STATISTICAL LIMITS OF DICTIONARY LEARNING: RANDOM MATRIX THEORY AND THE SPECTRAL REPLICA METHOD

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ABSTRACT. We consider increasingly complex models of matrix denoising and dictionary learning in the Bayes-optimal setting, in the challenging regime where the matrices to infer have a rank growing linearly with the system size. This is in contrast with most existing literature concerned with the low-rank (i.e., constant-rank) regime. We first consider a class of rotationally invariant matrix denoising problems whose mutual information and minimum mean-square error are computable using standard techniques from random matrix theory. Next, we analyze the more challenging models of dictionary learning. To do so we introduce a novel combination of the replica method from statistical mechanics together with random matrix theory, coined spectral replica method. It allows us to conjecture variational formulas for the mutual information between hidden representations and the noisy data as well as for the overlaps quantifying the optimal reconstruction error. The proposed methods reduce the number of degrees of freedom from $\Theta(N^2)$ (matrix entries) to $\Theta(N)$ (eigenvalues or singular values), and yield Coulomb gas representations of the mutual information which are reminiscent of matrix models in physics. The main ingredients are the use of HarishChandra-Itzykson-Zuber spherical integrals combined with a new replica symmetric decoupling ansatz at the level of the probability distributions of eigenvalues (or singular values) of certain overlap matrices.

1. INTRODUCTION

The simplest linear-rank matrix inference task, that we refer to as *matrix denoising*, is the problem of recovering the rotationally invariant full-rank matrix S from noisy observations Y generated as

$$Y = \sqrt{\lambda S} + \xi$$

where $\boldsymbol{\xi}$ is some Wigner gaussian noise matrix. In the random matrix theory (RMT) literature, typical problems are concerned with deriving spectral properties: spectral density and correlation functions of the eigenvalues or singular values of \boldsymbol{Y} , its bulk statistics, the fluctuations of its largest and smallest eigenvalues, potential universality properties, etc. The literature is too large to be exhaustive here and relevant references will be cited along the paper. We refer to [1,2] for generic good mathematic books, or [3–5] for a more physics-oriented presentation. In this paper we instead consider information-theoretic questions such as: "given a certain signal-to-noise λ , what is the mutual-information between the hidden matrix signal \boldsymbol{S} and the observed noisy data \boldsymbol{Y} ?", or "what is the statistically optimal reconstruction error on \boldsymbol{S} ?" We are interested in answering these questions in certain asymptotic large size limits. Despite the apparent simplicity of the model, these questions turn out to be highly non-trivial.

In matrix denoising we are "only" interested in the reconstruction of the matrix S. This allows to analyze the model using solely RMT. But there exist models where S possesses some additional internal structure other than the (possibly non-trivial) statistics of its spectrum and/or S may not

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be rotationally invariant. This is the case in the model we study next: *dictionary learning*, where a product structure arises.

Let M noisy N-dimensional data points $(\mathbf{Y}_j)_{j \leq M}$ be stacked as the columns of $\mathbf{Y} \in \mathbb{R}^{N \times M}$. The unsupervised dictionary learning task is to find a representation of this data \mathbf{Y} in the form

$$Y \propto ST^{\dagger} + Z$$
 .

The unknowns are both the "dictionary" $S \in \mathbb{R}^{N \times K}$ made of K features and the coefficients $T \in \mathbb{R}^{M \times K}$ in the decomposition of the clean data ST^{\dagger} in feature basis. Here Z represents undesired noise. We also analyze a symmetric/Hermitian version of the problem where one aims to find a positive-definite decomposition of Y in the form

$$Y arpropto X X^\dagger$$
 + $Z,$

where $X \in \mathbb{R}^{N \times M}$. The rich internal structure coming from the product between matrices requires new ideas for analysis: RMT alone does not seem sufficient for analyzing the optimal reconstruction performance on X, S, T themselves (instead of the products $ST^{\dagger}, XX^{\dagger}$ seen a individual matrices). This is where the statistical mechanics of spin glasses and the novel *spectral replica method* enter.

We will consider all models in the Bayes-optimal "matched setting" where Y is truly generated according to the model under study, and the statistician has perfect knowledge of this datagenerating model (i.e., knows the additive nature and statistics of the noise and therefore the likelihood) as well as the prior distributions underlying the hidden random matrix signals. The statistician can thus exploit this knowledge to write down the correct posterior distribution in order to perform inference. Each model will be analyzed both in the cases of real and complex matrices.

Given its fundamental nature and central role in signal processing and machine learning [6, 7], dictionary learning has generated a large body of work with applications in representation learning [8], sparse coding [9–11], robust principal components analysis [12, 13], sub-matrix localization [14], blind source separation [15], matrix completion [16, 17] and community detection [18–20]. Low-rank versions of dictionary learning have been introduced in statistics under the name of "spike models" as statistical models for sparse principal components analysis (PCA) [21–24]. These models in the low-rank (i.e., finite-rank) regime $M, N \to +\infty$ proportionally and $K = \Theta(1)$ (or $N \to +\infty$ while $M = \Theta(1)$ in the symmetric case) have become paradigms for the study of phase transition phenomena in the recovery of low-rank information hidden in noise. In PCA the classical rigorous results are due to Baik, Ben-Arous and Péché [25,26] who analyzed the performance of spectral algorithms. More recently, low-dimensional variational formulas for the mutual information and corresponding phase transitions at the level of the Bayes-optimal minimum mean-square error estimator, as well as the algorithmic transitions of message passing and gradient descent-based algorithms and their associated computational-to-statistical gaps, have been derived thanks to the global effort of an highly inter-disciplinary community [19, 27–51].

In contrast, much less is known in the challenging linear-rank regime studied here where $N, M, K \to +\infty$ at similar rates, so that rank (ST^{\dagger}) or rank (XX^{\dagger}) diverge linearly with N. References closely related to our work are [52, 53] which consider the very same setting. But we believe that the results found in these papers are only approximations, i.e., are "not correct" mean-field calculations and therefore do not yield asymptotically exact formulas. We will discuss the reasons why we think so and the differences with our approach in a dedicated section. Another important work is [54] which considers the same models as ours but focus on certain class of rotational invariant estimators instead of the information-theoretic performance.

Another very relevant literature concerns multi-matrix models from high-energy physics with applications in string theory, quantum gravity, quantum chromodynamics, fluctuating surfaces and map enumeration [55-66]. In certain aspects they are similar to matrix *inference* models like dictionary learning. E.g., in contrast to the low-dimensional order parameters of standard low-rank inference problems [67], in linear-rank regimes the order parameters are eigenvalues/singular values densities, as in multi-matrix models. Also, at first sight, the formulas found in the present contribution look very much like those appearing in these models, see [68]. It may thus be tempting to think that matrix inference models are special cases of known matrix models. This is *not* the case however. The presence of frozen, correlated randomness in inference, namely the data, radically changes the nature of the problem: new tools are needed. This essential difference prevents borrowing various important techniques from this field, but certain methods used in the analysis of matrix models will be crucial, in particular the use of spherical integrals [69, 70].

Concretely, having frozen data Y translates, as in spin glasses [71, 72], into the need to evaluate the expectation of the *logarithm* of the partition function with respect to it. This yields the behavior of the model for typical realizations of the signals and data. The difference is clear: the canonical two-matrix model from physics reads [57, 59, 68]

$$\ln \mathcal{Z}_{2MM} = \ln \int d\mathbf{A} d\mathbf{B} \exp \operatorname{Tr}[f(\mathbf{A}) + g(\mathbf{B}) + h(\mathbf{AB})] \quad \text{with} \quad \mathbf{A} = \mathbf{A}^{\dagger}, \ \mathbf{B} = \mathbf{B}^{\dagger},$$

and with f, g, h just depending on the spectra. Instead the free energy of matrix inference models (which is essentially the Shannon entropy of the data) will look like

(1)
$$\mathbb{E}_{\boldsymbol{Y}} \ln \mathcal{Z}_{INFER}(\boldsymbol{Y}) = \int d\boldsymbol{Y} \exp \operatorname{Tr} f(\boldsymbol{Y}) \ln \int d\boldsymbol{U} \exp \operatorname{Tr} [g(\boldsymbol{U}) + h(\boldsymbol{U}\boldsymbol{Y})]$$

This form will get even more complicated in non-symmetric multipartite systems such as the ST^{\dagger} -dictionary learning problem, with an integration over more matrices which are not necessarily symmetric/Hermitian. In addition, the presence of a quenched average in (1) is far from innocent. It generates a whole new level of difficulty, since the methods in the previous references, all relying on a direct saddle-point evaluation, do not apply [68]. This quenched average is the reason behind the fact that, even if only Hermitian matrices are present in the original inference model, non-Hermitian matrices will appear along the analysis. The role of the replica method combined with RMT is precisely to deal with these new difficulties, at a non-rigorous level.

Many derivations presented in this paper are based on heuristics, yet they are conjectured exact in proper asymptotic limits. We believe that some of our new methodology, in particular the spectral replica method, will pave the way to the analysis of a whole new class of inference and learning problems involving large linear-rank matrices and that remained inaccessible until now. Moreover, given the breadth of applications of such disordered matrix models in information processing systems but also physics, we believe that our results may have an impact in a broader context.

