_1\big) \tag{S76}$$
$$0 = \sqrt{\zeta}\psi\big(g_5 - g_6\tau_1\big) + \sqrt{n_0}\phi \tag{S77}$$
$$0 = -\zeta g_4 g_5 - g_6\big(\zeta\tau_1\sigma_{W_2}^2 + \phi\big) \tag{S78}$$
$$0 = \sqrt{\zeta}g_5\psi + \sqrt{n_0}\big(\phi - \zeta g_4\tau_2\big) \tag{S79}$$
$$0 = \phi - g_4\big(\tau_1\psi(\eta - \zeta) + \zeta\tau_2\psi + \phi\big) \tag{S80}$$
$$0 = -\zeta g_4\tau_2 - g_3\big(\zeta\tau_1\sigma_{W_2}^2 + \phi\big) + \phi \tag{S81}$$
$$0 = -\sqrt{\zeta}g_5\tau_1\psi - \sqrt{n_0}\tau_2\big(\zeta\tau_1\sigma_{W_2}^2 + \phi\big) \tag{S82}$$
$$0 = \sqrt{n_0}\big(\phi - g_3\big(\zeta\tau_1\sigma_{W_2}^2 + \phi\big)\big) - \sqrt{\zeta}g_6\tau_1\psi \tag{S83}$$
$$0 = \sqrt{n_0}\big(1 - \tau_1\big(\gamma + g_4(\eta - \zeta) + \sigma_{W_2}^2\big(\eta' + \zeta\big(g_3 - 1\big)\big)\big)\big) - \sqrt{\zeta}g_6\tau_1\psi\,. \tag{S84}$$

It is straightforward algebra to eliminate g_3, g_4, g_5 and g_6 from the above equations. A simple set of equations for τ_1 and τ_2 follows,

$$0 = \phi\left(\zeta\tau_2\tau_1 + \phi(\tau_2 - \tau_1)\right) + \zeta\tau_1\tau_2\psi\left(\gamma\tau_1 - 1\right) + \zeta\tau_1\tau_2\sigma_{W_2}^2\left(\zeta\left(\tau_2 - \tau_1\right)\psi + \tau_1\psi\eta' + \phi\right) \tag{S85}$$
$$0 = \zeta\tau_1^2\tau_2\left(\eta' - \eta\right)\sigma_{W_2}^2 + \zeta\tau_1\tau_2\left(\gamma\tau_1 - 1\right) - \left(\tau_2 - \tau_1\right)\phi\left(\zeta\left(\tau_2 - \tau_1\right) + \eta\tau_1\right)\,. \tag{S86}$$

Although these equations admit multiple solutions, the general results of [31, 40] guarantee that the correct root is given by the unique solutions $\tau_1, \tau_2 : \mathbb{C}^+ \to \mathbb{C}^+$ which are analytic in the upper half-plane.

It will prove useful to obtain expressions for $\tau_1'(\gamma)$ and $\tau_2'(\gamma)$. By differentiating eqns. (S85) and (S86) with respect to γ, we find

$$\tau_1' = -\frac{\zeta^2\tau_2^2\big(\psi\tilde{\tau}_1^2 - \phi^2\big)}{\psi\tilde{\tau}_1^2\big(\zeta^2\big(\tilde{\tau}_2 + 1\big)^2 + \phi\big(\zeta\tilde{\tau}_2 + \eta\big)\big(\zeta\tilde{\tau}_2\big(2\tilde{\tau}_2 + 3\big) + \eta\big)\big) + \zeta^2\phi^2\big(\tilde{\tau}_2 + 1\big)^2\big(\phi\tilde{\tau}_2^2 - 1\big)} \tag{S87}$$
$$\tau_2' = -\frac{\zeta\tau_2^2\big(\psi\tilde{\tau}_1^2(\zeta - \eta) - \zeta\phi^2\big(\tilde{\tau}_2 + 1\big)^2\big)}{\psi\tilde{\tau}_1^2\big(\zeta^2\big(\tilde{\tau}_2 + 1\big)^2 + \phi\big(\zeta\tilde{\tau}_2 + \eta\big)\big(\zeta\tilde{\tau}_2\big(2\tilde{\tau}_2 + 3\big) + \eta\big)\big) + \zeta^2\phi^2\big(\tilde{\tau}_2 + 1\big)^2\big(\phi\tilde{\tau}_2^2 - 1\big)}\,, \tag{S88}$$

where we have introduced some auxiliary variables to ease the presentation,

$$\tilde{\tau}_1 = \sigma_{W_2}^2\zeta\tau_2 + \phi\tilde{\tau}_2 \quad \text{and} \quad \tilde{\tau}_2 = -1 + \tau_2/\tau_1\,. \tag{S89}$$

S5 Exact asymptotics for the test loss

S5.1 Decomposition of terms

The test loss can be written as,

$$E_{\text{test}} = \mathbb{E}_{(\mathbf{x},y)}(y - \hat{y}(\mathbf{x}))^2 = E_1 + E_2 + E_3 \tag{S90}$$

with

$$E_1 = \mathbb{E}_{(\mathbf{x},\varepsilon)}\operatorname{tr}(y(\mathbf{x})y(\mathbf{x})^\top) + \mathbb{E}_{(\mathbf{x},\varepsilon)}\operatorname{tr}(N_0(\mathbf{x})N_0(\mathbf{x})^\top) \tag{S91}$$
$$E_2 = -2\mathbb{E}_{(\mathbf{x},\varepsilon)}\operatorname{tr}(K_{\mathbf{x}}^\top K^{-1}Y^\top y(\mathbf{x})) - 2\mathbb{E}_{(\mathbf{x},\varepsilon)}\operatorname{tr}(K_{\mathbf{x}}^\top K^{-1}N_0(X)^\top N_0(\mathbf{x})) \tag{S92}$$
$$E_3 = \mathbb{E}_{(\mathbf{x},\varepsilon)}\operatorname{tr}(K_{\mathbf{x}}^\top K^{-1}Y^\top Y K^{-1}K_{\mathbf{x}}) + \mathbb{E}_{(\mathbf{x},\varepsilon)}\operatorname{tr}(K_{\mathbf{x}}^\top K^{-1}N_0(X)^\top N_0(X)K^{-1}K_{\mathbf{x}})\,, \tag{S93}$$

where we have suppressed the terms linear in N_0 since they vanish owing to the linear dependence on the symmetric random variable W_2. The Neural Tangent Kernels $K = K(X, X)$ and $K_{\mathbf{x}} = K(X, \mathbf{x})$ are given by,

$$K = \sigma_{W_2}^2\left[(\eta' - \zeta)I_m + \frac{\zeta X^\top X}{n_0}\right] + \frac{F^\top F}{n_1} + \gamma I_m \qquad \text{and} \qquad K_{\mathbf{x}} = \frac{\sigma_{W_2}^2\zeta}{n_0}X^\top\mathbf{x} + \frac{1}{n_1}F^\top f\,. \tag{S94}$$

Remark 3. *In eqn.* (S46)*, we argued that the leading order behavior (all that is relevant for the test loss) of K_1 is relatively simple, leading to the expression for K in eqn.* (S94)*. Implicitly this requires that $\eta' \neq \zeta$, and similarly, in many of the expressions denominators are assumed to be nonzero. We handle degenerate expressions of this kind as special cases, but avoid details here to streamline the presentation.*

Using the cyclicity and linearity of the trace, the expectation over $\mathbf{x}$ requires the computation of

$$\mathbb{E}_{\mathbf{x}} K_{\mathbf{x}} K_{\mathbf{x}}^{\top}\,, \qquad \mathbb{E}_{\mathbf{x}} y(\mathbf{x}) K_{\mathbf{x}}^{\top}\,, \qquad \mathbb{E}_{\mathbf{x}} y(\mathbf{x}) y(\mathbf{x})^{\top}\,, \qquad \mathbb{E}_{\mathbf{x}} N_0(\mathbf{x}) K_{\mathbf{x}}^{\top}\,, \qquad \text{and} \quad \mathbb{E}_{\mathbf{x}} N_0(\mathbf{x}) N_0(\mathbf{x})^{\top}\,. \tag{S95}$$

As described in Sec. S3, without loss of generality we can consider the case of a linear teacher, so that $\eta_{\mathrm{T}} = \zeta_{\mathrm{T}} = 1$ and (S50) and (S49) become

$$y \to y^{\mathrm{lin}} = \frac{\sqrt{\zeta_{\mathrm{T}}}}{\sqrt{n_0 n_{\mathrm{T}}}} \omega \Omega \mathbf{x} + \sqrt{\eta_{\mathrm{T}} - \zeta_{\mathrm{T}}} \frac{1}{\sqrt{n_{\mathrm{T}}}} \omega \theta_y = \frac{1}{\sqrt{n_0 n_{\mathrm{T}}}} \omega \Omega \mathbf{x} \qquad \text{and} \qquad f \to f^{\mathrm{lin}} = \frac{\sqrt{\zeta}}{\sqrt{n_0}} W_1 \mathbf{x} + \sqrt{\eta - \zeta}\, \theta_f\,. \tag{S96}$$

Using these substitutions, the expectations over $\mathbf{x}$ are now trivial and we readily find,

$$\mathbb{E}_{\mathbf{x}} K_{\mathbf{x}} K_{\mathbf{x}}^{\top} = \frac{\sigma_{W_2}^4 \zeta^2}{n_0^2} X^{\top} X + \frac{\sigma_{W_2}^2 \zeta^{3/2}}{n_0^{3/2} n_1} (X^{\top} W_1^T F + F^{\top} W_1 X) + \frac{1}{n_1^2} F^{\top} \big(\frac{\zeta}{n_0} W_1 W_1^{\top} + (\eta - \zeta) I_{n_1}\big) F \tag{S97}$$

$$\mathbb{E}_{\mathbf{x}} y(\mathbf{x}) K_{\mathbf{x}}^{\top} = \frac{\sigma_{W_2}^2 \zeta}{n_0^{3/2} \sqrt{n_{\mathrm{T}}}} \omega \Omega X + \frac{\sqrt{\zeta}}{n_0 n_1 \sqrt{n_{\mathrm{T}}}} \omega \Omega W_1^{\top} F \tag{S98}$$

$$\mathbb{E}_{\mathbf{x}} y(\mathbf{x}) y(\mathbf{x})^{\top} = \frac{1}{n_0 n_{\mathrm{T}}} \omega \Omega \Omega^{\top} \omega^{\top} \tag{S99}$$

$$\mathbb{E}_{\mathbf{x}} N_0(\mathbf{x}) K_{\mathbf{x}}^{\top} = \frac{\sigma_{W_2}^2 \zeta^{3/2}}{n_0^{3/2} \sqrt{n_1}} W_2 W_1 X + \frac{1}{n_1^{3/2}} W_2 \big(\frac{\zeta}{n_0} W_1 W_1^{\top} + (\eta - \zeta) I_{n_1}\big) F \tag{S100}$$

$$\mathbb{E}_{\mathbf{x}} \operatorname{tr}(N_0(\mathbf{x}) N_0(\mathbf{x})^{\top}) = \sigma_{W_2}^2 \eta\,. \tag{S101}$$

One may interpret the substitutions in eqn. (S96) as a tool to calculate the expectations above to leading order as it leads to terms like eqn. (S51). Next we recall the substitution (S62),

$$Y \to \frac{1}{\sqrt{n_0 n_{\mathrm{T}}}} \omega \Omega X + \mathcal{E}\,. \tag{S102}$$

As above, we consider the leading order behavior with respect to the random variables ω, Ω, and W_2 using eqn. (S51) to find

$$\mathbb{E}_{\omega,\Omega,\mathcal{E}} \left[Y^{\top} Y\right] = \frac{1}{n_0} X^{\top} X + \sigma_{\varepsilon}^2 I_m \tag{S103}$$

$$\mathbb{E}_{\omega,\Omega,\mathcal{E},W_2} \left[Y^{\top} \mathbb{E}_{\mathbf{x}} y(\mathbf{x}) K_{\mathbf{x}}^{\top}\right] = \frac{\sigma_{W_2}^2 \zeta}{n_0^2} X^{\top} X + \frac{\sqrt{\zeta}}{n_0^{3/2} n_1} X^{\top} W_1^{\top} F \tag{S104}$$

$$\mathbb{E}_{W_2} \left[N_0(X)^{\top} N_0(X)\right] = \frac{\sigma_{W_2}^2}{n_1} F^{\top} F \tag{S105}$$

$$\mathbb{E}_{W_2} \left[N_0(X)^{\top} \mathbb{E}_{\mathbf{x}} N_0(\mathbf{x}) K_{\mathbf{x}}^{\top}\right] = \frac{\sigma_{W_2}^4 \zeta^{3/2}}{n_0^{3/2} n_1} F^{\top} W_1 X + \frac{\sigma_{W_2}^2}{n_1^2} F^{\top} \big(\frac{\zeta}{n_0} W_1 W_1^{\top} + (\eta - \zeta) I_{n_1}\big) F\,. \tag{S106}$$

$$F \to F^{\mathrm{lin}} = \frac{\sqrt{\zeta}}{\sqrt{n_0}} W_1 X + \sqrt{\eta - \zeta}\, \Theta_F\,, \tag{S107}$$

we can write,

$$\frac{\sqrt{\zeta}}{\sqrt{n_0}} F^{\top} W_1 X + \frac{\sqrt{\zeta}}{\sqrt{n_0}} X^{\top} W_1^{\top} F = F^{\top} F + \frac{\zeta}{n_0} X^{\top} W_1^{\top} W_1 X - (\eta - \zeta) \Theta_F^{\top} \Theta_F\,. \tag{S108}$$

Putting these pieces together, we have

$$E_1 = 1 + \nu\sigma_{W_2}^2\eta \tag{S109}$$
$$E_2 = E_{21} + \nu E_{22} \tag{S110}$$
$$E_3 = E_{31} + E_{32} + \nu E_{33}\,, \tag{S111}$$

where $\nu = 0$ with centering and $\nu = 1$ without it,

$$E_{21} = -\mathbb{E}\,\mathrm{tr}\left(2\frac{\sigma_{W_2}^2\zeta}{n_0^2}XK^{-1}X^\top + \frac{1}{n_0n_1}FK^{-1}F^\top + \frac{\zeta}{n_0^2n_1}W_1XK^{-1}X^\top W_1^\top - \frac{\eta-\zeta}{n_0n_1}\Theta_F K^{-1}\Theta_F^\top\right) \tag{S112}$$
$$E_{22} = -\frac{2\sigma_{W_2}^2}{n_1}\mathbb{E}\,\mathrm{tr}\left(\frac{\sigma_{W_2}^2\zeta^{3/2}}{n_0^{3/2}}K^{-1}F^\top W_1X + \frac{\zeta}{n_0n_1}K^{-1}F^\top W_1W_1^\top F + \frac{\eta-\zeta}{n_1}K^{-1}F^\top F\right) \tag{S113}$$
$$E_{31} = \sigma_\varepsilon^2\mathbb{E}\,\mathrm{tr}\left(K^{-1}\Sigma_3K^{-1}\right) \tag{S114}$$
$$E_{32} = \frac{1}{n_0}\mathbb{E}\,\mathrm{tr}\left(XK^{-1}\Sigma_3K^{-1}X^\top\right) \tag{S115}$$
$$E_{33} = \frac{\sigma_{W_2}^2}{n_1}\mathbb{E}\,\mathrm{tr}\left(FK^{-1}\Sigma_3K^{-1}F^\top\right)\,, \tag{S116}$$

and,

$$\Sigma_3 = \frac{\sigma_{W_2}^4\zeta^2}{n_0^2}X^\top X + \big(\frac{\sigma_{W_2}^2\zeta}{n_0n_1} + \frac{\eta-\zeta}{n_1^2}\big)F^\top F + \frac{\zeta}{n_0n_1^2}F^\top W_1W_1^\top F + \frac{\sigma_{W_2}^2\zeta^2}{n_0^2n_1}X^\top W_1^\top W_1X - \frac{\sigma_{W_2}^2\zeta(\eta-\zeta)}{n_0n_1}\Theta_F^\top\Theta_F\,. \tag{S117}$$

S5.2 Linear pencils

Repeated application of the Schur complement formula for block matrix inversion establishes the following representations for $E_{21}, E_{22}, E_{31}, E_{32}, E_{33}$.

S5.2.1 E_{21}

A linear pencil for E_{21} follows from the representation,

$$E_{21} = \mathrm{tr}(U_{21}^TQ_{21}^{-1}V_{21})\,, \tag{S118}$$

where,

$$U_{21}^T = \begin{pmatrix} 0 & -\frac{2\zeta I_{n_0}\sigma_{W_2}^2}{n_0} & 0 & 0 & 0 & \frac{(\eta-\zeta)I_{n_1}}{n_0} & 0 & 0 & 0 & 0 & 0 & -\frac{I_{n_1}}{n_0} & 0 & 0 \end{pmatrix} \tag{S119}$$
$$V_{21}^T = \begin{pmatrix} 0 & 0 & 0 & -\frac{\sqrt{n_0}n_1I_{n_0}}{\sqrt{\zeta}} & 0 & 0 & 0 & 0 & 0 & I_{n_1} & 0 & 0 & 0 & 0 \end{pmatrix} \tag{S120}$$

and,

$$Q_{21} = \begin{pmatrix} Q_{21}^{11} & 0 & 0 \\ 0 & Q_{21}^{22} & Q_{21}^{23} \\ 0 & 0 & Q_{21}^{33} \end{pmatrix} \tag{S121}$$

with,

$$Q_{21}^{11} = \begin{pmatrix} I_m\left(\gamma + \sigma_{W_2}^2\left(\eta'-\zeta\right)\right) & \frac{\zeta X^\top\sigma_{W_2}^2}{n_0} & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} \\ -X & I_{n_0} & 0 & 0 \\ -\sqrt{\eta-\zeta}\Theta_F & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & I_{n_1} & 0 \\ 0 & 0 & -W_1^\top & I_{n_0} \end{pmatrix} \tag{S122}$$

$$
Q_{21}^{22} = \begin{pmatrix} I_m\left(\gamma + \sigma_{W_2}^2\left(\eta' - \zeta\right)\right) & 0 & \frac{\zeta X^\top \sigma_{W_2}^2}{n_0} & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} \\ -\Theta_F & I_{n_1} & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}\sqrt{\eta-\zeta}} & 0 & 0 \\ -X & 0 & I_{n_0} & 0 & 0 \\ -\sqrt{\eta-\zeta}\Theta_F & 0 & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & I_{n_1} & \\ 0 & 0 & 0 & -W_1^\top & I_{n_0} \end{pmatrix} \tag{S123}
$$

$$
Q_{21}^{23} = \begin{pmatrix} -\Theta_F^\top & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\sqrt{\zeta}W_1}{\sqrt{n_0}(\eta-\zeta)} & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ I_{n_1} & 0 & 0 & 0 & 0 \end{pmatrix} \tag{S124}
$$

$$
Q_{21}^{33} = \begin{pmatrix} -\sqrt{\eta-\zeta}\Theta_F^\top & I_m\left(\gamma + \sigma_{W_2}^2\left(\eta' - \zeta\right)\right) & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\zeta X^\top \sigma_{W_2}^2}{n_0} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} \\ 0 & -\sqrt{\eta-\zeta}\Theta_F & I_{n_1} & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & 0 \\ 0 & -X & 0 & I_{n_0} & 0 \\ n_1 W_1^\top & 0 & -W_1^\top & 0 & I_{n_0} \end{pmatrix}. \tag{S125}
$$

S5.2.2 E_{22}

A linear pencil for E_{22} follows from the representation,

$$
E_{22} = \operatorname{tr}(U_{22}^T Q_{22}^{-1} V_{22}) \,, \tag{S126}
$$

where,

$$
U_{22}^T = \begin{pmatrix} 0 & -\frac{2\sqrt{\zeta}I_{n_1}\sigma_{W_2}^2\left(n_0(\eta-\zeta)+\zeta n_1\sigma_{W_2}^2\right)}{n_0^{3/2}n_1} & 0 & \frac{2(\zeta-\eta)I_{n_1}\sigma_{W_2}^2}{n_1} & 0 & 0 & 0 \end{pmatrix} \tag{S127}
$$

$$
V_{22}^T = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -n_1 I_{n_1} & 0 \end{pmatrix} \tag{S128}
$$

and,

$$
Q_{22} = \begin{pmatrix} I_{n_0} & 0 & -X & 0 & 0 & 0 & 0 \\ -W_1 & I_{n_1} & 0 & 0 & -\frac{\sqrt{n_0}W_1}{\sqrt{\zeta}n_1\sigma_{W_2}^2} & 0 & 0 \\ \frac{\zeta X^\top \sigma_{W_2}^2}{n_0} & 0 & I_m\left(\gamma+\sigma_{W_2}^2\left(\eta'-\zeta\right)\right) & 0 & 0 & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} \\ 0 & 0 & -\sqrt{\eta-\zeta}\Theta_F & I_{n_1} & \frac{W_1}{n_1\sigma_{W_2}^2} & 0 & 0 \\ 0 & -\frac{\sqrt{\zeta}W_1^\top}{\sqrt{n_0}} & 0 & -W_1^\top & I_{n_0} & 0 & 0 \\ -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & 0 & -\sqrt{\eta-\zeta}\Theta_F & 0 & 0 & I_{n_1} & 0 \\ 0 & 0 & 0 & 0 & 0 & -W_1^\top & I_{n_0} \end{pmatrix}. \tag{S129}
$$

S5.2.3 E_{31}

A linear pencil for E_{31} follows from the representation,

$$
E_{31} = \operatorname{tr}(U_{31}^T Q_{31}^{-1} V_{31}) \,, \tag{S130}
$$

where,

$$
U_{31}^T = \begin{pmatrix} m\sigma_\varepsilon^2 I_m & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad V_{31}^T = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & I_m & 0 & 0 \end{pmatrix} \tag{S131}
$$

and, for $\beta = \big(n_0(\zeta-\eta) - \zeta n_1 \sigma_{W_2}^2\big)$,

$$Q_{31} = \begin{pmatrix} I_m\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) & \frac{\zeta X^\top \sigma_{W_2}^2}{n_0} & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} & -\frac{\zeta^2 X^\top \sigma_{W_2}^4}{n_0^2} & 0 & \frac{\sqrt{\eta-\zeta}\Theta_F^\top \beta}{n_0 n_1^2} & \frac{\sqrt{\zeta}X^\top \beta}{n_0^{3/2} n_1^2} \\ -X & I_{n_0} & 0 & 0 & 0 & 0 & 0 & 0 \\ -\sqrt{\eta-\zeta}\Theta_F & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & I_{n_1} & 0 & 0 & -\frac{\zeta\sqrt{\eta-\zeta}\Theta_F \sigma_{W_2}^2}{n_0} & 0 & \frac{\zeta W_1}{n_0 n_1} \\ 0 & 0 & -W_1^\top & I_{n_0} & 0 & 0 & \frac{\zeta W_1^\top \sigma_{W_2}^2}{n_0} & 0 \\ 0 & 0 & 0 & 0 & I_{n_0} & -X & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\zeta X^\top \sigma_{W_2}^2}{n_0} & I_m\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & -\sqrt{\eta-\zeta}\Theta_F & I_{n_1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -W_1^\top & I_{n_0} \end{pmatrix}. \tag{S132}$$

