Abstract

Double descent refers to the phase transition that is exhibited by the generalization error of unregularized learning models when varying the ratio between the number of parameters and the number of training samples. The recent success of highly over-parameterized machine learning models such as deep neural networks has motivated a theoretical analysis of the double descent phenomenon in classical models such as linear regression which can also generalize well in the over-parameterized regime. We build on recent advances in Randomized Numerical Linear Algebra (RandNLA) to provide the first exact non-asymptotic expressions for double descent of the minimum norm linear estimator. Our approach involves constructing what we call a surrogate random design to replace the standard i.i.d. design of the training sample. This surrogate design admits exact expressions for the mean squared error of the estimator while preserving the key properties of the standard design. We also establish an exact implicit regularization result for over-parameterized training samples. In particular, we show that, for the surrogate design, the implicit bias of the unregularized minimum norm estimator precisely corresponds to solving a ridge-regularized least squares problem on the population distribution.

1 Introduction

Classical statistical learning theory asserts that to achieve generalization one must use training sample size that sufficiently exceeds the complexity of the learning model, where the latter is typically represented by the number of parameters (or some related structural parameter) [FHT01]. In particular, this seems to suggest the conventional wisdom that one should not use models that fit the training data exactly. However, modern machine learning practice often seems to go against this intuition, using models with so many parameters that the training data can be perfectly interpolated, in which case the training error vanishes. It has been shown that models such as deep neural networks, as well as certain so-called interpolating kernels and decision trees, can generalize well in this regime. In particular, recent work [BHMM19] empirically demonstrated a
phase transition in generalization performance of learning models which occurs at an *interpolation threshold*, i.e., a point where training error goes to zero (as one varies the ratio between the model complexity and the sample size). Moving away from this threshold in either direction tends to reduce the generalization error, leading to the so-called *double descent* curve.

To understand this surprising phenomenon, in perhaps the simplest possible setting, we study it in the context of linear or least squares regression. Consider a full rank $n \times d$ data matrix $X$ and a vector $y$ of responses corresponding to each of the $n$ data points (the rows of $X$), where we wish to find the best linear model $Xw \approx y$, parameterized by a $d$-dimensional vector $w$. The simplest example of an estimator that has been shown to exhibit the double descent phenomenon [BHX19] is the Moore-Penrose estimator, $\hat{w} = X^+y$: in the so-called over-determined regime, i.e., when $n > d$, it corresponds to the least squares solution, i.e., $\arg\min_w \|Xw - y\|^2$; and in the under-determined regime (also known as over-parameterized or interpolating), i.e., when $n < d$, it corresponds to the minimum norm solution to the linear system $Xw = y$. Given the ubiquity of linear regression and the Moore-Penrose solution, e.g., in kernel-based machine learning, studying the performance of this estimator can shed some light on the effects of over-parameterization/interpolation in machine learning more generally. Of particular interest are results that are exact (i.e., not upper/lower bounds) and non-asymptotic (i.e., for large but still finite $n$ and $d$).

We build on methods from Randomized Numerical Linear Algebra (RandNLA) in order to obtain exact non-asymptotic expressions for the mean squared error (MSE) of the Moore-Penrose estimator (see Theorem 1). This provides a precise characterization of the double descent phenomenon for perhaps the simplest and most ubiquitous regression problem. In obtaining these results, we are able to provide precise formulas for the *implicit regularization* induced by minimum norm solutions of under-determined training samples, relating it to classical ridge regularization (see Theorem 2). This result has been observed empirically for RandNLA methods [Mah11], but it has also been shown in deep learning [Ney17] and machine learning [Mah12] more generally. To obtain our precise results, we use a somewhat non-standard random design, which we term surrogate random design (see Section 2 for a detailed discussion), and which we expect will be of more general interest. In Theorem 3 and Section 5 we show, both theoretically and empirically, that our surrogate design accurately preserves the key properties of the original design when the data distribution is a multivariate Gaussian.

1.1 Main results: double descent and implicit regularization

As the performance metric in our analysis, we use the *mean squared error* (MSE), defined as $\text{MSE}[\hat{w}] = \mathbb{E}[\|\hat{w} - w^*\|^2]$, where $w^*$ is a fixed underlying linear model of the responses. In analyzing the MSE, we make the following standard assumption on the response noise.

**Assumption 1** (Homoscedastic noise). *Responses are $y(x) = x^T w^* + \xi$ where $\xi \sim \mathcal{N}(0,\sigma^2)$.*

Our main result provides an exact expression for the MSE of the Moore-Penrose estimator under our surrogate design denoted $S^\mu_n$, where $\mu$ is the $d$-variate distribution of the row vector $x^\top$ and $n$ is the sample size (details in Section 2). This surrogate is used in place of the standard $n \times d$ random design $X \sim \mu^n$, where $n$ data points (the rows of $X$) are sampled independently from $\mu$. Unlike for the standard design, our MSE formula is fully expressible as a function of the covariance matrix $\Sigma_\mu = \mathbb{E}_\mu[xx^\top]$. To state our main result, we need an additional minor assumption on $\mu$ which is
satisfied by most standard continuous distributions such as any multivariate Gaussian with positive definite covariance matrix.

**Assumption 2** (General position). For $1 \leq n \leq d$, if $X \sim \mu^n$, then $\text{rank}(X) = n$ almost surely.

Under Assumptions 1 and 2, we can establish our first main result, stated as the following theorem.

**Theorem 1** (Exact non-asymptotic MSE). If the response noise is homoscedastic with variance $\sigma^2$ (Assumption 1) and $\mu$ is in general position (Assumption 2), then for $X \sim S^\mu_n$ (Definition 4) and $\bar{y}_i = y(X_i)$, we have

$$\text{MSE}[\hat{X}^\dagger \hat{y}] = \begin{cases} 
\sigma^2 \text{tr}((\Sigma_{\mu} + \lambda_n I)^{-1}) \cdot \frac{1 - \alpha_n}{d - n} + \frac{w^* \Sigma_{\mu} + \lambda_n I)^{-1} w^*}{\text{tr}((\Sigma_{\mu} + \lambda_n I)^{-1})} \cdot (d - n), & \text{for } n < d, \\
\sigma^2 \text{tr}(\Sigma_{\mu}^{-1}), & \text{for } n = d, \\
\sigma^2 \text{tr}(\Sigma_{\mu}^{-1}) \cdot \frac{1 - \beta_n}{n - d}, & \text{for } n > d,
\end{cases}$$

where $\lambda_n \geq 0$ satisfies $\text{tr}(\Sigma_{\mu} (\Sigma_{\mu} + \lambda_n I)^{-1}) = n$, while $\alpha_n = \det(\Sigma_{\mu} (\Sigma_{\mu} + \lambda_n I)^{-1})$ and $\beta_n = e^{d-n}$.  

**Definition 1.** We will use $\mathcal{M}(\Sigma_{\mu}, w^*, \sigma^2, n)$ to denote the above expressions for $\text{MSE}[\hat{X}^\dagger \hat{y}]$.

For illustration, we plot these MSE expressions in Figure 1a, comparing them with empirical estimates. The plots show that varying the spectral decay of $\Sigma$ that our theory aligns well with the empirical estimates, whereas previously, no such theory was available except for special cases such as $\Sigma = I$ (more details in Theorem 3 and Section 5). The plots show that varying the spectral decay of $\Sigma$ has a significant effect on the shape of the curve in the under-determined regime. We use the horizontal line to denote the MSE of the null estimator $\text{MSE}[0] = \|w^*\|^2 = 1$. When the eigenvalues of $\Sigma$ decay rapidly, then the Moore-Penrose estimator suffers less error than the null estimator for some values of $n < d$, and the curve exhibits a local optimum in this regime.

One important aspect of Theorem 1 comes from the relationship between $n$ and the parameter $\lambda_n$, which together satisfy $n = \text{tr}(\Sigma_{\mu} (\Sigma_{\mu} + \lambda_n I)^{-1})$. This expression is precisely the classical notion of effective dimension for ridge regression regularized with $\lambda_n$ [AM15], and it arises here even though there is no explicit ridge regularization in the problem being considered in Theorem 1. The global solution to the ridge regression task (i.e., $\ell_2$-regularized least squares) with parameter $\lambda$ is defined as:

$$\argmin_w \left\{ \mathbb{E}_{\mu,y}[(x^\top w - y(x))^2] + \lambda\|w\|^2 \right\} = (\Sigma_{\mu} + \lambda I)^{-1} v_{\mu,y},$$

where $v_{\mu,y} = \mathbb{E}_{\mu,y}[y(x) x]$.

When Assumption 1 holds, then $v_{\mu,y} = \Sigma_{\mu} w^*$, however ridge-regularized least squares is well-defined for much more general response models. Our second result makes a direct connection between the (expectation of the) unregularized minimum norm solution on the sample and the global ridge-regularized solution. While the under-determined regime (i.e., $n < d$) is of primary interest to us, for completeness we state this result for arbitrary values of $n$ and $d$. Note that, just like the definition of regularized least squares, this theorem applies more generally than Theorem 1, in that it does not require the responses to follow any linear model as in Assumption 1.
(a) Surrogate MSE expressions (Theorem 1) closely match numerical estimates even for non-isotropic features. Eigenvalue decay leads to a steeper descent curve in the under-determined regime ($n < d$).

(b) The mean of the estimator $\mathbf{X}^T \mathbf{y}$ exhibits shrinkage which closely matches the shrinkage of a ridge-regularized least squares optimum (theory lines), as characterized by Theorem 2.

Figure 1: Illustration of the main results for $d = 100$ and $\mu = \mathcal{N}(\mathbf{0}, \Sigma)$ where $\Sigma$ is diagonal with eigenvalues decaying exponentially and scaled so that $\text{tr}(\Sigma^{-1}) = d$. We use our surrogate formulas to plot (a) the MSE (Theorem 1) and (b) the norm of the expectation (Theorem 2) of the Moore-Penrose estimator (theory lines), accompanied by the empirical estimates based on the standard i.i.d. design (error bars are three times the standard error of the mean). We consider three different condition numbers $\kappa$ of $\Sigma$, with isotropic corresponding to $\kappa = 1$, i.e., $\Sigma = \mathbf{I}$. In all cases, we use $\sigma^2 = \|\mathbf{w}^*\| = 1$ with $\mathbf{w}^* = \frac{1}{\sqrt{d}} \mathbf{1}$.