Organization: In Section 2 we start by analyzing the simplest linear-rank matrix inference model using RMT techniques, namely, denoising of an Hermitian rotationally invariant matrix. Two special cases (one only being non-trivial) can be completely treated, in the sense of deriving explicit enough formulas to draw a phase diagram. In Section 3 we provide generic systematic expansions of the previously derived formulas in the low (and to some extent high) signal-to-noise regimes. Section 4 generalizes the analysis to the case of non-Hermitian matrix denoising. Section 5 is devoted to the analysis of Hermitian (i.e., positive-definite) dictionary learning. Starting from this section, RMT tools do not suffice anymore, and we introduce the spectral replica method to go beyond.

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The first part of this section reduces the model to effective Coulomb gases of singular values, while the second one expresses it in terms of eigenvalues. We also discuss the main differences with previous attempts to analyse this model. Finally in Section 6, we consider the non-symmetric case of dictionary learning. Appendix A recalls known facts about full-rank spherical integrals which are of crucial importance in our analyses. Appendix B derives a generic formula for the minimum mean-square error in matrix denoising. In Appendix C we discuss how our formulas can be re-expressed in terms of densities order parameters. The last Appendix D provides the necessary MATHEMATICA codes to reproduce our numerical results.

Notations: Let the field $\mathbb{K} = \mathbb{R}$ if $\beta = 1$ or $\mathbb{K} = \mathbb{C}$ if $\beta = 2$, where β refers to the Dyson index. The symbol \dagger corresponds to the transpose \top in the real case $\beta = 1$ or to the transpose conjugate when $\beta = 2$, the conjugate being $\overline{z} := \Re z - i \Im z$ with $\Re z$ and $\Im z$ the real and imaginary parts of $z \in \mathbb{C}$ and i = $\sqrt{-1}$. Vectors and matrices are in bold. Vectors are columns by default and their transpose (conjugate) x^{\dagger} are row vectors. When no confusion can arise we denote the trace $\operatorname{Tr} f(A) = \operatorname{Tr} [f(A)]$ so, e.g., $\operatorname{Tr} A^2 = \operatorname{Tr} [A^2]$ or $\operatorname{Tr} AB = \operatorname{Tr} [AB]$. Similarly $\mathbb{E} X^2 = \mathbb{E} (X)^2 = \mathbb{E} [X^2] \ge (\mathbb{E} X)^2 = \mathbb{E} [X]^2$. The usual inner product between (possibly complex) vectors $\sum_i \bar{x}_i y_i$ is denoted $\boldsymbol{x}^{\dagger} \boldsymbol{y}$ or $\langle \bar{\boldsymbol{x}}, \boldsymbol{y} \rangle$ (with $\bar{x} = x$ if x is real); the matrix inner product is $\text{Tr}X^{\dagger}Y$. The usual L^2 vector (squared) norm is $\sum_i |x_i|^2 = \|\boldsymbol{x}\|^2$. Every sum or product over $j \leq t$ means over $j = 1, \ldots, t$. We will often drop parentheses, e.g., $\exp \cdots = \exp(\cdots)$. Depending on the context, the symbol \propto means "equality up to a normalization", "equality up to an irrelevant additive constant" or "proportional to". We denote $[N] := \{1, \ldots, N\}$. For a diagonal matrix Σ we will write the diagonal elements with a single index $\Sigma_i := \Sigma_{ii}$. For a diagonalizable matrix **A** the diagonal matrix of eigenvalues is $\lambda^A = \lambda_A$ and the individual eigenvalues are λ_i^A ; similarly for a generic matrix **B** the matrix of singular values is $\sigma^B = \sigma_B$ (with the singular values on the main diagonal) and the individual singular values are σ_i^B . We generically denote ρ_A the asymptotic limit of the empirical distribution of eigenvalues or singular values of a matrix A. Symbol \mathcal{P} refers to the set of probability densities with finite support. A matrix M with elements $M_{i,j}$ may also be written $[M_{ij}]$ or $[M_{cd}]$. Finally, the symbol $x \sim y$ means equality in distribution for two random variables; $x \sim p$ instead means that x is a sample from p whenever p is a probability distribution or a sample from p(x)dx if p is a probability density function.

2. Denoising of an Hermitian rotationally invariant matrix

Before considering the richer dictionary learning models, we start with the simplest possible model of inference of a large matrix: linear-rank rotationally invariant matrix denoising. It will only require known tools from random matrix theory.

2.1. The model. Let a matrix signal $\mathbf{S} = \mathbf{S}^{\dagger} \in \mathbb{K}^{N \times N}$ with $\mathbf{S} \sim P_{S,N}$ for some known prior distribution (which in general does not factorize over the matrix entries), and $\boldsymbol{\xi} = \boldsymbol{\xi}^{\dagger} \in \mathbb{K}^{N \times N}$ a standard Wigner noise matrix with probability density function (p.d.f.)

$$dP_{\boldsymbol{\xi},N}(\boldsymbol{\xi}) = C_N d\boldsymbol{\xi} \exp \operatorname{Tr} \left[-\frac{\beta N}{4} \boldsymbol{\xi}^2 \right]$$

with C_N the normalization factor. Consider a matrix denoising problem with data $\mathbf{Y} = \mathbf{Y}^{\dagger} \in \mathbb{K}^{N \times N}$ generated according to the observation model

(2)
$$Y = \sqrt{\lambda}S + \xi$$

The hidden matrix S to recover from the data is rotationally invariant in the sense that it is drawn from a prior distribution such that

$$dP_{S,N}(S) = dP_{S,N}(O^{\dagger}SO)$$

for any orthogonal ($\beta = 1$) or unitary ($\beta = 2$) matrix \boldsymbol{O} . It can thus be diagonalized as $\boldsymbol{S} = \tilde{\boldsymbol{U}}^{\dagger} \lambda^{S} \tilde{\boldsymbol{U}}$ where $\tilde{\boldsymbol{U}} \sim \mu_{N}^{(\beta)}$ with $\mu_{N}^{(\beta)}$ the normalized Haar measure over the orthogonal group $\mathcal{O}(N)$ if $\beta = 1$ or over the unitary group $\mathcal{U}(N)$ if $\beta = 2$. Matrix \boldsymbol{S} has $O(1/\sqrt{N})$ entries. This scaling for the entries of \boldsymbol{S} and of the Wigner matrix are such that the (real) eigenvalues of $\boldsymbol{S}, \boldsymbol{\xi}$ and therefore \boldsymbol{Y} remain O(1) in the limit $N \to +\infty$. The joint probability density function (j.p.d.f.) of eigenvalues of the matrix \boldsymbol{Y} generated according to model (2) is rigorously established in the case where \boldsymbol{S} has independent entries (which we do *not* necessarily assume), and is obtaind with techniques of a similar flavor as our strategy (i.e., based on the use of spherical integrals) [73]; see also [1] for an approach based on Dyson's Brownian motion.

The above model defines a random matrix ensemble for Y which is linked to the Rosenzweig-Porter random matrix model [74] from condensed matter. A generalized version of it has a rich behavior with a localization transition and regions with "multifractal eigenstates", see [75–78]. The regime we are interested in, namely with both λ^S and the eigenvalues of ξ being order 1, corresponds precisely to the critical scaling regime where a recently discovered transition from non-ergodic extended states to ergodic extended states happens in the model (i.e., the transition towards multifractality), see the discussion on the regime $\gamma = 1$ in [77]. We find the connection with inference particularly intriguing and the results of this paper may thus may be of independent interest in this context. In particular, if there is an information-theoretic transition in this inference problem it may happen to be connected to the $\gamma = 1$ ergodicity-breaking transition found in [77].