S5.2.4 E_{32}

A linear pencil for E_{32} follows from the representation,

$$E_{32} = \mathrm{tr}(U_{32}^T Q_{32}^{-1} V_{32})\,, \tag{S133}$$

where,

$$U_{32}^T = \begin{pmatrix} 0 & I_{n_0} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad V_{32}^T = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{n_0}n_1 I_{n_0}}{\sqrt{\zeta}} \end{pmatrix} \tag{S134}$$

and, for $\beta = \big(n_0(\zeta-\eta) - \zeta n_1 \sigma_{W_2}^2\big)$

$$Q_{32} = \begin{pmatrix} I_m\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) & 0 & \frac{\zeta X^\top \sigma_{W_2}^2}{n_0} & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} & -\frac{\zeta^2 X^\top \sigma_{W_2}^4}{n_0^2} & 0 & \frac{\sqrt{\eta-\zeta}\Theta_F^\top \beta}{n_0 n_1^2} & 0 \\ -X & I_{n_0} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -X & 0 & I_{n_0} & 0 & 0 & 0 & 0 & \frac{\sqrt{\zeta}W_1^\top}{\sqrt{n_0}n_1} & 0 \\ -\sqrt{\eta-\zeta}\Theta_F & 0 & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & I_{n_1} & 0 & 0 & -\frac{\zeta\sqrt{\eta-\zeta}\Theta_F \sigma_{W_2}^2}{n_0} & 0 & 0 \\ 0 & 0 & 0 & -W_1^\top & I_{n_0} & 0 & 0 & W_1^\top\left(\frac{\eta-\zeta}{n_1}+\frac{\zeta\sigma_{W_2}^2}{n_0}\right) & 0 \\ 0 & 0 & 0 & 0 & 0 & I_{n_0} & -X & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\zeta X^\top \sigma_{W_2}^2}{n_0} & I_m\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & -\sqrt{\eta-\zeta}\Theta_F & I_{n_1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -W_1^\top & I_{n_0} \end{pmatrix}. \tag{S135}$$

S5.2.5 E_{33}

A linear pencil for E_{33} follows from the representation,

$$E_{33} = \mathrm{tr}(U_{33}^T Q_{33}^{-1} V_{33})\,, \tag{S136}$$

where,

$$U_{33}^T = \begin{pmatrix} 0 & I_{n_1}\sigma_{W_2}^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{S137}$$

$$V_{33}^T = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -n_1 I_{n_1} & 0 \end{pmatrix} \tag{S138}$$

and, for $\beta = \big(n_0(\zeta-\eta) - \zeta n_1 \sigma_{W_2}^2\big)$,

$$Q_{33} = \begin{pmatrix}
I_m\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) & 0 & 0 & \frac{\zeta X^\top \sigma_{W_2}^2}{n_0} & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} & -\frac{\zeta^2 X^\top \sigma_{W_2}^4}{n_0^2} & 0 & \frac{\sqrt{\eta-\zeta}\Theta_F^\top \beta}{n_0 n_1^2} & 0 & 0 \\
-\sqrt{\eta-\zeta}\Theta_F & I_{n_1} & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-X & 0 & I_{n_0} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-X & 0 & 0 & I_{n_0} & 0 & 0 & 0 & 0 & \frac{\sqrt{\zeta}W_1^\top}{\sqrt{n_0}n_1} & 0 & 0 \\
-\sqrt{\eta-\zeta}\Theta_F & 0 & 0 & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & I_{n_1} & 0 & 0 & -\frac{\zeta\sqrt{\eta-\zeta}\Theta_F\sigma_{W_2}^2}{n_0} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -W_1^\top & I_{n_0} & 0 & 0 & W_1^\top\left(\frac{\eta-\zeta}{n_1}+\frac{\zeta\sigma_{W_2}^2}{n_0}\right) & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & I_{n_0} & -X & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{\zeta X^\top \sigma_{W_2}^2}{n_0} & I_m\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) & 0 & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} \\
0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & -\sqrt{\eta-\zeta}\Theta_F & I_{n_1} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & -\sqrt{\eta-\zeta}\Theta_F & 0 & I_{n_1} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -W_1^\top & I_{n_0}
\end{pmatrix}. \tag{S139}$$

S5.3 Operator-valued Stieltjes transform

Even though the individual error terms $E_{21}, E_{22}, E_{31}, E_{32}, E_{33}$ can be written as the trace of self-adjoint matrices, the individual Q matrices are not themselves self-adjoint. However, by enlarging the dimensionality by a factor of two, equivalent self-adjoint representations can easily be constructed. To do so, we simply utilize the identity,

$$U^T Q V = \bar{U}^\top \bar{Q} \bar{V} \equiv \begin{pmatrix} \frac{1}{2}U^\top & V^\top \end{pmatrix} \begin{pmatrix} 0 & Q^\top \\ Q & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{2}U \\ V \end{pmatrix}. \tag{S140}$$

Observe that $\bar{Q}_{21}, \bar{Q}_{22}, \bar{Q}_{31}, \bar{Q}_{32}$ and $\bar{Q}_{33}$ are all self-adjoint block matrices whose blocks are either constants or proportional to one of $\{X, X^\top, W_1, W_1^\top, \Theta_F, \Theta_F^\top\}$; let us denote the constant terms as Z. As such, we can directly utilize the results of [31, 40] to compute the error terms in question.

For each linear pencil, the corresponding error term can be extracted from the operator-valued Stieltjes transform $G : M_d(\mathbb{C})^+ \to M_d(\mathbb{C})^+$, which is a solution of the equation,

$$ZG = I_d + \eta(G)G\,, \tag{S141}$$

where d is the number of blocks, $\eta : M_d(\mathbb{C}) \to M_d(\mathbb{C})$ defined by

$$[\eta(D)]_{ij} = \sum_{kl} \sigma(i,k;l,j)\alpha_k D_{kl}\,, \tag{S142}$$

where α_k is dimensionality of the kth block and $\sigma(i,k;l,k)$ denotes the covariance between the entries of the ij block of $\bar{Q}$ and entries of the kl block of $\bar{Q}$. Eqn. (S141) may admit many solutions, but there is a unique solution such that Im$G \succ 0$ for Im$Z \succ 0$.

The constants Z, the entries of σ, and therefore the equations (S142) are manifest by inspection of the block matrix representations for Q. Although the matrix representations are too large to reproduce here, we can nevertheless extract the equations satisfied by each entry of G, which we present in the subsequent sections.

S5.3.1 E_{21}

The equations satisfied by the operator-valued Stieltjes transform G of $\bar{Q}_{21}$ induce the following structure on G,

$$G = \begin{pmatrix} 0 & G_{12} \\ G_{12}^\top & 0 \end{pmatrix}, \tag{S143}$$

where,

$$G_{12} = \begin{pmatrix} g_8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & g_9 & 0 & g_6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & g_{11} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & g_{12} & 0 & g_{10} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & g_8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & g_1 & 0 & g_5 & 0 & g_4 & 0 & g_7 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & g_9 & 0 & g_6 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_{11} & 0 & g_3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & g_{12} & 0 & g_{10} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_8 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_2 & 0 & g_{11} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_9 & g_6 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_{12} & g_{10} \end{pmatrix}, \tag{S144}$$

and the independent entry-wise component functions g_i combine to produce the error E_{21} through the relation,

$$E_{21} = \frac{g_4(\eta - \zeta)}{n_0} + \frac{2\sqrt{\zeta} g_6 \sqrt{n_0} \sigma_{W_2}^2}{\psi} - \frac{g_2}{n_0}\,, \tag{S145}$$

and themselves satisfy the following system of polynomial equations,

$$0 = 1 - g_1 \tag{S146a}$$

$$0 = \sqrt{\zeta} g_9 g_{11} \sqrt{n_0} - g_{12}\psi \tag{S146b}$$

$$0 = \sqrt{\zeta} g_6 g_{11} \sqrt{n_0} - g_{10}\psi + \psi \tag{S146c}$$

$$0 = g_7(\eta - \zeta) + \sqrt{\zeta} g_6 g_{11} \sqrt{n_0} \tag{S146d}$$

$$0 = g_8 g_{11} n_0 \sqrt{\eta - \zeta} - g_3 \phi\big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) \tag{S146e}$$

$$0 = -\sqrt{\zeta} g_8 g_9 \psi - g_6 \sqrt{n_0} \phi\big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) \tag{S146f}$$

$$0 = -\sqrt{\zeta} g_8 g_{12} \psi - \big(g_{10} - 1\big) \sqrt{n_0} \phi\big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) \tag{S146g}$$

$$0 = g_6 \sqrt{n_0} \phi\big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) + g_8\big(\sqrt{\zeta} g_{10} \psi + \zeta g_6 \sqrt{n_0} \sigma_{W_2}^2\big) \tag{S146h}$$

$$0 = g_8 g_{11} \psi(\eta - \zeta) - \phi\big(g_5 \sqrt{\eta - \zeta} - \sqrt{\zeta} g_6 g_{11} \sqrt{n_0}\big)\big(\sigma_{W_2}^2 (\zeta - \eta') - \gamma\big) \tag{S146i}$$

$$0 = \big(g_9 - 1\big) \sqrt{n_0} \phi\big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) + g_8\big(\sqrt{\zeta} g_{12} \psi + \zeta g_9 \sqrt{n_0} \sigma_{W_2}^2\big) \tag{S146j}$$

$$0 = g_1 g_8 n_0 \sqrt{\eta - \zeta} + g_3\big(g_8 \psi(\zeta - \eta) + \phi\big(\sqrt{\zeta} g_6 \sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big)\big) \tag{S146k}$$

$$0 = \sqrt{\zeta} g_{10} g_{11} \sqrt{n_0} \phi\big(\sigma_{W_2}^2 (\zeta - \eta') - \gamma\big) + g_{12} \psi\big(\gamma\phi + \sigma_{W_2}^2 \big(-\zeta\phi + \phi\eta' + \zeta g_8\big)\big) \tag{S146l}$$

$$0 = g_{11}\big(g_8 \psi(\zeta - \eta) + \phi\big(\sqrt{\zeta} g_6 \sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big)\big) + \phi\big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) \tag{S146m}$$

$$0 = g_{11} n_0 \big(g_8 \psi(\eta - \zeta) + \sqrt{\zeta} g_6 \sqrt{n_0} \phi\big(\sigma_{W_2}^2 (\zeta - \eta') - \gamma\big)\big) - g_2 \psi\phi\big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) \tag{S146n}$$

$$0 = g_9 \psi\big(\gamma\phi + \sigma_{W_2}^2 \big(\phi(\eta' - \zeta) + \zeta g_8\big)\big) - \phi\big(\sqrt{\zeta} g_6 g_{11} \sqrt{n_0} + \psi\big)\big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) \tag{S146o}$$

$$0 = g_8\big(-\sqrt{\zeta} g_{12} \psi - \sqrt{n_0}\big(\gamma + g_{11}(\eta - \zeta) + \sigma_{W_2}^2 \big(\eta' + \zeta\big(g_9 - 1\big)\big)\big)\big) + \sqrt{n_0}\big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) \tag{S146p}$$

$$0 = \sqrt{\zeta} g_1 g_6 \sqrt{n_0} \phi\big(\sigma_{W_2}^2 (\zeta - \eta') - \gamma\big) - g_7(\zeta - \eta)\big(g_8 \psi(\zeta - \eta) + \phi\big(\sqrt{\zeta} g_6 \sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big)\big) \tag{S146q}$$

$$\begin{aligned} 0 = {} & g_1 n_0 \big(g_8 \psi(\eta - \zeta) + \sqrt{\zeta} g_6 \sqrt{n_0} \phi\big(\sigma_{W_2}^2 (\zeta - \eta') - \gamma\big)\big) + g_2 \psi\big(g_8 \psi(\zeta - \eta) \\ & + \phi\big(\sqrt{\zeta} g_6 \sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big)\big) \end{aligned} \tag{S146r}$$

$$\begin{aligned} 0 = {} & g_1\big(g_8 \psi(\eta - \zeta) + \sqrt{\zeta} g_6 \sqrt{n_0} \phi\big(\sigma_{W_2}^2 (\zeta - \eta') - \gamma\big)\big) + g_5 \sqrt{\eta - \zeta}\big(g_8 \psi(\eta - \zeta) \\ & - \phi\big(\sqrt{\zeta} g_6 \sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big)\big) \end{aligned} \tag{S146s}$$

$$
\begin{aligned}
0 &= n_0\big(-\zeta g_5 g_8 \psi\sqrt{\eta-\zeta} + \eta g_5 g_8 \psi \sqrt{\eta-\zeta} + g_8\psi(\zeta-\eta)\big(g_7(\zeta-\eta)-g_1\big) \\
&\quad + \sqrt{\zeta} g_6 \sqrt{n_0}\phi\big(g_7(\zeta-\eta)+g_1\big)\big(\gamma+\sigma_{W_2}^2(\eta'-\zeta)\big)\big) + g_4\psi\phi(\zeta-\eta)\big(\gamma+\sigma_{W_2}^2(\eta'-\zeta)\big) && \text{(S146t)}\\
0 &= \sqrt{n_0}\sqrt{\eta-\zeta}\big(g_1 g_8\sqrt{n_0}\psi(\eta-\zeta) + \sqrt{\zeta} g_1 g_6 n_0 \phi\big(\gamma+\sigma_{W_2}^2(\eta'-\zeta)\big) - \sqrt{\zeta} g_2 g_6 \psi\phi\big(\gamma+\sigma_{W_2}^2(\eta'-\zeta)\big)\big) \\
&\quad + g_3\psi(\zeta-\eta)\big(g_8\psi(\eta-\zeta) + \sqrt{\zeta} g_6\sqrt{n_0}\phi\big(\sigma_{W_2}^2(\zeta-\eta')-\gamma\big)\big) + g_4\psi(-\phi)(\eta-\zeta)^{3/2}\big(\gamma+\sigma_{W_2}^2(\eta'-\zeta)\big)\,. && \text{(S146u)}
\end{aligned}
$$

After some straightforward algebra, one can eliminate all g_i except for g_6 and g_8, which satisfy coupled polynomial equations. Those equations can be shown to be identical to eqn. (S66) by invoking the change of variables,

$$
g_6 = -\frac{\sqrt{\zeta}\psi}{\sqrt{n_0}\phi}\tau_2\,, \quad \text{and} \quad g_8 = \big(\gamma+\sigma_{W_2}^2(\eta'-\zeta)\big)\tau_1\,. \tag{S147}
$$

In terms of these variables, the error E_{21} is given by,

$$
E_{21} = 2(\tau_2/\tau_1 - 1)\,. \tag{S148}
$$

S5.3.2 E_{22}

The equations satisfied by the operator-valued Stieltjes transform G of $\bar{Q}_{22}$ induce the following structure on G,

$$
G = \begin{pmatrix} 0 & G_{12} \\ G_{12}^\top & 0 \end{pmatrix}\,, \tag{S149}
$$

where,

$$
G_{12} = \begin{pmatrix}
g_{11} & 0 & 0 & 0 & 0 & 0 & g_7 \\
0 & g_5 & 0 & g_2 & 0 & g_9 & 0 \\
0 & 0 & g_{10} & 0 & 0 & 0 & 0 \\
0 & g_3 & 0 & g_4 & 0 & g_8 & 0 \\
g_{14} & 0 & 0 & 0 & g_1 & 0 & g_6 \\
0 & 0 & 0 & 0 & 0 & g_{13} & 0 \\
g_{14} & 0 & 0 & 0 & 0 & 0 & g_{12}
\end{pmatrix}\,, \tag{S150}
$$

and the independent entry-wise component functions g_i combine to produce the error E_{22} through the relation,

$$
E_{22} = \frac{2\sqrt{\zeta} g_9 \sigma_{W_2}^2\big(\psi(\eta-\zeta)+\zeta\sigma_{W_2}^2\big)}{\sqrt{n_0}\psi} + 2 g_8(\eta-\zeta)\sigma_{W_2}^2\,, \tag{S151}
$$

and themselves satisfy the following system of polynomial equations,

$$
\begin{aligned}
0 &= \sqrt{\zeta} g_{11} g_{13}\sqrt{n_0} - g_{14}\psi && \text{(S152a)}\\
0 &= \sqrt{\zeta} g_7 g_{13}\sqrt{n_0} - g_{12}\psi + \psi && \text{(S152b)}\\
0 &= g_1\psi\big(g_3\sqrt{n_0} - \sqrt{\zeta} g_4\big) - g_3\sqrt{n_0}\sigma_{W_2}^2 && \text{(S152c)}\\
0 &= -g_1\psi\big(\sqrt{\zeta} g_5 + g_3\sqrt{n_0}\big) - g_3\sqrt{n_0}\sigma_{W_2}^2 && \text{(S152d)}\\
0 &= g_1\psi\big(g_5\sqrt{n_0} - \sqrt{\zeta} g_2\big) - \sqrt{\zeta} g_2\sigma_{W_2}^2 && \text{(S152e)}\\
0 &= g_1\psi\big(\sqrt{\zeta} g_2 + g_4\sqrt{n_0}\big) - \sqrt{\zeta} g_2\sigma_{W_2}^2 && \text{(S152f)}\\
0 &= g_1\psi\big(g_5\sqrt{n_0} - \sqrt{\zeta} g_2\big) - \big(g_5-1\big)\sqrt{n_0}\sigma_{W_2}^2 && \text{(S152g)}\\
0 &= -g_1\psi\big(\sqrt{\zeta} g_2 + g_4\sqrt{n_0}\big) - \big(g_4-1\big)\sqrt{n_0}\sigma_{W_2}^2 && \text{(S152h)}\\
0 &= g_1\psi\big(g_3\sqrt{n_0} - \sqrt{\zeta} g_4\big) - \sqrt{\zeta}\big(g_4-1\big)\sigma_{W_2}^2 && \text{(S152i)}\\
0 &= g_1\psi\big(\sqrt{\zeta} g_5 + g_3\sqrt{n_0}\big) - \sqrt{\zeta}\big(g_5-1\big)\sigma_{W_2}^2 && \text{(S152j)}\\
0 &= -\sqrt{\zeta} g_{10} g_{11}\psi - g_7\sqrt{n_0}\phi\big(\gamma+\sigma_{W_2}^2(\eta'-\zeta)\big) && \text{(S152k)}
\end{aligned}
$$

$$0 = -\sqrt{\zeta} g_{10} g_{14} \psi - g_6 \sqrt{n_0} \phi \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) \tag{S152l}$$
$$0 = -\sqrt{\zeta} g_{10} g_{14} \psi - (g_{12} - 1) \sqrt{n_0} \phi \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) \tag{S152m}$$
$$0 = g_1 \big(-\zeta g_2 + \sqrt{\zeta} (g_5 - g_4) \sqrt{n_0} + g_3 n_0 \big) - \sqrt{\zeta} (g_1 - 1) \sqrt{n_0} \sigma_{W_2}^2 \tag{S152n}$$
$$0 = g_1 \psi \big(\sqrt{\zeta} g_9 + g_8 \sqrt{n_0} \big) + \sqrt{\zeta} (g_7 g_{13} n_0 - g_9) \sigma_{W_2}^2 + g_6 g_{13} \sqrt{n_0} \psi \tag{S152o}$$
$$0 = g_7 \sqrt{n_0} \phi \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) + g_{10} \big(\sqrt{\zeta} g_{12} \psi + \zeta g_7 \sqrt{n_0} \sigma_{W_2}^2 \big) \tag{S152p}$$
$$0 = (g_{11} - 1) \sqrt{n_0} \phi \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) + g_{10} \big(\sqrt{\zeta} g_{14} \psi + \zeta g_{11} \sqrt{n_0} \sigma_{W_2}^2 \big) \tag{S152q}$$
$$0 = \sqrt{\zeta} g_{12} g_{13} \sqrt{n_0} \phi \big(\sigma_{W_2}^2 (\zeta - \eta') - \gamma \big) + g_{14} \psi \big(\gamma \phi + \sigma_{W_2}^2 (-\zeta \phi + \phi \eta' + \zeta g_{10}) \big) \tag{S152r}$$
$$0 = g_{13} \big(g_{10} \psi (\zeta - \eta) + \phi \big(\sqrt{\zeta} g_7 \sqrt{n_0} - 1 \big) \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta) \big) \big) + \phi \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta) \big) \tag{S152s}$$
$$0 = g_6 \psi \big(-\zeta g_2 + \sqrt{\zeta} (g_5 - g_4) \sqrt{n_0} + g_3 n_0 \big) + \sqrt{\zeta} \sqrt{n_0} \sigma_{W_2}^2 \big(g_7 \big(\zeta g_9 + \sqrt{\zeta} (g_5 + g_8) \sqrt{n_0} + g_3 n_0 \big) - g_6 \psi \big) \tag{S152t}$$
$$0 = g_{11} \psi \big(\gamma \phi + \sigma_{W_2}^2 \big(\phi (\eta' - \zeta) + \zeta g_{10} \big) \big) - \phi \big(\sqrt{\zeta} g_7 g_{13} \sqrt{n_0} + \psi \big) \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta) \big) \tag{S152u}$$
$$0 = g_{10} \big(-\sqrt{\zeta} g_{14} \psi - \sqrt{n_0} \big(\gamma + g_{13} (\eta - \zeta) + \sigma_{W_2}^2 \big(\eta' + \zeta (g_{11} - 1) \big) \big) \big) + \sqrt{n_0} \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta) \big) \tag{S152v}$$
$$\begin{aligned} 0 = {} & g_{14} \psi \big(-\zeta g_2 + \sqrt{\zeta} (g_5 - g_4) \sqrt{n_0} + g_3 n_0 \big) + \sqrt{\zeta} \sqrt{n_0} \sigma_{W_2}^2 \big(g_{11} \big(\zeta g_9 \\ & + \sqrt{\zeta} (g_5 + g_8) \sqrt{n_0} + g_3 n_0 \big) - g_{14} \psi \big) \end{aligned} \tag{S152w}$$
$$\begin{aligned} 0 = {} & \sqrt{\zeta} g_6 g_{13} \sqrt{n_0} \phi \big(\sigma_{W_2}^2 (\zeta - \eta') - \gamma \big) - g_1 \phi \big(\zeta g_9 + \sqrt{\zeta} (g_5 + g_8) \sqrt{n_0} + g_3 n_0 \big) \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta) \big) \\ & + g_{14} \psi \big(\gamma \phi + \sigma_{W_2}^2 (-\zeta \phi + \phi \eta' + \zeta g_{10}) \big) \end{aligned} \tag{S152x}$$
$$\begin{aligned} 0 = {} & g_1 \psi \phi \big(\sqrt{\zeta} g_9 + g_8 \sqrt{n_0} \big) \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta) \big) + \sqrt{n_0} \big(\sigma_{W_2}^2 \big(g_{10} g_{13} \psi (\eta - \zeta) + g_8 \phi \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta) \big) \big) \\ & + g_6 g_{13} \psi \phi \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta) \big) \big) \end{aligned} \tag{S152y}$$
$$\begin{aligned} 0 = {} & \sqrt{\zeta} g_8 \sigma_{W_2}^2 \big(g_{10} \psi (\eta - \zeta) - \phi \big(\sqrt{\zeta} g_7 \sqrt{n_0} - 1 \big) \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta) \big) \big) - g_3 \sqrt{n_0} \phi \big(\sqrt{\zeta} g_7 \sqrt{n_0} \sigma_{W_2}^2 + g_6 \psi \big) \\ & \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta) \big) + \sqrt{\zeta} g_4 \psi \big(g_6 \phi \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta) \big) + g_{10} (\eta - \zeta) \sigma_{W_2}^2 \big) \end{aligned} \tag{S152z}$$
$$\begin{aligned} 0 = {} & \sqrt{\zeta} g_9 \sigma_{W_2}^2 \big(g_{10} \psi (\eta - \zeta) - \phi \big(\sqrt{\zeta} g_7 \sqrt{n_0} - 1 \big) \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta) \big) \big) - g_5 \sqrt{n_0} \phi \big(\sqrt{\zeta} g_7 \sqrt{n_0} \sigma_{W_2}^2 + g_6 \psi \big) \\ & \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta) \big) + \sqrt{\zeta} g_2 \psi \big(g_6 \phi \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta) \big) + g_{10} (\eta - \zeta) \sigma_{W_2}^2 \big) \end{aligned} \tag{S152aa}$$

After some straightforward algebra, one can eliminate all g_i except for g_7 and g_{10}, which satisfy coupled polynomial equations. Those equations can be shown to be identical to eqn. (S66) by invoking the change of variables,

$$g_7 = -\frac{\sqrt{\zeta} \psi}{\sqrt{n_0} \phi} \tau_2 \,, \quad \text{and} \quad g_{10} = \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta) \big) \tau_1 \,. \tag{S153}$$