**Theorem 2** (Implicit regularization of Moore-Penrose estimator). For $\mu$ satisfying\(^1\) Assumption 2 and any $y(\cdot)$ such that $\mathbf{v}_{\mu,y} = \mathbb{E}_{\mu,y}[y(\mathbf{x}) \mathbf{x}]$ is well-defined, if $\mathbf{X} \sim S_{\mu}^n$ and $\bar{y}_i = y(\bar{x}_i)$, then

$$
\mathbb{E}[\bar{X}^T \bar{y}] = \begin{cases} 
(\Sigma_{\mu} + \lambda_n \mathbf{I})^{-1}\mathbf{v}_{\mu,y} & \text{for } n < d, \\
\Sigma_{\mu}^{-1}\mathbf{v}_{\mu,y} & \text{for } n \geq d,
\end{cases}
$$

where, as in Theorem 1, $\lambda_n$ is chosen so that the effective dimension $\text{tr}(\Sigma_{\mu}(\Sigma_{\mu} + \lambda_n \mathbf{I})^{-1})$ equals $n$.

That is, when $n < d$, the Moore-Penrose estimator (which itself is not regularized), computed on the random training sample, in expectation equals the global ridge-regularized least squares solution of the underlying regression problem. Moreover, $\lambda_n$, i.e., the amount of implicit $\ell_2$-regularization, is controlled by the degree of over-parameterization in such a way as to ensure that $n$ becomes the ridge effective dimension (a.k.a. the effective degrees of freedom).

We illustrate this result in Figure 1b, plotting the norm of the expectation of the Moore-Penrose estimator. As for the MSE, our surrogate theory aligns well with the empirical estimates for i.i.d. Gaussian designs, showing that the shrinkage of the unregularized estimator in the under-determined regime matches the implicit ridge-regularization characterized by Theorem 2. While

\(^1\)The proof of Theorem 2 can be easily extended to probability measures $\mu$ that do not satisfy Assumption 2 (such as discrete distributions). We include this assumption here to simplify the presentation.
the shrinkage is a linear function of the sample size $n$ for isotropic features (i.e., $\Sigma = I$), it exhibits a non-linear behavior for other spectral decays. Such implicit regularization has been studied previously [MO11, PM11, GM14, Mah12]; it has been observed empirically for RandNLA sampling algorithms [Mah11, MMY15]; and it has also received attention more generally within the context of neural networks [Ney17]. While our implicit regularization result is limited to the Moore-Penrose estimator, this new connection (and others, described below) between the minimum norm solution of an unregularized under-determined system and a ridge-regularized least squares solution offers a simple interpretation for the implicit regularization observed in modern machine learning architectures.

Our exact non-asymptotic expressions in Theorem 1 and our exact implicit regularization results in Theorem 2 are derived for the surrogate design, but Figure 1 suggests that they accurately describe the MSE (up to lower order terms) also under the standard i.i.d. design $X \sim \mu n$, particularly when $\mu$ is a multivariate Gaussian. As a third result, we can verify this in the cases where there exist known expressions for the MSE under the i.i.d. design (standard Gaussian for the under-determined setting, and arbitrary Gaussian for the over-determined one).

**Theorem 3** (Asymptotic consistency of surrogate design). Let $\rho = n/d \neq 1$, $X \sim \mu n$ and $y_i = y(x_i)$ satisfy Assumption 1. If $d \geq c_\rho = \frac{2}{|1-\rho|}$ and

$$
\mu = \begin{cases} 
N(0, I) & \text{when } n < d - 1, \\
N(0, \Sigma), \Sigma > 0 & \text{when } n > d + 1,
\end{cases}
$$

then the absolute difference between surrogate expressions and the true MSE is bounded as follows:

$$
\left| \text{MSE}[X^\top y] - \mathcal{M}(\Sigma, w^*, \sigma^2, n) \right| \leq \frac{c_\rho}{d} \cdot \mathcal{M}(\Sigma, w^*, \sigma^2, n).
$$

**Remark 1.** For $n$ equal to $d - 1$, $d$ or $d + 1$, the true MSE under Gaussian random design can be infinite, whereas the surrogate MSE is finite and has a closed form expression.

Empirical estimates given in Figure 1 suggest that the consistency of surrogate expressions holds much more generally than it is stated above. Based on a detailed empirical analysis described in Section 5.2, we conjecture that an asymptotic consistency result of the form similar to the statement of Theorem 3 holds true in the under-determined regime without the assumption that $\Sigma = I$. In this case, no formula is known for MSE$[X^\top y]$, whereas the expressions for the surrogate Gaussian design naturally extend.

### 1.2 Key techniques: surrogate designs and determinant preserving matrices

The standard random design model for linear regression assumes that each pair $(x_i^\top, y_i)$ is drawn independently, where the row vector $x_i^\top$ comes from some $d$-variate distribution $\mu$ and $y_i = y(x_i)$ is a random response variable drawn conditionally on $x_i$. Precise theoretical analysis of under-determined regression in this setting poses significant challenges, even in such special cases as the Moore-Penrose estimator and a Gaussian data distribution $\mu$. Rather than trying to directly analyze the usual i.i.d. random design $X \sim \mu n$ described above, we modify it slightly by introducing the notion of a surrogate random design, $\tilde{X} \sim S^\mu_n$. Informally, the goal of a surrogate random design is to modify an original design to capture the main properties of the original design, while being “nicer” for theoretical or empirical analysis. In particular, here, we will modify the distribution of matrix $X$ so as to:
1. closely preserve the behavior of the Moore-Penrose estimator from the i.i.d. design; and
2. obtain exact expressions for double descent in terms of the mean squared error.

A key element in the construction of our surrogate designs involves rescaling the measure $X \sim \mu^n$ by the pseudo-determinant $\text{pdet}(XX^\top)$, i.e., a product of the non-zero eigenvalues. A similar type of determinantal design was suggested in prior work [DWH19b], but it was restricted there only to $n \geq d$. We broaden this definition by not only allowing the sample size to be less than $d$, but also allowing it to be randomized. Our definition of a determinantal design matrix $\bar{X}$ follows by expressing $E_r F_p \bar{X} q s$ for any real-valued function $F_p \bar{X} q s$ as (see Definition 2):

$$E_r F_p \bar{X} q s \propto E[\text{pdet}(XX^\top)F(X)],$$

where $X \sim \mu^K$ and $K$ is a random variable. Then, we define (in Definition 3) our surrogate design $S^n_\mu$ for each $n > 0$ as a determinantal design with a carefully chosen random variable $K$, so that the expected sample size is equal to $n$ and so that it is possible to derive closed form expressions for the MSE. We achieve this by using modifications of the Poisson distribution to construct the variable $K$.

The key technical contribution that allows us to derive the MSE for determinantal designs is the concept of \textit{determinant preserving random matrices}, a notion that we expect to be useful more generally. Specifically, in Section 3 we define a class of $d \times d$ random matrices $A$ for which taking the determinant commutes with taking the expectation, for the matrix itself and any of its square submatrices (see Definition 4):

$$E[\det(A_{\mathcal{I},\mathcal{J}})] = \det(E[A_{\mathcal{I},\mathcal{J}}]) \text{ for all } \mathcal{I}, \mathcal{J} \subseteq [d] \text{ s.t. } |\mathcal{I}| = |\mathcal{J}|.$$

Not all random matrices satisfy this property, however many interesting and non-trivial examples can be found. Constructing these examples is facilitated by the closure properties that this class enjoys. In particular, if $A$ and $B$ are determinant preserving and independent, then $A + B$ and $AB$ are also determinant preserving (see Lemma 3). We use these techniques to prove a number of determinantal expectation formulas. For example, we show that if $X \sim \mu^K$, where $K$ is a Poisson random variable, then:

(Lemma 4) $E[\det(X^\top X)] = \det(E[X^\top X])$,

(Lemma 6) $E[\det(XX^\top)] = e^{-E[K]} \det(I + E[X^\top X])$.

These formulas are used to derive the normalization constants for our surrogate design distribution, which are later used in proving Theorems 1 and 2.

1.3 Related work

There is a large body of related work, which for simplicity we cluster into three groups.

\textbf{Double descent.} The double descent phenomenon (a term introduced by [BHMM19]) corresponds to the phase transition in the generalization error that occurs when the ratio between the model complexity and the sample size crosses the so-called interpolation threshold. It has been observed empirically in a number of learning models, including neural networks [BHMM19, GJS+19], kernel methods [BMM18, BRT19], nearest neighbor models [BHM18], and decision trees.
The theoretical analysis of double descent, and more broadly the generalization properties of interpolating estimators, have primarily focused on various forms of linear regression. The most comparable to our work are [BLLT19, LR19] and [HMRT19], who provide non-asymptotic upper/lower bounds and asymptotic formulas, respectively, for the generalization error of the Moore-Penrose estimator under essentially the same i.i.d. random design setting as ours. On the other hand, [MVSS19] provide bounds for the error of the ideal linear interpolator (instead of the minimum norm one). Note that while we analyze the classical mean squared error, many works focus on the squared prediction error instead (some of them still refer to it as the MSE). Another line of literature deals with linear regression in the so-called misspecified setting, where the set of observed features does not match the feature space in which the response model is linear [BHX19, HMRT19, Mit19, MM19b], e.g., when the learner observes a random subset of $d$ features from a larger population. This is an important distinction, because it allows varying the model complexity by changing the number of observed features while keeping the linear model fixed (see further discussion in Section 6). We believe that our results can be extended to this important setting, and we leave this as a direction for future work.

**RandNLA.** Randomized numerical linear algebra [Mah11, DM16, DM17] has traditionally focused on obtaining algorithmic improvements for tasks such as least squares and low-rank approximation via techniques that include sketching [Sar06] and i.i.d. leverage score sampling [DMM06]. However, there has been growing interest in understanding the statistical properties of these randomized methods [MMY15, RM16], for example looking at the mean squared error of the least squares estimator obtained via i.i.d. subsampling under the standard linear response model. Determinantal sampling methods (a.k.a. volume sampling, or determinantal point processes), which first found their way into RandNLA in the context of low-rank approximation [DRVW06], have been recently shown to combine strong worst-case guarantees with elegant statistical properties. In particular, [DW17] showed that the least-squares estimator subsampled via the so-called size $d$ volume sampling (loosely corresponding to the special case of our surrogate design $S^n_\mu$ where $n = d$) is an unbiased estimator that admits exact formulas for both the expected square loss (a worst-case metric) and the mean squared error (a statistical metric). These results were developed further by [DWH18, DWH19a, DCMW19], however they were still limited to the over-determined setting (with the exception of [DW18a, DLM19] who gave upper bounds on the mean squared error of the ridge estimator under different determinantal samplings). Also in the over-determined setting, [DWH19b] provided evidence for the fact that determinantal rescaling can be used to modify the original data distribution (particularly, a multivariate Gaussian) without a significant distortion to the estimator, while making certain statistical quantities expressible analytically. We take this direction further by analyzing the unregularized least squares estimator in the under-determined setting which is less well understood, partly due to the presence of implicit regularization.