We consider a generic j.p.d.f. $p_{S,N}(\lambda^S)$ of eigenvalues which is symmetric¹ (i.e., invariant under any permutation of the entries of λ^S) and whose one-point marginal is assumed to weakly converge as $N \to +\infty$ to a well defined measure ρ_S with finite support and without point masses; in particular \boldsymbol{S} needs to be full-rank. We discuss at the end of this section how to overcome this latter constraint. Generically, rotational invariance implies that the prior over $\boldsymbol{S} = \tilde{\boldsymbol{U}}^{\dagger} \lambda^S \tilde{\boldsymbol{U}}$ can be decomposed as

(3)
$$dP_{S,N}(\boldsymbol{S}) = d\mu_N^{(\beta)}(\tilde{\boldsymbol{U}}) \, dp_{S,N}(\boldsymbol{\lambda}^S)$$

A (rather generic) special case of rotationally invariant measures for the signal are those of the form

(4)
$$dP_{S,N}(\boldsymbol{S}) \propto d\mu_N^{(\beta)}(\tilde{\boldsymbol{U}}) \, d\boldsymbol{\lambda}^S \exp \operatorname{Tr} \left[-\frac{\beta N}{4} V(\boldsymbol{\lambda}^S) \right] |\Delta_N(\boldsymbol{\lambda}^S)|^{\beta}$$

for a rotation invariant matrix potential $\text{Tr}V(S) = \text{Tr}V(\lambda^S)$, and where the Vandermonde determinant for a $N \times N$ diagonal matrix A with diagonal entries $(A_i)_{i \leq N}$ reads

(5)
$$\Delta_N(\boldsymbol{A}) \coloneqq \prod_{i< j}^{1,N} (A_i - A_j) = \det[(A_c)^{d-1}]$$

In this case the eigenvalues j.p.d.f. has the form

(6)
$$p_{S,N}(\boldsymbol{\lambda}^S) \propto \exp \operatorname{Tr} \left[-\frac{\beta N}{4} V(\boldsymbol{\lambda}^S) \right] |\Delta_N(\boldsymbol{\lambda}^S)|^{\beta}.$$

The case of a standard real symmetric or complex Hermitian Wigner matrices then corresponds to $V(\boldsymbol{\lambda}^S) = \boldsymbol{\lambda}_S^2$. Wishart matrices $\boldsymbol{S} = \boldsymbol{X} \boldsymbol{X}^{\dagger}$ with $\boldsymbol{X} \in \mathbb{K}^{N \times M}$ have a density for $N \leq M$ corresponding to $V(\boldsymbol{\lambda}^S) = 2(1 - M/N - 1/N + 2/(\beta N)) \ln \boldsymbol{\lambda}^S + 2(M/N) \boldsymbol{\lambda}^S$ (see more details later in Section 3).

¹We require symmetry except in the trivial case $p_{S,N}(\lambda^S) = \delta(\lambda^S - \lambda_0^S)$ for some fixed λ_0^S .

The main object of interest is the mutual information between data and signal:

$$I(\mathbf{Y}; \mathbf{S}) = H(\mathbf{Y}) - H(\mathbf{Y} \mid \mathbf{S})$$

= $H(\mathbf{Y}) - H(\boldsymbol{\xi})$
= $-\mathbb{E}_{\mathbf{Y}} \ln \int dP_{S,N}(\mathbf{s}) C_N \exp \operatorname{Tr} \left[-\frac{\beta N}{4} (\mathbf{Y} - \sqrt{\lambda} \mathbf{s})^2 \right] + \mathbb{E} \ln C_N \exp \operatorname{Tr} \left[-\frac{\beta N}{4} \boldsymbol{\xi}^2 \right]$
(7) = $-\mathbb{E}_{\mathbf{Y}} \ln \int dP_{S,N}(\mathbf{s}) \exp \frac{\beta N}{2} \operatorname{Tr} \left[\sqrt{\lambda} \mathbf{s} \mathbf{Y} - \frac{\lambda}{2} \mathbf{s}^2 \right] + \frac{\beta \lambda N}{4} \mathbb{E} \operatorname{Tr} \mathbf{S}^2.$

2.2. Free entropy and mutual information through random matrix theory. We define the free entropy $f_N = f_N(\mathbf{Y})$ as minus the first term in (7) divided by N^2 , without the expectation. The mutual information will directly be deduced from the free entropy, and using that the later is expected to concentrate onto its \mathbf{Y} -average. Using the eigen-decomposition $\mathbf{s} = \mathbf{U}^{\dagger} \boldsymbol{\lambda}^s \mathbf{U}$ the free entropy reads

$$f_{N} \coloneqq \frac{1}{N^{2}} \ln \int dP_{S,N}(\boldsymbol{s}) \exp \frac{\beta N}{2} \operatorname{Tr} \left[\sqrt{\lambda} \boldsymbol{s} \boldsymbol{Y} - \frac{\lambda}{2} \boldsymbol{s}^{2} \right]$$
$$= \frac{1}{N^{2}} \ln \int dp_{S,N}(\boldsymbol{\lambda}^{s}) \exp \left[-\frac{\beta \lambda N}{4} \operatorname{Tr} \boldsymbol{\lambda}_{s}^{2} \right] \int d\mu_{N}^{(\beta)}(\boldsymbol{U}) \exp \frac{\beta \sqrt{\lambda}}{2} N \operatorname{Tr} \left[\boldsymbol{U}^{\dagger} \boldsymbol{\lambda}^{s} \boldsymbol{U} \boldsymbol{Y} \right]$$
$$(8) \qquad = \frac{1}{N^{2}} \ln \int d\boldsymbol{\lambda}^{s} \exp N^{2} \left(\frac{1}{N^{2}} \ln p_{S,N}(\boldsymbol{\lambda}^{s}) - \frac{\beta \lambda}{4N} \operatorname{Tr} \boldsymbol{\lambda}_{s}^{2} + I_{N}^{(\beta)}(\boldsymbol{\lambda}^{s}, \boldsymbol{\lambda}^{Y}, \sqrt{\lambda}) \right).$$

There appears the HarishChandra-Itzykson-Zuber (HCIZ) spherical integral [70,79], which is only a function of the eigenspectra of its arguments: for $N \times N$ symmetric/Hermitian matrices \boldsymbol{A} and \boldsymbol{B} ,

(9)
$$I_N^{(\beta)}(\boldsymbol{A}, \boldsymbol{B}, \gamma) = I_N^{(\beta)}(\boldsymbol{\lambda}^A, \boldsymbol{\lambda}^B, \gamma) \coloneqq \frac{1}{N^2} \ln \int d\mu_N^{(\beta)}(\boldsymbol{U}) \exp \frac{\beta \gamma}{2} N \operatorname{Tr} \left[\boldsymbol{U}^{\dagger} \boldsymbol{\lambda}^A \boldsymbol{U} \boldsymbol{\lambda}^B \right]$$

where the integration is over $\mathcal{O}(N)$ when $\beta = 1$ or $\mathcal{U}(N)$ when $\beta = 2$. We recall known facts about it in Appendix A. It has a well-defined limit [79,80]:

$$I^{(\beta)}[\rho_A,\rho_B,\gamma] \coloneqq \lim_{N \to +\infty} I_N^{(\beta)}(\boldsymbol{\lambda}^A,\boldsymbol{\lambda}^B,\gamma),$$

where ρ_A, ρ_B are the asymptotic *densities* of eigenvalues (i.e., one-point correlation functions) of Aand B, respectively. In the present case, the eigenvalues λ^Y of the data matrix Y and associated asymptotic density ρ_Y are fixed by the model; λ^Y can be simulated and ρ_Y can be obtained using free probability, see, e.g., [81,82]. Thus, a standard saddle-point argument leads to the following conjecture for the free entropy $f_N = f_N(Y)$ as $N \to +\infty$.

Conjecture 1 (Free entropy of Hermitian rotationally invariant matrix denoising). The free entropy of model (2) verifies

(10)
$$f_N = \sup_{\boldsymbol{\lambda}^s \in \mathbb{R}^N} \left\{ \frac{1}{N^2} \ln p_{S,N}(\boldsymbol{\lambda}^s) - \frac{\beta \lambda}{4N} \operatorname{Tr} \boldsymbol{\lambda}_s^2 + I_N^{(\beta)}(\boldsymbol{\lambda}^s, \boldsymbol{\lambda}^Y, \sqrt{\lambda}) \right\} + \tau_N$$

Assuming there exists a functional Γ depending only on the asymptotic density of eigenvalues ρ_s associated with λ^s and such that

$$\Gamma[\rho_s] = \lim_{N \to +\infty} \frac{1}{N^2} \ln p_{S,N}(\boldsymbol{\lambda}^s)$$

we get, in terms of the density of eigenvalues,

$$f_N \to \sup_{\rho_s \in \mathcal{P}} \left\{ \Gamma[\rho_s] - \frac{\beta \lambda}{4} \int d\rho_s(x) \, x^2 + I^{(\beta)}[\rho_s, \rho_Y, \sqrt{\lambda}] \right\} + \tau.$$

The optimization is over the set \mathcal{P} of probability densities with finite support. The constants τ_N and τ fix the constraint $f_N(\lambda = 0) = 0$ (the spherical integral cancels when $\lambda = 0$):

$$\tau_N \coloneqq -\sup_{\boldsymbol{\lambda}^s \in \mathbb{R}^N} \frac{1}{N^2} \ln p_{S,N}(\boldsymbol{\lambda}^s) + o_N(1) \quad and \ its \ limit \quad \tau \coloneqq -\sup_{\rho_s \in \mathcal{P}} \Gamma[\rho_s]$$

For the typical form of eigenvalues density (6) we have

$$\frac{1}{N^2} \ln p_{S,N}(\boldsymbol{\lambda}^s) = \frac{\beta}{2N^2} \sum_{i\neq j}^{1,N} \ln |\lambda_i^s - \lambda_j^s| - \frac{\beta}{4N} \operatorname{Tr} V(\boldsymbol{\lambda}^s)$$

and the functional

$$\Gamma[\rho_s] = \frac{\beta}{2} \int d\rho_s(x) \, d\rho_s(y) \ln |x-y| - \frac{\beta}{4} \int d\rho_s(x) \, V(x).$$

Because we do not rigorously control the saddle-point estimation we state the result as a conjecture, but it should not be out of reach to turn it into a theorem using techniques as in [68].