The error E_{22} is then given by,

$$E_{22} = 2\zeta \left(\frac{\tau_2}{\tau_1} - 1 \right) + \frac{2\psi \big(\zeta (\tau_2 - \tau_1) + \eta \tau_1 \big)^2 \big((\tau_2 - \tau_1) \phi + \zeta \tau_1 \tau_2 \sigma_{W_2}^2 \big)}{\zeta \tau_1^2 \tau_2 \phi} \,. \tag{S154}$$

S5.3.3 E_{31}

The equations satisfied by the operator-valued Stieltjes transform G of $\bar{Q}_{31}$ induce the following structure on G,

$$G = \begin{pmatrix} 0 & G_{12} \\ G_{12}^\top & 0 \end{pmatrix} \,, \tag{S155}$$

where,

$$G_{12} = \begin{pmatrix} g_5 & 0 & 0 & 0 & 0 & g_2 & 0 & 0 \\ 0 & g_6 & 0 & g_1 & g_3 & 0 & 0 & g_4 \\ 0 & 0 & g_8 & 0 & 0 & 0 & g_{12} & 0 \\ 0 & g_{11} & 0 & g_7 & g_{10} & 0 & 0 & g_9 \\ 0 & 0 & 0 & 0 & g_6 & 0 & 0 & g_1 \\ 0 & 0 & 0 & 0 & 0 & g_5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & g_8 & 0 \\ 0 & 0 & 0 & 0 & g_{11} & 0 & 0 & g_7 \end{pmatrix}, \tag{S156}$$

and the independent entry-wise component functions g_i give the error E_{31} through the relation,

$$E_{31} = \frac{g_2 n_0 \sigma_\varepsilon^2}{\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big)}, \tag{S157}$$

and themselves satisfy the following system of polynomial equations,

$$0 = \sqrt{\zeta} g_6 g_8 \sqrt{n_0} - g_{11}\psi \tag{S158a}$$

$$0 = \sqrt{\zeta} g_1 g_8 \sqrt{n_0} - g_7\psi + \psi \tag{S158b}$$

$$0 = -\sqrt{\zeta} g_5 g_6 \psi - g_1\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S158c}$$

$$0 = -\sqrt{\zeta} g_5 g_{11}\psi - \big(g_7 - 1\big)\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S158d}$$

$$0 = -\zeta g_7 g_8 \psi + \sqrt{\zeta}\sqrt{n_0}\big(\big(g_4 g_8 + g_1 g_{12}\big)n_0 - \zeta g_1 g_8 \sigma_{W_2}^2\big) - g_9 n_0 \psi \tag{S158e}$$

$$0 = g_1\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) + g_5\big(\sqrt{\zeta} g_7\psi + \zeta g_1\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S158f}$$

$$0 = \sqrt{\zeta} g_6 g_{12} n_0^{3/2} - g_8\big(\zeta g_{11}\psi + \sqrt{\zeta}\sqrt{n_0}\big(\zeta g_6 \sigma_{W_2}^2 - g_3 n_0\big)\big) - g_{10} n_0 \psi \tag{S158g}$$

$$0 = \big(g_6 - 1\big)\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) + g_5\big(\sqrt{\zeta} g_{11}\psi + \zeta g_6\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S158h}$$

$$0 = \sqrt{\zeta} g_7 g_8 \sqrt{n_0}\phi\big(\sigma_{W_2}^2\big(\zeta - \eta'\big) - \gamma\big) + g_{11}\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_5\big)\big) \tag{S158i}$$

$$0 = g_8\big(g_5\psi(\zeta - \eta) + \phi\big(\sqrt{\zeta} g_1\sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big)\big) + \phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S158j}$$

$$0 = g_6\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_5\big)\big) - \phi\big(\sqrt{\zeta} g_1 g_8\sqrt{n_0} + \psi\big)\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S158k}$$

$$0 = g_5\big(\sqrt{\zeta} g_{11}\psi + \sqrt{n_0}\big(\gamma + g_8(\eta - \zeta) + \sigma_{W_2}^2\big(\eta' + \zeta\big(g_6 - 1\big)\big)\big)\big) - \sqrt{n_0}\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S158l}$$

$$\begin{aligned} 0 = {} & \sqrt{\zeta} g_5\psi\big(g_6\big(\psi(\eta - \zeta) + \zeta\sigma_{W_2}^2\big) - g_3 n_0\big) - \sqrt{n_0}\big(\sqrt{\zeta} g_2 g_6\sqrt{n_0}\psi + g_4 n_0\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \\ & + \zeta g_1 g_8\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big)\big) \end{aligned} \tag{S158m}$$

$$\begin{aligned} 0 = {} & \sqrt{\zeta} g_5\psi\big(g_{11}\big(\psi(\eta - \zeta) + \zeta\sigma_{W_2}^2\big) - g_{10} n_0\big) - \sqrt{n_0}\big(\sqrt{\zeta} g_2 g_{11}\sqrt{n_0}\psi + g_9 n_0\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \\ & + \zeta g_7 g_8\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big)\big) \end{aligned} \tag{S158n}$$

$$\begin{aligned} 0 = {} & g_5\big(-\sqrt{\zeta} g_9 n_0\psi + \zeta\sqrt{n_0}\sigma_{W_2}^2\big(\zeta g_1\sigma_{W_2}^2 - g_4 n_0\big) + \sqrt{\zeta} g_7\psi\big(\psi(\eta - \zeta) + \zeta\sigma_{W_2}^2\big)\big) \\ & - n_0\big(g_4\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) + g_2\big(\sqrt{\zeta} g_7\psi + \zeta g_1\sqrt{n_0}\sigma_{W_2}^2\big)\big) \end{aligned} \tag{S158o}$$

$$\begin{aligned} 0 = {} & g_5\big(-\sqrt{\zeta} g_{10} n_0\psi + \zeta\sqrt{n_0}\sigma_{W_2}^2\big(\zeta g_6\sigma_{W_2}^2 - g_3 n_0\big) + \sqrt{\zeta} g_{11}\psi\big(\psi(\eta - \zeta) + \zeta\sigma_{W_2}^2\big)\big) \\ & - n_0\big(g_3\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) + g_2\big(\sqrt{\zeta} g_{11}\psi + \zeta g_6\sqrt{n_0}\sigma_{W_2}^2\big)\big) \end{aligned} \tag{S158p}$$

$$\begin{aligned} 0 = {} & g_2 g_8 n_0\psi(\eta - \zeta) - g_5\psi(\zeta - \eta)\big(g_8\psi(\zeta - \eta) + g_{12} n_0\big) - \sqrt{n_0}\phi\big(g_{12}\big(\sqrt{\zeta} g_1 n_0 - \sqrt{n_0}\big) \\ & + \sqrt{\zeta} g_8\big(g_4 n_0 - \zeta g_1\sigma_{W_2}^2\big)\big)\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) + \zeta g_7 g_8\psi\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \end{aligned} \tag{S158q}$$

$$\begin{aligned} 0 = {} & g_2 n_0\big(-\sqrt{\zeta} g_{11}\psi - \sqrt{n_0}\big(\gamma + g_8(\eta - \zeta) + \sigma_{W_2}^2\big(\eta' + \zeta\big(g_6 - 1\big)\big)\big)\big) + g_5\big(\sqrt{n_0}\big(g_8\psi(\zeta - \eta)^2 \\ & + g_{12} n_0(\zeta - \eta) - \sqrt{\zeta} g_{10}\sqrt{n_0}\psi - \zeta g_3 n_0\sigma_{W_2}^2 + \zeta^2 g_6\sigma_{W_2}^4\big) + \sqrt{\zeta} g_{11}\psi\big(\psi(\eta - \zeta) + \zeta\sigma_{W_2}^2\big)\big) \end{aligned} \tag{S158r}$$

$$0 = g_3 n_0\psi\big(\gamma\phi + \sigma_{W_2}^2\big(\phi\big(\eta' - \zeta\big) + \zeta g_5\big)\big) - \sqrt{\zeta}\big(g_4 g_8 n_0^{3/2}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big)$$

$$+ g_1\sqrt{n_0}\phi\big(g_{12}n_0 - \zeta g_8\sigma_{W_2}^2\big)\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) + \sqrt{\zeta}g_6\psi\sigma_{W_2}^2\big(\zeta g_5\sigma_{W_2}^2 - g_2n_0\big)\big) \tag{S158s}$$

$$0 = g_{10}n_0\psi\big(\gamma\phi + \sigma_{W_2}^2\big(\phi(\eta' - \zeta) + \zeta g_5\big)\big) - \sqrt{\zeta}\big(g_7g_{12}n_0^{3/2}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big)$$
$$+ g_8\sqrt{n_0}\phi\big(g_9n_0 - \zeta g_7\sigma_{W_2}^2\big)\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) + \sqrt{\zeta}g_{11}\psi\sigma_{W_2}^2\big(\zeta g_5\sigma_{W_2}^2 - g_2n_0\big)\big) \tag{S158t}$$

After some straightforward algebra, one can eliminate all g_i except for g_1 and g_5, which satisfy coupled polynomial equations. Those equations can be shown to be identical to eqn. (S66) by invoking the change of variables,

$$g_1 = -\frac{\sqrt{\zeta}\psi}{\sqrt{n_0}\phi}\tau_2\,, \quad \text{and} \quad g_5 = \big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big)\tau_1\,. \tag{S159}$$

The error E_{31} can then be written in terms of τ_1 and its derivative τ_1' (S87),

$$E_{31} = \sigma_\varepsilon^2\big(- \tau_1'/\tau_1^2 - 1\big)\,. \tag{S160}$$

S5.3.4 E_{32}

The equations satisfied by the operator-valued Stieltjes transform G of $\bar{Q}_{32}$ induce the following structure on G,

$$G = \begin{pmatrix} 0 & G_{12} \\ G_{12}^\top & 0 \end{pmatrix}\,, \tag{S161}$$

where,

$$G_{12} = \begin{pmatrix}
g_9 & 0 & 0 & 0 & 0 & 0 & g_6 & 0 & 0 \\
0 & g_1 & g_3 & 0 & g_4 & g_7 & 0 & 0 & g_2 \\
0 & 0 & g_{10} & 0 & g_4 & g_{13} & 0 & 0 & g_5 \\
0 & 0 & 0 & g_{12} & 0 & 0 & 0 & g_{16} & 0 \\
0 & 0 & g_{15} & 0 & g_{11} & g_{14} & 0 & 0 & g_8 \\
0 & 0 & 0 & 0 & 0 & g_{10} & 0 & 0 & g_4 \\
0 & 0 & 0 & 0 & 0 & 0 & g_9 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & g_{12} & 0 \\
0 & 0 & 0 & 0 & 0 & g_{15} & 0 & 0 & g_{11}
\end{pmatrix}\,, \tag{S162}$$

and the independent entry-wise component functions g_i give the error E_{32} through the relation,

$$E_{32} = -g_2n_0^{3/2}/(\sqrt{\zeta}\psi)\,, \tag{S163}$$

and themselves satisfy the following system of polynomial equations,

$$0 = \sqrt{\zeta}g_{10}g_{12}\sqrt{n_0} - g_{15}\psi \tag{S164a}$$
$$0 = \sqrt{\zeta}g_4g_{12}\sqrt{n_0} - g_{11}\psi + \psi \tag{S164b}$$
$$0 = -\sqrt{\zeta}g_9g_{10}\psi - g_4\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S164c}$$
$$0 = -\sqrt{\zeta}g_9g_{15}\psi - \big(g_{11} - 1\big)\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S164d}$$
$$0 = -\sqrt{\zeta}g_9\psi - \sqrt{\zeta}g_3g_9\psi - g_4\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S164e}$$
$$0 = -\sqrt{\zeta}g_6g_{10}\psi - \sqrt{\zeta}g_9g_{13}\psi - g_5\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S164f}$$
$$0 = -\sqrt{\zeta}g_9g_{14}\psi - \sqrt{\zeta}g_6g_{15}\psi - g_8\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S164g}$$
$$0 = \sqrt{\zeta}g_5g_{12}n_0 + \sqrt{\zeta}g_4\big(g_{16}n_0 + g_{12}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big)\big) + g_8\sqrt{n_0}(-\psi) \tag{S164h}$$
$$0 = g_4\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) + g_9\big(\sqrt{\zeta}g_{11}\psi + \zeta g_4\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S164i}$$
$$0 = g_3\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) + g_9\big(\sqrt{\zeta}g_{15}\psi + \zeta g_{10}\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S164j}$$
$$0 = \sqrt{\zeta}g_{12}g_{13}n_0 + \sqrt{\zeta}g_{10}\big(g_{16}n_0 + g_{12}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big)\big) + g_{14}\sqrt{n_0}(-\psi) \tag{S164k}$$

$$0 = (g_{10} - 1)\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_9\big(\sqrt{\zeta}g_{15}\psi + \zeta g_{10}\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S164l}$$

$$0 = -\sqrt{\zeta}\big((g_1 + g_3)g_6 + g_7 g_9\big)\psi - \gamma g_2\sqrt{n_0}\phi + \zeta g_2\sqrt{n_0}\phi\sigma_{W_2}^2 + g_2\sqrt{n_0}(-\phi)\eta'\sigma_{W_2}^2 \tag{S164m}$$

$$0 = \sqrt{\zeta}g_{11}g_{12}\sqrt{n_0}\phi\big(\sigma_{W_2}^2(\zeta - \eta') - \gamma\big) + g_{15}\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_9\big)\big) \tag{S164n}$$

$$0 = g_{12}\big(g_9\psi(\zeta - \eta) + \phi\big(\sqrt{\zeta}g_4\sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big) + \phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S164o}$$

$$0 = g_{10}\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_9\big)\big) - \phi\big(\sqrt{\zeta}g_4 g_{12}\sqrt{n_0} + \psi\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S164p}$$

$$0 = g_9\big(\sqrt{\zeta}g_{15}\psi + \sqrt{n_0}\big(\gamma + g_{12}(\eta - \zeta) + \sigma_{W_2}^2\big(\eta' + \zeta(g_{10} - 1)\big)\big)\big) - \sqrt{n_0}\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S164q}$$

$$0 = -\sqrt{\zeta}g_4 g_{12}\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_3\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_9\big)\big) + \zeta g_9\psi\sigma_{W_2}^2 \tag{S164r}$$

$$0 = g_7 n_0\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_6\big(\sqrt{\zeta}g_{15}\sqrt{n_0}\psi + \zeta g_{10}n_0\sigma_{W_2}^2\big) + g_9\big(\sqrt{\zeta}g_{14}\sqrt{n_0}\psi + \zeta\sigma_{W_2}^2\big(g_{13}n_0 - \zeta g_{10}\sigma_{W_2}^2\big)\big) \tag{S164s}$$

$$\begin{aligned}0 &= \gamma g_2 n_0\phi + \sqrt{\zeta}g_8 g_9\sqrt{n_0}\psi + g_6\big(\sqrt{\zeta}g_{11}\sqrt{n_0}\psi + \zeta g_4 n_0\sigma_{W_2}^2\big) - \zeta g_2 n_0\phi\sigma_{W_2}^2 + \zeta g_5 g_9 n_0\sigma_{W_2}^2\\&\quad + g_2 n_0\phi\eta'\sigma_{W_2}^2 - \zeta^2 g_4 g_9\sigma_{W_2}^4\end{aligned} \tag{S164t}$$

$$\begin{aligned}0 &= g_6\big(-\sqrt{\zeta}g_{15}\sqrt{n_0}\psi - n_0\big(\gamma + g_{12}(\eta - \zeta) + \sigma_{W_2}^2\big(\eta' + \zeta(g_{10} - 1)\big)\big)\big) + g_9\big(g_{12}\psi(\zeta - \eta)^2\\&\quad + g_{16}n_0(\zeta - \eta) - \sqrt{\zeta}g_{14}\sqrt{n_0}\psi - \zeta g_{13}n_0\sigma_{W_2}^2 + \zeta^2 g_{10}\sigma_{W_2}^4\big)\end{aligned} \tag{S164u}$$

$$\begin{aligned}0 &= \gamma g_5 n_0\phi + \sqrt{\zeta}g_8 g_9\sqrt{n_0}\psi + \sqrt{\zeta}g_6 g_{11}\sqrt{n_0}\psi + \zeta g_4\big(g_6 n_0\sigma_{W_2}^2 + g_{12}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) - \zeta g_9\sigma_{W_2}^4\big)\\&\quad - \zeta g_5 n_0\phi\sigma_{W_2}^2 + \zeta g_5 g_9 n_0\sigma_{W_2}^2 + g_5 n_0\phi\eta'\sigma_{W_2}^2\end{aligned} \tag{S164v}$$

$$\begin{aligned}0 &= \gamma g_{13}n_0\phi + \sqrt{\zeta}g_6 g_{15}\sqrt{n_0}\psi + \zeta g_{10}\big(g_6 n_0\sigma_{W_2}^2 + g_{12}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) - \zeta g_9\sigma_{W_2}^4\big)\\&\quad + g_9\big(\sqrt{\zeta}g_{14}\sqrt{n_0}\psi + \zeta g_{13}n_0\sigma_{W_2}^2\big) - \zeta g_{13}n_0\phi\sigma_{W_2}^2 + g_{13}n_0\phi\eta'\sigma_{W_2}^2\end{aligned} \tag{S164w}$$

$$\begin{aligned}0 &= -\sqrt{\zeta}g_{12}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big(\sqrt{n_0}\big(g_8 n_0 + g_{11}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big)\big) - \sqrt{\zeta}g_{15}\psi\big)\\&\quad + g_{14}n_0\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_9\big)\big) - \sqrt{\zeta}g_{11}g_{16}n_0^{3/2}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + \zeta g_{15}\psi\sigma_{W_2}^2\big(g_6 n_0 - \zeta g_9\sigma_{W_2}^2\big)\end{aligned} \tag{S164x}$$

$$\begin{aligned}0 &= g_9\psi(-(\zeta - \eta))\big(g_{12}\psi(\zeta - \eta) + g_{16}n_0\big) - \sqrt{\zeta}g_4\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big(g_{16}n_0 + g_{12}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big)\big)\\&\quad + n_0\big(g_6 g_{12}\psi(\eta - \zeta) + \phi\big(g_{16} - \sqrt{\zeta}g_5 g_{12}\sqrt{n_0}\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big) + \zeta g_{10}g_{12}\psi\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\end{aligned} \tag{S164y}$$

$$\begin{aligned}0 &= g_{13}n_0\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_9\big)\big) - \sqrt{\zeta}g_4\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + \sqrt{\zeta}g_5 g_{12}n_0^{3/2}\phi\big(\sigma_{W_2}^2(\zeta - \eta') - \gamma\big)\\&\quad \big(g_{16}n_0 + g_{12}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big)\big) + \zeta g_{10}\psi\big(g_6 n_0\sigma_{W_2}^2 + g_{12}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) - \zeta g_9\sigma_{W_2}^4\big)\end{aligned} \tag{S164z}$$

$$\begin{aligned}0 &= -\gamma\sqrt{\zeta}g_2 g_{12}n_0^{3/2}\phi + \gamma g_7 n_0\psi\phi - \sqrt{\zeta}g_4\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big(g_{16}n_0 + g_{12}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big)\big)\\&\quad + \zeta g_3\psi\big(g_6 n_0\sigma_{W_2}^2 + g_{12}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) - \zeta g_9\sigma_{W_2}^4\big) + \zeta^{3/2}g_2 g_{12}n_0^{3/2}\phi\sigma_{W_2}^2 - \zeta^2 g_9\psi\sigma_{W_2}^4\\&\quad + n_0\phi\eta'\sigma_{W_2}^2\big(g_7\psi - \sqrt{\zeta}g_2 g_{12}\sqrt{n_0}\big) + \zeta g_6 n_0\psi\sigma_{W_2}^2 + \zeta g_7 g_9 n_0\psi\sigma_{W_2}^2 - \zeta g_7 n_0\psi\phi\sigma_{W_2}^2\end{aligned} \tag{S164aa}$$

After some straightforward algebra, one can eliminate all g_i except for g_4 and g_9, which satisfy coupled polynomial equations. Those equations can be shown to be identical to eqn. (S66) by invoking the change of variables,

$$g_4 = -\frac{\sqrt{\zeta}\psi}{\sqrt{n_0}\phi}\tau_2\,, \quad \text{and} \quad g_9 = \big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\tau_1\,. \tag{S165}$$

In terms of τ_1, τ_2, and τ_2' (S88), the error E_{32} is given by,

$$E_{32} = 1 - 2\tau_2/\tau_1 - \tau_2'/\tau_1^2\,. \tag{S166}$$

S5.3.5 E_{33}

The equations satisfied by the operator-valued Stieltjes transform G of $\bar{Q}_{32}$ induce the following structure on G,

$$G = \begin{pmatrix} 0 & G_{12} \\ G_{12}^\top & 0 \end{pmatrix}\,, \tag{S167}$$

where,

$$G_{12} = \begin{pmatrix} g_{13} & 0 & 0 & 0 & 0 & 0 & 0 & g_8 & 0 & 0 & 0 \\ 0 & g_1 & 0 & 0 & g_5 & 0 & 0 & 0 & g_{11} & g_3 & 0 \\ 0 & 0 & g_1 & g_4 & 0 & g_6 & g_9 & 0 & 0 & 0 & g_2 \\ 0 & 0 & 0 & g_{14} & 0 & g_6 & g_{17} & 0 & 0 & 0 & g_7 \\ 0 & 0 & 0 & 0 & g_{16} & 0 & 0 & 0 & g_{20} & g_{12} & 0 \\ 0 & 0 & 0 & g_{19} & 0 & g_{15} & g_{18} & 0 & 0 & 0 & g_{10} \\ 0 & 0 & 0 & 0 & 0 & 0 & g_{14} & 0 & 0 & 0 & g_6 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_{13} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_1 & g_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_{16} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & g_{19} & 0 & 0 & 0 & g_{15} \end{pmatrix}, \tag{S168}$$

and the independent entry-wise component functions g_i give the error E_{32} through the relation,