**Implicit regularization.** The term implicit regularization typically refers to the notion that approximate computation (e.g., rather than exactly minimizing a function $f$, instead running an approximation algorithm to get an approximately optimal solution) can implicitly lead to statistical regularization (e.g., exactly minimizing an objective of the form $f + \lambda g$, for some well-specified $\lambda$ and $g$). See [MO11, PM11, GM14] and references therein for early work on the topic; and see [Mah12] for an overview. More recently, often motivated by neural networks, there has been work on implicit regularization that typically considered SGD-based optimization algorithms. See, e.g., theoretical results on simplified models [NTS14, Ney17, SHN+18, GWB+17, ACHL19, KBMM19] as well as extensive empirical and phenomenological results on state-of-the-art neural network
models [MM18, MM19a]. The implicit regularization observed by us is different in that it is not caused by an inexact approximation algorithm (such as SGD) but rather by the selection of one out of many exact solutions (e.g., the minimum norm solution). In this context, most relevant are the asymptotic results of [LJB19] (which used the asymptotic risk results for ridge regression of [DW18b]) and [KLS18]. Our non-asymptotic results are also related to recent work in RandNLA on the expectation of the inverse [DM19] and generalized inverse [MDK19] of a subsampled matrix.

2 Surrogate random designs

In this section, we provide the definition of our surrogate random design $S^n_\mu$, where $\mu$ is a $d$-variate probability measure and $n$ is the sample size. This distribution is used in place of the standard random design $\mu^n$ consisting of $n$ row vectors drawn independently from $\mu$. Our surrogate design uses determinantal rescaling to alter the joint distribution of the vectors so that certain expected quantities (such as the mean squared error of the Moore-Penrose estimator) can be expressed in a closed form. We start by introducing notation.

**Preliminaries.** The set $\{1, \ldots, n\}$ will be denoted by $[n]$. For an $n \times n$ matrix $A$, we use $p\text{det}(A)$ to denote the pseudo-determinant of $A$, which is the product of non-zero eigenvalues. For index subsets $I$ and $J$, we use $A_{I,J}$ to denote the submatrix of $A$ with rows indexed by $I$ and columns indexed by $J$. We may write $A_{I,*}$ to indicate that we take a subset of rows. We use $\text{adj}(A)$ to denote the adjugate of $A$, defined as follows: the $(i,j)$th entry of $\text{adj}(A)$ is $(-1)^{i+j} \det(A_{[n] \setminus (i), [n] \setminus (j)})$. We will use two useful identities related to the adjugate: (1) $\text{adj}(A) = \det(A) A^{-1}$ for invertible $A$, and (2) $\det(A + uv^T) = \det(A) + v^T \text{adj}(A) u$. For a probability measure $\mu$ over $\mathbb{R}^d$, we use $x^\top \sim \mu$ to denote a random row vector $x^\top$ sampled according to this distribution. We let $X \sim \mu^k$ denote a $k \times d$ random matrix with rows drawn i.i.d. according to $\mu$, and the $i$th row is denoted as $x_i^\top$. We also let $\Sigma_{\mu} = \mathbb{E}_\mu[xx^\top]$, where $\mathbb{E}_{\mu}$ refers to the expectation with respect to $x^\top \sim \mu$, assuming throughout that $\Sigma_{\mu}$ is well-defined and positive definite. We use Poisson($\gamma)_{\leq a}$ as the Poisson distribution restricted to values less than or equal to $a$, and a similar convention is used for the restriction to values greater or equal a. Finally, we use $\#(X)$ to denote the number of rows of $X$.

We now define a family of determinantal distributions over random matrices $\tilde{X}$, where not only the entries but also the number of rows is randomized. This randomized sample size is a crucial property of our designs that enables our analysis. Our definition follows by expressing $\mathbb{E}[F(X)]$ for real-valued functions $F : \bigcup_{k \geq 0} \mathbb{R}^{k \times d} \rightarrow \mathbb{R}$ (the expectation may be undefined for some functions).

**Definition 2.** Let $\mu$ satisfy Assumption 2 and let $K$ be a random variable over non-negative integers. A determinantal design $\tilde{X} \sim \text{Det}(\mu, K)$ is a distribution such that for any $F(\cdot)$ as above,

$$\mathbb{E}[F(\tilde{X})] \propto \mathbb{E}[p\text{det}(XX^\top) F(X)] \quad \text{for} \quad X \sim \mu^K.$$ 

Setting $F(\cdot)$ to 1, observe that the proportionality constant must be $1/\mathbb{E}[p\text{det}(XX^\top)]$. The above definition can be interpreted as rescaling the density function of $\mu^K$ by the pseudo-determinant, and then renormalizing it.

We now construct our surrogate design $S^n_\mu$ by appropriately selecting the random variable $K$. One might be tempted to use the obvious choice of $K = n$, but this does not result in simple closed form expressions for the MSE in the under-determined regime (i.e., $n < d$), which is the regime of primary interest to us. Instead, we derive our random variables $K$ from the Poisson distribution.

**Definition 3.** For $\mu$ satisfying Assumption 2, define surrogate design $S^n_\mu$ as $\text{Det}(\mu, K)$ where:
1. if \( n < d \), then \( K \sim \text{Poisson}(\gamma_n) \leq d \) with \( \gamma_n \) being the solution of \( n = \text{tr}(\Sigma_\mu(\Sigma_\mu + \frac{1}{\gamma_n} I)^{-1}) \),
2. if \( n = d \), then we simply let \( K = d \),
3. if \( n > d \), then \( K \sim \text{Poisson}(\gamma_n) \geq d \) with \( \gamma_n = n - d \).

Note that the under-determined case, i.e., \( n < d \), is restricted to \( K \leq d \) so that, under Assumption 2, \( \text{pdet}(XX^\top) = \text{det}(XX^\top) \) with probability 1. On the other hand in the over-determined case, i.e., \( n > d \), we have \( K \geq d \) so that \( \text{pdet}(XX^\top) = \text{det}(X^\top X) \). In the special case of \( n = d = K \) both of these equations are satisfied: \( \text{pdet}(XX^\top) = \text{det}(X^\top X) = \text{det}(XX^\top) = \text{det}(X)^2 \).

The first non-trivial property of the surrogate design \( S_\mu^n \) is that the expected sample size is in fact always equal to \( n \), which we prove at the end of this section.

**Lemma 1.** Let \( \bar{X} \sim S_\mu^n \) for any \( n > 0 \). Then, we have \( \mathbb{E}[\#(\bar{X})] = n \).

Our general template for computing expectations under a surrogate design \( \bar{X} \sim S_\mu^n \) is to use the following expressions based on the i.i.d. random design \( X \sim \mu^K \):

\[
\mathbb{E}[F(\bar{X})] = \begin{cases} 
\frac{\mathbb{E}[\text{det}(XX^\top)F(X)]}{\mathbb{E}[\text{det}(XX^\top)]} & K \sim \text{Poisson}(\gamma_n) \quad \text{for } n < d, \\
\frac{\mathbb{E}[\text{det}(X)^2F(X)]}{\mathbb{E}[\text{det}(X)^2]} & K = d \quad \text{for } n = d, \\
\frac{\mathbb{E}[\text{det}(X^\top X)F(X)]}{\mathbb{E}[\text{det}(X^\top X)]} & K \sim \text{Poisson}(\gamma_n) \quad \text{for } n > d.
\end{cases}
\]

These formulas follow from Definitions 2 and 3 because the determinants \( \text{det}(XX^\top) \) and \( \text{det}(X^\top X) \) are non-zero precisely in the regimes \( n \leq d \) and \( n \geq d \), respectively, which is why we can drop the restrictions on the range of the Poisson distribution. Crucially, the normalization constants for computing the expectations can be obtained using the following formulas: if \( X \sim \mu^K \) then

\begin{align*}
\text{(Lemma 6)} & \quad \mathbb{E}[\text{det}(XX^\top)] = e^{-\gamma_n} \text{det}(I + \gamma_n \Sigma_\mu) & \quad \text{for } K \sim \text{Poisson}(\gamma_n), \ n < d, \\
\text{(Lemma 5)} & \quad \mathbb{E}[\text{det}(X)^2] = d! \text{det}(\Sigma_\mu), & \quad \text{for } K = n = d, \\
\text{(Lemma 4)} & \quad \mathbb{E}[\text{det}(X^\top X)] = \text{det}(\gamma_n \Sigma_\mu), & \quad \text{for } K \sim \text{Poisson}(\gamma_n), \ n > d.
\end{align*}

**Remark 2.** We will use \( Z_{\mu}^n \) as a shorthand for the above normalization constants.

We prove Lemmas 4 and 6 in Section 3 by introducing the concept of determinant preserving random matrices. The lemmas play a crucial role in deriving a number of new expectation formulas for the under- and over-determined surrogate designs that we use to prove Theorems 1 and 2 in Section 4. On the other hand, Lemma 5 and the design \( S_\mu^d \) can be found in the literature [vdV65, DWH19b], and we will rely on those known results in this special case. Importantly, the \( n = d \) case offers a continuous transition between the under- and over-determined regimes because the distribution \( S_\mu^n \) converges to \( S_\mu^d \) when \( n \) approaches \( d \) from above and below. Another important property of the design \( S_\mu^d \) is that it can be used to construct an over-determined design for any \( n > d \). A similar version of this result was also previously shown by [DWH19b] for a different determinantal design.

**Lemma 2.** Let \( \bar{X} \sim S_\mu^d \) and \( X \sim \mu^K \), where \( K \sim \text{Poisson}(\gamma) \). Then the matrix composed of a random permutation of the rows from \( \bar{X} \) and \( X \) is distributed according to \( S_\mu^{d+\gamma} \).
Proof. Let \( \tilde{X} \) denote the matrix constructed from the permuted rows of \( \tilde{X} \) and \( X \). Letting \( Z \sim \mu^{K+d} \), we derive the expectation \( \mathbb{E}[F(\tilde{X})] \) by summing over the possible index subsets \( S \subseteq [K+d] \) that correspond to the rows coming from \( \tilde{X} \):

\[
\mathbb{E}[F(\tilde{X})] = \mathbb{E}\left[ \frac{1}{(K+d)!} \sum_{|S|=d} \mathbb{E}[\det(Z_{S,S})^2 F(Z) | K] \right] = \sum_{k=0}^{\infty} \frac{\gamma^k e^{-\gamma}}{k!} \frac{\gamma^d k!}{(k+d)!} \mathbb{E}\left[ \sum_{|S|=d} \det(Z_{S,S})^2 F(Z) | K = k \right]
\]

\[
= \sum_{k=0}^{\infty} \frac{\gamma^k e^{-\gamma}}{k!} \frac{\gamma^d}{(k+d)!} \mathbb{E}\left[ \det(Z^r F(Z) | K = k \right] ,
\]

where (\( * \)) uses the Cauchy-Binet formula to sum over all subsets \( S \) of size \( d \). Finally, since the sum shifts from \( k \) to \( k+d \), the last expression can be rewritten as \( \mathbb{E}[\det(X^r X) F(X)]/\det(\gamma \Sigma) \), where recall that \( X \sim \mu^K \) and \( K \sim \text{Poisson}(\gamma) \), matching the definition of \( S_{\mu}^d+\gamma \).