This free entropy was not averaged with respect to Y. But it is expected that additionally it is self-averaging as it depends only on the spectrum λ^{Y} of Y:

$$\mathbb{E}f_N = f_N + o_N(1).$$

Note that from this conjecture, the minimum mean-square error (MMSE) can be deduced using the I-MMSE relation for gaussian channels $[83]^2$

(11)
$$\frac{1}{N^2} \mathbb{E} \| \boldsymbol{S} - \mathbb{E} [\boldsymbol{S} \mid \boldsymbol{Y}] \|^2 = \frac{4}{\beta N^2} \frac{d}{d\lambda} I(\boldsymbol{Y}; \boldsymbol{S}) + O(1/N) = \frac{1}{N} \mathbb{E} \operatorname{Tr} \boldsymbol{\lambda}_S^2 - \frac{4}{\beta} \frac{d}{d\lambda} \mathbb{E} f_N + O(1/N).$$

Regularity of eigenvalues and singular values distributions. All along the paper we assume that all eigenvalues (and later singular values) distributions are such that empirical distributions of eigen/singular values converge weakly to well defined asymptotic probability densities with i) (possibly disconnected) finite support, and *ii*) without any point masses. Cases of distributions with point masses (such as a matrix **S** of rank lower than N with a point mass δ_0 in its eigenvalues distribution; for example a rank-deficient Wishart matrix with M > N) can be approximated by considering regularizations. If the original signal matrix, say $\mathbf{S} \in \mathbb{R}^{N \times N}$, has a rank $(\mathbf{S}) < N$ with a finite fraction of eigen/singular values strictly null, one may instead consider from the beginning the same inference model but with full-rank signal $S_{\varepsilon} := S + Z_{\varepsilon}$ where Z_{ε} is an independent rotationally invariant regularization with norm smaller than ε , such as a Wigner matrix with sufficiently small variance. In certain cases it should then be possible to obtain the j.p.d.f. of the resulting matrix ensemble. The asymptotic formulas for the free entropies and mutual informations are expected to be continuous in ε . Thus assuming that the convergence to the asymptotic value is uniform in ε , we can permute the $N \to +\infty$ and $\varepsilon \to 0_+$ limits to obtain the formulas for "non full-rank" cases and densities with point masses. For the rest of the paper, we will thus restrict all theoretical arguments to full-rank cases without point masses.

²The factor 4 that differs from the 2 in the usual I-MMSE relation [83] comes from the fact that the Wigner matrix to denoise has only a fraction $N(N+1)/(2N^2) = 1/2 + O(1/N)$ of independent entries. The O(1/N) correction comes from the diagonal terms in matrix S for which the signal-to-noise ratio is different than the one of the off-diagonal entries. The complex noise case of the I-MMSE relation is discussed in Section V.D of [83].

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Let us also mention that despite we focus on full-rank square models of matrix denoising (2) with S a $N \times N$ matrix, we believe that by combining our approach together with the idea of "quadratization of rectangular matrices" found in [84], and exploited, e.g., in [85,86], then it should not require too much work to generalize the results on matrix denoising of Sections 2 and 3 to the rectangular setting $S \in \mathbb{K}^{N \times M}$, $N \neq M$.

2.3. Simplifications in the Bayes-optimal setting using the Nishimori identity. The above conjecture has already reduced the computation of an integral over $\Theta(N^2)$ degrees of freedom (the matrix elements) onto an optimization problem over $\Theta(N)$ eigenvalues (or a functional optimization over a density). But we claim that because of the fact that we are in the Bayesian optimal setting the formula can be further simplified, see Conjecture 2 below. Indeed, because in this matched setting the posterior is the "correct" one, and as a consequence, a fundamental property known as the Nishimori identity holds. This identity states that for any well-behaved function $g: \mathbb{R}^{N \times N} \mapsto \mathbb{R}$ we have (here we state a restricted form of the most general identity found in [67])

(12)
$$\mathbb{E}\langle g(\boldsymbol{s})\rangle = \mathbb{E}g(\boldsymbol{S})$$

where the signal $S \sim P_{S,N}$, while s is a sample from the Bayes-optimal posterior j.p.d.f.

$$dP_{S|Y,N}(\boldsymbol{s} \mid \boldsymbol{Y}) = \frac{1}{\mathcal{Z}(\boldsymbol{Y})} dP_{S,N}(\boldsymbol{s}) \exp \operatorname{Tr} \left[-\frac{\beta N}{4} \left(\boldsymbol{Y} - \sqrt{\lambda} \boldsymbol{s} \right)^2 \right]$$

and the Gibbs-bracket $\langle \cdot \rangle$ is the associated expectation. In particular we have

(13)
$$\mathbb{E}\left\langle\frac{\mathrm{Tr}\boldsymbol{\lambda}_{s}^{k}}{N}\right\rangle = \mathbb{E}\frac{\mathrm{Tr}\boldsymbol{\lambda}_{S}^{k}}{N}$$

the kth moment of the empirical density of eigenvalues of the signal.

We now give an heuristic argument based on four steps and leading to Conjecture 2 below; we believe that this may be the starting point of a rigorous proof strategy. Let $\hat{\rho}_{s,N}$ be the empirical density of the eigenvalues λ^s of the posterior sample. Define its moments

$$m_{k,N} \coloneqq \int dx \, x^k \hat{\rho}_{s,N}(x) = \frac{\mathrm{Tr} \boldsymbol{\lambda}_s^k}{N}$$

- (1) First, note that in expression (8) the density $\hat{\rho}_{s,N}$ plays the role of an order parameter for a "mean-field" free entropy functional given by the exponent in the integrand in (8), or equivalently, by the functional to be extremized in Conjecture 1. Concretely, one can express the integrand in (8) entirely in terms of the moments $(m_{k,N})_{k\geq 1}$ (this point is briefly detailed in Appendix C).
- (2) Second, we assume that the extremizer $\hat{\rho}_{s,N}^*$ in Conjecture 1 is such that the corresponding moments $m_{k,N}^*$ are close to the Gibbs average $\langle m_{k,N} \rangle = N^{-1} \langle \operatorname{Tr}(\boldsymbol{\lambda}_s)^k \rangle$. In other words

$$m_{k,N}^* = \langle m_{k,N} \rangle + o_N(1).$$

This is a natural self-consistency hypothesis for any "replica-symmetric" mean-field theory, where the optimal value of the order parameter generally coincides with the Gibbs average (the reader may recall the solution of the Curie-Weiss model for the prime example of this mechanism). Replica symmetry, namely the self-averaging/concentration of the order parameters (the moments $(m_{k,N})_k$), is generically rigorously valid in Bayes-optimal inference of low-rank models [67, 87] and we think that this property extends to linear-rank regimes.

(3) Third, we assume that the Gibbs expectation of the moments concentrates with respect to the data $\mathbf{Y}: \langle m_{k,N} \rangle = \mathbb{E} \langle m_{k,N} \rangle + o_N(1)$. This translates to

$$\langle m_{k,N} \rangle = N^{-1} \mathbb{E} \langle \operatorname{Tr} \boldsymbol{\lambda}_s^k \rangle + o_N(1) = \mathbb{E} \langle (\lambda_1^s)^k \rangle + o_N(1).$$

This is again true in low-rank Bayes-optimal inference [67, 87].

(4) Finally, from the two previous points and the Nishimori identity (13) we conclude

$$m_{k,N}^* = \mathbb{E}(\lambda_1^S)^k + o_N(1).$$

We have thus found that, somewhat remarkably, the extremizer in Conjecture 1 is nothing else than the empirical density of eigenvalues of the signal $\hat{\rho}_{s,N}^* = \hat{\rho}_{S,N}$. Taking $N \to +\infty$, the argument becomes exact: the empirical densities $\hat{\rho}_{s,N}^* \to \rho_s^* = \rho_S$ the asymptotic density of eigenvalues of the signal; this gives the formula (14) below. In particular the supremum in both the non trivial term where the spherical integral appears in Conjecture 1 and the constant term τ_N (or τ in the case of infinite N) are the same. Consequently we obtain a greatly simplified expression for the mutual information using relation (7), the fact that $N^{-1}\text{Tr} S^2 = N^{-1}\text{Tr} \lambda_S^2$ concentrates onto $N^{-1}\mathbb{E}\text{Tr} S^2$ when $N \to +\infty$, and the concentration assumption for the free entropy $\mathbb{E}f_N = f_N + o_N(1)$. We also obtain a formula for the MMSE using the I-MMSE relation (11).