$$E_{33} = -g_3 n_0 \sigma_{W_2}^2/\psi\,, \tag{S169}$$

and themselves satisfy the following system of polynomial equations,

$$0 = \sqrt{\zeta} g_{14} g_{16} \sqrt{n_0} - g_{19}\psi \tag{S170a}$$
$$0 = \sqrt{\zeta} g_6 g_{16} \sqrt{n_0} - g_{15}\psi + \psi \tag{S170b}$$
$$0 = -\sqrt{\zeta} g_{13} g_{14}\psi - g_6\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S170c}$$
$$0 = -\sqrt{\zeta} g_{13} g_{19}\psi - \big(g_{15} - 1\big)\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S170d}$$
$$0 = -\sqrt{\zeta} g_{13}\psi - \sqrt{\zeta} g_4 g_{13}\psi - g_6\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S170e}$$
$$0 = -\sqrt{\zeta} g_8 g_{14}\psi - \sqrt{\zeta} g_{13} g_{17}\psi - g_7\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S170f}$$
$$0 = -\sqrt{\zeta} g_{13} g_{18}\psi - \sqrt{\zeta} g_8 g_{19}\psi - g_{10}\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S170g}$$
$$0 = g_{13} g_{16}\psi(\zeta - \eta) - \phi\big(g_5 - \sqrt{\zeta} g_6 g_{16}\sqrt{n_0}\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S170h}$$
$$0 = g_6\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_{13}\big(\sqrt{\zeta} g_{15}\psi + \zeta g_6\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S170i}$$
$$0 = g_4\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_{13}\big(\sqrt{\zeta} g_{19}\psi + \zeta g_{14}\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S170j}$$
$$0 = \big(g_{14} - 1\big)\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_{13}\big(\sqrt{\zeta} g_{19}\psi + \zeta g_{14}\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S170k}$$
$$0 = -\sqrt{\zeta}\big(\big(g_4 + 1\big)g_8 + g_9 g_{13}\big)\psi - \gamma g_2\sqrt{n_0}\phi + \zeta g_2\sqrt{n_0}\phi\sigma_{W_2}^2 + g_2\sqrt{n_0}(-\phi)\eta'\sigma_{W_2}^2 \tag{S170l}$$
$$0 = \sqrt{\zeta} g_{15} g_{16}\sqrt{n_0}\phi\big(\sigma_{W_2}^2(\zeta - \eta') - \gamma\big) + g_{19}\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_{13}\big)\big) \tag{S170m}$$
$$0 = g_{16}\big(g_{13}\psi(\zeta - \eta) + \phi\big(\sqrt{\zeta} g_6\sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big) + \phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S170n}$$
$$0 = g_{13}\big(\sqrt{\zeta} g_{19}\psi + \sqrt{n_0}\big(\gamma + g_{16}(\eta - \zeta) + \sigma_{W_2}^2\big(\eta' + \zeta\big(g_{14} - 1\big)\big)\big)\big) - \sqrt{n_0}\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S170o}$$
$$0 = g_{14}\psi\big(\gamma\phi + \sigma_{W_2}^2\big(\phi(\eta' - \zeta) + \zeta g_{13}\big)\big) - \phi\big(\sqrt{\zeta} g_6 g_{16}\sqrt{n_0} + \psi\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S170p}$$
$$0 = -\sqrt{\zeta} g_6 g_{16}\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_4\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_{13}\big)\big) + \zeta g_{13}\psi\sigma_{W_2}^2 \tag{S170q}$$
$$0 = \sqrt{\zeta}\big(g_7 g_{16} + g_6\big(g_{12} + g_{20}\big)\big)n_0 + g_{10}\sqrt{n_0}(-\psi) + \sqrt{\zeta} g_6\big(\psi(\zeta - \eta) - \zeta\sigma_{W_2}^2\big) + \sqrt{\zeta} g_5 g_6\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big) \tag{S170r}$$
$$0 = \sqrt{\zeta}\big(g_{16} g_{17} + g_{14}\big(g_{12} + g_{20}\big)\big)n_0 + g_{18}\sqrt{n_0}(-\psi) + \sqrt{\zeta} g_{14}\big(\psi(\zeta - \eta) - \zeta\sigma_{W_2}^2\big) + \sqrt{\zeta} g_5 g_{14}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big) \tag{S170s}$$
$$0 = g_{13}\psi(\zeta - \eta) + g_5\big(g_{13}\psi(\zeta - \eta) + \phi\big(\sqrt{\zeta} g_6\sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big) + \sqrt{\zeta} g_6\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S170t}$$
$$0 = g_9 n_0\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_8\big(\sqrt{\zeta} g_{19}\sqrt{n_0}\psi + \zeta g_{14} n_0\sigma_{W_2}^2\big) + g_{13}\big(\sqrt{\zeta} g_{18}\sqrt{n_0}\psi + \zeta\sigma_{W_2}^2\big(g_{17} n_0 - \zeta g_{14}\sigma_{W_2}^2\big)\big) \tag{S170u}$$
$$\begin{aligned} 0 = {} & \gamma g_2 n_0\phi + \sqrt{\zeta} g_{10} g_{13}\sqrt{n_0}\psi + g_8\big(\sqrt{\zeta} g_{15}\sqrt{n_0}\psi + \zeta g_6 n_0\sigma_{W_2}^2\big) - \zeta g_2 n_0\phi\sigma_{W_2}^2 \\ & + \zeta g_7 g_{13} n_0\sigma_{W_2}^2 + g_2 n_0\phi\eta'\sigma_{W_2}^2 - \zeta^2 g_6 g_{13}\sigma_{W_2}^4 \end{aligned} \tag{S170v}$$

$$
\begin{aligned}
0 &= g_{13}g_{16}\psi(-(\zeta-\eta))\big(\psi(\zeta-\eta)-\zeta\sigma_{W_2}^2\big) \\
&\quad -\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)\big(-\zeta g_{14}g_{16}\psi+\sqrt{\zeta}g_6g_{16}\sqrt{n_0}\big(\zeta\psi-\eta\psi-\zeta\sigma_{W_2}^2\big)-g_{20}n_0\big) \qquad \text{(S170w)}
\end{aligned}
$$

$$
\begin{aligned}
0 &= -\sqrt{\zeta}\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)\big(g_6\sqrt{n_0}\big(\zeta\psi-\eta\psi-\zeta\sigma_{W_2}^2\big)-\sqrt{\zeta}g_{14}\psi\big)+g_{20}n_0\big(g_{13}\psi(\eta-\zeta) \\
&\quad -\phi\big(\sqrt{\zeta}g_6\sqrt{n_0}-1\big)\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)\big)+g_{13}\psi(-(\zeta-\eta))\big(\psi(\zeta-\eta)-\zeta\sigma_{W_2}^2\big) \qquad \text{(S170x)}
\end{aligned}
$$

$$
\begin{aligned}
0 &= \big(\psi(\zeta-\eta)-\zeta\sigma_{W_2}^2\big)\big(g_{13}\psi(\eta-\zeta)+\sqrt{\zeta}g_6\sqrt{n_0}\phi\big(\sigma_{W_2}^2\big(\zeta-\eta'\big)-\gamma\big)\big)+n_0\big(g_{13}g_{20}\psi(\eta-\zeta) \\
&\quad +\phi\big(g_{11}-\sqrt{\zeta}g_6g_{20}\sqrt{n_0}\big)\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)\big)+\zeta g_4\psi\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) \qquad \text{(S170y)}
\end{aligned}
$$

$$
\begin{aligned}
0 &= \gamma g_7n_0\phi+\sqrt{\zeta}g_{10}g_{13}\sqrt{n_0}\psi+\sqrt{\zeta}g_8g_{15}\sqrt{n_0}\psi-\zeta g_7n_0\phi\sigma_{W_2}^2+\zeta g_6g_8n_0\sigma_{W_2}^2+\zeta g_7g_{13}n_0\sigma_{W_2}^2+g_7n_0\phi\eta'\sigma_{W_2}^2 \\
&\quad +\zeta g_6\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)+\zeta g_5g_6\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)-\zeta^2g_6g_{13}\sigma_{W_2}^4 \qquad \text{(S170z)}
\end{aligned}
$$

$$
\begin{aligned}
0 &= \gamma g_{17}n_0\phi+\sqrt{\zeta}g_{13}g_{18}\sqrt{n_0}\psi+\sqrt{\zeta}g_8g_{19}\sqrt{n_0}\psi-\zeta g_{17}n_0\phi\sigma_{W_2}^2+\zeta g_8g_{14}n_0\sigma_{W_2}^2+\zeta g_{13}g_{17}n_0\sigma_{W_2}^2+g_{17}n_0\phi\eta'\sigma_{W_2}^2 \\
&\quad +\zeta g_{14}\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)+\zeta g_5g_{14}\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)-\zeta^2g_{13}g_{14}\sigma_{W_2}^4 \qquad \text{(S170aa)}
\end{aligned}
$$

$$
\begin{aligned}
0 &= g_5\big(\psi(\zeta-\eta)-\zeta\sigma_{W_2}^2\big)\big(g_{13}\psi(\eta-\zeta)+\sqrt{\zeta}g_6\sqrt{n_0}\phi\big(\sigma_{W_2}^2\big(\zeta-\eta'\big)-\gamma\big)\big)+n_0\big(\phi\big(g_3-\sqrt{\zeta}\big(g_6g_{12}+g_2g_{16}\big)\sqrt{n_0}\big) \\
&\quad \big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)-\big(g_{12}g_{13}+g_8g_{16}\big)\psi(\zeta-\eta)\big)+\zeta g_4g_5\psi\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) \qquad \text{(S170ab)}
\end{aligned}
$$

$$
\begin{aligned}
0 &= \big(\psi(\zeta-\eta)-\zeta\sigma_{W_2}^2\big)\big(g_{13}\psi(\eta-\zeta)+\sqrt{\zeta}g_6\sqrt{n_0}\phi\big(\sigma_{W_2}^2\big(\zeta-\eta'\big)-\gamma\big)\big)+g_5\big(g_{13}\psi(-(\zeta-\eta))\big(\psi(\zeta-\eta)-\zeta\sigma_{W_2}^2\big) \\
&\quad -\sqrt{\zeta}\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)\big(g_6\sqrt{n_0}\big(\zeta\psi-\eta\psi-\zeta\sigma_{W_2}^2\big)-\sqrt{\zeta}g_{14}\psi\big)\big)+g_{11}n_0\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) \\
&\quad +\zeta g_4\psi\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) \qquad \text{(S170ac)}
\end{aligned}
$$

$$
\begin{aligned}
0 &= g_{12}n_0\big(g_{13}\psi(\eta-\zeta)-\phi\big(\sqrt{\zeta}g_6\sqrt{n_0}-1\big)\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)\big)-g_{16}\big(g_8n_0\psi(\zeta-\eta)+\sqrt{\zeta}g_7n_0^{3/2}\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) \\
&\quad +\zeta g_{13}\psi(\zeta-\eta)\sigma_{W_2}^2\big)+g_5\big(g_{13}\psi(-(\zeta-\eta))\big(\psi(\zeta-\eta)-\zeta\sigma_{W_2}^2\big) \\
&\quad -\sqrt{\zeta}\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)\big(g_6\sqrt{n_0}\big(\zeta\psi-\eta\psi-\zeta\sigma_{W_2}^2\big)-\sqrt{\zeta}g_{14}\psi\big)\big) \qquad \text{(S170ad)}
\end{aligned}
$$

$$
\begin{aligned}
0 &= \gamma\sqrt{\zeta}g_7g_{16}n_0^{3/2}\phi+\gamma\sqrt{\zeta}g_6g_{20}n_0^{3/2}\phi+g_8g_{16}n_0\psi(\zeta-\eta)+\zeta g_{13}g_{20}n_0\psi-\eta g_{13}g_{20}n_0\psi \\
&\quad +g_{12}n_0\big(g_{13}\psi(\zeta-\eta)+\phi\big(\sqrt{\zeta}g_6\sqrt{n_0}-1\big)\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)\big)-\zeta^{3/2}g_7g_{16}n_0^{3/2}\phi\sigma_{W_2}^2-\zeta^{3/2}g_6g_{20}n_0^{3/2}\phi\sigma_{W_2}^2 \\
&\quad +\sqrt{\zeta}\big(g_7g_{16}+g_6g_{20}\big)n_0^{3/2}\phi\eta'\sigma_{W_2}^2+\zeta^2g_{13}g_{16}\psi\sigma_{W_2}^2-\zeta\eta g_{13}g_{16}\psi\sigma_{W_2}^2 \qquad \text{(S170ae)}
\end{aligned}
$$

$$
\begin{aligned}
0 &= -\gamma g_8n_0-\sqrt{\zeta}g_{13}g_{18}\sqrt{n_0}\psi-\sqrt{\zeta}g_8g_{19}\sqrt{n_0}\psi+\zeta g_{12}g_{13}n_0+\zeta g_8g_{16}n_0+\zeta g_{13}g_{20}n_0-\eta g_{12}g_{13}n_0 \\
&\quad -\eta g_8g_{16}n_0-\eta g_{13}g_{20}n_0+\zeta g_8n_0\sigma_{W_2}^2-\zeta g_8g_{14}n_0\sigma_{W_2}^2-\zeta g_{13}g_{17}n_0\sigma_{W_2}^2-g_8n_0\eta'\sigma_{W_2}^2+\zeta^2g_{13}g_{14}\sigma_{W_2}^4 \\
&\quad +\zeta^2g_{13}g_{16}\sigma_{W_2}^2+g_{13}(\zeta-\eta)\big(\psi(\zeta-\eta)-\zeta\sigma_{W_2}^2\big)+g_5g_{13}(\zeta-\eta)\big(\zeta\psi-\eta\psi-\zeta\sigma_{W_2}^2\big)-\zeta\eta g_{13}g_{16}\sigma_{W_2}^2 \qquad \text{(S170af)}
\end{aligned}
$$

$$
\begin{aligned}
0 &= \gamma\sqrt{\zeta}g_5g_7n_0^{3/2}\phi+\gamma\sqrt{\zeta}g_6g_{11}n_0^{3/2}\phi+\zeta g_5g_8n_0\psi+\zeta g_{11}g_{13}n_0\psi-\eta g_5g_8n_0\psi-\eta g_{11}g_{13}n_0\psi \\
&\quad +g_3n_0\big(g_{13}\psi(\zeta-\eta)+\phi\big(\sqrt{\zeta}g_6\sqrt{n_0}-1\big)\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)\big)+n_0\big(g_8\psi(\zeta-\eta) \\
&\quad +\sqrt{\zeta}g_2\sqrt{n_0}\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)\big)-\zeta^{3/2}g_5g_7n_0^{3/2}\phi\sigma_{W_2}^2-\zeta^{3/2}g_6g_{11}n_0^{3/2}\phi\sigma_{W_2}^2+\sqrt{\zeta}g_5g_7n_0^{3/2}\phi\eta'\sigma_{W_2}^2 \\
&\quad +\sqrt{\zeta}g_6g_{11}n_0^{3/2}\phi\eta'\sigma_{W_2}^2+\zeta^2g_5g_{13}\psi\sigma_{W_2}^2-\zeta\eta g_5g_{13}\psi\sigma_{W_2}^2 \qquad \text{(S170ag)}
\end{aligned}
$$

$$
\begin{aligned}
0 &= -\sqrt{\zeta}g_6\sqrt{n_0}\phi\big(\psi(\zeta-\eta)-\zeta\sigma_{W_2}^2\big)\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)-\sqrt{\zeta}g_5g_6\sqrt{n_0}\phi\big(\psi(\zeta-\eta)-\zeta\sigma_{W_2}^2\big)\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) \\
&\quad +g_9n_0\psi\big(\gamma\phi+\sigma_{W_2}^2\big(\phi\big(\eta'-\zeta\big)+\zeta g_{13}\big)\big)+\zeta g_4\psi\big(g_8n_0\sigma_{W_2}^2+g_5\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)-\zeta g_{13}\sigma_{W_2}^4\big) \\
&\quad -\sqrt{\zeta}\big(g_2g_{16}+g_6\big(g_{12}+g_{20}\big)\big)n_0^{3/2}\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)+\zeta\psi\sigma_{W_2}^2\big(g_8n_0-\zeta g_{13}\sigma_{W_2}^2\big) \\
&\quad +\zeta g_4\psi\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) \qquad \text{(S170ah)}
\end{aligned}
$$

$$
\begin{aligned}
0 &= -\gamma\sqrt{\zeta}g_6g_{12}n_0^{3/2}\phi-\gamma\sqrt{\zeta}g_7g_{16}n_0^{3/2}\phi-\gamma\sqrt{\zeta}g_6g_{20}n_0^{3/2}\phi+\gamma g_{17}n_0\psi\phi-\sqrt{\zeta}\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) \\
&\quad \big(g_6\sqrt{n_0}\big(\zeta\psi-\eta\psi-\zeta\sigma_{W_2}^2\big)-\sqrt{\zeta}g_{14}\psi\big)-\sqrt{\zeta}g_5\phi\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)\big(g_6\sqrt{n_0}\big(\zeta\psi-\eta\psi-\zeta\sigma_{W_2}^2\big)-\sqrt{\zeta}g_{14}\psi\big) \\
&\quad +\zeta^{3/2}g_6g_{12}n_0^{3/2}\phi\sigma_{W_2}^2+\zeta^{3/2}g_7g_{16}n_0^{3/2}\phi\sigma_{W_2}^2+\zeta^{3/2}g_6g_{20}n_0^{3/2}\phi\sigma_{W_2}^2-n_0\phi\eta'\sigma_{W_2}^2\big(\sqrt{\zeta}\big(g_7g_{16}+g_6\big(g_{12}+g_{20}\big)\big)\sqrt{n_0}
\end{aligned}
$$

$$- g_{17}\psi\big) + \zeta g_8 g_{14} n_0 \psi \sigma_{W_2}^2 + \zeta g_{13} g_{17} n_0 \psi \sigma_{W_2}^2 - \zeta g_{17} n_0 \psi \phi \sigma_{W_2}^2 - \zeta^2 g_{13} g_{14} \psi \sigma_{W_2}^4 \tag{S170ai}$$

$$0 = -\gamma\sqrt{\zeta} g_{12} g_{15} n_0^{3/2}\phi - \gamma\sqrt{\zeta} g_{10} g_{16} n_0^{3/2}\phi - \gamma\sqrt{\zeta} g_{15} g_{20} n_0^{3/2} + \gamma g_{18} n_0 \psi\phi - \sqrt{\zeta}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)$$
$$\big(g_{15}\sqrt{n_0}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big) - \sqrt{\zeta} g_{19}\psi\big) - \sqrt{\zeta} g_5 \phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big(g_{15}\sqrt{n_0}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big) - \zeta g_{18} n_0 \psi\phi\sigma_{W_2}^2$$
$$- \sqrt{\zeta} g_{19}\psi\big) + \zeta^{3/2} g_{12} g_{15} n_0^{3/2}\phi\sigma_{W_2}^2 + \zeta^{3/2} g_{10} g_{16} n_0^{3/2}\phi\sigma_{W_2}^2 + \zeta^{3/2} g_{15} g_{20} n_0^{3/2}\phi\sigma_{W_2}^2 - \zeta^2 g_{13} g_{19}\psi\sigma_{W_2}^4$$
$$- n_0\phi\eta'\sigma_{W_2}^2\big(\sqrt{\zeta}\big(g_{10} g_{16} + g_{15}\big(g_{12} + g_{20}\big)\big)\sqrt{n_0} - g_{18}\psi\big) + \zeta g_{13} g_{18} n_0 \psi\sigma_{W_2}^2 + \zeta g_8 g_{19} n_0 \psi\sigma_{W_2}^2 \tag{S170aj}$$

After some straightforward algebra, one can eliminate all g_i except for g_6 and g_{13}, which satisfy coupled polynomial equations. Those equations can be shown to be identical to eqn. (S66) by invoking the change of variables,

$$g_6 = -\frac{\sqrt{\zeta}\psi}{\sqrt{n_0}\phi}\tau_2\,, \quad \text{and} \quad g_{13} = \big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\tau_1\,. \tag{S171}$$

In terms of τ_1, τ_2, and their derivatives τ_1' (S87), τ_2' (S88), the error E_{33} is given by,

$$E_{33} = \sigma_{W_2}^2\left[\left(\tau_1 + (\sigma_{W_2}^2(\eta' - \zeta) + \gamma)\tau_1' + \sigma_{W_2}^2\zeta\tau_2'\right)/\tau_1^2 - \eta\right] - E_{22}\,. \tag{S172}$$

S6 Exact asymptotics for bias and variance terms

Following Sec. S1, for each random variable in question we introduce an iid copy of it denoted by a tilde. Using this simplifying notation and recalling $P = \{W_1, W_2\}$ we have,

$$B = \mathbb{E}_{(\mathbf{x},y)}(y - \mathbb{E}_{(P,X,\varepsilon)}\hat{y}(\mathbf{x}; P, X, \varepsilon))^2 \tag{S173}$$
$$= \mathbb{E}_{(\mathbf{x},y)}\mathbb{E}_{(P,X,\varepsilon)}\mathbb{E}_{(\tilde{P},\tilde{X},\tilde{\varepsilon})}(y - \hat{y}(\mathbf{x}; P, X, \varepsilon))(y - \hat{y}(\mathbf{x}; \tilde{P}, \tilde{X}, \tilde{\varepsilon})) \tag{S174}$$
$$= 1 + E_{21} + H_{000}\,, \tag{S175}$$

where E_{21} was computed previously and H_{000} and the other H_{ijk}(also defined above) are,

$$H_{000} = \mathbb{E}\hat{y}(\mathbf{x}; P, X, \varepsilon)\hat{y}(\mathbf{x}; \tilde{P}, \tilde{X}, \tilde{\varepsilon}) \tag{S176}$$
$$H_{001} = \mathbb{E}\hat{y}(\mathbf{x}; P, X, \varepsilon)\hat{y}(\mathbf{x}; \tilde{P}, \tilde{X}, \varepsilon) \tag{S177}$$
$$H_{010} = \mathbb{E}\hat{y}(\mathbf{x}; P, X, \varepsilon)\hat{y}(\mathbf{x}; \tilde{P}, X, \tilde{\varepsilon}) \tag{S178}$$
$$H_{011} = \mathbb{E}\hat{y}(\mathbf{x}; P, X, \varepsilon)\hat{y}(\mathbf{x}; \tilde{P}, X, \varepsilon) \tag{S179}$$
$$H_{100} = \mathbb{E}\hat{y}(\mathbf{x}; P, X, \varepsilon)\hat{y}(\mathbf{x}; P, \tilde{X}, \tilde{\varepsilon}) \tag{S180}$$
$$H_{101} = \mathbb{E}\hat{y}(\mathbf{x}; P, X, \varepsilon)\hat{y}(\mathbf{x}; P, \tilde{X}, \varepsilon) \tag{S181}$$
$$H_{110} = \mathbb{E}\hat{y}(\mathbf{x}; P, X, \varepsilon)\hat{y}(\mathbf{x}; P, X, \tilde{\varepsilon}) \tag{S182}$$
$$H_{111} = \mathbb{E}\hat{y}(\mathbf{x}; P, X, \varepsilon)\hat{y}(\mathbf{x}; P, X, \varepsilon)\,, \tag{S183}$$

where the expectations are over $\mathbf{x}, P, X, \varepsilon, \tilde{P}, \tilde{X}$, and $\tilde{\varepsilon}$. Recalling the definition of $\hat{y}$,

$$\hat{y}(\mathbf{x}; P, X, \varepsilon) := N_0(\mathbf{x}; P) + (Y(X, \epsilon) - N_0(X; P))K(X, X; P)^{-1}K(X, \mathbf{x}; P) \tag{S184}$$

and the techniques described in the previous section, it is straightforward to analyze each of the above terms, which we do in the following subsections. To aid those calculations, we first note that, similar to above, we can write,

$$\mathbb{E}_{\mathbf{x}}K(X, \mathbf{x}; P)K(\mathbf{x}, \tilde{X}; \tilde{P}) = \frac{\sigma_{W_2}^4\zeta^2}{n_0^2}X^\top\tilde{X} + \frac{\sigma_{W_2}^2\zeta^{3/2}}{n_0^{3/2}n_1}(X^\top W_1^T\tilde{F} + F^\top\tilde{W}_1\tilde{X}) + \frac{\zeta}{n_0 n_1^2}F^\top W_1\tilde{W}_1^\top\tilde{F} \tag{S185}$$
$$= (\frac{\sigma_{W_2}^2\zeta}{n_0}X^\top + \frac{\zeta}{\sqrt{n_0}n_1}F^\top W_1)(\frac{\sigma_{W_2}^2\zeta}{n_0}\tilde{X}^\top + \frac{\sqrt{\zeta}}{\sqrt{n_0}n_1}\tilde{F}^\top\tilde{W}_1)^\top \tag{S186}$$

$$\mathbb{E}_{\mathbf{x}} K(X,\mathbf{x};P)K(\mathbf{x},X;\tilde{P}) = (\frac{\sigma_{W_2}^2\zeta}{n_0}X^\top + \frac{\zeta}{\sqrt{n_0}n_1}F^\top W_1)(\frac{\sigma_{W_2}^2\zeta}{n_0}X^\top + \frac{\sqrt{\zeta}}{\sqrt{n_0}n_1}f(\tilde{W}_1 X)^\top \tilde{W}_1)^\top \tag{S187}$$

$$\mathbb{E}_{\mathbf{x}} K(X,\mathbf{x};P)K(\mathbf{x},\tilde{X};P) = (\frac{\sigma_{W_2}^2\zeta}{n_0}X^\top + \frac{\zeta}{\sqrt{n_0}n_1}F^\top W_1)(\frac{\sigma_{W_2}^2\zeta}{n_0}\tilde{X}^\top + \frac{\sqrt{\zeta}}{\sqrt{n_0}n_1}f(W_1\tilde{X})^\top W_1)^\top + \frac{\eta-\zeta}{n_1^2}F^\top f(W_1\tilde{X}) \tag{S188}$$