We now return to the proof of Lemma 1, where we establish that the expected sample size of \( S_{\mu}^n \) is indeed \( n \).

Proof. (of Lemma 1) The result is obvious when \( n = d \), whereas for \( n > d \) it is an immediate consequence of Lemma 2. Finally, for \( n < d \) the expected sample size follows as a corollary of a more general expectation formula proven in Section 4, which states that

\[
(\text{Lemma 8}) \quad \mathbb{E}[I - \tilde{X}^\dagger \tilde{X}] = (\gamma_n \Sigma + I)^{-1},
\]

where \( \tilde{X}^\dagger \tilde{X} \) is the orthogonal projection onto the subspace spanned by the rows of \( \tilde{X} \). Since the rank of this subspace is equal to the number of the rows, we have \( \#(\tilde{X}) = \text{tr}(\tilde{X}^\dagger \tilde{X}) \), so

\[
\mathbb{E}[\#(X)] = d - \text{tr}((\gamma_n \Sigma + I)^{-1}) = \text{tr}(\gamma_n \Sigma \gamma_n \Sigma + I)^{-1}) = n,
\]

which completes the proof.

\( \square \)

3 Determinant preserving random matrices

In this section, we introduce the key tool for computing expectation formulas of matrix determinants. It is used in our analysis of the surrogate design, and it should be of independent interest.

The key question motivating the following definition is: when does taking expectation commute with computing a determinant for a square random matrix?

Definition 4. A random \( d \times d \) matrix \( A \) is called determinant preserving (d.p.), if

\[
\mathbb{E}[\det(A_{\mathcal{I},\mathcal{J}})] = \det(\mathbb{E}[A_{\mathcal{I},\mathcal{J}}]) \quad \text{for all } \mathcal{I}, \mathcal{J} \subseteq [d] \text{ s.t. } |\mathcal{I}| = |\mathcal{J}|.
\]

Note that from the definition of an adjugate matrix (see Section 2) it immediately follows that if \( A \) is determinant preserving then adjugate commutes with expectation for this matrix:

\[
\mathbb{E}[(\text{adj}(A))_{i,j}] = \mathbb{E}[(-1)^{i+j} \det(A_{[d]\setminus\{i\},[d]\setminus\{j\}})]
\]

\[
= (-1)^{i+j} \det(\mathbb{E}[A_{[d]\setminus\{i\},[d]\setminus\{j\}})] = (\text{adj}(\mathbb{E}[A]))_{i,j}. \tag{1}
\]
We next give a few simple examples to provide some intuition. First, note that every $1 \times 1$ random matrix is determinant preserving simply because taking a determinant is an identity transformation in one dimension. Similarly, every fixed matrix is determinant preserving because in this case taking the expectation is an identity transformation. In all other cases, however, Definition 4 has to be verified more carefully. Further examples (positive and negative) follow.

**Example 1.** If $A$ has i.i.d. Gaussian entries $a_{ij} \sim \mathcal{N}(0, 1)$, then $A$ is d.p. because $E[\det(A)] = 0$.

In fact, it can be shown that all random matrices with independent entries are determinant preserving. However, this is not a necessary condition.

**Example 2.** Let $A = sZ$, where $Z$ is fixed with rank $r$, and $s$ is a scalar random variable. Then for $|I| = |J| = r$ we have

$$E[\det(sZ_{I,J})] = E[s'] \det(Z_{I,J}) = \det((E[s'])^{\frac{1}{2}}Z_{I,J}),$$

so if $r = 1$ then $A$ is determinant preserving, whereas if $r > 1$ and $\text{Var}[s] > 0$ then it is not.

To construct more complex examples, we show that determinant preserving random matrices are closed under addition and multiplication. The proof of this result is an extension of an argument given by [DM19] (Lemma 7) for computing the expected determinant of the sum of rank-1 random matrices.

**Lemma 3.** If $A, B$ are independent and d.p. then $A + B$ and $AB$ are also determinant preserving.

**Proof.** First, we show that $A + uv^T$ is d.p. for any fixed $u, v \in \mathbb{R}^d$. Below, we use a standard identity for the rank one update of a determinant: $\det(A + uv^T) = \det(A) + v^T \text{adj}(A)u$. It follows that for any $I$ and $J$ of the same size,

$$E[\det(A_{I,J} + u_I v_J^T)] = E[\det(A_{I,J}) + v_J^T \text{adj}(A_{I,J})u_I]$$

$$\overset{(*)}{=} E[\det(A_{I,J})] + v_J^T \text{adj}(E[A_{I,J}])u_I$$

$$= \det(E[A_{I,J} + u_I v_J^T]),$$

where $(*)$ used (1), i.e., the fact that for d.p. matrices, adjugate commutes with expectation. Crucially, through the definition of an adjugate this step implicitly relies on the assumption that all the square submatrices of $A_{I,J}$ are also determinant preserving. Iterating this, we get that $A + Z$ is d.p. for any fixed $Z$. We now show the same for $A + B$:

$$E[\det(A_{I,J} + B_{I,J})] = E\left[E[\det(A_{I,J} + B_{I,J}) | B]\right]$$

$$\overset{(*)}{=} E[\det(E[A_{I,J}] + B_{I,J})]$$

$$= \det(E[A_{I,J} + B_{I,J}]),$$

where $(*)$ uses the fact that after conditioning on $B$ we can treat it as a fixed matrix. Next, we
show that $AB$ is determinant preserving via the Cauchy-Binet formula:

$$
\mathbb{E}[\det((AB)_{I,J})] = \mathbb{E}[\det(A_{I,*}B_{*,J})]
= \mathbb{E}
\left[
\sum_{S: |S| = |I|} \det(A_{I,S}) \det(B_{S,J})
\right]
= \sum_{S: |S| = |I|} \det(\mathbb{E}[A]_{I,S}) \det(\mathbb{E}[B]_{S,J})
= \det(\mathbb{E}[A]_{I,*} \mathbb{E}[B]_{*,J}),
$$

where recall that $A_{I,*}$ denotes the submatrix of $A$ consisting of its (entire) rows indexed by $I$. \hfill □

Finally, we introduce another important class of d.p. matrices: a sum of i.i.d. rank-1 random matrices with the number of i.i.d. samples being a Poisson random variable. Our use of the Poisson distribution is crucial for the below result to hold. It is an extension of an expectation formula given by [Der19] for sampling from discrete distributions.

**Lemma 4.** If $K$ is a Poisson random variable and $A, B$ are random $K \times d$ matrices whose rows are sampled as an i.i.d. sequence of joint pairs of random vectors, then $A^\top B$ is d.p., and in particular,

$$
\mathbb{E}
\left[
\det(A^\top B)
\right]
= \det(\mathbb{E}[A^\top B]).
$$

To prove the above result, we will use the following lemma, many variants of which appeared in the literature (e.g., [vdV65]). We use the one given by [DWH19a].

**Lemma 5 ([DWH19a]).** If the rows of random matrices $A, B \in \mathbb{R}^{k \times d}$ are sampled as an i.i.d. sequence of $k \geq d$ pairs of joint random vectors, then

$$
k^d \mathbb{E}
\left[
\det(A^\top B)
\right]
= k^d \det(\mathbb{E}[A^\top B]).
$$

(2)

Here, we use the following standard shorthand: $k^d = \frac{k!}{(k-d)!} = k(k-1) \cdots (k-d+1)$. Note that the above result almost looks like we are claiming that the matrix $A^\top B$ is d.p., but in fact it is not because $k^d \neq k^d$. The difference in those factors is precisely what we are going to correct with the Poisson random variable. We now present the proof of Lemma 4.

**Proof.** (of Lemma 4) Without loss of generality, it suffices to check Definition 4 with both $I$ and $J$ equal $[d]$. We first expand the expectation by conditioning on the value of $K$ and letting $\gamma = \mathbb{E}[K]$:

$$
\mathbb{E}[\det(A^\top B)]
= \sum_{k=0}^{\infty} \mathbb{E}[\det(A^\top B) \mid K = k] \Pr(K = k)
= \sum_{k=d}^{\infty} \frac{k! (k-d)!}{(k-d)!} \det(\mathbb{E}[A^\top B \mid K = k]) \frac{\gamma^{k-d} e^{-\gamma}}{k!}
= \sum_{k=d}^{\infty} \left(\frac{\gamma}{k}\right)^d \det(\mathbb{E}[A^\top B \mid K = k]) \frac{\gamma^{k-d} e^{-\gamma}}{(k-d)!}.
$$
Note that $\frac{1}{k} \mathbb{E}[\mathbf{A}^\top \mathbf{B} \mid K = k] = \mathbb{E}[\mathbf{A}^\top \mathbf{B}]$, which is independent of $k$. Thus we can rewrite the above expression as:

$$\det(\mathbb{E}[\mathbf{A}^\top \mathbf{B}]) \sum_{k=d}^{\infty} \frac{\gamma^{k-d}e^{-\gamma}}{(k-d)!} = \det(\mathbb{E}[\mathbf{A}^\top \mathbf{B}]) \sum_{k=0}^{\infty} \frac{\gamma^k e^{-\gamma}}{k!} = \det(\mathbb{E}[\mathbf{A}^\top \mathbf{B}]),$$

which concludes the proof. \( \square \)

Finally we use Lemma 4 combined with Lemma 3 to show the expectation formula needed for obtaining the normalization constant of the under-determined surrogate design (proven by setting $\mathbf{A} = \mathbf{B} = \mathbf{X} \sim \mu^K$). Note that the below result is more general than the normalization constant requires, because it allows the matrices $\mathbf{A}$ and $\mathbf{B}$ to be different. In fact, we will use this more general statement later on in our analysis.