Conjecture 2 (Mutual information of Hermitian rotationally invariant matrix denoising). Let $\lambda^s \in \mathbb{R}^N$ be the eigenvalues of a random matrix $\mathbf{s} \sim P_{S,N}$, i.e., $\lambda^s \sim p_{S,N}$. The mutual information of model (2) verifies

$$\frac{1}{N^2}I(\boldsymbol{Y};\boldsymbol{S}) = \frac{\beta\lambda}{2N} \operatorname{Tr} \boldsymbol{\lambda}_s^2 - I_N^{(\beta)}(\boldsymbol{\lambda}^s, \boldsymbol{\lambda}^Y, \sqrt{\lambda}) + o_N(1).$$

By introducing the density of eigenvalues we get

(14)
$$\frac{1}{N^2}I(\boldsymbol{Y};\boldsymbol{S}) \to \frac{\beta\lambda}{2} \int d\rho_s(x) \, x^2 - I^{(\beta)}[\rho_s,\rho_Y,\sqrt{\lambda}]$$

where ρ_s is the asymptotic spectral density of $\boldsymbol{s} \sim P_{S,N}$.

We deduce from (11) and a convexity argument (as $(I(\mathbf{Y}; \mathbf{S}))_N$ is a sequence of concave functions in λ) that the minimum mean-square error verifies

(15)
$$\frac{1}{N^2} \mathbb{E} \| \boldsymbol{S} - \mathbb{E} [\boldsymbol{S} \mid \boldsymbol{Y}] \|^2 = \frac{2}{N} \mathbb{E} \operatorname{Tr} \boldsymbol{\lambda}_S^2 - \frac{4}{\beta} \frac{d}{d\lambda} I_N^{(\beta)}(\boldsymbol{\lambda}^S, \boldsymbol{\lambda}^Y, \sqrt{\lambda}) + o_N(1),$$

or, working with the eigenvalues densities,

$$\frac{1}{N^2} \mathbb{E} \|\boldsymbol{S} - \mathbb{E} [\boldsymbol{S} \mid \boldsymbol{Y}] \|^2 \to 2 \int d\rho_S(x) \, x^2 - \frac{4}{\beta} \frac{d}{d\lambda} I^{(\beta)} [\rho_S, \rho_Y, \sqrt{\lambda}].$$

Remark 1: The spherical integral $I^{(\beta)}$ or $I_N^{(\beta)}$ is difficult to compute. One route is to try using the HCIZ formula, but it is known that the ratio of determinants involved in the formula (see Appendix A) is notoriously difficult to evaluate analytically or even numerically. Another one is to employ its asymptotic hydrodynamic description [79, 80] but this is challenging too. The

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HCIZ formula can be evaluated exactly in very special cases (e.g., the uniform and Wigner cases below) or perturbatively (see Section 3), or approximated by using sampling techniques [88]. We wish to point out that an easy and nice application of the HCIZ formula is to check that the asymptotic mutual information obtained in Conjecture 2 is the same for a signal S or its centered (trace-less) version $S - I_{d,N} N^{-1} \text{Tr} S$ (where $I_{d,N}$ is the identity of size N); this can be checked using basic properties of determinants. We know a-priori that this must be so because in the Bayesian-optimal case the statistician knows the asymptotic value of $N^{-1}\text{Tr} S \to \mathbb{E}\lambda_1^s$ (which is nothing else than the first moment of distribution of the signal) and can subtract it from the data matrix, so information-theoretically this has no influence.

Remark 2: Conjecture 2 was first obtained in the thesis of C. Schmidt [53] in the real case $\beta = 1$ (see Appendix 7). But what we believe are crucial steps and justifications were completely omitted in his derivation, and it is not obvious to us how the final (correct) result was obtained. In particular, [53] jumps from equation (8) to the final Conjecture 2 without justification (see the transition from equation (A.79) to (A.83) in Appendix 7 of [53]).

Remark 3: The formula for the MMSE involves the derivative of the HCIZ formula with respect to λ . This can be computed in cases where some expression for the asymptotic value $I^{(\beta)}[\rho_S, \rho_Y, \sqrt{\lambda}]$ is known. This is for example the case for the sanity checks of the next paragraphs, and also in terms of perturbative expansions presented in Section 3 for small and large signal-to-noise ratio. It is possible to deduce from the HCIZ formula an expression for the derivative directly in terms of the eigenvalues and eigenvectors of \mathbf{Y} . While this is not directly used in the present paper it could be of interest in numerical approaches and for the analysis of the various variational problems in this paper. For this reason we include it in Appendix B.

Let us comment on an a-priori quite surprising observation. Consider three scenarios for the prior over the eigenvalues λ^{S} of the signal:

- (1) The prior over the eigenvalues is of the form (6). When $N \to +\infty$ (which can be thought of as a vanishing temperature limit), strongly coupled eigenvalues λ^S drawn according to $p_{S,N}(\lambda^S)$ freeze into a configuration of minimal energy (which includes the external potential V plus the long range Coulomb repulsion due to the Vandermonde). The resulting one-point marginal is a non-trivial density ρ_S .
- (2) The prior is factorized as $p_{S,N}(\boldsymbol{\lambda}^S) = \prod_{i \leq N} \rho_S(\lambda_i^S)$, where ρ_S corresponds to the asymptotic marginal from the prior in case (1). In this case the prior does not induce any sort of interaction among eigenvalues and fluctuations survive as $N \to +\infty$: the "temperature remains finite" and no freezing phenomenon occurs.
- (3) The eigenvalues are deterministic and given to the statistician, i.e., $p_{S,N}(\lambda^S) = \delta(\lambda^S \lambda_0^S)$, where the fixed configuration λ_0^S has an empirical density converging to ρ_S .

By construction these three priors have the same one-point marginals (in the large size limit). For example, in the Wigner case, (1) would correspond to (6) with $V(\lambda^S) = \lambda_S^2$, and case (2) to $p_{S,N}(\lambda^S) = \prod_{i \leq N} (4 - (\lambda_i^S)^2)^{1/2}/(2\pi)$ a product of semicircle laws. For case (3) one can generate a typical sample from priors (1) or (2) and fix it. For the Wishart ensemble it would correspond

to $V(\boldsymbol{\lambda}^S) = 2(1 - M/N - 1/N + 2/(\beta N)) \ln \boldsymbol{\lambda}^S + 2(M/N)\boldsymbol{\lambda}^S$ in (6) for case (1), and $p_{S,N}(\boldsymbol{\lambda}^S) = \prod_{i \leq N} \rho_{MP}(\boldsymbol{\lambda}^S_i)$ a product of Marcenko-Pastur laws (31).

Now, we claim that in all three cases Conjecture 2 holds without any difference apart from possible $o_N(1)$ corrections. Indeed, in case (3) the integration over λ^s in (8) is trivial and it gives directly Conjecture 2. In case (2) if one plugs $p_{S,N}(\lambda^S) = \prod_{i \leq N} \rho_S(\lambda_i^S)$ in formula (10) the term $N^{-2} \ln p_{S,N}(\lambda^s) = o_N(1)$, so one may think that the prior has no influence on the formula. But this is not true, because the influence of this prior manifests itself through the data \boldsymbol{Y} which strongly depends on it. Going again through the four points above leading to the simplified Conjecture 2, one can see that they all remain valid. And because the moments $\mathbb{E}(\lambda_1^S)^k$ are the same in scenarios (1) and (2) (and (3) as well), the last point based on the Nishimori identity (13) identifies the same maximizing $(m_{k,N}^s)$, i.e., the same optimal density $\rho_s^s \to \rho_S$.

Let us provide an alternative information-theoretic counting argument in order to obtain Conjecture 2 "directly" without going through all the previous steps, and that justifies a-posteriori the equivalence of these seemingly very different situations at the level of the mutual information (which is thus insensitive to possible strong correlations between the eigenvalues of S and only depends on their density). By the chain rule for mutual information it can be decomposed as (recall $S = \tilde{U}^{\dagger} \lambda^{S} \tilde{U}$)

$$\frac{1}{N^2}I(\boldsymbol{Y};\boldsymbol{S}) = \frac{1}{N^2}I(\boldsymbol{Y};(\tilde{\boldsymbol{U}},\boldsymbol{\lambda}^S)) = \frac{1}{N^2}I(\boldsymbol{Y};\tilde{\boldsymbol{U}}\mid\boldsymbol{\lambda}^S) + \frac{1}{N^2}I(\boldsymbol{Y};\boldsymbol{\lambda}^S).$$

Now, because there are only N unknowns for the eigenvalues while there are N(N-1)/2 for the angles defining the eigenbasis \tilde{U} , the second term in the right-hand side in the above decomposition is O(1/N). Thus, at leading order $O(N^2)$, the mutual information $I(\boldsymbol{Y}; \boldsymbol{S})$ and the one given the eigenvalues $I(\boldsymbol{Y}; \tilde{\boldsymbol{U}} \mid \boldsymbol{\lambda}^S)$ are equal. Said differently, there are so much fewer eigenvalues $\boldsymbol{\lambda}^S$ than angular degrees of freedom and data points that their inference has comparably negligible cost. In particular in $I(\boldsymbol{Y}; \tilde{\boldsymbol{U}} \mid \boldsymbol{\lambda}^S)$ the set of eigenvalues is given, so that their correlations does not matter and the mutual information can only depend on their density ρ_S . Since the priors (1)–(3) above have the same density the corresponding mutual informations are identical. Finally, note that by the same arguments we also have that $I(\boldsymbol{Y}; \tilde{\boldsymbol{U}} \mid \boldsymbol{\lambda}^S)$ (and thus $I(\boldsymbol{Y}; \boldsymbol{S})$ too) is equal, at leading order in N, to $I(\boldsymbol{Y}; \tilde{\boldsymbol{U}}) = I(\sqrt{\lambda} \tilde{\boldsymbol{U}}^{\dagger} \boldsymbol{\lambda}^S \tilde{\boldsymbol{U}} + \boldsymbol{\xi}; \tilde{\boldsymbol{U}})$.