S6.1 H_{000}

$$\begin{aligned}
H_{000} &= \mathbb{E}\hat{y}(\mathbf{x};P,X,\varepsilon)\hat{y}(\mathbf{x};\tilde{P},\tilde{X},\tilde{\varepsilon}) && \text{(S189)}\\
&= \mathbb{E}K(\mathbf{x},\tilde{X};\tilde{P})K(\tilde{X},\tilde{X};\tilde{P})^{-1}Y(\tilde{X},\tilde{\varepsilon})^\top Y(X,\varepsilon)K(X,X;P)^{-1}K(X,\mathbf{x};P) && \text{(S190)}\\
&= \mathbb{E}\,\mathrm{tr}\left(K(\tilde{X},\tilde{X};\tilde{P})^{-1}\tilde{X}^\top X K(X,X;P)^{-1}K(X,\mathbf{x};P)K(\mathbf{x},\tilde{X};\tilde{P})\right) && \text{(S191)}\\
&= \mathbb{E}\,\mathrm{tr}\left(K(\tilde{X},\tilde{X};\tilde{P})^{-1}\tilde{X}^\top X K(X,X;P)^{-1}(\frac{\sigma_{W_2}^2\zeta}{n_0}X^\top + \frac{\sqrt{\zeta}}{\sqrt{n_0}n_1}F^\top W_1)(\frac{\sigma_{W_2}^2\zeta}{n_0}\tilde{X}^\top + \frac{\sqrt{\zeta}}{\sqrt{n_0}n_1}\tilde{F}^\top\tilde{W}_1)^\top\right) && \text{(S192)}\\
&= \mathrm{tr}\left(XK^{-1}(\frac{\sigma_{W_2}^2\zeta}{n_0}X^\top + \frac{\sqrt{\zeta}}{\sqrt{n_0}n_1}F^\top W_1)\right)^2 && \text{(S193)}\\
&\equiv E_4 && \text{(S194)}
\end{aligned}$$

A linear pencil for E_4 follows from the representation,

$$E_4 = \mathrm{tr}(U_4^T Q_4^{-1} V_4)^2\,, \tag{S195}$$

where,

$$U_4^T = \begin{pmatrix} 0 & \frac{\zeta I_{n_0}\sigma_{W_2}^2}{n_0} & 0 & 0 & \frac{\sqrt{\zeta}I_m}{\sqrt{n_0}n_1}\end{pmatrix}\,,\quad V_4^T = \begin{pmatrix} 0 & -\frac{n_0 I_{n_0}}{\zeta\sigma_{W_2}^2} & 0 & 0 & \frac{\sqrt{n_0}n_1 I_m}{\sqrt{\zeta}}\end{pmatrix} \tag{S196}$$

and,

$$Q_4 = \begin{pmatrix}
I_m\big(\gamma+\sigma_{W_2}^2(\eta'-\zeta)\big) & \frac{\zeta X^\top\sigma_{W_2}^2}{n_0} & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} & 0\\
-X & I_{n_0} & 0 & 0 & 0\\
-\sqrt{\eta-\zeta}\Theta_F & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & I_{n_1} & 0 & 0\\
0 & 0 & -W_1^\top & I_{n_0} & 0\\
0 & 0 & 0 & 0 & I_m
\end{pmatrix}. \tag{S197}$$

The equations satisfied by the operator-valued Stieltjes transform G of $\bar{Q}_4$ induce the following structure on G,

$$G = \begin{pmatrix} 0 & G_{12}\\ G_{12}^\top & 0\end{pmatrix}\,, \tag{S198}$$

where,

$$G_{12} = \begin{pmatrix}
g_3 & 0 & 0 & 0 & 0\\
0 & g_4 & 0 & g_2 & 0\\
0 & 0 & g_6 & 0 & 0\\
0 & g_7 & 0 & g_5 & 0\\
0 & 0 & 0 & 0 & g_1
\end{pmatrix}\,, \tag{S199}$$

and the independent entry-wise component functions g_i give the error E_4 through the relation,

$$E_4 = (g_1 - g_4)^2\,, \tag{S200}$$

and themselves satisfy the following system of polynomial equations,

$$0 = 1 - g_1 \tag{S201a}$$

$$0 = \sqrt{\zeta} g_4 g_6 \sqrt{n_0} - g_7 \psi \tag{S201b}$$

$$0 = \sqrt{\zeta} g_2 g_6 \sqrt{n_0} - g_5 \psi + \psi \tag{S201c}$$

$$0 = -\sqrt{\zeta} g_3 g_4 \psi - g_2 \sqrt{n_0} \phi \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) \tag{S201d}$$

$$0 = -\sqrt{\zeta} g_3 g_7 \psi - (g_5 - 1) \sqrt{n_0} \phi \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) \tag{S201e}$$

$$0 = g_2 \sqrt{n_0} \phi \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) + g_3 \big(\sqrt{\zeta} g_5 \psi + \zeta g_2 \sqrt{n_0} \sigma_{W_2}^2\big) \tag{S201f}$$

$$0 = (g_4 - 1) \sqrt{n_0} \phi \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) + g_3 \big(\sqrt{\zeta} g_7 \psi + \zeta g_4 \sqrt{n_0} \sigma_{W_2}^2\big) \tag{S201g}$$

$$0 = \sqrt{\zeta} g_5 g_6 \sqrt{n_0} \phi \big(\sigma_{W_2}^2 (\zeta - \eta') - \gamma\big) + g_7 \psi \big(\gamma \phi + \sigma_{W_2}^2 \big(-\zeta \phi + \phi \eta' + \zeta g_3\big)\big) \tag{S201h}$$

$$0 = g_6 \big(g_3 \psi (\zeta - \eta) + \phi \big(\sqrt{\zeta} g_2 \sqrt{n_0} - 1\big) \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big)\big) + \phi \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) \tag{S201i}$$

$$0 = g_3 \big(\sqrt{\zeta} g_7 \psi + \sqrt{n_0} \big(\gamma + g_6 (\eta - \zeta) + \sigma_{W_2}^2 \big(\eta' + \zeta (g_4 - 1)\big)\big)\big) - \sqrt{n_0} \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) \tag{S201j}$$

$$0 = g_4 \psi \big(\gamma \phi + \sigma_{W_2}^2 \big(-\zeta \phi + \phi \eta' + \zeta g_3\big)\big) - \phi \big(\sqrt{\zeta} g_2 g_6 \sqrt{n_0} + \psi\big) \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) \tag{S201k}$$

After some straightforward algebra, one can eliminate all g_i except for g_2 and g_3, which satisfy coupled polynomial equations. Those equations can be shown to be identical to eqn. (S66) by invoking the change of variables,

$$g_2 = -\frac{\sqrt{\zeta}\psi}{\sqrt{n_0}\phi} \tau_2 \,, \quad \text{and} \quad g_3 = \big(\gamma + \sigma_{W_2}^2 (\eta' - \zeta)\big) \tau_1 \,. \tag{S201l}$$

In terms of the related variables defined in eqn. (S89), the error E_4 is given by,

$$E_4 = \tilde{\tau}_2^2 \,. \tag{S201m}$$

S6.2 H_{001}

$$\begin{aligned}
H_{001} &= \mathbb{E} \hat{y}(\mathbf{x}; P, X, \varepsilon) \hat{y}(\mathbf{x}; \tilde{P}, \tilde{X}, \varepsilon) && \text{(S202)}\\
&= \mathbb{E} K(\mathbf{x}, \tilde{X}; \tilde{P}) K(\tilde{X}, \tilde{X}; \tilde{P})^{-1} Y(\tilde{X}, \varepsilon)^\top Y(X, \varepsilon) K(X, X; P)^{-1} K(X, \mathbf{x}; P) && \text{(S203)}\\
&= \mathbb{E} \operatorname{tr} \big(K(\tilde{X}, \tilde{X}; \tilde{P})^{-1} \tilde{X}^\top X K(X, X; P)^{-1} K(X, \mathbf{x}; P) K(\mathbf{x}, \tilde{X}; \tilde{P})\big) && \text{(S204)}\\
&= H_{000} && \text{(S205)}
\end{aligned}$$

S6.3 H_{010}

$$\begin{aligned}
H_{010} &= \mathbb{E} \hat{y}(\mathbf{x}; P, X, \varepsilon) \hat{y}(\mathbf{x}; \tilde{P}, X, \tilde{\varepsilon}) && \text{(S206)}\\
&= \mathbb{E} K(\mathbf{x}, X; \tilde{P}) K(X, X; \tilde{P})^{-1} Y(X, \tilde{\varepsilon})^\top Y(X, \varepsilon) K(X, X; P)^{-1} K(X, \mathbf{x}; P) && \text{(S207)}\\
&= \mathbb{E} \operatorname{tr} \big(K(X, X; \tilde{P})^{-1} X^\top X K(X, X; P)^{-1} K(X, \mathbf{x}; P) K(\mathbf{x}, X; \tilde{P})\big) && \text{(S208)}\\
&= \mathbb{E} \operatorname{tr} \Big(K(X, X; \tilde{P})^{-1} X^\top X K(X, X; P)^{-1} K(X, \mathbf{x}; P) K(\mathbf{x}, X; \tilde{P}) && \text{(S209)}\\
&\qquad \times \big(\frac{\sigma_{W_2}^2 \zeta}{n_0} X^\top + \frac{\zeta}{\sqrt{n_0} n_1} F^\top W_1\big) \big(\frac{\sigma_{W_2}^2 \zeta}{n_0} X^\top + \frac{\sqrt{\zeta}}{\sqrt{n_0} n_1} f(\tilde{W}_1 X)^\top \tilde{W}_1\big)^\top \Big) && \text{(S210)}\\
&\equiv E_5 \,. && \text{(S211)}
\end{aligned}$$

A linear pencil for E_5 follows from the representation,

$$E_5 = \operatorname{tr}(U_5^T Q_5^{-1} V_5) \,, \tag{S212}$$

where,

$$U_5^T = \begin{pmatrix} 0 & \frac{I_{n_0}}{m} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad V_5^T = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{n_0} n_1 I_{n_0}}{\sqrt{\zeta}} \end{pmatrix} \tag{S213}$$

and,

$$Q_5 = \begin{pmatrix}
I_m\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) & 0 & \frac{\zeta X^\top \sigma_{W_2}^2}{n_0} & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} & -\frac{\zeta^2 m X^\top \sigma_{W_2}^4}{n_0^2} & 0 & 0 & 0 \\
-X & I_{n_0} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-X & 0 & I_{n_0} & 0 & 0 & 0 & 0 & \frac{\sqrt{\zeta}m\tilde{W}_1^\top}{\sqrt{n_0}n_1} & 0 \\
-\sqrt{\eta-\zeta}\Theta_F & 0 & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & I_{n_1} & 0 & \frac{\zeta^{3/2} m W_1 \sigma_{W_2}^2}{n_0^{3/2}} & 0 & 0 & 0 \\
0 & 0 & 0 & -W_1^\top & I_{n_0} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & I_{n_0} & -X & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{\zeta X^\top \sigma_{W_2}^2}{n_0} & I_m\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) & \frac{\sqrt{\eta-\zeta}\tilde{\Theta}_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} \\
0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{\zeta}\tilde{W}_1}{\sqrt{n_0}} & -\sqrt{\eta-\zeta}\tilde{\Theta}_F & I_{n_1} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -\tilde{W}_1^\top & I_{n_0}
\end{pmatrix}. \tag{S214}$$

The equations satisfied by the operator-valued Stieltjes transform G of $\bar{Q}_5$ induce the following structure on G,

$$G = \begin{pmatrix} 0 & G_{12} \\ G_{12}^\top & 0 \end{pmatrix}, \tag{S215}$$

where,

$$G_{12} = \begin{pmatrix}
g_9 & 0 & 0 & 0 & 0 & 0 & g_6 & 0 & 0 \\
0 & g_1 & g_5 & 0 & g_8 & g_3 & 0 & 0 & g_2 \\
0 & 0 & g_{10} & 0 & g_8 & g_{13} & 0 & 0 & g_7 \\
0 & 0 & 0 & g_{12} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & g_{15} & 0 & g_{11} & g_{14} & 0 & 0 & g_4 \\
0 & 0 & 0 & 0 & 0 & g_{10} & 0 & 0 & g_8 \\
0 & 0 & 0 & 0 & 0 & 0 & g_9 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & g_{12} & 0 \\
0 & 0 & 0 & 0 & 0 & g_{15} & 0 & 0 & g_{11}
\end{pmatrix}, \tag{S216}$$

and the independent entry-wise component functions g_i give the error E_5 through the relation,

$$E_5 = -\frac{g_2\sqrt{n_0}\phi}{\sqrt{\zeta}\psi}, \tag{S217}$$

and themselves satisfy the following system of polynomial equations,

$$0 = 1 - g_1 \tag{S218a}$$
$$0 = \sqrt{\zeta}g_{10}g_{12}\sqrt{n_0} - g_{15}\psi \tag{S218b}$$
$$0 = \sqrt{\zeta}g_8 g_{12}\sqrt{n_0} - g_{11}\psi + \psi \tag{S218c}$$
$$0 = \sqrt{\zeta}g_{12}\sqrt{n_0}\big(g_7\phi - \zeta g_8\sigma_{W_2}^2\big) - g_4\psi\phi \tag{S218d}$$
$$0 = \sqrt{\zeta}g_{12}\sqrt{n_0}\big(g_{13}\phi - \zeta g_{10}\sigma_{W_2}^2\big) - g_{14}\psi\phi \tag{S218e}$$
$$0 = -\sqrt{\zeta}g_9 g_{10}\psi - g_8\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S218f}$$
$$0 = -\sqrt{\zeta}g_9 g_{15}\psi - \big(g_{11} - 1\big)\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S218g}$$
$$0 = -\sqrt{\zeta}g_1 g_9\psi - \sqrt{\zeta}g_5 g_9\psi - g_8\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S218h}$$
$$0 = -\sqrt{\zeta}g_6 g_{10}\psi - \sqrt{\zeta}g_9 g_{13}\psi - g_7\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S218i}$$

$$0 = -\sqrt{\zeta} g_9 g_{14} \psi - \sqrt{\zeta} g_6 g_{15} \psi - g_4 \sqrt{n_0} \phi\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) \tag{S218j}$$
$$0 = g_8 \sqrt{n_0} \phi\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) + g_9 \big(\sqrt{\zeta} g_{11} \psi + \zeta g_8 \sqrt{n_0} \sigma_{W_2}^2\big) \tag{S218k}$$
$$0 = g_5 \sqrt{n_0} \phi\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) + g_9 \big(\sqrt{\zeta} g_{15} \psi + \zeta g_{10} \sqrt{n_0} \sigma_{W_2}^2\big) \tag{S218l}$$
$$0 = \big(g_{10} - 1\big) \sqrt{n_0} \phi\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) + g_9 \big(\sqrt{\zeta} g_{15} \psi + \zeta g_{10} \sqrt{n_0} \sigma_{W_2}^2\big) \tag{S218m}$$
$$0 = -\sqrt{\zeta}\big(\big(g_1 + g_5\big) g_6 + g_3 g_9\big) \psi - \gamma g_2 \sqrt{n_0} \phi + \zeta g_2 \sqrt{n_0} \phi \sigma_{W_2}^2 + g_2 \sqrt{n_0} (-\phi) \eta' \sigma_{W_2}^2 \tag{S218n}$$
$$0 = \sqrt{\zeta} g_{11} g_{12} \sqrt{n_0} \phi\big(\sigma_{W_2}^2 \big(\zeta - \eta'\big) - \gamma\big) + g_{15} \psi\big(\gamma \phi + \sigma_{W_2}^2 \big(-\zeta \phi + \phi \eta' + \zeta g_9\big)\big) \tag{S218o}$$
$$0 = g_{12}\big(g_9 \psi(\zeta - \eta) + \phi\big(\sqrt{\zeta} g_8 \sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big)\big) + \phi\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) \tag{S218p}$$
$$0 = g_{10} \psi\big(\gamma \phi + \sigma_{W_2}^2 \big(-\zeta \phi + \phi \eta' + \zeta g_9\big)\big) - \phi\big(\sqrt{\zeta} g_8 g_{12} \sqrt{n_0} + \psi\big)\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) \tag{S218q}$$
$$0 = g_9\big(\sqrt{\zeta} g_{15} \psi + \sqrt{n_0}\big(\gamma + g_{12}(\eta - \zeta) + \sigma_{W_2}^2 \big(\eta' + \zeta\big(g_{10} - 1\big)\big)\big)\big) - \sqrt{n_0}\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) \tag{S218r}$$
$$0 = -\sqrt{\zeta} g_8 g_{12} \sqrt{n_0} \phi\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) + g_5 \psi\big(\gamma \phi + \sigma_{W_2}^2 \big(-\zeta \phi + \phi \eta' + \zeta g_9\big)\big) + \zeta g_1 g_9 \psi \sigma_{W_2}^2 \tag{S218s}$$
$$0 = \sqrt{\zeta} g_4 g_9 \psi \phi + \sqrt{n_0}\big(g_2 \phi^2 \big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) + \zeta g_9 \sigma_{W_2}^2 \big(g_7 \phi - \zeta g_8 \sigma_{W_2}^2\big)\big) + g_6\big(\sqrt{\zeta} g_{11} \psi \phi + \zeta g_8 \sqrt{n_0} \phi \sigma_{W_2}^2\big) \tag{S218t}$$
$$\begin{aligned} 0 &= g_6 \phi\big(\sqrt{\zeta} g_{15} \psi + \sqrt{n_0}\big(\gamma + g_{12}(\eta - \zeta) + \sigma_{W_2}^2 \big(\eta' + \zeta\big(g_{10} - 1\big)\big)\big)\big) \\ &\quad + g_9\big(\sqrt{\zeta} g_{14} \psi \phi + \zeta \sqrt{n_0} \sigma_{W_2}^2 \big(g_{13} \phi - \zeta g_{10} \sigma_{W_2}^2\big)\big) \end{aligned} \tag{S218u}$$
$$0 = \phi\big(g_3 \sqrt{n_0} \phi\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) + g_6\big(\sqrt{\zeta} g_{15} \psi + \zeta g_{10} \sqrt{n_0} \sigma_{W_2}^2\big)\big) + g_9\big(\sqrt{\zeta} g_{14} \psi \phi + \zeta \sqrt{n_0} \sigma_{W_2}^2 \big(g_{13} \phi - \zeta g_{10} \sigma_{W_2}^2\big)\big) \tag{S218v}$$
$$\begin{aligned} 0 &= \phi\big(\sqrt{n_0}\big(\zeta g_{10} g_{12} + g_{13} \phi\big)\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) + g_6\big(\sqrt{\zeta} g_{15} \psi + \zeta g_{10} \sqrt{n_0} \sigma_{W_2}^2\big)\big) \\ &\quad + g_9\big(\sqrt{\zeta} g_{14} \psi \phi + \zeta \sqrt{n_0} \sigma_{W_2}^2 \big(g_{13} \phi - \zeta g_{10} \sigma_{W_2}^2\big)\big) \end{aligned} \tag{S218w}$$
$$\begin{aligned} 0 &= \sqrt{\zeta} g_4 g_9 \psi \phi + \sqrt{n_0}\big(g_7 \phi\big(\gamma \phi + \sigma_{W_2}^2 \big(-\zeta \phi + \phi \eta' + \zeta g_9\big)\big) + \zeta g_8\big(g_{12} \phi\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) - \zeta g_9 \sigma_{W_2}^4\big)\big) \\ &\quad + g_6\big(\sqrt{\zeta} g_{11} \psi \phi + \zeta g_8 \sqrt{n_0} \phi \sigma_{W_2}^2\big) \end{aligned} \tag{S218x}$$
$$\begin{aligned} 0 &= \sqrt{\zeta} g_{12} \phi\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big)\big(\sqrt{\zeta} g_{15} \psi + \sqrt{n_0}\big(\zeta g_{11} \sigma_{W_2}^2 - g_4 \phi\big)\big) + g_{14} \psi \phi\big(\gamma \phi + \sigma_{W_2}^2 \big(-\zeta \phi + \phi \eta' + \zeta g_9\big)\big) \\ &\quad + \zeta g_{15} \psi \sigma_{W_2}^2 \big(g_6 \phi - \zeta g_9 \sigma_{W_2}^2\big) \end{aligned} \tag{S218y}$$
$$\begin{aligned} 0 &= \phi\big(g_{13} \psi\big(\gamma \phi + \sigma_{W_2}^2 \big(-\zeta \phi + \phi \eta' + \zeta g_9\big)\big) - \sqrt{\zeta} g_{12} \sqrt{n_0}\big(g_7 \phi - \zeta g_8 \sigma_{W_2}^2\big)\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big)\big) \\ &\quad + \zeta g_{10} \psi\big(g_{12} \phi\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) - \zeta g_9 \sigma_{W_2}^4 + g_6 \phi \sigma_{W_2}^2\big) \end{aligned} \tag{S218z}$$
$$\begin{aligned} 0 &= -\sqrt{\zeta} g_2 g_{12} \sqrt{n_0} \phi^2 \big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) + \zeta \sigma_{W_2}^2 \big(\sqrt{\zeta} g_8 g_{12} \sqrt{n_0} \phi\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) + g_1 \psi\big(g_6 \phi - \zeta g_9 \sigma_{W_2}^2\big)\big) \\ &\quad + g_3 \psi \phi\big(\gamma \phi + \sigma_{W_2}^2 \big(\phi\big(\eta' - \zeta\big) + \zeta g_9\big)\big) + \zeta g_5 \psi\big(g_{12} \phi\big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) - \zeta g_9 \sigma_{W_2}^4 + g_6 \phi \sigma_{W_2}^2\big) \end{aligned} \tag{S218aa}$$

After some straightforward algebra, one can eliminate all g_i except for g_8 and g_9, which satisfy coupled polynomial equations. Those equations can be shown to be identical to eqn. (S66) by invoking the change of variables,

$$g_8 = -\frac{\sqrt{\zeta}\psi}{\sqrt{n_0}\phi} \tau_2\,, \quad \text{and} \quad g_9 = \big(\gamma + \sigma_{W_2}^2 \big(\eta' - \zeta\big)\big) \tau_1\,. \tag{S219}$$

In terms of the related variables defined in eqn. (S89), the error E_4 is given by,

$$E_5 = \tilde{\tau}_2^2 (1 + \phi + 2\tilde{\tau}_2 \phi)/(1 - \tilde{\tau}_2^2 \phi)\,. \tag{S220}$$

S6.4 H_{011}

$$\begin{aligned} H_{011} &= \mathbb{E} \hat{y}(\mathbf{x}; P, X, \varepsilon) \hat{y}(\mathbf{x}; \tilde{P}, X, \tilde{\varepsilon}) && \text{(S221)} \\ &= \mathbb{E} K(\mathbf{x}, X; \tilde{P}) K(X, X; \tilde{P})^{-1} Y(X, \tilde{\varepsilon})^\top Y(X, \varepsilon) K(X, X; P)^{-1} K(X, \mathbf{x}; P) && \text{(S222)} \end{aligned}$$

$$= \mathbb{E}\,\mathrm{tr}\left(K(X,X;\tilde{P})^{-1}(X^\top X + \sigma_\varepsilon^2 n_1 I_m)K(X,X;P)^{-1}K(X,\mathbf{x};P)K(\mathbf{x},X;\tilde{P})\right) \tag{S223}$$

$$= \mathbb{E}\,\mathrm{tr}\Big(K(X,X;\tilde{P})^{-1}(X^\top X + \sigma_\varepsilon^2 n_1 I_m)K(X,X;P)^{-1}K(X,\mathbf{x};P)K(\mathbf{x},X;\tilde{P}) \tag{S224}$$

$$\times (\frac{\sigma_{W_2}^2\zeta}{n_0}X^\top + \frac{\zeta}{\sqrt{n_0}n_1}F^\top W_1)(\frac{\sigma_{W_2}^2\zeta}{n_0}X^\top + \frac{\sqrt{\zeta}}{\sqrt{n_0}n_1}f(\tilde{W}_1X)^\top\tilde{W}_1)^\top\Big) \tag{S225}$$

$$\equiv H_{010} + E_6\,, \tag{S226}$$

where,

$$E_6 = \sigma_\varepsilon^2 n_1 \mathbb{E}\,\mathrm{tr}\Big(K(X,X;\tilde{P})^{-1}K(X,X;P)^{-1} \tag{S227}$$

$$\times (\frac{\sigma_{W_2}^2\zeta}{n_0}X^\top + \frac{\zeta}{\sqrt{n_0}n_1}F^\top W_1)(\frac{\sigma_{W_2}^2\zeta}{n_0}X^\top + \frac{\sqrt{\zeta}}{\sqrt{n_0}n_1}f(\tilde{W}_1X)^\top\tilde{W}_1)^\top\Big)\,. \tag{S228}$$