**Lemma 6.** If $K$ is a Poisson random variable and $\mathbf{A}$, $\mathbf{B}$ are random $K \times d$ matrices whose rows are sampled as an i.i.d. sequence of joint pairs of random vectors, then

$$\mathbb{E}[\det(\mathbf{A} \mathbf{B}^\top)] = e^{-\mathbb{E}[K]} \det(\mathbf{I} + \mathbb{E}[\mathbf{B}^\top \mathbf{A}]).$$

**Proof.** By Lemma 4, the matrix $\mathbf{B}^\top \mathbf{A}$ is determinant preserving. Applying Lemma 3 we conclude that $\mathbf{I} + \mathbf{B}^\top \mathbf{A}$ is also d.p., so

$$\det(\mathbf{I} + \mathbb{E}[\mathbf{B}^\top \mathbf{A}]) = \mathbb{E}[\det(\mathbf{I} + \mathbf{B}^\top \mathbf{A})] = \mathbb{E}[\det(\mathbf{I} + \mathbf{A} \mathbf{B}^\top)],$$

where the second equality is known as Sylvester’s Theorem. We now use the following standard determinantal formula.

**Lemma 7 ([KT12]).** For any $k \times d$ matrices $\mathbf{A}, \mathbf{B}$ we have $\det(\mathbf{I} + \mathbf{A} \mathbf{B}^\top) = \sum_{S \subseteq [k]} \det(\mathbf{A}_{S,*} \mathbf{B}_{S,*}^\top)$. We rewrite the expectation of $\det(\mathbf{I} + \mathbf{A} \mathbf{B}^\top)$ by applying the lemma. Letting $\gamma = \mathbb{E}[K]$, we obtain:

$$\mathbb{E}[\det(\mathbf{I} + \mathbf{A} \mathbf{B}^\top)] = \mathbb{E}\left[ \sum_{S \subseteq [k]} \mathbb{E}[\det(\mathbf{A}_{S,*} \mathbf{B}_{S,*}^\top) \mid K]\right]$$

$$= \sum_{i=0}^{\infty} \frac{\gamma^i e^{-\gamma}}{i!} \sum_{k=0}^{\infty} \frac{k^k}{i!} \mathbb{E}[\det(\mathbf{A} \mathbf{B}^\top) \mid K = i]$$

$$= \sum_{i=0}^{\infty} \frac{\gamma^i e^{-\gamma}}{i!} \mathbb{E}[\det(\mathbf{A} \mathbf{B}^\top) \mid K = i] \sum_{k=0}^{\infty} \frac{\gamma^k}{k!}$$

$$= \sum_{i=0}^{\infty} \frac{\gamma^i e^{-\gamma}}{i!} \mathbb{E}[\det(\mathbf{A} \mathbf{B}^\top) \mid K = i] \sum_{k=0}^{\infty} \frac{\gamma^{k-i}}{(k-i)!}$$

$$= \mathbb{E}[\det(\mathbf{A} \mathbf{B}^\top)] \cdot e^{\gamma},$$

where $(\ast)$ follows from the exchangeability of the rows of $\mathbf{A}$ and $\mathbf{B}$, which implies that the distribution of $\mathbf{A}_{S,*} \mathbf{B}_{S,*}^\top$ is the same for all subsets $S$ of a fixed size $k$. \( \square \)
4 Expectation formulas for surrogate designs

In this section we prove a number of expectation formulas for determinantal surrogate designs, which we then use to prove Theorems 1 and 2. In the process, we derive closed form expressions for $E_{\mathbf{\bar{X}}^\dagger \mathbf{X}}$, i.e., the expectation of the orthogonal projection onto the subspace spanned by the the rows of $\mathbf{\bar{X}}$, and for $E[\text{tr}(\mathbf{\bar{X}}^\dagger \mathbf{X})^\dagger]$, the trace of the pseudo-inverse of the sample covariance matrix. To our knowledge, neither of these quantities admit closed form expressions for standard i.i.d. random designs such as Gaussian with general covariance (except for the isotropic case).

4.1 Proof of Theorem 1

Let $y(x)$ follow the homoscedastic noise model with variance $\sigma^2$ (Assumption 1). Recall that we have $\mathbf{\bar{X}} \sim S^n_\mu$ and $\mathbf{\bar{y}}_i = y(\mathbf{\bar{x}}_i) = \mathbf{\bar{x}}_i^\dagger w^* + \xi_i$, where $\xi_i \sim \mathcal{N}(0, \sigma^2)$. A standard decomposition of the MSE of the Moore-Penrose estimator proceeds as follows:

$$
\text{MSE}[\mathbf{\bar{X}}^\dagger \mathbf{\bar{y}}] = E[\|\mathbf{\bar{X}}^\dagger (\mathbf{\bar{X}} w^* + \xi) - w^*\|^2] \\
= E[\mathbf{\bar{X}}^\dagger \xi^2] + E[\|\mathbf{\bar{X}}^\dagger (\mathbf{\bar{X}} - I) w^*\|^2] \\
= \sigma^2 E[\text{tr}((\mathbf{\bar{X}}^\dagger \mathbf{\bar{X}})^\dagger)] + w^* E[I - \mathbf{\bar{X}}^\dagger \mathbf{\bar{X}}] w^*.
$$

Thus, our task is to find closed form expressions for the two expectations above. If $n \geq d$, then the latter goes away because when $\mathbf{\bar{X}}$ has full column rank then $I - \mathbf{\bar{X}}^\dagger \mathbf{\bar{X}} = 0$. When $n < d$, this expectation is given in the following result.

**Lemma 8.** If $\mathbf{\bar{X}} \sim S^n_\mu$ and $n < d$, then we have

$$E[I - \mathbf{\bar{X}}^\dagger \mathbf{\bar{X}}] = (\gamma_n \Sigma_\mu + I)^{-1}.$$ 

The proof of Lemma 8 is deferred to Section 4.2 because it follows as a corollary of a more general result (Lemma 11). We next derive the second expectation needed to compute the MSE. The under- and over-determined cases are proven separately, starting with the former.

**Lemma 9.** If $\mathbf{\bar{X}} \sim S^n_\mu$ for $n < d$, then we have

$$E[\text{tr}((\mathbf{\bar{X}}^\dagger \mathbf{\bar{X}})^\dagger)] = \gamma_n (1 - \det((\frac{1}{\gamma_n} I + \Sigma_\mu)^{-1} \Sigma_\mu)).$$

**Proof.** Let $\mathbf{X} \sim \mu^K$ for $K \sim \text{Poisson}(\gamma_n)$. Note that if $\det(\mathbf{XX}^\dagger) > 0$ then using the fact that $\det(\mathbf{A})A^{-1} = \text{adj}(\mathbf{A})$ for any invertible matrix $\mathbf{A}$, we can write:

$$
\det(\mathbf{XX}^\dagger) \text{tr}((\mathbf{X}^\dagger \mathbf{X})^\dagger) = \det(\mathbf{XX}^\dagger) \text{tr}((\mathbf{XX}^\dagger)^{-1}) \\
= \text{tr}(\text{adj}(\mathbf{XX}^\dagger)) \\
= \sum_{i=1}^{K} \det(\mathbf{X}_{-i} \mathbf{X}_{-i}^\dagger),
$$

where $\mathbf{X}_{-i}$ is a shorthand for $\mathbf{X}_{[K]\backslash \{(i)\},\mu}$. Assumption 2 ensures that $\Pr\{\det(\mathbf{XX}^\dagger) > 0\} = 1$, which
allows us to write:

\[
Z_n^\mu \cdot \mathbb{E}\left[\text{tr}\left((\tilde{X}^\top \tilde{X})^\dagger\right)\right] = \mathbb{E}\left[\sum_{i=1}^{K} \det(X_{i, \cdot} X_{i, \cdot}^\top) \mid \det(XX^\top) > 0\right] \cdot \frac{1}{\Pr\{\det(XX^\top) > 0\}}
\]

\[
= \sum_{k=0}^{d} \frac{\gamma_n^kk^{-\gamma_n}}{k!} \mathbb{E}\left[\sum_{i=1}^{k} \det(X_{i, \cdot} X_{i, \cdot}^\top) \mid K = k\right]
\]

\[
= \sum_{k=0}^{d} \frac{\gamma_n^kk^{-\gamma_n}}{k!} k \mathbb{E}[\det(XX^\top) \mid K = k - 1]
\]

\[
= \gamma_n \sum_{k=0}^{d-1} \frac{\gamma_n^kk^{-\gamma_n}}{k!} \mathbb{E}[\det(XX^\top) \mid K = k]
\]

\[
= \gamma_n \left(\mathbb{E}[\det(XX^\top)] - \frac{\gamma_n^d e^{-\gamma_n}}{d!} \mathbb{E}[\det(X)^2 \mid K = d]\right) \tag{1}
\]

\[
\overset{(*)}{=} \gamma_n \left(\gamma^{-\gamma_n} \det(I + \gamma_n \Sigma) - e^{-\gamma_n} \det(\gamma_n \Sigma)\right),
\]

where \((*)\) uses Lemma 6 for the first term and Lemma 5 for the second term. We obtain the desired result by dividing both sides by \(Z_n^\mu = e^{-\gamma_n} \det(I + \gamma_n \Sigma)\).

In the over-determined regime, a more general matrix expectation formula can be shown (omitting the trace). The following result is related to an expectation formula derived by [DWH19b], however they use a slightly different determinantal design so the results are incomparable.

**Lemma 10.** If \(\tilde{X} \sim S_n^\mu\) and \(n > d\), then we have

\[
\mathbb{E}\left[(\tilde{X}^\top \tilde{X})^\dagger\right] = \Sigma_{\mu}^{-1} \cdot \frac{1 - e^{-\gamma_n}}{\gamma_n}.
\]

**Proof.** Let \(X \sim \mu^K\) for \(K \sim \text{Poisson}(\gamma_n)\). Assumption 2 implies that for \(K \neq d - 1\) we have

\[
\det(X^\top X)(X^\top X)^\dagger = \adj(X^\top X),
\]

however when \(k = d - 1\) then (3) does not hold because \(\det(X^\top X) = 0\) while \(\adj(X^\top X)\) may be non-zero. It follows that:

\[
Z_n^{\mu} \cdot \mathbb{E}\left[(\tilde{X}^\top \tilde{X})^\dagger\right] = \mathbb{E}\left[\det(X^\top X)(X^\top X)^\dagger\right]
\]

\[
= \mathbb{E}\left[\adj(X^\top X)\right] - \gamma_n^{d-1} e^{-\gamma_n} \mathbb{E}\left[\adj(X^\top X) \mid K = d - 1\right]
\]

\[
= \adj(\gamma_n \Sigma_{\mu}) - \gamma_n^{d-1} \gamma^{-\gamma_n} \adj(\gamma_n \Sigma_{\mu})\tag{1}
\]

\[
= \det(\gamma_n \Sigma_{\mu}) \Sigma_{\mu}^{-1} \cdot \frac{1 - e^{-\gamma_n}}{\gamma_n},
\]

where the first term in (\(\ast\)) follows from Lemma 6 and (1), whereas the second term comes from Lemma 2.3 of [DWH19b]. Dividing both sides by \(Z_n^{\mu} = \det(\gamma_n \Sigma_{\mu})\) completes the proof. \(\square\)
Finally, applying the closed form expressions from Lemmas 8, 9 and 10, we derive the formula for the MSE and prove Theorem 1.