2.4. A sanity check: the case of a Wigner signal. Consider the problem of denoising a Wigner matrix: S is itself a standard Wigner with same distribution as the noise $\boldsymbol{\xi}$. So $V(S) = S^2$ in (4). The data \boldsymbol{Y} is therefore also a centered Wigner matrix with law

$$P(\mathbf{Y}) \propto \exp \operatorname{Tr} \left[-\frac{\beta N}{4(1+\lambda)} \mathbf{Y}^2 \right]$$

whose asymptotic spectral density is a semicircle of width $\sigma_Y \coloneqq \sqrt{1 + \lambda}$. This case is completely decoupled in the sense that each i.i.d. entry of the matrix \boldsymbol{S} is corrupted independently by an i.i.d. gaussian noise, so we should recover the known formulas for scalar decoupled gaussian channels [83]. This can be verified as follows: in this case the supremum over ρ_s in Conjecture 1 is attained for ρ_s being itself a semicircle of width $\sigma_s = 1$. Note that in this particular case, this can be deduced without making use of the Nishimori identity by realizing that whenever $\lambda \to +\infty$ or $\lambda \to 0_+$ it has to be so. Indeed in the noiseless limit $\lambda \to +\infty$ the posterior is peaked on the ground-truth signal \boldsymbol{S} and thus a sample \boldsymbol{s} will match it and have the same spectrum $\boldsymbol{\lambda}^s = \boldsymbol{\lambda}^S$ whose density is a semicircle of width 1. In the opposite completely noisy limit limit $\lambda = 0$, a sample from the posterior is simply

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drawn according to the prior $P_{S,N}$ which is the law of a standard Wigner matrix. Therefore in both cases the density ρ_s is a semicircle of width 1, but only in the second case the actual eigenvalues will match those of S. For any intermediate value of λ the eigenvalues λ^s will be in a mixture that polarize more towards λ^S as λ increases, but which maintains the same asymptotic *density*. In the complex case $\beta = 2$, the asymptotic spherical integral $I^{(2)}[\rho_s, \rho_Y, \sqrt{\lambda}]$ has a closed expression when evaluated for two semicircle laws [89]:

(16)
$$I^{(2)}[\rho_s, \rho_Y, \sqrt{\lambda}] = \frac{1}{2} \Big(\sqrt{4\sigma(\lambda)^4 + 1} - 1 - \ln\left(1 + \sqrt{4\sigma(\lambda)^4 + 1}\right) + \ln 2 \Big),$$

where $\sigma(\lambda)^2 := \sqrt{\lambda}\sigma_Y \sigma_s = \sqrt{\lambda(1+\lambda)}$. Moreover, according to "Zuber's $\frac{1}{2}$ -rule" [90] we can simply relate the real case $\beta = 1$ to the complex one $\beta = 2$:

(17)
$$I^{(1)}[\rho_s, \rho_Y, \sqrt{\lambda}] = \frac{1}{2} I^{(2)}[\rho_s, \rho_Y, \sqrt{\lambda}]$$

Using that the second moment $\mathbb{E}(\lambda_1^S)^2 = \int_{-2}^2 dx \, x^2 \sqrt{4 - x^2}/(2\pi) = 1$ we reach from Conjecture 2 the expected expression:

(18)
$$\frac{1}{N^2}I(\boldsymbol{Y};\boldsymbol{S}) \to \frac{\beta}{4}\left(2\lambda + 1 - \sqrt{4\lambda(1+\lambda)+1} + \ln\left(1 + \sqrt{4\lambda(1+\lambda)+1}\right) - \ln 2\right) = \frac{\beta}{4}\ln(1+\lambda).$$

The minimum mean-square error is thus

(19)
$$\frac{1}{N^2} \mathbb{E} \| \boldsymbol{S} - \mathbb{E} [\boldsymbol{S} \mid \boldsymbol{Y}] \|^2 \to \frac{1}{1+\lambda}$$

So we recover the formulas of [83]. Note that in the present case, the convergence \rightarrow in the above identities are actually equalities for any N (but our derivation here is asymptotic in nature).

2.5. An explicit model with uniform spectral distribution. We consider model (2) with λ^{S} being a uniform permutation of equally spaced eigenvalues in $[-\sqrt{3}, \sqrt{3})$:

(20)
$$p_{S,N}(\boldsymbol{\lambda}^{S}) = \frac{1}{N!} \mathbf{1} \Big(\boldsymbol{\lambda}^{S} \in \Pi \Big(\sqrt{\gamma} \Big(-\frac{1}{2}, \frac{1}{N} - \frac{1}{2}, \frac{2}{N} - \frac{1}{2}, \dots, \frac{1}{2} - \frac{1}{N} \Big) \Big) \Big)$$

where, letting $v \in \mathbb{R}^N$, $\Pi(v)$ is the set of all N! permutations of v, $\mathbf{1}(\cdot)$ is the indicator function and $\gamma = \gamma_N \to 12$ enforces $\operatorname{Tr} \lambda_S^2 = N$. The advantage of this model is that the HCIZ integral appearing in Conjecture 2 is explicit when $\beta = 2$. Let $\lambda^s \sim p_{S,N}$. The HCIZ integral (see Appendix A) does not depend on the ordering of the eigenvalues, therefore we can consider the increasing ordering $\lambda_i^s = \sqrt{\gamma}(i-1)/N - \sqrt{\gamma}/2$. Denote $\sigma := \gamma \lambda$. The HCIZ formula then gives (because the ratio of determinants is non-negative we can insert an absolute value)

$$N^{2}I_{N}^{(2)}(\boldsymbol{\lambda}^{s},\sqrt{\lambda}\boldsymbol{\lambda}^{Y},1) = \ln\frac{\prod_{k\leq N-1}k!}{N^{N(N-1)/2}} + \ln\left|\frac{\det[(\exp\sqrt{\sigma}\lambda_{j}^{Y})^{i-1}\exp(-N\sqrt{\sigma}\lambda_{j}^{Y}/2)]}{\Delta_{N}(\boldsymbol{\lambda}^{S})\Delta_{N}(\sqrt{\lambda}\boldsymbol{\lambda}^{Y})}\right|$$
$$= \ln\frac{\prod_{k\leq N-1}k!}{N^{N(N-1)/2}} + \ln\left|\frac{\det[(\exp\sqrt{\sigma}\lambda_{j}^{Y})^{i-1}]}{\Delta_{N}(\boldsymbol{\lambda}^{S})\Delta_{N}(\sqrt{\lambda}\boldsymbol{\lambda}^{Y})}\right| - \frac{N}{2}\sqrt{\sigma}\operatorname{Tr}\boldsymbol{\lambda}^{Y}.$$

The matrix $[(\exp \sqrt{\sigma \lambda_i^Y})^{i-1}]$ is a generalized Vandermonde, and thus

$$\det[(\exp\sqrt{\sigma\lambda_j^Y})^{i-1}] = \prod_{i< j}^{1,N} (\exp\sqrt{\sigma\lambda_i^Y} - \exp\sqrt{\sigma\lambda_j^Y}).$$

The mutual information from Conjecture 2 then reads:

(21)
$$\frac{1}{N^2}I(\boldsymbol{Y};\boldsymbol{S}) = \lambda - \frac{1}{N^2}\sum_{i$$

The MMSE can then be obtained using the I-MMSE relation (11):

$$\frac{\beta}{N^2} \mathbb{E} \| \boldsymbol{S} - \mathbb{E} [\boldsymbol{S} \mid \boldsymbol{Y}] \|^2 = 4 - \frac{4}{N^2} \sum_{i < j}^{1,N} \frac{e^{\sqrt{\sigma}\lambda_i^Y} \frac{d}{d\lambda} (\sqrt{\sigma}\lambda_i^Y) - e^{\sqrt{\sigma}\lambda_j^Y} \frac{d}{d\lambda} (\sqrt{\sigma}\lambda_j^Y)}{e^{\sqrt{\sigma}\lambda_i^Y} - e^{\sqrt{\sigma}\lambda_j^Y}} + \frac{1}{\lambda} + \frac{4}{N^2} \sum_{i < j}^{1,N} \frac{\frac{d}{d\lambda} (\lambda_i^Y - \lambda_j^Y)}{\lambda_i^Y - \lambda_j^Y} + \sqrt{\frac{\gamma}{\lambda}} \frac{1}{N} \operatorname{Tr} \boldsymbol{\lambda}^Y + \frac{2\sqrt{\sigma}}{N} \sum_{i \leq N} \frac{d}{d\lambda} \lambda_i^Y + o_N(1).$$