A linear pencil for E_6 follows from the representation,

$$E_6 = \mathrm{tr}(U_6^T Q_6^{-1} V_6)\,, \tag{S229}$$

where,

$$U_6^T = \begin{pmatrix}\sigma_\varepsilon^2 I_m & 0 & 0 & 0 & 0 & 0 & 0 & 0\end{pmatrix}\,, \quad V_6^T = \begin{pmatrix}0 & 0 & 0 & 0 & 0 & \frac{I_m}{\gamma+\sigma_{W_2}^2(\eta'-\zeta)} & 0 & 0\end{pmatrix} \tag{S230}$$

and,

$$Q_6 = \begin{pmatrix}
I_m\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) & \frac{\zeta X^\top\sigma_{W_2}^2}{n_0} & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} & -\frac{\zeta^2 m X^\top\sigma_{W_2}^4}{n_0^2} & 0 & -\frac{\zeta^{3/2}mX^\top\sigma_{W_2}^2}{n_0^{3/2}n_1} & 0 \\
-X & I_{n_0} & 0 & 0 & 0 & 0 & 0 & 0 \\
-\sqrt{\eta-\zeta}\Theta_F & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & I_{n_1} & 0 & \frac{\zeta^{3/2}mW_1\sigma_{W_2}^2}{n_0^{3/2}} & 0 & \frac{\zeta m W_1}{n_0 n_1} & 0 \\
0 & 0 & -W_1^\top & I_{n_0} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & I_{n_0} & -X & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{\zeta X^\top\sigma_{W_2}^2}{n_0} & I_m\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} & \frac{\sqrt{\eta-\zeta}\tilde{\Theta}_F^\top}{n_1} \\
0 & 0 & 0 & 0 & 0 & 0 & I_{n_0} & -\tilde{W}_1^\top \\
0 & 0 & 0 & 0 & -\frac{\sqrt{\zeta}\tilde{W}_1}{\sqrt{n_0}} & -\sqrt{\eta-\zeta}\tilde{\Theta}_F & 0 & I_{n_1}
\end{pmatrix}\,. \tag{S231}$$

The equations satisfied by the operator-valued Stieltjes transform G of $\bar{Q}_6$ induce the following structure on G,

$$G = \begin{pmatrix}0 & G_{12}\\ G_{12}^\top & 0\end{pmatrix}\,, \tag{S232}$$

where,

$$G_{12} = \begin{pmatrix}
g_5 & 0 & 0 & 0 & 0 & g_2 & 0 & 0 \\
0 & g_6 & 0 & g_3 & g_1 & 0 & g_4 & 0 \\
0 & 0 & g_8 & 0 & 0 & 0 & 0 & 0 \\
0 & g_{11} & 0 & g_7 & g_{10} & 0 & g_9 & 0 \\
0 & 0 & 0 & 0 & g_6 & 0 & g_3 & 0 \\
0 & 0 & 0 & 0 & 0 & g_5 & 0 & 0 \\
0 & 0 & 0 & 0 & g_{11} & 0 & g_7 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & g_8
\end{pmatrix}\,, \tag{S233}$$

and the independent entry-wise component functions g_i give the error E_6 through the relation,

$$E_6 = \frac{g_2\sigma_\varepsilon^2}{\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big)}\,, \tag{S234}$$

and themselves satisfy the following system of polynomial equations,

$$0 = \sqrt{\zeta} g_6 g_8 \sqrt{n_0} - g_{11}\psi \tag{S235a}$$
$$0 = \sqrt{\zeta} g_3 g_8 \sqrt{n_0} - g_7\psi + \psi \tag{S235b}$$
$$0 = -\sqrt{\zeta} g_5 g_6 \psi - g_3 \sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S235c}$$
$$0 = -\zeta g_7 g_8 \psi + \sqrt{\zeta} g_8 \sqrt{n_0}\big(g_4\phi - \zeta g_3 \sigma_{W_2}^2\big) - g_9\psi\phi \tag{S235d}$$
$$0 = -\sqrt{\zeta} g_5 g_{11}\psi - \big(g_7 - 1\big)\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S235e}$$
$$0 = -\zeta g_8 g_{11}\psi + \sqrt{\zeta} g_8 \sqrt{n_0}\big(g_1\phi - \zeta g_6 \sigma_{W_2}^2\big) + g_{10}\psi(-\phi) \tag{S235f}$$
$$0 = g_3\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_5\big(\sqrt{\zeta} g_7\psi + \zeta g_3\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S235g}$$
$$0 = \big(g_6 - 1\big)\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_5\big(\sqrt{\zeta} g_{11}\psi + \zeta g_6\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S235h}$$
$$0 = \sqrt{\zeta} g_7 g_8\sqrt{n_0}\phi\big(\sigma_{W_2}^2(\zeta - \eta') - \gamma\big) + g_{11}\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_5\big)\big) \tag{S235i}$$
$$0 = g_8\big(g_5\psi(\zeta - \eta) + \phi\big(\sqrt{\zeta} g_3\sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big) + \phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S235j}$$
$$0 = g_6\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_5\big)\big) - \phi\big(\sqrt{\zeta} g_3 g_8\sqrt{n_0} + \psi\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S235k}$$
$$0 = g_5\big(\sqrt{\zeta} g_{11}\psi + \sqrt{n_0}\big(\gamma + g_8(\eta - \zeta) + \sigma_{W_2}^2\big(\eta' + \zeta\big(g_6 - 1\big)\big)\big)\big) - \sqrt{n_0}\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S235l}$$
$$0 = \sqrt{\zeta} g_2 g_{11}\psi\phi + \sqrt{n_0}\phi\big(\zeta g_7 g_8 + g_9\phi\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + \sqrt{\zeta} g_5\psi\big(g_{10}\phi - \zeta g_{11}\sigma_{W_2}^2\big) \tag{S235m}$$
$$\begin{aligned}0 = {} & g_2\phi\big(\sqrt{\zeta} g_{11}\psi + \sqrt{n_0}\big(\gamma + g_8(\eta - \zeta) + \sigma_{W_2}^2\big(\eta' + \zeta\big(g_6 - 1\big)\big)\big)\big) \\ & + g_5\big(\sqrt{\zeta} g_{10}\psi\phi - \zeta\sigma_{W_2}^2\big(\sqrt{\zeta} g_{11}\psi + \sqrt{n_0}\big(\zeta g_6\sigma_{W_2}^2 - g_1\phi\big)\big)\big)\end{aligned} \tag{S235n}$$
$$\begin{aligned}0 = {} & g_4\sqrt{n_0}\phi^2\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_2\big(\sqrt{\zeta} g_7\psi\phi + \zeta g_3\sqrt{n_0}\phi\sigma_{W_2}^2\big) + g_5\big(\sqrt{\zeta} g_9\psi\phi \\ & - \zeta\sigma_{W_2}^2\big(\sqrt{\zeta} g_7\psi + \sqrt{n_0}\big(\zeta g_3\sigma_{W_2}^2 - g_4\phi\big)\big)\big)\end{aligned} \tag{S235o}$$
$$\begin{aligned}0 = {} & -\sqrt{\zeta} g_8\sqrt{n_0}\phi\big(g_9\phi - \zeta g_7\sigma_{W_2}^2\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_{10}\psi\phi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_5\big)\big) \\ & + \zeta g_{11}\psi\sigma_{W_2}^2\big(g_2\phi - \zeta g_5\sigma_{W_2}^2\big)\end{aligned} \tag{S235p}$$
$$\begin{aligned}0 = {} & \phi\big(g_1\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_2\big(\sqrt{\zeta} g_{11}\psi + \zeta g_6\sqrt{n_0}\sigma_{W_2}^2\big)\big) + g_5\big(\sqrt{\zeta} g_{10}\psi\phi \\ & - \zeta\sigma_{W_2}^2\big(\sqrt{\zeta} g_{11}\psi + \sqrt{n_0}\big(\zeta g_6\sigma_{W_2}^2 - g_1\phi\big)\big)\big)\end{aligned} \tag{S235q}$$
$$\begin{aligned}0 = {} & \sqrt{\zeta} g_1 g_5\psi\phi + \sqrt{\zeta} g_2 g_6\psi\phi + \gamma\zeta g_3 g_8\sqrt{n_0}\phi + \gamma g_4\sqrt{n_0}\phi^2 - \zeta^2 g_3 g_8\sqrt{n_0}\phi\sigma_{W_2}^2 + \sqrt{n_0}\phi\eta'\sigma_{W_2}^2\big(\zeta g_3 g_8 + g_4\phi\big) \\ & - \zeta g_4\sqrt{n_0}\phi^2\sigma_{W_2}^2 - \zeta^{3/2} g_5 g_6\psi\sigma_{W_2}^2\end{aligned} \tag{S235r}$$
$$\begin{aligned}0 = {} & -\sqrt{\zeta} g_4 g_8\sqrt{n_0}\phi^2\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + \zeta\sigma_{W_2}^2\big(\sqrt{\zeta} g_3 g_8\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) - \zeta g_5 g_6\psi\sigma_{W_2}^2 + g_2 g_6\psi\phi\big) \\ & + g_1\psi\phi\big(\gamma\phi + \sigma_{W_2}^2\big(\phi(\eta' - \zeta) + \zeta g_5\big)\big)\end{aligned} \tag{S235s}$$
$$\tag{S235t}$$

After some straightforward algebra, one can eliminate all g_i except for g_3 and g_5, which satisfy coupled polynomial equations. Those equations can be shown to be identical to eqn. (S66) by invoking the change of variables,

$$g_3 = -\frac{\sqrt{\zeta}\psi}{\sqrt{n_0}\phi}\tau_2\,, \quad \text{and} \quad g_5 = \big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big)\tau_1\,. \tag{S236}$$

In terms of the related variables defined in eqn. (S89), the error E_6 is given by,

$$E_6 = \sigma_\varepsilon^2\phi\tilde{\tau}_2^2/(1 - \tilde{\tau}_2^2\phi) \tag{S237}$$

S6.5 H_{100}

$$H_{100} = \mathbb{E}\hat{y}(\mathbf{x}; P, X, \varepsilon)\hat{y}(\mathbf{x}; P, \tilde{X}, \tilde{\varepsilon}) \tag{S238}$$

$$
\begin{aligned}
&= \mathbb{E}\Big[N_0(\mathbf{x};P)N_0(\mathbf{x};P)^\top + K(\mathbf{x},\tilde{X};P)K(\tilde{X},\tilde{X};P)^{-1}Y(\tilde{X},\tilde{\varepsilon})^\top Y(X,\varepsilon)K(X,X;P)^{-1}K(X,\mathbf{x};P)\\
&\quad + K(\mathbf{x},\tilde{X};\mathbb{P})K(\tilde{X},\tilde{X};P)^{-1}N_0(\tilde{X})^\top N_0(X)K(X,X;P)^{-1}K(X,\mathbf{x};P)\\
&\quad - N_0(\mathbf{x};P)N_0(X;P)K(X,X;P)^{-1}K(X,\mathbf{x};P) - N_0(\mathbf{x};P)N_0(\tilde{X};P)K(\tilde{X},\tilde{X};P)^{-1}K(\tilde{X},\mathbf{x};P)\Big] \qquad \text{(S239)}\\
&= \nu\sigma_{W_2}^2\eta + \nu E_{22} + \mathbb{E}\,\mathrm{tr}\,\big(K(\tilde{X},\tilde{X};P)^{-1}(\tilde{X}^\top X + \nu\frac{\sigma_{W_2}^2}{n_1}f(W_1\tilde{X})^T F)K(X,X;P)^{-1}K(X,\mathbf{x};P)K(\mathbf{x},\tilde{X};P)\big) \qquad \text{(S240)}\\
&= \nu\sigma_{W_2}^2\eta + \nu E_{22} + \mathbb{E}\,\mathrm{tr}\,\Big(K(\tilde{X},\tilde{X};P)^{-1}(\tilde{X}^\top X + \nu\frac{\sigma_{W_2}^2}{n_1}f(W_1\tilde{X})^T F)K(X,X;P)^{-1} \qquad \text{(S241)}\\
&\qquad \times (\frac{\sigma_{W_2}^2\zeta}{n_0}X^\top + \frac{\zeta}{\sqrt{n_0}n_1}F^\top W_1)(\frac{\sigma_{W_2}^2\zeta}{n_0}\tilde{X}^\top + \frac{\sqrt{\zeta}}{\sqrt{n_0}n_1}f(W_1\tilde{X})^\top W_1)^\top\Big) \qquad \text{(S242)}\\
&\equiv \nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{71} + \nu E_{72}\,, \qquad \text{(S243)}
\end{aligned}
$$

where, E_{22} is given above and,

$$
\begin{aligned}
E_{71} &= \mathbb{E}\,\mathrm{tr}\,\Big(K(\tilde{X},\tilde{X};P)^{-1}\tilde{X}^\top X K(X,X;P)^{-1}\big(\frac{\eta-\zeta}{n_1^2}f(W_1X)^\top f(W_1\tilde{X}) \qquad \text{(S244)}\\
&\qquad + (\frac{\sigma_{W_2}^2\zeta}{n_0}X^\top + \frac{\zeta}{\sqrt{n_0}n_1}F^\top W_1)(\frac{\sigma_{W_2}^2\zeta}{n_0}\tilde{X}^\top + \frac{\sqrt{\zeta}}{\sqrt{n_0}n_1}f(W_1\tilde{X})^\top W_1)^\top\big)\Big) \qquad \text{(S245)}\\
E_{72} &= \frac{\sigma_{W_2}^2}{n_1}\mathbb{E}\,\mathrm{tr}\,\Big(K(\tilde{X},\tilde{X};P)^{-1}f(W_1\tilde{X})^T F K(X,X;P)^{-1}\big(\frac{\eta-\zeta}{n_1^2}f(W_1X)^\top f(W_1\tilde{X}) \qquad \text{(S246)}\\
&\qquad + (\frac{\sigma_{W_2}^2\zeta}{n_0}X^\top + \frac{\zeta}{\sqrt{n_0}n_1}F^\top W_1)(\frac{\sigma_{W_2}^2\zeta}{n_0}\tilde{X}^\top + \frac{\sqrt{\zeta}}{\sqrt{n_0}n_1}f(W_1\tilde{X})^\top W_1)^\top\big)\Big)\,. \qquad \text{(S247)}
\end{aligned}
$$

S6.5.1 E_{71}

A linear pencil for E_{71} follows from the representation,

$$
E_{71} = \mathrm{tr}(U_{71}^T Q_{71}^{-1} V_{71})\,, \qquad \text{(S248)}
$$

where,

$$
U_{71}^T = \begin{pmatrix} 0 & \frac{I_{n_0}}{m} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \qquad \text{(S249)}
$$

$$
V_{71}^T = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{n_0}n_1 I_{n_0}}{\sqrt{\zeta}} \end{pmatrix} \qquad \text{(S250)}
$$

and, for $\beta = \big(n_0(\zeta-\eta) - \zeta n_1\sigma_{W_2}^2\big)$,

$$
Q_{71} = \begin{pmatrix}
I_m\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) & 0 & \frac{\zeta X^\top\sigma_{W_2}^2}{n_0} & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} & -\frac{\zeta^2 m X^\top\sigma_{W_2}^4}{n_0^2} & 0 & 0 & 0\\
-X & I_{n_0} & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
-X & 0 & I_{n_0} & 0 & 0 & 0 & 0 & \frac{\sqrt{\zeta}mW_1^\top}{\sqrt{n_0}n_1} & 0\\
-\sqrt{\eta-\zeta}\Theta_F & 0 & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & I_{n_1} & 0 & -\frac{\sqrt{\zeta}mW_1\beta}{n_0^{3/2}n_1} & \frac{m(\eta-\zeta)^{3/2}\tilde{\Theta}_F}{n_1} & 0 & 0\\
0 & 0 & 0 & -W_1^\top & I_{n_0} & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & I_{n_0} & -\tilde{X} & 0 & 0\\
0 & 0 & 0 & 0 & 0 & \frac{\zeta\sigma_{W_2}^2\tilde{X}^\top}{n_0} & I_m\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) & \frac{\sqrt{\eta-\zeta}\tilde{\Theta}_F^\top}{n_1} & \frac{\sqrt{\zeta}\tilde{X}^\top}{\sqrt{n_0}n_1}\\
0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & -\sqrt{\eta-\zeta}\tilde{\Theta}_F & I_{n_1} & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -W_1^\top & I_{n_0}
\end{pmatrix}. \qquad \text{(S251)}
$$

The equations satisfied by the operator-valued Stieltjes transform G of $\bar{Q}_{71}$ induce the following structure on G,

$$G = \begin{pmatrix} 0 & G_{12} \\ G_{12}^\top & 0 \end{pmatrix}, \tag{S252}$$

where,

$$G_{12} = \begin{pmatrix} g_8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & g_1 & g_3 & 0 & g_5 & g_6 & 0 & 0 & g_2 \\ 0 & 0 & g_9 & 0 & g_5 & g_{12} & 0 & 0 & g_4 \\ 0 & 0 & 0 & g_{11} & 0 & 0 & 0 & g_{15} & 0 \\ 0 & 0 & g_{14} & 0 & g_{10} & g_{13} & 0 & 0 & g_7 \\ 0 & 0 & 0 & 0 & 0 & g_9 & 0 & 0 & g_5 \\ 0 & 0 & 0 & 0 & 0 & 0 & g_8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_{11} & 0 \\ 0 & 0 & 0 & 0 & 0 & g_{14} & 0 & 0 & g_{10} \end{pmatrix}, \tag{S253}$$

and the independent entry-wise component functions g_i give the error E_{71} through the relation,

$$E_{71} = -\frac{g_2\sqrt{n_0}\phi}{\sqrt{\zeta}\psi}, \tag{S254}$$

and themselves satisfy the following system of polynomial equations,

$$0 = 1 - g_1 \tag{S255a}$$
$$0 = \sqrt{\zeta}g_9g_{11}\sqrt{n_0} - g_{14}\psi \tag{S255b}$$
$$0 = \sqrt{\zeta}g_5g_{11}\sqrt{n_0} - g_{10}\psi + \psi \tag{S255c}$$
$$0 = -\sqrt{\zeta}g_6g_8\psi - g_2\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S255d}$$
$$0 = -\sqrt{\zeta}g_8g_9\psi - g_5\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S255e}$$
$$0 = -\sqrt{\zeta}g_8g_{12}\psi - g_4\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S255f}$$
$$0 = -\sqrt{\zeta}g_8g_{13}\psi - g_7\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S255g}$$
$$0 = -\sqrt{\zeta}g_8g_{14}\psi - (g_{10} - 1)\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S255h}$$
$$0 = -\sqrt{\zeta}g_1g_8\psi - \sqrt{\zeta}g_3g_8\psi - g_5\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S255i}$$
$$0 = g_3\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_8\big(\sqrt{\zeta}g_{14}\psi + \zeta g_9\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S255j}$$
$$0 = g_5\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_8\big(\sqrt{\zeta}g_{10}\psi + \zeta g_5\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S255k}$$
$$0 = \sqrt{\zeta}\sqrt{n_0}\big(g_5\big(g_{11}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big) + g_{15}\phi\big) + g_4g_{11}\phi\big) - g_7\psi\phi \tag{S255l}$$
$$0 = \sqrt{\zeta}\sqrt{n_0}\big(g_9\big(g_{11}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big) + g_{15}\phi\big) + g_{11}g_{12}\phi\big) - g_{13}\psi\phi \tag{S255m}$$
$$0 = (g_9 - 1)\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_8\big(\sqrt{\zeta}g_{14}\psi + \zeta g_9\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S255n}$$
$$0 = \sqrt{\zeta}g_7g_8\psi\phi + \sqrt{n_0}\big(g_2\phi^2\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + \zeta g_8\sigma_{W_2}^2\big(g_4\phi - \zeta g_5\sigma_{W_2}^2\big)\big) \tag{S255o}$$
$$0 = \sqrt{\zeta}g_{10}g_{11}\sqrt{n_0}\phi\big(\sigma_{W_2}^2(\zeta - \eta') - \gamma\big) + g_{14}\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_8\big)\big) \tag{S255p}$$
$$0 = g_{11}\big(g_8\psi(\zeta - \eta) + \phi\big(\sqrt{\zeta}g_5\sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big) + \phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S255q}$$
$$0 = g_6\sqrt{n_0}\phi^2\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_8\big(\sqrt{\zeta}g_{13}\psi\phi + \zeta\sqrt{n_0}\sigma_{W_2}^2\big(g_{12}\phi - \zeta g_9\sigma_{W_2}^2\big)\big) \tag{S255r}$$
$$0 = g_9\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_8\big)\big) - \phi\big(\sqrt{\zeta}g_5g_{11}\sqrt{n_0} + \psi\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S255s}$$
$$0 = g_8\big(\sqrt{\zeta}g_{14}\psi + \sqrt{n_0}\big(\gamma + g_{11}(\eta - \zeta) + \sigma_{W_2}^2\big(\eta' + \zeta(g_9 - 1)\big)\big)\big) - \sqrt{n_0}\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S255t}$$
$$0 = -\sqrt{\zeta}g_5g_{11}\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_3\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_8\big)\big) + \zeta g_1g_8\psi\sigma_{W_2}^2 \tag{S255u}$$

$$0 = \sqrt{n_0}\phi\big(\zeta g_9 g_{11} + g_{12}\phi\big)\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) + g_8\big(\sqrt{\zeta}g_{13}\psi\phi + \zeta\sqrt{n_0}\sigma_{W_2}^2\big(g_{12}\phi - \zeta g_9\sigma_{W_2}^2\big)\big) \tag{S255v}$$

$$0 = \sqrt{\zeta}g_7 g_8\psi\phi + \sqrt{n_0}\big(g_4\phi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_8\big)\big) + \zeta g_5\big(g_{11}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) - \zeta g_8\sigma_{W_2}^4\big)\big) \tag{S255w}$$

$$\begin{aligned} 0 = {} & g_8\psi(-(\zeta - \eta))\big(g_{11}\psi(\zeta - \eta) + g_{15}\phi\big) - \phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \\ & \big(-\zeta g_9 g_{11}\psi + \sqrt{\zeta}\sqrt{n_0}\big(g_5\big(g_{11}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big) + g_{15}\phi\big) + g_4 g_{11}\phi\big) - g_{15}\phi\big) \end{aligned} \tag{S255x}$$

$$\begin{aligned} 0 = {} & \phi\big(g_{12}\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_8\big)\big) - \sqrt{\zeta}\sqrt{n_0}\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \\ & \big(g_5\big(g_{11}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big) + g_{15}\phi\big) + g_4 g_{11}\phi\big)\big) + \zeta g_9\psi\big(g_{11}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) - \zeta g_8\sigma_{W_2}^4\big) \end{aligned} \tag{S255y}$$

$$\begin{aligned} 0 = {} & \sqrt{\zeta}\big(-g_{10}g_{15}\sqrt{n_0}\phi^2\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) - g_{11}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big)\big(\sqrt{n_0}\big(g_{10}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big) + g_7\phi\big) \\ & - \sqrt{\zeta}g_{14}\psi\big) - \zeta^{3/2}g_8 g_{14}\psi\sigma_{W_2}^4\big) + g_{13}\psi\phi\big(\gamma\phi + \sigma_{W_2}^2\big(\phi\big(\eta' - \zeta\big) + \zeta g_8\big)\big) \end{aligned} \tag{S255z}$$

$$\begin{aligned} 0 = {} & \sqrt{\zeta}\big(-\gamma\zeta g_5 g_{11}\sqrt{n_0}\psi\phi + \gamma\eta g_5 g_{11}\sqrt{n_0}\psi\phi - \gamma g_5 g_{15}\sqrt{n_0}\phi^2 - g_2 g_{11}\sqrt{n_0}\phi^2\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \\ & + \gamma\zeta g_5 g_{11}\sqrt{n_0}\phi\sigma_{W_2}^2 + \zeta^2 g_5 g_{11}\sqrt{n_0}\psi\phi\sigma_{W_2}^2 - \zeta^2 g_5 g_{11}\sqrt{n_0}\phi\sigma_{W_2}^4 \\ & + g_5\sqrt{n_0}\phi\eta'\sigma_{W_2}^2\big(g_{11}\big(-\zeta\psi + \eta\psi + \zeta\sigma_{W_2}^2\big) - g_{15}\phi\big) - \zeta\eta g_5 g_{11}\sqrt{n_0}\psi\phi\sigma_{W_2}^2 + \zeta g_5 g_{15}\sqrt{n_0}\phi^2\sigma_{W_2}^2 \\ & + \sqrt{\zeta}g_3\psi\big(g_{11}\phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) - \zeta g_8\sigma_{W_2}^4\big) - \zeta^{3/2}g_1 g_8\psi\sigma_{W_2}^4\big) \\ & + g_6\psi\phi\big(\gamma\phi + \sigma_{W_2}^2\big(\phi\big(\eta' - \zeta\big) + \zeta g_8\big)\big) \end{aligned} \tag{S255aa}$$