Proof. (of Theorem 1) First, assume that \( n < d \), in which case we have \( \gamma_n = \frac{1}{\chi_n} \) and moreover

\[
\begin{align*}
  n &= \text{tr}(\Sigma_\mu(\Sigma_\mu + \lambda_n I)^{-1}) \\
  &= \text{tr}((\Sigma_\mu + \lambda_n I - \lambda_n I)(\Sigma_\mu + \lambda_n I)^{-1}) \\
  &= d - \lambda_n \text{tr}((\Sigma_\mu + \lambda_n I)^{-1}),
\end{align*}
\]

so we can write \( \lambda_n \) as \((d - n)/\text{tr}((\Sigma_\mu + \lambda_n I)^{-1})\). From this and Lemmas 8 and 9, we obtain the desired expression, where recall that \( \alpha_n = \det(\Sigma_\mu(\Sigma_\mu + \frac{1}{\gamma_n})^{-1}) \):

\[
\text{MSE}[\bar{X}_i^\dagger \bar{y}] = \sigma^2 \gamma_n (1 - \alpha_n) + \frac{1}{\gamma_n} w^* \Sigma_\mu w^* (\Sigma_\mu + \frac{1}{\gamma_n} I)^{-1} \Sigma_\mu \Sigma_\mu (\Sigma_\mu + \lambda_n I)^{-1},
\]

(b) \( \alpha_2 \text{tr}((\Sigma_\mu + \lambda_n I)^{-1}) \frac{1 - \alpha_n}{d - n} + (d - n) \frac{w^* \Sigma_\mu w^* (\Sigma_\mu + \lambda_n I)^{-1} \Sigma_\mu (\Sigma_\mu + \lambda_n I)^{-1}}{\text{tr}((\Sigma_\mu + \lambda_n I)^{-1})}.
\]

While the expression given after (a) is simpler than the one after (b), the latter better illustrates how the MSE depends on the sample size \( n \) and the dimension \( d \). Now, assume that \( n > d \). In this case, we have \( \gamma_n = n - d \) and apply Lemma 10:

\[
\text{MSE}[\bar{X}_i^\dagger \bar{y}] = \sigma^2 \text{tr}(\Sigma_\mu^{-1}) \frac{1 - e^{-\gamma_n}}{\gamma_n} = \sigma^2 \text{tr}(\Sigma_\mu^{-1}) \frac{1 - \beta_n}{n - d}.
\]

The case of \( n = d \) was shown by [DWH19b] (Theorem 2.12). This concludes the proof.

4.2 Proof of Theorem 2

Recall that our goal is to compute the expected value of \( \bar{X}_i^\dagger \bar{y} \) under the surrogate design \( S_{\mu}^n \). Similarly as for Theorem 1, the case of \( n = d \) was shown by [DWH19b] (Theorem 2.10). We break the rest down into the under-determined case \((n < d)\) and the over-determined case \((n > d)\), starting with the former. Recall that we do not require any modeling assumptions on the responses.

Lemma 11. If \( \bar{X} \sim S_{\mu}^n \) and \( n < d \), then for any \( y(\cdot) \) such that \( E_{\mu,y}[y(x)x] \) is well-defined, denoting \( \bar{y}_i \) as \( y(x_i) \), we have

\[
E[\bar{X}_i^\dagger \bar{y}] = (\Sigma_\mu + \frac{1}{\gamma_n} I)^{-1} E_{\mu,y}[y(x)x].
\]

Proof. Let \( X \sim \mu^K \) for \( K \sim \text{Poisson}(\gamma_n) \) and denote \( y(x_i) \) as \( y_i \). Note that when \( \det(XX^\top) > 0 \), then the \( j \)th entry of \( X_i \bar{y} \) equals \( f_j^y \Sigma_\mu (XX^\top)^{-1} \bar{y} \), where \( f_j \) is the \( j \)th column of \( X \), so:

\[
\det(XX^\top) (X_i \bar{y})_j = \det(XX^\top) f_j^y (XX^\top)^{-1} \bar{y} = \det(XX^\top + y f_j^\top) - \det(XX^\top).
\]
If $\det(XX^\top) = 0$, then also $\det(XX^\top + yf_j^\top) = 0$, so we can write:

$$Z_n^\mu \cdot \mathbb{E}[(\tilde{X}^\top \tilde{y})_j] = \mathbb{E}[\det(XX^\top)(X^\top y)_j]$$

$$= \mathbb{E}[\det(XX^\top + yf_j^\top) - \det(XX^\top)]$$

$$= \mathbb{E}[\det([X, y][X, f_j]^\top)] - \mathbb{E}[\det(XX^\top)]$$

$$= \left(1\right)e^{-\gamma_n} \det\left(I + \gamma_n \mathbb{E}_{\mu, y}\left[\begin{pmatrix} xx^\top & x y(x) \\ x_j x_j^\top & x_j y(x) \end{pmatrix}\right]\right) - e^{-\gamma_n} \det(I)$$

$$= \left(2\right)e^{-\gamma_n} \det(I + \gamma_n \Sigma_{\mu}) \left(\mathbb{E}_{\mu, y}[\gamma_n x_j y(x)] - \mathbb{E}_{\mu}[\gamma_n x_j x_j^\top](I + \gamma_n \Sigma_{\mu})^{-1}\mathbb{E}_{\mu, y}[\gamma_n x y(x)]\right),$$

where (1) uses Lemma 6 twice, with the first application involving two different matrices $A = [X, y]$ and $B = [X, f_j]$, whereas (2) is a standard determinantal identity (see Fact 2.14.2 in [Ber11]). Dividing both sides by $Z_n^\mu$ and letting $\mathbf{v}_{\mu, y} = \mathbb{E}_{\mu, y}[y(x) \mathbf{x}]$, we obtain that:

$$\mathbb{E}[(\tilde{X}^\top \tilde{y})] = \gamma_n \mathbf{v}_{\mu, y} - \frac{\gamma_n^2 \Sigma_{\mu}(I + \gamma_n \Sigma_{\mu})^{-1}\mathbf{v}_{\mu, y}}{\gamma_n(I - \gamma_n \Sigma_{\mu}(I + \gamma_n \Sigma_{\mu})^{-1})\mathbf{v}_{\mu, y}} - \gamma_n(I + \gamma_n \Sigma_{\mu})^{-1}\mathbf{v}_{\mu, y},$$

which completes the proof. □

We return to Lemma 8 from Section 4.1, regarding the expected orthogonal projection onto the complement of the row-span of $\tilde{X}$, i.e., $\mathbb{E}[I - \tilde{X}^\top \tilde{X}]$, which follows as a corollary of Lemma 11.

**Proof.** (of Lemma 8) We let $y(x) = x_j$ for each $j \in [d]$ and apply Lemma 11 d times, obtaining:

$$I - \mathbb{E}[\tilde{X}^\top \tilde{X}] = I - (\Sigma_{\mu} + \frac{1}{\gamma_n} I)^{-1}\Sigma_{\mu},$$

from which the result follows by simple algebraic manipulation. □

We move on to the over-determined case, where the ridge regularization of adding the identity to $\Sigma_{\mu}$ vanishes. Recall that we assume throughout the paper that $\Sigma_{\mu}$ is invertible.

**Lemma 12.** If $X \sim S_n^d$ and $n > d$, then for any real-valued random function $y(\cdot)$ such that $\mathbb{E}_{\mu, y}[y(x) \mathbf{x}]$ is well-defined, denoting $\bar{y}_i$ as $y(\mathbf{x}_i)$, we have

$$\mathbb{E}[(\tilde{X}^\top \tilde{y})] = \Sigma_{\mu}^{-1}\mathbb{E}_{\mu, y}[y(x) \mathbf{x}].$$

**Proof.** Let $X \sim \mu^K$ for $K \sim \text{Poisson}(\gamma_n)$ and denote $y_i = y(\mathbf{x}_i)$. Similarly as in the proof of Lemma 11, we note that when $\det(X^\top X) > 0$, then the $j$th entry of $X^\top y$ equals $e_j^\top (X^\top X)^{-1} X^\top y$, where $e_j$ is the $j$th standard basis vector, so:

$$\det(X^\top X)(X^\top y)_j = \det(X^\top X) e_j^\top (X^\top X)^{-1} X^\top y = \det(X^\top X + X^\top ye_j^\top) - \det(X^\top X).$$

If $\det(X^\top X) = 0$, then also $\det(X^\top X + X^\top ye_j^\top) = 0$. We proceed to compute the expectation:

$$Z_n^\mu \cdot \mathbb{E}[(\tilde{X}^\top \tilde{y})] = \mathbb{E}[\det(X^\top X)(X^\top y)_j]$$

$$= \mathbb{E}[\det(X^\top X + X^\top ye_j^\top)] - \det(X^\top X)$$

$$= \mathbb{E}[\det(X^\top (X + ye_j^\top))] - \mathbb{E}[\det(X^\top X)]$$

$$\overset{(a)}{=} \gamma_n \mathbb{E}_{\mu, y}[x(x + y(x)e_j)^\top] - \det(\gamma_n \Sigma_{\mu})$$

$$= \det(\gamma_n \Sigma_{\mu} + \gamma_n \mathbb{E}_{\mu, y}[x y(x)e_j^\top]) - \det(\gamma_n \Sigma_{\mu})$$

$$= \det(\gamma_n \Sigma_{\mu}) \cdot \gamma_n e_j^\top (\gamma_n \Sigma_{\mu})^{-1}\mathbb{E}_{\mu, y}[y(x) \mathbf{x}],$$

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where \((*)\) uses Lemma 4 twice (the first time, with \(A = X\) and \(B = X + y\epsilon^T\)). Dividing both sides by \(Z_n^\mu = \det(\gamma_n\Sigma_\mu)\) concludes the proof. \(\Box\)

We combine Lemmas 11 and 12 to obtain the proof of Theorem 2.