Introducing the Y-eigenvectors $Y \psi_i^Y = \lambda_i^Y \psi_i^Y$, the Hellmann-Feynman theorem implies

$$\frac{d}{d\lambda}\lambda_i^Y = \frac{1}{2\sqrt{\lambda}}(\boldsymbol{\psi}_i^Y)^{\dagger}\boldsymbol{S}\boldsymbol{\psi}_i^Y =: \frac{1}{2\sqrt{\lambda}}p_i$$

where S is the ground-truth in (2) (not to be confused with s, another independent sample from $P_{S,N}$). As a consequence we finally obtain the explicit expression

$$\frac{\beta}{N^{2}} \mathbb{E} \| \boldsymbol{S} - \mathbb{E} [\boldsymbol{S} | \boldsymbol{Y}] \|^{2} = 4 - \frac{2\sqrt{\gamma}}{N^{2}} \sum_{i < j}^{1,N} \frac{e^{\sqrt{\sigma}\lambda_{i}^{Y}} (\frac{1}{\sqrt{\lambda}}\lambda_{i}^{Y} + p_{i}) - e^{\sqrt{\sigma}\lambda_{j}^{Y}} (\frac{1}{\sqrt{\lambda}}\lambda_{j}^{Y} + p_{j})}{e^{\sqrt{\sigma}\lambda_{i}^{Y}} - e^{\sqrt{\sigma}\lambda_{j}^{Y}}} + \frac{1}{\lambda} + \frac{2}{\sqrt{\lambda}N^{2}} \sum_{i < j}^{1,N} \frac{p_{i} - p_{j}}{\lambda_{i}^{Y} - \lambda_{j}^{Y}} + \sqrt{\frac{\gamma}{\lambda}} \frac{1}{N} \operatorname{Tr} \boldsymbol{\lambda}^{Y} + \frac{\sqrt{\gamma}}{N} \sum_{i \leq N} p_{i} + o_{N}(1).$$

Let us introduce the asymptotic spectral densities ρ_s and ρ_Y associated with the matrices s and Y. Then the above expression reads, in the large size limit $N \to +\infty$,

(23)
$$\frac{1}{N^2}I(\boldsymbol{Y};\boldsymbol{S}) \to \lambda + \frac{\ln\lambda\gamma}{4} + \frac{1}{2}\int d\rho_Y(x)\,d\rho_Y(y)\ln\left|\frac{x-y}{\exp x\sqrt{\lambda\gamma} - \exp y\sqrt{\lambda\gamma}}\right|.$$

We used that

$$\frac{1}{N^2} \sum_{i$$

so these two terms asymptotically cancel each other. We also used that \mathbf{Y} , as a sum of asymptotically trace-less matrices, is asymptotically trace-less too and therefore the term $\int d\rho_Y(x) x = 0$.

Note that, as explained below Conjecture 2, we could have fixed from the beginning one arbitrary permutation of the eigenvalues: $p_{S,N}(\lambda^S) = \delta(\lambda^S - \sqrt{\gamma}(-1/2, 1/N - 1/2, 2/N - 1/2, \ldots, 1/2 - 1/N))$, instead of considering the uniform measure (20) over permutations. This would have lead to the same calculations which is easily seen. What is less trivial to see, because in that case we could not simplify anymore the HCIZ formula using the generalized Vandermonde form, is that the result would be asymptotically the same if the prior was instead uniform but not necessarily equally spaced, i.e., $p_{S,N} = \mathcal{U}[-\sqrt{3}, \sqrt{3})^{\otimes N}$.

The λ -dependent data spectral distribution ρ_Y can be obtained from free probability as follows; we refer to [81,91] for clean definitions, domains of definitions and properties of the functions we



FIGURE 1. Left: Asymptotic $N \to +\infty$ spectral density $\rho_Y(x)$ (red) for the denoising model (2) with $\lambda = 20$ and a signal S with uniform eigenvalues in $[-\sqrt{3}, \sqrt{3})$. It is compared to the empirical spectral density of Y for a realization of size N = 5000 (blue). Right: The same for a smaller signal-to-noise ratio $\lambda = 2$. As expected, the spectrum ressembles more the semicircle law in that case. The density does approach Wigner's semicircle law of radius 2 as $\lambda \to 0_+$.

are going to use now. The complex-valued Green function (or minus Stieljes transform) associated with ρ , whose domain is the complex plane minus the support of ρ , is

$$G_{\rho}(z) \coloneqq \int d\rho(x) \frac{1}{z - x}$$

The Blue function is its functional inverse verifying $B_{\rho}(G_{\rho}(z)) = G_{\rho}(B_{\rho}(z)) = z$. Then the complex valued R-transform is defined as

$$R_{\rho}(z) = B_{\rho}(z) - \frac{1}{z} = \sum_{i \ge 1} k_i z^{i-1}$$

where the coefficients $(k_i)_{i\geq 1}$ in its series expansion are the so-called free cumulants associated with density ρ . Asymptotically, the matrix $\sqrt{\lambda} S$ has eigenvalue density $\rho_{\sqrt{\lambda}S}$ which is the uniform distribution in $[-\sqrt{3\lambda}, \sqrt{3\lambda})$. The associated Green function is

$$G_{\rho_{\sqrt{\lambda}S}}(z) = \frac{1}{2\sqrt{3\lambda}} \ln \frac{z + \sqrt{3\lambda}}{z - \sqrt{3\lambda}}, \quad \text{thus} \quad \mathcal{R}_{\rho_{\sqrt{\lambda}S}}(z) = \sqrt{3\lambda} \coth(z\sqrt{3\lambda}) - \frac{1}{z}.$$

The R-transform of the standard Wigner semicircle law is the identity: $R_{\rho_Z}(z) = z$. Finally, by additivity of the R-transform for asymptotically free random matrices, the R-transform of the spectral density of the data matrix is

$$R_{\rho_Y}(z) = R_{\rho_{\sqrt{\lambda}S}}(z) + R_{\rho_Z}(z) = \sqrt{3\lambda} \coth(z\sqrt{3\lambda}) - \frac{1}{z} + z$$

Its Blue function is thus $B_{\rho_Y}(z) = \sqrt{3\lambda} \coth(z\sqrt{3\lambda}) + z$ from which we get a transcendental equation for its Green function:

(24)
$$z = \sqrt{3\lambda} \coth(G_{\rho_Y}(z)\sqrt{3\lambda}) + G_{\rho_Y}(z).$$



FIGURE 2. Main: The abciss corresponds to the signal-to-noise ratio λ in model (2). The blue dots correspond to the mutual information (MI) for the uniform spectrum case evaluated from (21) for N = 1000 averaged over 100 independent realizations: the orange dots are the MMSE in the same monte-carlo experiment, evaluated from (22). The pink dots correspond to the asymptotic $N \to +\infty$ mutual information for the uniform spectrum case evaluated from (23). The finite N and asymptotic $N \rightarrow +\infty$ values of the mutual information match very closely as can be seen from the superposition of the pink and blue dots. The red dashed line is the mutual information for the Wigner signal case (18) and the black one the MMSE (19). All is for $\beta = 2$. The curves for the uniform and semicircle laws match surprisingly well but are actually different. Inset: These curves quantify the relative difference between the empirical curves (the blue or orange dots) for the uniform case and the (dashed) curves for the Wigner case. The relative difference is typically of order $O(10^{-3})$. When comparing instead the $N \to +\infty$ curve for the uniform case (pink dots) to the Wigner mutual information so that any finite size effects are removed, a difference of the same order survives (which is much higher than the expected numerical precision for these computations). This confirms that the curves are *not* exactly the same.

This equation can be solved numerically using a complex non-linear solver. A MATHEMATICA code to do so is provided in Appendix D. From its solution we can access the spectral density:

(25)
$$\rho_Y(x) = \frac{1}{\pi} \lim_{\varepsilon \to 0} |\Im G_{\rho_Y}(x - i\varepsilon)|$$

Figure 1 shows in red the asymptotic prediction from the spectrum extracted from the numerical solution of (24) and (25). It almost perfectly matches the empirical density of eigenvalues of \boldsymbol{Y} for realisations of the model for large sizes, see the blue histograms.

Given a signal-to-noise ratio λ , we can compute the mutual information in the large size limit $N \rightarrow +\infty$ using formulas (23), (24) and (25). This yields the pink dots of Figure 2. The blue dots are instead for the mutual information for large realizations of the model (2) for a S with a uniform spectrum, see formula (21). The orange dots are for the MMSE for that case, see formula (22).

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These curves are compared to the case of Wigner signal and match surprisingly well up to relative differences of $O(10^{-3})$. But our perturbative expansions of the next section as well as the comparison with the asymptotic predictions from (23) show that this difference, even if small, is not just due to numerical imprecisions: the curves really are different even in the large size limit. Yet, it is very interesting to observe that the simple (decoupled) case of matrix denoising with S a Wigner matrix allows us to very accurately approximate the information-theoretic quantities of the much less trivial setting where S has a uniform spectrum (and therefore the matrix elements of S are dependent, as opposed to the Wigner case). Further investigation around this fact is needed and left for future work.