After some straightforward algebra, one can eliminate all g_i except for g_5 and g_8, which satisfy coupled polynomial equations. Those equations can be shown to be identical to eqn. (S66) by invoking the change of variables,

$$g_5 = -\frac{\sqrt{\zeta}\psi}{\sqrt{n_0}\phi}\tau_2\,, \quad \text{and} \quad g_8 = \big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big)\tau_1\,. \tag{S256}$$

In terms of the related variables defined in eqn. (S89), the error E_{71} is given by,

$$\begin{aligned} E_{71} &= \frac{\psi\tilde{\tau}_1^2\big(2\zeta\tilde{\tau}_2 + \eta\big) + \zeta\phi^2\tilde{\tau}_2^2}{\zeta\big(\phi^2 - \psi\tilde{\tau}_1^2\big)} && \text{(S257)} \\ &= \tau_2'/\tau_1' - 2\tau_2/\tau_1 + 1\,. && \text{(S258)} \end{aligned}$$

S6.5.2 E_{72}

A linear pencil for E_{72} follows from the representation,

$$E_{72} = \operatorname{tr}(U_{72}^T Q_{72}^{-1} V_{72})\,, \tag{S259}$$

where,

$$\begin{aligned} U_{72}^T &= \begin{pmatrix} 0 & \frac{I_{n_1}}{m} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} && \text{(S260)} \\ V_{72}^T &= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -n_1 I_{n_1} & 0 \end{pmatrix} && \text{(S261)} \end{aligned}$$

and, for $\beta = \big(n_0(\zeta-\eta) - \zeta n_1 \sigma_{W_2}^2\big)$,

$$Q_{72} = \begin{pmatrix} I_m\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) & 0 & 0 & \frac{\zeta X^\top \sigma_{W_2}^2}{n_0} & \frac{\sqrt{\eta-\zeta}\Theta_F^\top}{n_1} & \frac{\sqrt{\zeta}X^\top}{\sqrt{n_0}n_1} & -\frac{\zeta^2 m X^\top \sigma_{W_2}^4}{n_0^2} & 0 & 0 & 0 & 0 \\ -\sqrt{\eta-\zeta}\Theta_F & I_{n_1} & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -X & 0 & I_{n_0} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -X & 0 & 0 & I_{n_0} & 0 & 0 & 0 & 0 & \frac{\sqrt{\zeta}mW_1^\top}{\sqrt{n_0}n_1} & 0 & 0 \\ -\sqrt{\eta-\zeta}\Theta_F & 0 & 0 & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & I_{n_1} & 0 & -\frac{\sqrt{\zeta}mW_1\beta}{n_0^{3/2}n_1} & \frac{m(\eta-\zeta)^{3/2}\tilde{\Theta}_F}{n_1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -W_1^\top & I_{n_0} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & I_{n_0} & -\tilde{X} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\zeta\sigma_{W_2}^2\tilde{X}^\top}{n_0} & I_m\big(\gamma+\sigma_{W_2}^2\big(\eta'-\zeta\big)\big) & 0 & \frac{\sqrt{\eta-\zeta}\tilde{\Theta}_F^\top}{n_1} & \frac{\sqrt{\zeta}\tilde{X}^\top}{\sqrt{n_0}n_1} \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & -\sqrt{\eta-\zeta}\tilde{\Theta}_F & I_{n_1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{\zeta}W_1}{\sqrt{n_0}} & -\sqrt{\eta-\zeta}\tilde{\Theta}_F & 0 & I_{n_1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -W_1^\top & I_{n_0} \end{pmatrix} . \tag{S262}$$

The equations satisfied by the operator-valued Stieltjes transform G of $\bar{Q}_{72}$ induce the following structure on G,

$$G = \begin{pmatrix} 0 & G_{12} \\ G_{12}^\top & 0 \end{pmatrix} , \tag{S263}$$

where,

$$G_{12} = \begin{pmatrix} g_{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & g_1 & 0 & 0 & g_6 & 0 & 0 & 0 & g_{11} & g_3 & 0 \\ 0 & 0 & g_1 & g_4 & 0 & g_7 & g_8 & 0 & 0 & 0 & g_2 \\ 0 & 0 & 0 & g_{13} & 0 & g_7 & g_{16} & 0 & 0 & 0 & g_5 \\ 0 & 0 & 0 & 0 & g_{15} & 0 & 0 & 0 & g_{19} & g_{10} & 0 \\ 0 & 0 & 0 & g_{18} & 0 & g_{14} & g_{17} & 0 & 0 & 0 & g_9 \\ 0 & 0 & 0 & 0 & 0 & 0 & g_{13} & 0 & 0 & 0 & g_7 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_{12} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_1 & g_6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & g_{15} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & g_{18} & 0 & 0 & 0 & g_{14} \end{pmatrix} , \tag{S264}$$

and the independent entry-wise component functions g_i give the error E_{72} through the relation,

$$E_{72} = -\frac{\phi g_3}{\psi} , \tag{S265}$$

and themselves satisfy the following system of polynomial equations,

$$0 = 1 - g_1 \tag{S266a}$$
$$0 = -\zeta g_{13} g_{15} \psi - g_{19} \phi \tag{S266b}$$
$$0 = \sqrt{\zeta} g_{13} g_{15} \sqrt{n_0} - g_{18} \psi \tag{S266c}$$
$$0 = \sqrt{\zeta} g_7 g_{15} \sqrt{n_0} - g_{14} \psi + \psi \tag{S266d}$$
$$0 = g_{11}(-\phi) - \zeta\big(g_1 g_4 + g_6 g_{13}\big)\psi \tag{S266e}$$
$$0 = -\sqrt{\zeta} g_8 g_{12} \psi - g_2 \sqrt{n_0} \phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S266f}$$
$$0 = -\sqrt{\zeta} g_{12} g_{13} \psi - g_7 \sqrt{n_0} \phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S266g}$$
$$0 = -\sqrt{\zeta} g_{12} g_{16} \psi - g_5 \sqrt{n_0} \phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S266h}$$
$$0 = -\sqrt{\zeta} g_{12} g_{17} \psi - g_9 \sqrt{n_0} \phi\big(\gamma + \sigma_{W_2}^2\big(\eta' - \zeta\big)\big) \tag{S266i}$$

$$0 = -\sqrt{\zeta}g_{12}g_{18}\psi - (g_{14}-1)\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S266j}$$

$$0 = -\sqrt{\zeta}g_1g_{12}\psi - \sqrt{\zeta}g_4g_{12}\psi - g_7\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S266k}$$

$$0 = g_{12}g_{15}\psi(\zeta-\eta) - \phi\big(g_6 - \sqrt{\zeta}g_7g_{15}\sqrt{n_0}\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S266l}$$

$$0 = g_7\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_{12}\big(\sqrt{\zeta}g_{14}\psi + \zeta g_7\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S266m}$$

$$0 = g_4\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_{12}\big(\sqrt{\zeta}g_{18}\psi + \zeta g_{13}\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S266n}$$

$$0 = \sqrt{\zeta}\sqrt{n_0}\big(g_7\big(g_{15}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big) + (g_{10}+g_{19})\phi\big) + g_5g_{15}\phi\big) - g_9\psi\phi \tag{S266o}$$

$$0 = (g_{13}-1)\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_{12}\big(\sqrt{\zeta}g_{18}\psi + \zeta g_{13}\sqrt{n_0}\sigma_{W_2}^2\big) \tag{S266p}$$

$$0 = \sqrt{\zeta}\sqrt{n_0}\big(g_{13}\big(g_{15}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big) + g_{19}\phi\big) + g_{10}g_{13}\phi + g_{15}g_{16}\phi\big) - g_{17}\psi\phi \tag{S266q}$$

$$0 = \sqrt{\zeta}g_9g_{12}\psi\phi + \sqrt{n_0}\big(g_2\phi^2\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + \zeta g_{12}\sigma_{W_2}^2\big(g_5\phi - \zeta g_7\sigma_{W_2}^2\big)\big) \tag{S266r}$$

$$0 = \sqrt{\zeta}g_{14}g_{15}\sqrt{n_0}\phi\big(\sigma_{W_2}^2(\zeta - \eta') - \gamma\big) + g_{18}\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_{12}\big)\big) \tag{S266s}$$

$$0 = g_{15}\big(g_{12}\psi(\zeta-\eta) + \phi\big(\sqrt{\zeta}g_7\sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big) + \phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S266t}$$

$$0 = g_8\sqrt{n_0}\phi^2\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_{12}\big(\sqrt{\zeta}g_{17}\psi\phi + \zeta\sqrt{n_0}\sigma_{W_2}^2\big(g_{16}\phi - \zeta g_{13}\sigma_{W_2}^2\big)\big) \tag{S266u}$$

$$0 = g_{13}\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_{12}\big)\big) - \phi\big(\sqrt{\zeta}g_7g_{15}\sqrt{n_0} + \psi\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S266v}$$

$$0 = g_{12}\big(\sqrt{\zeta}g_{18}\psi + \sqrt{n_0}\big(\gamma + g_{15}(\eta-\zeta) + \sigma_{W_2}^2\big(\eta' + \zeta(g_{13}-1)\big)\big)\big) - \sqrt{n_0}\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S266w}$$

$$0 = g_{12}g_{19}\psi(\zeta-\eta) - \phi\big(g_{11} - \sqrt{\zeta}g_7g_{19}\sqrt{n_0}\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + \zeta g_1g_4\psi\big(\sigma_{W_2}^2(\zeta - \eta') - \gamma\big) \tag{S266x}$$

$$0 = g_{19}\big(g_{12}\psi(\zeta-\eta) + \phi\big(\sqrt{\zeta}g_7\sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big) - \zeta g_1g_{13}\psi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \tag{S266y}$$

$$0 = -\sqrt{\zeta}g_7g_{15}\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_4\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_{12}\big)\big) + \zeta g_1g_{12}\psi\sigma_{W_2}^2 \tag{S266z}$$

$$0 = \sqrt{n_0}\phi\big(\zeta(g_1+g_6)g_{13} + g_{16}\phi\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) + g_{12}\big(\sqrt{\zeta}g_{17}\psi\phi + \zeta\sqrt{n_0}\sigma_{W_2}^2\big(g_{16}\phi - \zeta g_{13}\sigma_{W_2}^2\big)\big) \tag{S266aa}$$

$$\begin{aligned}0 = {}& g_6\big(g_{12}\psi(\zeta-\eta) + \phi\big(\sqrt{\zeta}g_7\sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big) + g_1\big(g_{12}\psi(\zeta-\eta) \\ & + \sqrt{\zeta}g_7\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big)\end{aligned} \tag{S266ab}$$

$$\begin{aligned}0 = {}& \sqrt{\zeta}g_9g_{12}\psi\phi + \sqrt{n_0}\big(g_5\phi\big(\gamma\phi + \sigma_{W_2}^2\big(\phi(\eta'-\zeta) + \zeta g_{12}\big)\big) + \zeta g_7\big(g_1\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \\ & + g_6\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) - \zeta g_{12}\sigma_{W_2}^4\big)\big)\end{aligned} \tag{S266ac}$$

$$\begin{aligned}0 = {}& g_{12}\psi(-(\zeta-\eta))\big(g_{15}\psi(\zeta-\eta) + g_{19}\phi\big) - \sqrt{\zeta}\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) \\ & \big(g_7\big(g_{15}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big) + g_{19}\phi\big) + g_5g_{15}\phi\big) + g_{10}\phi\big(g_{12}\psi(\eta-\zeta) \\ & - \phi\big(\sqrt{\zeta}g_7\sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big)\end{aligned} \tag{S266ad}$$

$$\begin{aligned}0 = {}& g_{15}\big(g_{12}\psi^2\big(-(\zeta-\eta)^2\big) - \sqrt{\zeta}\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big(g_7\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big) + g_5\phi\big)\big) \\ & + g_{10}\phi\big(g_{12}\psi(\eta-\zeta) - \phi\big(\sqrt{\zeta}g_7\sqrt{n_0} - 1\big)\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big) + \zeta g_6g_{13}\psi\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\end{aligned} \tag{S266ae}$$

$$\begin{aligned}0 = {}& \zeta g_{10}g_{12}\psi - \eta g_{10}g_{12}\psi + \gamma\sqrt{\zeta}g_7g_{10}\sqrt{n_0}\phi + \gamma\sqrt{\zeta}g_2g_{15}\sqrt{n_0}\phi - \zeta^{3/2}g_7g_{10}\sqrt{n_0}\phi\sigma_{W_2}^2 \\ & - \zeta^{3/2}g_2g_{15}\sqrt{n_0}\phi\sigma_{W_2}^2 + \sqrt{\zeta}(g_7g_{10} + g_2g_{15})\sqrt{n_0}\phi\eta'\sigma_{W_2}^2 + \zeta g_4g_6\psi\big(\sigma_{W_2}^2(\zeta - \eta') - \gamma\big) \\ & - g_3\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\end{aligned} \tag{S266af}$$

$$\begin{aligned}0 = {}& \phi\big(g_8\psi\big(\gamma\phi + \sigma_{W_2}^2\big(-\zeta\phi + \phi\eta' + \zeta g_{12}\big)\big) - \sqrt{\zeta}\sqrt{n_0}\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big(g_7\big(g_{15}\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big) \\ & + (g_{10}+g_{19})\phi\big) + g_2g_{15}\phi\big)\big) + \zeta g_1\psi\big(g_4\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) - \zeta g_{12}\sigma_{W_2}^4\big) \\ & + \zeta g_4\psi\big(g_6\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big) - \zeta g_{12}\sigma_{W_2}^4\big)\end{aligned} \tag{S266ag}$$

$$\begin{aligned}0 = {}& g_6\big(g_{12}\psi^2\big(-(\zeta-\eta)^2\big) - \sqrt{\zeta}\sqrt{n_0}\phi\big(\gamma + \sigma_{W_2}^2(\eta' - \zeta)\big)\big(g_7\big(\zeta\psi - \eta\psi - \zeta\sigma_{W_2}^2\big) + g_5\phi\big)\big) \\ & + \phi\big(g_{11}\big(g_{12}\psi(\eta-\zeta) + \sqrt{\zeta}g_7\sqrt{n_0}\phi\big(\sigma_{W_2}^2(\zeta - \eta') - \gamma\big)\big) + \sqrt{\zeta}g_1g_2\sqrt{n_0}\phi\big(\sigma_{W_2}^2(\zeta - \eta') - \gamma\big)\big)\end{aligned}$$

$$
\begin{aligned}
&+ g_3\phi\big(g_{12}\psi(\eta-\zeta) - \phi\big(\sqrt{\zeta}g_7\sqrt{n_0}-1\big)\big(\gamma+\sigma_{W_2}^2(\eta'-\zeta)\big)\big) && \text{(S266ah)}\\
0 =\,& \sqrt{\zeta}\big(-\gamma\zeta g_{14}g_{15}\sqrt{n_0}\psi\phi + \gamma\eta g_{14}g_{15}\sqrt{n_0}\psi\phi - \gamma g_{10}g_{14}\sqrt{n_0}\phi^2 - \gamma g_9 g_{15}\sqrt{n_0}\phi^2 - \gamma g_{14}g_{19}\sqrt{n_0}\phi^2 \\
&+ \gamma\zeta g_{14}g_{15}\sqrt{n_0}\phi\sigma_{W_2}^2 + \zeta^2 g_{14}g_{15}\sqrt{n_0}\psi\phi\sigma_{W_2}^2 - \zeta^2 g_{14}g_{15}\sqrt{n_0}\phi\sigma_{W_2}^4 \\
&- \sqrt{n_0}\phi\eta'\sigma_{W_2}^2\big(g_{14}\big(g_{15}\big(\zeta\psi-\eta\psi-\zeta\sigma_{W_2}^2\big)+g_{19}\phi\big)+g_{10}g_{14}\phi+g_9g_{15}\phi\big) - \zeta\eta g_{14}g_{15}\sqrt{n_0}\psi\phi\sigma_{W_2}^2 \\
&+ \zeta g_{10}g_{14}\sqrt{n_0}\phi^2\sigma_{W_2}^2 + \zeta g_9 g_{15}\sqrt{n_0}\phi^2\sigma_{W_2}^2 + \zeta g_{14}g_{19}\sqrt{n_0}\phi^2\sigma_{W_2}^2 + \sqrt{\zeta}g_1g_{18}\psi\phi\big(\gamma+\sigma_{W_2}^2(\eta'-\zeta)\big) \\
&+ \sqrt{\zeta}g_6g_{18}\psi\phi\big(\gamma+\sigma_{W_2}^2(\eta'-\zeta)\big) - \zeta^{3/2}g_{12}g_{18}\psi\sigma_{W_2}^4\big) + g_{17}\psi\phi\big(\gamma\phi+\sigma_{W_2}^2\big(\phi(\eta'-\zeta)+\zeta g_{12}\big)\big) && \text{(S266ai)}\\
0 =\,& \gamma g_{16}\psi\phi^2 - \gamma\zeta^{3/2}g_7g_{15}\sqrt{n_0}\psi\phi + \gamma\sqrt{\zeta}\eta g_7g_{15}\sqrt{n_0}\psi\phi - \gamma\sqrt{\zeta}g_7g_{10}\sqrt{n_0}\phi^2 - \gamma\sqrt{\zeta}g_5g_{15}\sqrt{n_0}\phi^2 \\
&- \gamma\sqrt{\zeta}g_7g_{19}\sqrt{n_0}\phi^2 + \gamma\zeta^{3/2}g_7g_{15}\sqrt{n_0}\phi\sigma_{W_2}^2 - \zeta^{3/2}\eta g_7g_{15}\sqrt{n_0}\psi\phi\sigma_{W_2}^2 + \zeta^{3/2}g_7g_{10}\sqrt{n_0}\phi^2\sigma_{W_2}^2 \\
&+ \zeta^{3/2}g_5g_{15}\sqrt{n_0}\phi^2\sigma_{W_2}^2 + \zeta^{3/2}g_7g_{19}\sqrt{n_0}\phi^2\sigma_{W_2}^2 + \zeta^{5/2}g_7g_{15}\sqrt{n_0}\psi\phi\sigma_{W_2}^2 - \zeta^{5/2}g_7g_{15}\sqrt{n_0}\phi\sigma_{W_2}^4 \\
&+ \phi\eta'\sigma_{W_2}^2\big(g_{16}\psi\phi - \sqrt{\zeta}\sqrt{n_0}\big(g_7\big(g_{15}\big(\zeta\psi-\eta\psi-\zeta\sigma_{W_2}^2\big)+(g_{10}+g_{19})\phi\big)+g_5g_{15}\phi\big)\big) \\
&+ \zeta g_1g_{13}\psi\phi\big(\gamma+\sigma_{W_2}^2(\eta'-\zeta)\big) + \zeta g_6g_{13}\psi\phi\big(\gamma+\sigma_{W_2}^2(\eta'-\zeta)\big) - \zeta^2g_{12}g_{13}\psi\sigma_{W_2}^4 - \zeta g_{16}\psi\phi^2\sigma_{W_2}^2 \\
&+ \zeta g_{12}g_{16}\psi\phi\sigma_{W_2}^2 && \text{(S266aj)}
\end{aligned}
$$

After some straightforward algebra, one can eliminate all g_i except for g_7 and g_{12}, which satisfy coupled polynomial equations. Those equations can be shown to be identical to eqn. (S66) by invoking the change of variables,

$$
g_7 = -\frac{\sqrt{\zeta}\psi}{\sqrt{n_0}\phi}\tau_2\,, \quad \text{and} \quad g_{12} = \big(\gamma+\sigma_{W_2}^2(\eta'-\zeta)\big)\tau_1\,. \tag{S267}
$$

In terms of the related variables defined in eqn. (S89), the error E_{72} is given by,

$$
\begin{aligned}
E_{72} &= -\frac{\psi\tilde\tau_1^2\big(2\zeta\psi\tilde\tau_1(\zeta-2\eta)+\phi\big(\zeta^2\psi-\zeta\eta(\psi+1)-\eta^2\psi\big)\big)}{2\zeta\phi\big(\phi^2-\psi\tilde\tau_1^2\big)} + \frac{\psi^2\tilde\tau_1^2(\zeta-\eta)^3}{2\zeta^2\big(\tilde\tau_2+1\big)^2\big(\psi\tilde\tau_1^2-\phi^2\big)} \\
&\quad + \frac{\psi\tilde\tau_1\tilde\tau_2\big(\psi\tilde\tau_1+\phi\big)\big(\zeta\tilde\tau_1+\eta\phi\big)}{\phi^3-\psi\phi\tilde\tau_1^2} + \frac{\psi^2\tilde\tau_1^2(\zeta-\eta)^2\big(\tilde\tau_1+\phi\big)}{\zeta\phi\big(\tilde\tau_2+1\big)\big(\phi^2-\psi\tilde\tau_1^2\big)} + \frac{\zeta\tilde\tau_2^2\big(\psi\tilde\tau_1+\phi\big)^2}{2\big(\phi^2-\psi\tilde\tau_1^2\big)} && \text{(S268)}\\
&= -T_2/\tau_1' - E_{22} - \eta\sigma_{W_2}^2\,, && \text{(S269)}
\end{aligned}
$$

where T_2 is given in eqn. (S65).