Proof. (of Theorem 2) The case of \(n = d\) follows directly from the result of [DWH19a] (Theorem 2.10). Assume that \(n < d\). Then we have \(\gamma_n = \frac{1}{\lambda_n}\), so the result follows from Lemma 11. If \(n > d\), then the result follows from Lemma 12. \(\Box\)

5 Asymptotic consistency of surrogate Gaussian designs

In this section we compare the MSE expressions obtained for the surrogate design with the true MSE of the standard i.i.d. design for the case where \(\mu\) is a centered Gaussian distribution \(N(0, \Sigma)\). First, we theoretically compare the analytical expressions available in certain cases for the i.i.d. design with their surrogate equivalents, showing that the surrogate expressions are asymptotically consistent (Theorem 3). In fact, we show even more: that the surrogate expressions provide a multiplicative approximation for the true MSE with the error decaying at the rate of \(O(1/d)\). However, this result does not cover the under-determined setting for a non-isotropic Gaussian, because to the best of our knowledge, analytical expressions for the i.i.d. design are not available there. To address this case, which is of primary interest to us, we perform thorough empirical analysis showing that our surrogate expressions are asymptotically consistent, with the error decaying as \(O(1/d)\), in all of the non-isotropic Gaussian test-cases that we evaluated. Based on this, we formulate Conjectures 1 and 2, regarding the asymptotic behavior of the pseudo-inverse of the singular Wishart distribution and of a random Gaussian projection, that are of independent interest to multivariate statistics.

5.1 Proof of Theorem 3

Once again, we break down the proof into under- and over-determined cases, starting with the former. Note that in this case we require that the covariance be equal to identity.

Lemma 13. Let \(\rho = n/d\), \(X \sim N(0, I)^n\) and \(y_i = y(x_i)\) under Assumption 1. If \(d > n + 1\) then

\[
0 \leq \frac{\text{MSE}[X^\dagger y] - M(I, w^*, \sigma^2, n)}{M(I, w^*, \sigma^2, n)} \leq \frac{1}{d} \cdot \frac{1}{1 - \rho - \frac{1}{d}} + 3\rho^d.
\]

Proof. We first recall the standard decomposition of MSE\([X^\dagger y]\):

\[
\text{MSE}[X^\dagger y] = \sigma^2 E[\text{tr}((X^T X)^\dagger)] + w^*\text{tr}(I - E[X^\dagger X])w^*.
\]

Since the rows of \(X\) are standard normal random variables, \(XX^\dagger\) is an \(n \times n\) Wishart random matrix with \(d > n + 1\) degrees of freedom. Using the formula for the mean of the Inverse-Wishart distribution, it follows that

\[
E[\text{tr}((X^\dagger X)^\dagger)] = E[\text{tr}((XX^\dagger)^{-1})] = \frac{n}{d - n - 1}.
\]

Note that \(X^\dagger X\) is a uniformly random projection matrix so by rotational symmetry it follows that

\[
w^*\text{E}[X^\dagger X]w^* = \text{E}[\|X^\dagger X w^*\|^2] = \frac{n}{d} \|w^*\|^2.
\]

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Putting this together we obtain that

\[ \text{MSE}[X^\dagger y] = \frac{\sigma^2 n}{d - n} + \|w^*\|^2 \frac{d - n}{d}. \]

On the other hand, the surrogate MSE expression can be derived by observing that for \( \Sigma = I \) we have \( \text{tr}((\Sigma + \lambda_n I)^{-1}) = d/(1 + \lambda_n) = n \) (see definition of \( \lambda_n \) in Theorem 1):

\[ M(I, w^*, \sigma^2, n) = \sigma^2 n \cdot \frac{1 - \alpha_n}{d - n} + \|w^*\|^2 \frac{d - n}{d}. \]

Note that the second term is the same in both cases, even though this may not be true for non-isotropic Gaussians. We now compute the normalized difference between the expressions,

\[ \frac{\text{MSE}[X^\dagger y] - M(I, w^*, \sigma^2, n)}{M(I, w^*, \sigma^2, n)} = \frac{\sigma^2 n \cdot \frac{1}{d - n} - \frac{1 - \alpha_n}{d - n}}{\sigma^2 n \cdot \frac{1 - \alpha_n}{d - n} + \|w^*\|^2 \frac{d - n}{d}} \]

\[ \leq \frac{d - n}{1 - \alpha_n} \left( \frac{1}{d - n - 1} - \frac{1 - \alpha_n}{d - n} \right) \]

\[ = \frac{d - n}{d - n - 1} + \frac{\alpha_n}{1 - \alpha_n} \left( \frac{1}{d - n - 1} \right). \]

Let \( \rho = n/d \). Then \( \frac{1}{d - n - 1} = \frac{1}{d} \cdot \frac{1}{1 - \rho - \frac{1}{d}} \) and moreover \( \alpha_n = (\frac{d - 2}{d})^d = (\frac{n}{d})^d = \rho^d \). From the assumption that \( d > n + 1 \), we conclude that \( \alpha_n \leq (\frac{d - 2}{d})^d \leq e^{-2} \) so that \( \frac{\alpha_n}{1 - \alpha_n} (1 + \frac{1}{d - n - 1}) \leq \frac{2\alpha_n}{1 - \alpha_n} \leq 3 \rho^d \). This shows the right-hand-side inequality of the theorem. That fact that \( \text{MSE}[X^\dagger y] \geq M(I, w^*, \sigma^2, n) \) follows easily.

**Lemma 14.** Let \( \rho = n/d \), \( X \sim \mathcal{N}(0, \Sigma)^n \) and \( y_i = y(x_i) \) under Assumption 1. If \( n > d + 1 \) then

\[ 0 \leq \frac{\text{MSE}[X^\dagger y] - M(\Sigma, w^*, \sigma^2, n)}{M(\Sigma, w^*, \sigma^2, n)} \leq \frac{1}{d} \cdot \frac{1}{\rho - 1 - \frac{1}{d}} + 3(e^{-1})^d. \]

**Proof.** The MSE for the over-determined Gaussian design can be derived by using the formula for the mean of the Inverse-Wishart distribution:

\[ \text{MSE}[X^\dagger y] = \sigma^2 \text{tr}(\mathbb{E}([X^\top X]^{-1})) = \frac{\sigma^2 \text{tr}(\Sigma^{-1})}{n - d - 1}. \]

To compute the normalized difference we follow similar derivations as in the proof of Lemma 13:

\[ \frac{\text{MSE}[X^\dagger y] - M(\Sigma, w^*, \sigma^2, n)}{M(\Sigma, w^*, \sigma^2, n)} = \frac{n - d}{1 - \beta_n} \left( \frac{1}{n - d - 1} - \frac{1 - \beta_n}{n - d} \right) \]

\[ \leq \frac{1}{d} \cdot \frac{1}{\rho - 1 - \frac{1}{d}} + \frac{2\beta_n}{1 - \beta_n}. \]

Recall that \( \beta_n = e^{d-n} = (e^{-1})^d \) and for \( n - d \geq 2 \) we have \( \frac{2}{1 - \beta_n} \leq 3. \) The desired inequalities follow immediately.
Theorem 3 now follows as a consequence of Lemmas 13 and 14.

**Proof.** (of Theorem 3) Since \( \frac{1}{d} \leq \frac{1}{3}|1 - \rho| \) and \( e^{-|1-\rho|d} \leq \frac{1}{2d|1-\rho|} \), it follows that
\[
\frac{1}{d} \cdot \frac{1}{|1-\rho| - \frac{1}{d}} + 3(e^{-|1-\rho|d}) \leq \frac{1}{d} \cdot \frac{1}{|1-\rho| - \frac{1}{d}} + \frac{3}{2d|1-\rho|} = c_d.
\]
The case of \( n > d + 1 \) now follows from Lemma 14. Also, since \( \rho \leq e^{\rho - 1} \), for \( n < d - 1 \) we have \( 3^d \leq 3(e^{-|1-\rho|d}) \), so the same bound follows from Lemma 13. \( \square \)

### 5.2 Empirical analysis of asymptotic consistency

Theorem 3 states that our surrogate expressions for the MSE under certain Gaussian designs are asymptotically consistent with the multiplicative error rate of \( O(1/d) \). In this section, we show strong empirical evidence that this fact extends to the setting not covered by the theorem: under-determined regime (i.e., \( n < d \)) with a non-isotropic Gaussian distribution (i.e., \( \Sigma \neq \mathbf{I} \)). We break down our analysis into verifying two conjectures which are of independence interest to multivariate Gaussian analysis. The first conjecture addresses the variance term in the MSE and postulates an asymptotically consistent formula for the expected Moore-Penrose pseudo-inverse of the singular Wishart distribution. Recall that matrix \( \mathbf{W} \sim \mathcal{W}(\Sigma, n) \) is distributed according to the Wishart distribution with \( n \) degrees of freedom if it can be decomposed as \( \mathbf{W} = \mathbf{X}^\top \mathbf{X} \), where \( \mathbf{X} \sim \mathcal{N}(\mathbf{0}, \Sigma)^n \).

**Conjecture 1** (Pseudo-inverse of singular Wishart). *Fix \( n/d < 1 \) and let \( \mathbf{W} \sim \mathcal{W}(\Sigma, n) \), where \( \Sigma \) is \( d \times d \) positive definite with condition number bounded by a constant. Then:*
\[
\frac{\mathbb{E}[\text{tr}(\mathbf{W}^\top)]}{\mathcal{V}(\Sigma, n)} - 1 = O(1/d) \quad \text{for} \quad \mathcal{V}(\Sigma, n) = \text{tr}((\Sigma + \lambda_n \mathbf{I})^{-1}) \frac{1 - \alpha_n}{d - n}, \tag{4}
\]
*where \( \lambda_n \geq 0 \) satisfies \( n = \text{tr}(\Sigma(\Sigma + \lambda_n \mathbf{I})^{-1}) \) and \( \alpha_n = \det(\Sigma(\Sigma + \lambda_n \mathbf{I})^{-1}) \).*

Our second conjecture involves the projection onto the orthogonal complement of a Gaussian sample \( \mathbf{X} \), i.e., the matrix \( \mathbf{I} - \mathbf{X}^\top \mathbf{X} \), and addresses the bias term in the MSE.

**Conjecture 2** (Gaussian orthogonal projection). *Fix \( n/d < 1 \) and let \( \mathbf{X} \sim \mathcal{N}(\mathbf{0}, \Sigma)^n \), where \( \Sigma \) is \( d \times d \) positive definite with condition number bounded by a constant. Then:
\[
\sup_{\mathbf{w} \in \mathbb{R}^d \setminus \{\mathbf{0}\}} \left| \frac{\mathbf{w}^\top \mathbb{E}[\mathbf{I} - \mathbf{X}^\top \mathbf{X}] \mathbf{w}}{\mathbf{w}^\top \mathcal{B}(\Sigma, n) \mathbf{w}} - 1 \right| = O(1/d) \quad \text{for} \quad \mathcal{B}(\Sigma, n) = (\Sigma + \lambda_n \mathbf{I})^{-1} \frac{d - n}{\text{tr}((\Sigma + \lambda_n \mathbf{I})^{-1})}, \tag{5}
\]
*where \( \lambda_n \geq 0 \) satisfies \( n = \text{tr}(\Sigma(\Sigma + \lambda_n \mathbf{I})^{-1}) \).*

Note that the surrogate expression for the mean squared error can be written as:
\[
\mathcal{M}(\Sigma_\mu, \mathbf{w}^*, \sigma^2, n) = \sigma^2 \mathcal{V}(\Sigma_\mu, n) + \mathbf{w}^* \mathbf{w}^\top \mathcal{B}(\Sigma_\mu, n) \mathbf{w}^*.
\]
So, if the conjectures are true, this would immediately imply that the asymptotic consistency claim given in Theorem 3 for the surrogate Gaussian MSE extends to the under-determined setting with arbitrary covariance \( \Sigma \).