S6.6 H_{101}

$$
\begin{aligned}
H_{101} &= \mathbb{E}\hat y(\mathbf{x};P,X,\varepsilon)\hat y(\mathbf{x};P,\tilde X,\varepsilon) && \text{(S270)}\\
&= \mathbb{E}\Big[N_0(\mathbf{x};P)N_0(\mathbf{x};P)^\top + K(\mathbf{x},\tilde X;\mathbb{P})K(\tilde X,\tilde X;P)^{-1}Y(\tilde X,\varepsilon)^\top Y(X,\varepsilon)K(X,X;P)^{-1}K(X,\mathbf{x};P) \\
&\quad + K(\mathbf{x},\tilde X;\mathbb{P})K(\tilde X,\tilde X;P)^{-1}N_0(\tilde X)^\top N_0(X)K(X,X;P)^{-1}K(X,\mathbf{x};P) \\
&\quad - N_0(\mathbf{x};P)N_0(X;P)K(X,X;P)^{-1}K(X,\mathbf{x};P) - N_0(\mathbf{x};P)N_0(\tilde X;P)K(\tilde X,\tilde X;P)^{-1}K(\tilde X,\mathbf{x};P)\Big] && \text{(S271)}\\
&= \nu\sigma_{W_2}^2\eta + \nu E_{22} + \mathbb{E}\,\mathrm{tr}\,\Big(K(\tilde X,\tilde X;P)^{-1}(\tilde X^\top X + \nu\frac{\sigma_{W_2}^2}{n_1}f(W_1\tilde X)^T F)K(X,X;P)^{-1}K(X,\mathbf{x};P)K(\mathbf{x},\tilde X;P)\Big) && \text{(S272)}\\
&= H_{100}\,, && \text{(S273)}
\end{aligned}
$$

S6.7 H_{110}

$$\begin{aligned}
H_{110} &= \mathbb{E}\hat{y}(\mathbf{x}; P, X, \varepsilon)\hat{y}(\mathbf{x}; P, X, \tilde{\varepsilon}) && \text{(S274)}\\
&= \mathbb{E}\Big[N_0(\mathbf{x}; P)N_0(\mathbf{x}; P)^\top + K(\mathbf{x}, ; \mathbb{P})K(X, X; P)^{-1}Y(X, \tilde{\varepsilon})^\top Y(X, \varepsilon)K(X, X; P)^{-1}K(X, \mathbf{x}; P)\\
&\quad + K(\mathbf{x}, X; \mathbb{P})K(X, X; P)^{-1}N_0(X)^\top N_0(X)K(X, X; P)^{-1}K(X, \mathbf{x}; P)\\
&\quad - 2N_0(\mathbf{x}; P)N_0(X; P)K(X, X; P)^{-1}K(X, \mathbf{x}; P)\Big] && \text{(S275)}\\
&= \mathbb{E}\Big[N_0(\mathbf{x}; P)N_0(\mathbf{x}; P)^\top + K(\mathbf{x}, ; \mathbb{P})K(X, X; P)^{-1}X^\top XK(X, X; P)^{-1}K(X, \mathbf{x}; P)\\
&\quad + K(\mathbf{x}, X; \mathbb{P})K(X, X; P)^{-1}N_0(X)^\top N_0(X)K(X, X; P)^{-1}K(X, \mathbf{x}; P)\\
&\quad - 2N_0(\mathbf{x}; P)N_0(X; P)K(X, X; P)^{-1}K(X, \mathbf{x}; P)\Big] && \text{(S276)}\\
&= \nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{32} + \nu E_{33} && \text{(S277)}
\end{aligned}$$

S6.8 H_{111}

$$\begin{aligned}
H_{111} &= \mathbb{E}\hat{y}(\mathbf{x}; P, X, \varepsilon)\hat{y}(\mathbf{x}; P, X, \varepsilon) && \text{(S278)}\\
&= \mathbb{E}\Big[N_0(\mathbf{x}; P)N_0(\mathbf{x}; P)^\top + K(\mathbf{x}, ; \mathbb{P})K(X, X; P)^{-1}Y(X, \varepsilon)^\top Y(X, \varepsilon)K(X, X; P)^{-1}K(X, \mathbf{x}; P)\\
&\quad + K(\mathbf{x}, X; \mathbb{P})K(X, X; P)^{-1}N_0(X)^\top N_0(X)K(X, X; P)^{-1}K(X, \mathbf{x}; P)\\
&\quad - 2N_0(\mathbf{x}; P)N_0(X; P)K(X, X; P)^{-1}K(X, \mathbf{x}; P)\Big] && \text{(S279)}\\
&= \mathbb{E}\Big[N_0(\mathbf{x}; P)N_0(\mathbf{x}; P)^\top + K(\mathbf{x}, ; \mathbb{P})K(X, X; P)^{-1}(X^\top X + \sigma_\varepsilon^2 n_1 I_m)K(X, X; P)^{-1}K(X, \mathbf{x}; P)\\
&\quad + K(\mathbf{x}, X; \mathbb{P})K(X, X; P)^{-1}N_0(X)^\top N_0(X)K(X, X; P)^{-1}K(X, \mathbf{x}; P)\\
&\quad - 2N_0(\mathbf{x}; P)N_0(X; P)K(X, X; P)^{-1}K(X, \mathbf{x}; P)\Big] && \text{(S280)}\\
&= \nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{31} + E_{32} + \nu E_{33} && \text{(S281)}
\end{aligned}$$

S6.9 Combining results: asymptotic variance terms

Summarizing the above result, we have,

$$\begin{aligned}
H_{000} &= E_4\\
H_{001} &= E_4\\
H_{010} &= E_5\\
H_{011} &= E_5 + E_6\\
H_{100} &= \nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{71} + \nu E_{72}\\
H_{101} &= \nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{71} + \nu E_{72}\\
H_{110} &= \nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{32} + \nu E_{33}\\
H_{111} &= \nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{31} + E_{32} + \nu E_{33}\,,
\end{aligned}$$

which using eqn. (S18) gives,

$$B = 1 + E_{21} + E_4$$

$$
\begin{aligned}
&= \tau_2^2/\tau_1^2 \\
V_P &= H_{100} - H_{000} \\
&= \nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{71} + \nu E_{72} - E_4 \\
&= E_{71} - E_4 - \nu T_2/\tau_1' \\
&= \tau_2'/\tau_1' + 2\tau_2/\tau_1 - 1 - (\tau_2/\tau_1 - 1)^2 - \nu T_2/\tau_1' \\
&= \tau_2'/\tau_1' - B - \nu T_2/\tau_1' \\
V_X &= H_{010} - H_{000} \\
&= E_5 - E_4 \\
&= \phi\tilde{\tau}_2^2\big(\tilde{\tau}_2 + 1\big)^2/(1 - \phi\tilde{\tau}_2^2) \\
&= \phi B(\tau_1 - \tau_2)^2/(\tau_1^2 - \phi(\tau_1 - \tau_2)^2) \\
V_{\boldsymbol{\varepsilon}} &= H_{001} - H_{000} \\
&= 0 \\
V_{PX} &= H_{110} - H_{010} - H_{100} + H_{000} \\
&= \nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{32} + \nu E_{33} - E_5 - (\nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{71} + \nu E_{72}) + E_4 \\
&= E_{32} - E_{71} - E_5 + E_4 + \nu(E_{33} - E_{72}) \\
&= 1 - 2\tau_2/\tau_1 - \tau_2'/\tau_1^2 - (\tau_2'/\tau_1' - 2\tau_2/\tau_1 + 1) - V_X \\
&\quad + \nu\left[\sigma_{W_2}^2\left[\left(\tau_1 + (\sigma_{W_2}^2(\eta' - \zeta) + \gamma)\tau_1' + \sigma_{W_2}^2\zeta\tau_2'\right)/\tau_1^2 - \eta\right] - E_{22} - (T_2 - E_{22} - \eta\sigma_{W_2}^2))\right] \\
&= -\tau_2'/\tau_1^2 - \tau_2'/\tau_1' - V_X + \nu\left[\sigma_{W_2}^2\left[\left(\tau_1 + (\sigma_{W_2}^2(\eta' - \zeta) + \gamma)\tau_1' + \sigma_{W_2}^2\zeta\tau_2'\right)/\tau_1^2\right] - T_2)\right] \\
&= -\tau_2'/\tau_1^2 - B - V_P - V_X + \nu T_2/(\gamma\tau_1)^2 \\
V_{P\boldsymbol{\varepsilon}} &= H_{101} - H_{001} - H_{100} + H_{000} \\
&= \nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{71} + \nu E_{72} - E_4 - (\nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{71} + \nu E_{72}) + E_4 \\
&= 0 \\
V_{X\boldsymbol{\varepsilon}} &= H_{011} - H_{001} - H_{010} + H_{000} \\
&= E_5 + E_6 - E_4 - E_5 + E_4 \\
&= E_6 \\
&= \sigma_\varepsilon^2\phi\tilde{\tau}_2^2/(1 - \tilde{\tau}_2^2\phi) \\
&= \sigma_\varepsilon^2 V_X/B \\
V_{PX\boldsymbol{\varepsilon}} &= \nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{31} + E_{32} + \nu E_{33} - (E_5 + E_6) - (\nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{71} + \nu E_{72}) \\
&\quad - (\nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{32} + \nu E_{33}) + E_4 + E_5 + \nu\sigma_{W_2}^2\eta + \nu E_{22} + E_{71} + \nu E_{72} - E_4 \\
&= E_{31} - E_6 \\
&= \sigma_\varepsilon^2\big(-\tau_1'/\tau_1^2 - 1\big) - V_{X\boldsymbol{\varepsilon}}\,.
\end{aligned}
$$

Therefore, we have established the main result, Theorem S3.

S7 Proof of Corollary 1

S7.1 Bias is non-increasing

In terms of the auxiliary variables $\tilde{\tau}_1$ and $\tilde{\tau}_2$ defined in eqn. (S89), the coupled equations defining τ_1 and τ_2, eqn. (S42), simplify to

$$0 = \gamma\phi\tilde{\tau}_2 - \gamma\tilde{\tau}_1 + \sigma_{W_2}^2\left(\tilde{\tau}_2\left(\zeta\phi\tilde{\tau}_2 + \zeta + \phi\eta'\right) + \tilde{\tau}_1\left(\eta - \eta'\right) + \zeta\right) \tag{S282}$$

$$0 = \left(\tilde{\tau}_1 - \phi\tilde{\tau}_2\right)\left(\psi\tilde{\tau}_1\left(\zeta\tilde{\tau}_2 + \eta\right) + \zeta\phi\left(\tilde{\tau}_2 + 1\right)\right) + \zeta\phi\tilde{\tau}_1\left(\tilde{\tau}_2 + 1\right)\sigma_{W_2}^2\,. \tag{S283}$$

Eliminating $\tilde{\tau}_1$ from these equations gives,

$$\begin{aligned}\zeta\phi\left(\tilde{\tau}_2 + 1\right)\left(\left(\eta - \eta'\right)\sigma_{W_2}^2 - \gamma\right)\left(\tilde{\tau}_2\left(\zeta\phi\tilde{\tau}_2 + \phi(\gamma + \eta) + \zeta\right) + \sigma_{W_2}^2\left(\tilde{\tau}_2\left(\zeta\phi\tilde{\tau}_2 + \zeta + \phi\eta'\right) + \zeta\right) + \zeta\right)\\ = \psi\left(\zeta\tilde{\tau}_2 + \eta\right)\left(\tilde{\tau}_2\left(\zeta\phi\tilde{\tau}_2 + \zeta + \eta\phi\right) + \zeta\right)\left(\gamma\phi\tilde{\tau}_2 + \sigma_{W_2}^2\left(\tilde{\tau}_2\left(\zeta\phi\tilde{\tau}_2 + \zeta + \phi\eta'\right) + \zeta\right)\right)\end{aligned} \tag{S284}$$

Specializing to the random feature kernel ($\sigma_{W_2} = 0$), the equation becomes,

$$\left(\tilde{\tau}_2\left(\zeta\psi\tilde{\tau}_2 + \zeta + \eta\psi\right) + \zeta\right)\left(\tilde{\tau}_2\left(\zeta\phi\tilde{\tau}_2 + \zeta + \eta\phi\right) + \zeta\right) = -\gamma\zeta\phi\tilde{\tau}_2\left(\tilde{\tau}_2 + 1\right)\,. \tag{S285}$$

In the ridgeless limit, $\gamma = 0$, and the quartic equation factorizes into the product of two quadratic polynomials. The root of these equations that respects the conditions of Lemma 1 is given by

$$\tilde{\tau}_2 = \frac{-\zeta - \eta\omega + \sqrt{(\zeta + \eta\omega)^2 - 4\zeta^2\omega}}{2\zeta\omega}\,, \tag{S286}$$

where $\omega = \max\{\phi, \psi\}$. Next, recall from Theorem 1 that $B = \tau_2^2/\tau_1^2 = (1 + \tilde{\tau}_2)^2$ so that

$$\frac{\partial B}{\partial n_1} = -\frac{\psi^2}{n_0}\frac{\partial B}{\partial\psi}(1 + \tilde{\tau}_2)^2 = -2\frac{\psi^2}{n_0}(1 + \tilde{\tau}_2)\frac{\partial\tilde{\tau}_2}{\partial\psi}\,. \tag{S287}$$

To show that $\partial B/\partial n_1 \leq 0$, we show that $(1 + \tilde{\tau}_2) \geq 0$ and that $\partial\tilde{\tau}_2/\partial\psi \geq 0$. First of all,

$$\begin{aligned}1 + \tilde{\tau}_2 &= 1 + \frac{-\zeta - \eta\omega + \sqrt{(\zeta + \eta\omega)^2 - 4\zeta^2\omega}}{2\zeta\omega} &\text{(S288)}\\ &= \frac{-(-2\zeta\omega + \zeta + \eta\omega) + \sqrt{(\zeta + \eta\omega)^2 - 4\zeta^2\omega}}{2\zeta\omega} &\text{(S289)}\\ &\geq \frac{-\sqrt{(-2\zeta\omega + \zeta + \eta\omega)^2} + \sqrt{(\zeta + \eta\omega)^2 - 4\zeta^2\omega}}{2\zeta\omega} &\text{(S290)}\\ &= \frac{-\sqrt{(\zeta + \eta\omega)^2 - 4\zeta^2\omega - 4\zeta(\eta - \zeta)\omega^2} + \sqrt{(\zeta + \eta\omega)^2 - 4\zeta^2\omega}}{2\zeta\omega} \geq 0\,, &\text{(S291)}\end{aligned}$$

where we used the relation $\eta \geq \zeta$ which was proved in [26]. As for the derivative, note that $\partial\tilde{\tau}_2/\partial\psi = 0$ if $\psi < \phi$ and otherwise,

$$\begin{aligned}\frac{\partial\tilde{\tau}_2}{\partial\psi} &= \frac{-(-2\zeta\omega + \zeta + \eta\omega) + \sqrt{(\zeta + \eta\omega)^2 - 4\zeta^2\omega}}{2\omega^2\sqrt{(\zeta + \eta\omega)^2 - 4\zeta^2\omega}} &\text{(S292)}\\ &\geq \frac{-\sqrt{(-2\zeta\omega + \zeta + \eta\omega)^2} + \sqrt{(\zeta + \eta\omega)^2 - 4\zeta^2\omega}}{2\omega^2\sqrt{(\zeta + \eta\omega)^2 - 4\zeta^2\omega}} &\text{(S293)}\\ &= \frac{-\sqrt{(\zeta + \eta\omega)^2 - 4\zeta^2\omega - 4\zeta(\eta - \zeta)\omega^2} + \sqrt{(\zeta + \eta\omega)^2 - 4\zeta^2\omega}}{2\omega^2\sqrt{(\zeta + \eta\omega)^2 - 4\zeta^2\omega}} &\text{(S294)}\\ &\geq 0\,. &\text{(S295)}\end{aligned}$$

Therefore we have shown that

$$\frac{\partial B}{\partial n_1} \leq 0\,, \tag{S296}$$

i.e. the bias B is monotonically decreasing.

S7.2 Behavior near the interpolation boundary

From inspection of the expressions in Theorem 1, the bias and variance terms depend on τ_1 and τ_2 through four ratios, τ_2/τ_1, τ_2'/τ_1', τ_2'/τ_1^2 and τ_1'/τ_1^2. In the ridgeless ($\gamma = 0$) limit, these ratios can all be expressed in terms of $\tilde{\tau}_2$ by using eqns. (S87), (S88), (S89) and (S285).

We examine the behavior near the interpolation thereshold $\phi = \psi$ by taking the limit from both directions. It is straightforward algebraic substitution to show that for $\phi < \psi$,

$$\frac{\tau_2}{\tau_1} = \frac{\tau_2'}{\tau_1'} = 1 + \tilde{\tau}_2\,, \quad \frac{\tau_1'}{\tau_1^2} = \frac{\zeta\left(\tilde{\tau}_2+1\right)}{(\phi-\psi)\tilde{\tau}_2\left(\zeta\tilde{\tau}_2+\eta\right)}\,, \quad \frac{\tau_2'}{\tau_1^2} = \frac{\zeta\left(\tilde{\tau}_2+1\right)^2}{(\phi-\psi)\tilde{\tau}_2\left(\zeta\tilde{\tau}_2+\eta\right)}\,. \tag{S297}$$

From eqn. (S286), we see that $\tilde{\tau}_2$ is finite when $\phi = \psi$ so that the terms in eqn. (S297) obey,

$$\frac{\tau_2}{\tau_1} = \frac{\tau_2'}{\tau_1'} = \mathcal{O}(1)\,, \quad \frac{\tau_1'}{\tau_1^2} = \mathcal{O}\left(\frac{1}{\phi-\psi}\right)\,, \quad \frac{\tau_2'}{\tau_1^2} = \mathcal{O}\left(\frac{1}{\phi-\psi}\right)\,. \tag{S298}$$

Turning now to the case of $\phi > \psi$, similar algebraic substitutions yield,

$$\frac{\tau_2}{\tau_1} = \tilde{\tau}_2 + 1 \tag{S299}$$

$$\frac{\tau_2'}{\tau_1'} = \frac{\zeta^2\tilde{\tau}_2\left(\tilde{\tau}_2^2(-\psi+\phi+1)+3\tilde{\tau}_2+2\right)+\zeta\eta\left(\tilde{\tau}_2^3(\psi-\phi)+\tilde{\tau}_2^2(\phi-\psi)+\tilde{\tau}_2+1\right)+\eta^2\tilde{\tau}_2^2(\psi-\phi)}{\zeta\left(\zeta\tilde{\tau}_2\left(\tilde{\tau}_2^2(\phi-\psi)+\tilde{\tau}_2+2\right)+\eta\tilde{\tau}_2^2(\phi-\psi)+\eta\right)} \tag{S300}$$

$$\frac{\tau_1'}{\tau_1^2} = \frac{\zeta\left(\tilde{\tau}_2+1\right)}{\tilde{\tau}_2(\psi-\phi)\left(\zeta\tilde{\tau}_2+\eta\right)} - \frac{\zeta\tilde{\tau}_2\left(\tilde{\tau}_2+1\right)}{\zeta\tilde{\tau}_2\left(\tilde{\tau}_2+2\right)+\eta} \tag{S301}$$

$$\frac{\tau_2'}{\tau_1^2} = \frac{\zeta\left(\tilde{\tau}_2+1\right)^2}{\tilde{\tau}_2(\psi-\phi)\left(\zeta\tilde{\tau}_2+\eta\right)} + \frac{\tilde{\tau}_2\left(\tilde{\tau}_2+1\right)(\eta-\zeta)}{\zeta\tilde{\tau}_2\left(\tilde{\tau}_2+2\right)+\eta}\,. \tag{S302}$$

We can isolate the pole at $\phi = \psi$ by examining the relevant functions of $\tilde{\tau}_2$. In particular, substituting the solution (S286) gives,

$$\frac{\tau_2'}{\tau_1'}\Big|_{\psi=\phi} = \frac{\sqrt{(\zeta+\eta\phi)^2-4\zeta^2\phi}+2\zeta\phi-\zeta-\eta\phi}{2\zeta\phi} \tag{S303}$$

which is evidently finite when $\phi = \psi$ and,

$$\frac{\tilde{\tau}_2\left(\tilde{\tau}_2+1\right)}{\zeta\tilde{\tau}_2\left(\tilde{\tau}_2+2\right)+\eta} = \frac{2\zeta\phi}{(\zeta+\eta\phi)\sqrt{(\zeta+\eta\phi)^2-4\zeta^2\phi}+(\zeta+\eta\phi)^2-4\zeta^2\phi} \tag{S304}$$

whose denominator is a sum of non-negative terms that only vanishes if $\phi = 1$ and $\eta = \zeta$, i.e. the activation function is linear. Therefore, we find for $\phi > \psi$ the same behavior as for $\phi < \psi$, namely,

$$\frac{\tau_2}{\tau_1} = \frac{\tau_2'}{\tau_1'} = \mathcal{O}(1)\,, \quad \frac{\tau_1'}{\tau_1^2} = \mathcal{O}\left(\frac{1}{\phi-\psi}\right)\,, \quad \frac{\tau_2'}{\tau_1^2} = \mathcal{O}\left(\frac{1}{\phi-\psi}\right)\,. \tag{S305}$$

Altogether, we conclude that as $\phi \to \psi$,

$$B = \mathcal{O}(1)\,, \quad V_P = \mathcal{O}(1)\,, \quad V_X = \mathcal{O}(1)\,, \quad V_{X\varepsilon} = \mathcal{O}(1)\,, \quad V_{PX} = \mathcal{O}\left(\frac{1}{\phi-\psi}\right)\,, \quad V_{PX\varepsilon} = \mathcal{O}\left(\frac{1}{\phi-\psi}\right)\,, \tag{S306}$$

i.e. the only divergent terms are V_{PX} and $V_{PX\varepsilon}$.

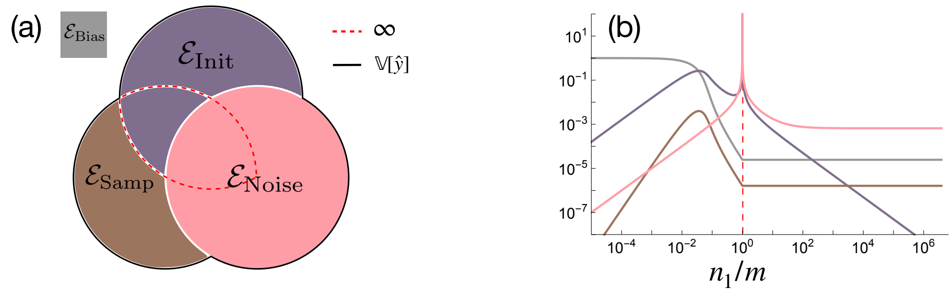


Figure S3: The multivariate variance decomposition of [35]. Following the setup of Fig. 1, panel (a) depicts the decomposition with a Venn diagram and panel (b) shows plots of the individual terms as functions of the overparameterization ratio n_1/m. The total variance is partitioned into three terms in a sequential manner, breaking the symmetry of the random variables and failing to account for their interactions. Since it is those interactions that cause the divergences (see Corollary 1), it is not possible to unambiguously attribute the divergences to a univariate source of variance, despite the the observed spikes in $\mathcal{E}_{\text{Noise}}$ and $\mathcal{E}_{\text{Init}}$.

S8 The Bias-Variance Decomposition of d'Ascoli *et al.* [35]

While finalizing this manuscript, we became aware of a related work [35] that similarly proposes and calculates a multivariate variance decomposition in order to examine the origins of double descent. Their approach is sequential in nature, first defining $\mathcal{E}_{\text{Noise}}$ to be the (expected) variance conditional on P and X, then $\mathcal{E}_{\text{Init}}$ to be the remaining variance conditional on X, and finally $\mathcal{E}_{\text{Samp}}$ to be the remaining variance. In terms of our fine-grained decomposition, their expressions read,

$$\mathcal{E}_{\text{Bias}} = B\,, \quad \mathcal{E}_{\text{Init}} = V_P + V_{PX}\,, \quad \mathcal{E}_{\text{Samp}} = V_X\,, \quad \mathcal{E}_{\text{Noise}} = V_{PX\varepsilon} + V_{X_\varepsilon} + V_{P\varepsilon} + V_\varepsilon\,. \tag{S307}$$

Fig. S3(a) illustrates their decomposition in terms of a Venn diagram and Fig. S3(b) shows how the components of their decomposition behave as the number of random features varies, similarly to Figs. 1 and S2. Note that their total bias and total variance agree with ours, and that their decomposition also resolves the two separate divergent terms at the interpolation threshold (since $\mathcal{E}_{\text{Noise}}$ contains $V_{PX\varepsilon}$ and $\mathcal{E}_{\text{Init}}$ contains V_{PX}). However, because their decomposition is not fully multivariate, the resulting areas do not necessarily possess the interpretations one might expect from the names "noise variance," "initialization variance," and "sampling variance." For example, the divergence in $\mathcal{E}_{\text{Noise}}$ ultimately comes from the contribution of $V_{PX\varepsilon}$, which vanishes when you ensemble over initial parameters, for example. This strong dependence on the parameters does not seem like a desirable property of a quantity designed to measure the variance due to noise. Similarly, the divergence of $\mathcal{E}_{\text{Init}}$ can be eliminated by ensembling (bagging) over different training samples, which also seems like a undesirable property of "initialization variance." The underlying reason for these inconsistent interpretations is that the divergences ultimately arise from the *interaction* terms V_{PX} and $V_{PX\varepsilon}$, but these interactions are not captured in their decomposition.