Furthermore, both of these conjectures are related to open problems which have been extensively studied in the literature. With respect to Conjecture 1, [Sri03] first derived the probability density
function of a singular Wishart distribution, and [CF11] computed the first and second moments of
generalized inverses of a singular Wishart distribution. However, for the Moore-Penrose pseudo-
inverse and arbitrary covariance $\Sigma$, [CF11] claims that the quantities required to express the mean
“do not have tractable closed-form representation.” Conjecture 2 has connections to directional
statistics. Using the SVD, we have the equivalent representation $X^\top X = V V^\top$ where $V$ is an
element of the Stiefel manifold $V_{n,d}$ (i.e., orthonormal $n$-frames in $\mathbb{R}^d$). The distribution of $V$
is known as the matrix angular central Gaussian (MACG) distribution [Chi90]. While prior work has
considered high dimensional limit theorems [Chi91] as well as density estimation and hypothesis
testing [Chi98] on $V_{n,d}$, they only analyzed the invariant measure (which corresponds in our setting
to $\Sigma = I$), and to our knowledge a closed form expression of $E[r V V^\top s]$ where $V$ is distributed
according to MACG with arbitrary $\Sigma$ remains an open question.

For verifying these two conjectures, it suffices to only consider diagonal covariance matrices $\Sigma$
This is because if $\Sigma = Q D Q^\top$ is its eigendecomposition and $X \sim \mathcal{N}(0, Q D Q^\top)^n$, then we have
for $W \sim \mathcal{W}(\Sigma, n)$ that $W \overset{d}{=} X^\top X$ and hence, defining $\tilde{X} \sim \mathcal{N}(0, D)^n$, by linearity and unitary
invariance of trace,

$$E[tr(W^\top)] = tr(E[(X^\top X)^\top]) = tr(QE[(\tilde{X}^\top \tilde{X})^\top]Q^\top) = tr(E[(\tilde{X}^\top \tilde{X})^\top]) = E[tr((\tilde{X}^\top \tilde{X})^\top)].$$

Similarly, we have that $E[X^\top X] = Q E[\tilde{X}^\top \tilde{X}] Q^\top$, and a simple calculation shows that the expression
in Conjecture 2 is also independent of the choice of matrix $Q$. Thus, we empirically validate our
conjectures for diagonal matrices $\Sigma$ with several different eigenvalue decay profiles. Denoting
$\lambda_1, \ldots, \lambda_d$ as the eigenvalues of $\Sigma$, we consider the following decays:

- **diag_linear**: linear decay, $\lambda_i = b - ai$;
- **diag_exp**: exponential decay, $\lambda_i = b 10^{-ai}$;
- **diag_poly**: fixed-degree polynomial decay, $\lambda_i = (b - ai)^2$;
- **diag_poly_2**: variable-degree polynomial decay, $\lambda_i = bi^{-a}$.

The constants $a$ and $b$ are chosen to ensure $\lambda_{\max}(\Sigma) = 1$ and $\lambda_{\min}(\Sigma) = 10^{-4}$ (i.e., the condition
number $\kappa(\Sigma) = 10^4$ remains constant). Figure 2 illustrates an example of these decay profiles for
$d = 100$.

![Figure 2: Scree-plots of $\Sigma$ for the eigenvalue decays examined in our empirical valuations. Here $d = 100$ for visualization, whereas our experiments increase $d$ while preserving the ratio $n/d$ and the decay profile, with $\lambda_{\max}(\Sigma) = 1$ to $\lambda_{\min}(\Sigma) = 10^{-4}$.](image)
We verify our conjectures by increasing \(d\) while keeping the aspect ratio \(n/d\) fixed and examining the rate of decay of the quantities asserted in the conjectures. As no closed form expressions are available for the expectations in the conjectures, we estimate \(\mathbb{E}[\text{tr}(W^\dagger)]\) (for Conjecture 1) and \(\mathbb{E}[I - X^\dagger X]\) (for Conjecture 2) through Monte Carlo sampling. To ensure that estimation noise is sufficiently small, we continually increase the number of Monte Carlo samples until the bootstrap confidence intervals are within \(\pm 12.5\%\) of the quantities in (4) and (5). We found that while Conjecture 1 required a relatively small number of trials (up to one thousand), estimation noise was much larger in Conjecture 2 and necessitated over two million trials to obtain good estimates near \(d = 100\).

Figure 3: Empirical verification of Conjecture 1. We show the quantity \(|\mathbb{E}[\text{tr}(W^\dagger)]\mathcal{V}(\Sigma, n)^{-1} - 1|\) as \(d\) increases for various aspect ratios \(n/d\). Consistent with our conjecture, an \(O(1/d)\) decay (linear with slope \(-1\) on a log-log plot) is exhibited across all eigenvalue decay profiles and aspect ratios investigated.

The results of empirically validating Conjecture 1 are illustrated in Figure 3, where we performed Monte Carlo estimation of \(\mathbb{E}[\text{tr}(W^\dagger)]\) and \(\mathbb{E}[I - X^\dagger X]\) as \(d\) increases from 10 to 1000, across a range of aspect ratios \(n/d\) and eigenvalue decay profiles for \(\Sigma\). Confidence intervals are estimated by bootstrapping. We observe that on log-log axes all of the plots are decreasing with a linear \(-1\) slope, consistent with the \(O(1/d)\) rate predicted by Conjecture 1.

Conjecture 2 is handled similarly, by sampling \(X \sim \mu^n\) where \(\mu = \mathcal{N}(0, \Sigma)\) to obtain a Monte Carlo estimate of \(\mathbb{E}[I - X^\dagger X]\). To handle the supremum over \(w\), notice that we can rewrite (5) as a spectral norm

\[
\sup_{w \in \mathbb{R}^n \setminus \{0\}} \left| \frac{w^\dagger \mathbb{E}[I - X^\dagger X]w}{w^\dagger \mathcal{B}(\Sigma, n)w} - 1 \right| = \|\mathbb{E}[I - X^\dagger X]\mathcal{B}(\Sigma, n)^{-1} - I\|.
\]

(6)

Confidence intervals can now be constructed using existing methods for constructing operator norm confidence intervals, and our results use the bootstrapping method described in [LEM19].

Figure 4 shows how \(\|\mathbb{E}[I - X^\dagger X]\mathcal{B}(\Sigma, n)^{-1} - I\|\) decays as we hold the aspect ratio \(n/d\) fixed and increase \(d\) between 10 and 100 across the listed eigenvalue decay profiles and aspect ratios. Again, we observe on log-log axes a linear decay with slope \(-1\) consistent with the \(O(1/d)\) rate posed by Conjecture 2. Note that the range of \(d\) is smaller than in Figure 3 because the large number of Monte Carlo samples (up to two million) required for this experiment made the computations much more expensive.
Figure 4: Empirical results validating Conjecture 2. We show how $\|E[I - X^\top X]B(\Sigma, n)^{-1} - I\|$ (which by Equation 6 is equal to the quantity controlled by Conjecture 2) decays as $d$ increases and observe a linear slope consistent with the conjectured $O(1/d)$ rate.

6 Conclusions

We derived exact non-asymptotic expressions for the MSE of the Moore-Penrose estimator in the standard regression task, reproducing the double descent phenomenon as the sample size crosses between the under- and over-determined regime. To achieve this, we modified the standard i.i.d. random design distribution using a determinantal rescaling to obtain a surrogate design which admits exact MSE expressions, while capturing the key properties of the i.i.d. design. We also provided a result that relates the expected value of the Moore-Penrose estimator of a training sample in the under-determined regime (i.e., the minimum norm solution) to the ridge-regularized least squares solution for the population distribution, thereby providing an interpretation for the implicit regularization resulting from over-parameterization.

An important technical issue is that, in this work, we focus on the classical well-specified linear regression task, where the underlying response model is linear with respect to the observed feature space. A significant effort in the related literature (see Section 1.3) has been directed towards a number of misspecified linear regression tasks, where the set of $d$ observed features is different than the set of $D$ features which define the linear model (typically, $d \ll D$). Crucially, unlike in the well-specified task, here it is possible to vary the number of observed features without changing the underlying linear model. Recent work [HIMRT19] has compared how varying the feature dimension affects the (asymptotic) generalization error for both well-specified and misspecified tasks, however their analysis was limited to certain special settings such as an isotropic data distribution. As an additional point of comparison, in Figure 5 we plot the MSE expressions of Theorem 1 for our well-specified setting when varying the feature dimension $d$. The model is chosen just like in Figure 1, where the covariances $\Sigma_{\mu}$ are diagonal with condition number $\kappa$ and exponentially decaying spectrum scaled so that $\text{tr}(\Sigma_{\mu}^{-1}) = d$. We also use $\sigma^2 = 1$ and $w^* = \frac{1}{\sqrt{d}} 1_d$. Qualitatively,
our plots follow the trends outlined by [HMRT19] for the isotropic case (i.e., $\kappa = 1$), but the spectral decay of the covariance matrix (captured by our new MSE expressions) does have a significant effect on the descent curve in the under-determined regime. Note that the plots achieve their minimum as $d$ goes to zero because in the well-specified task as the complexity of the prediction model decreases, so does the complexity of the true response model. Nevertheless, even in the well-specified setting we achieve non-trivial generalization in the under-determined regime, as seen by the fact that the MSE curve goes below the error of the null estimator, $\text{MSE}[\mathbf{0}] = \|\mathbf{w}^*\|^2 = 1$.

Our work opens up a number of new directions for future research. Most obviously, this includes extending our surrogate analysis to the misspecified linear regression discussed above. In addition, in Section 5, we provided two conjectures, the goal of which is to bound the difference between the results obtained for our surrogate designs and the true values corresponding to the i.i.d. design, in the case of multivariate Gaussians. We believe that addressing these conjectures will have a broader impact on our understanding of non-isotropic Gaussian designs. Finally, it remains open whether the analysis we provided for the mean squared error can be reproduced in the context of mean squared prediction error, which is relevant in many machine learning tasks.

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