3. Perturbative expansions for Hermitian matrix denoising

We exploit perturbative expansions of the HCIZ integral, for small [92] and large [89] λ , to discuss the corresponding expansions of the mutual information and MMSE as predicted by Conjecture 2. In this section we only consider complex cases $\beta = 2$, for which expansions of the HCIZ integral have been worked out.

3.1. Small signal-to-noise regime. Let \boldsymbol{A} and \boldsymbol{B} two hermitian $N \times N$ matrices. We use an expansion of the HCIZ integral (9) in the complex case $I_N^{(2)}(\boldsymbol{A}, \boldsymbol{B}, \sqrt{\lambda})$ in terms of moments

$$\theta_p \coloneqq \lim_{N \to +\infty} \frac{1}{N} \operatorname{Tr} \boldsymbol{A}^p = \lim_{N \to +\infty} \frac{1}{N} \sum_{i \le N} (\lambda_i^A)^p \quad \text{and} \quad \bar{\theta}_p \coloneqq \lim_{N \to +\infty} \frac{1}{N} \operatorname{Tr} \boldsymbol{B}^p = \lim_{N \to +\infty} \frac{1}{N} \sum_{i \le N} (\lambda_i^B)^p$$

for integer $p \ge 1$. Note that by concentration θ_p is also equal to $\lim_{N\to+\infty} N^{-1}\mathbb{E}\operatorname{Tr} \mathbf{A}^p$ and similarly for $\bar{\theta}_p$. We assume that \mathbf{A} and \mathbf{B} are *trace-less*, i.e., $\theta_1 = \bar{\theta}_1 = 0$. Then, according to [92],

(26)
$$\lim_{N \to +\infty} I_N^{(2)}(\boldsymbol{A}, \boldsymbol{B}, \sqrt{\lambda}) = I^{(2)}[\rho_A, \rho_B, \sqrt{\lambda}] = \sum_{n \ge 2} \lambda^{\frac{n}{2}} F_n(\boldsymbol{A}, \boldsymbol{B})$$

with (terms up to n = 8 are explicitly derived in [92] and diagrammatic rules are given for higher orders; see also Appendix D for their complete expressions)

(27)
$$\begin{cases} F_2 &= \frac{1}{2}\theta_2\theta_2, \\ F_3 &= \frac{1}{3}\theta_3\bar{\theta}_3, \\ F_4 &= \frac{3}{4}\theta_2\bar{\theta}_2 - \frac{1}{2}\theta_2^2\bar{\theta}_4 - \frac{1}{2}\theta_4\bar{\theta}_2^2 + \frac{1}{4}\theta_4\bar{\theta}_4 \end{cases}$$

We will also make use of the derivatives with respect to the moments $\bar{\theta}_p$. These read

$$\frac{\partial}{\partial \bar{\theta}_p} I^{(2)}[\rho_A, \rho_B, \sqrt{\lambda}] = \frac{\bar{D}_p}{p} \quad \text{for} \quad p \ge 2, \quad \text{with} \quad \begin{cases} \bar{D}_2 &= \lambda \theta_2 + \lambda^2 \frac{1}{2} (3\theta_2 - 4\theta_4 \bar{\theta}_2) + O(\lambda^{5/2}), \\ \bar{D}_3 &= \lambda^{3/2} \theta_3 + O(\lambda^{5/2}), \\ \bar{D}_4 &= -\lambda^2 (2\theta_2^2 - \theta_4) + O(\lambda^3). \end{cases}$$

where the higher order corrections come from the structure of F_5 and F_6 and can be worked out from [92].

These formulas are applied for $\mathbf{A} = \mathbf{S}$ and $\mathbf{B} = \mathbf{Y} = \sqrt{\lambda}\mathbf{S} + \boldsymbol{\xi}$ with $N^{-1}\text{Tr}\mathbf{S} = o_N(1)$ and $N^{-1}\text{Tr}\mathbf{Y} = o_N(1)$. As explained in Remark 1 after Conjecture 2 the mutual information remains the same if we center the signal to make \mathbf{S} and \mathbf{Y} trace-less. Although this is not necessary, and one can work out the expansion for a non-centered signal and data, this turns out to be a major

simplification in the ensuing calculations. For the mutual information, according to Conjecture 2 we find the expansion when $\beta = 2$:

(28)
$$\lim_{N \to +\infty} \frac{1}{N^2} I(\boldsymbol{Y}; \boldsymbol{S}) = \lambda \theta_2 - \sum_{n \ge 2} \lambda^{\frac{n}{2}} F_r$$

and for the MMSE

(29)

$$\lim_{N \to +\infty} \frac{\beta}{N^2} \mathbb{E} \| \boldsymbol{S} - \mathbb{E} [\boldsymbol{S} | \boldsymbol{Y}] \|^2 = 4\theta_2 - 4 \frac{\partial}{\partial \lambda} I^{(2)} [\rho_S, \rho_Y, \sqrt{\lambda}] - 4 \sum_{p \ge 2} \frac{\partial}{\partial \bar{\theta}_p} I^{(2)} [\rho_S, \rho_Y, \sqrt{\lambda}] \frac{d\theta_p}{d\lambda}$$

$$= 4\theta_2 - 4 \sum_{n \ge 2} \frac{n}{2} \lambda^{\frac{n}{2} - 1} F_n - 4 \sum_{p \ge 2} \frac{\bar{D}_p}{p} \frac{d\bar{\theta}_p}{d\lambda}.$$

In these expressions F_n and D_p are given by their expansions in terms of the moments

$$\begin{cases} \theta_p &= \lim_{N \to +\infty} N^{-1} \mathrm{Tr} \boldsymbol{S}^p = \lim_{N \to +\infty} N^{-1} \mathbb{E} \mathrm{Tr} \boldsymbol{S}^p, \\ \bar{\theta}_p &= \lim_{N \to +\infty} N^{-1} \mathrm{Tr} \boldsymbol{Y}^p = \lim_{N \to +\infty} N^{-1} \mathbb{E} \mathrm{Tr} \boldsymbol{Y}^p, \end{cases}$$

which themselves are polynomials in $\sqrt{\lambda}$. To go further we must fix a specific model of interest.

Example 1 (Wigner signal): Let $\boldsymbol{\xi} = \boldsymbol{\xi}^{\dagger} \in \mathbb{C}^{N \times N}$, $\boldsymbol{\xi} \sim \exp \operatorname{Tr}\left[-\frac{N}{2}\boldsymbol{\xi}^{2}\right]$ a standard Hermitian Wigner matrix; this corresponds to a potential $V(x) = x^{2}$ in (4). Take an i.i.d. copy $\boldsymbol{\xi}'$ and set $\boldsymbol{S} = \boldsymbol{\xi}'$ and $\boldsymbol{Y} = \sqrt{\lambda}\boldsymbol{\xi}' + \boldsymbol{\xi}$. We note that $\boldsymbol{Y} \sim \sqrt{1+\lambda}\boldsymbol{\xi}$. Wigner's semicircle law

$$\rho_{\xi}(x) = \mathbf{1}(|x| \le 2) \frac{\sqrt{4 - x^2}}{2\pi}$$

implies for even moments (odd moments vanish)

$$\theta_{2p} = \lim_{N \to +\infty} \frac{1}{N} \mathbb{E} \operatorname{Tr} \boldsymbol{\xi}^{2p} = \frac{1}{p+1} \binom{2p}{p}, \quad \bar{\theta}_{2p} = \lim_{N \to +\infty} \frac{1}{N} \mathbb{E} \operatorname{Tr} \boldsymbol{Y}^{2p} = \frac{(1+\lambda)^p}{p+1} \binom{2p}{p}.$$

From $\theta_2 = 1$, $\theta_4 = 2$, $\theta_6 = 5$ and $\overline{\theta}_2 = 1 + \lambda$, $\overline{\theta}_4 = 2(1 + \lambda)^2$, $\overline{\theta}_6 = 5(1 + \lambda)^3$ we find

$$F_2 = \frac{1}{2}(1+\lambda),$$
 $F_4 = -\frac{1}{4}(1+\lambda)^2$ and $F_6 = \frac{1}{3}(1+\lambda)^3.$

From the expansion (28) for the mutual information we get

(30)
$$\lim_{N \to +\infty} \frac{1}{N^2} I(\boldsymbol{Y}; \boldsymbol{S}) = \frac{\lambda}{2} - \frac{\lambda^2}{4} + \frac{\lambda^3}{6} + O(\lambda^4)$$

We recognize the expansion of $\frac{1}{2}\ln(1+\lambda)$ and the result is consistent with (18).

Example 2 (Wishart signal): Consider $\mathbf{S} = \mathbf{X}\mathbf{X}^{\dagger}$ and $\mathbf{Y} = \sqrt{\lambda}\mathbf{X}\mathbf{X}^{\dagger} + \boldsymbol{\xi}$, where the noise $\boldsymbol{\xi} \in \mathbb{C}^{N \times N}$ is an Hermitian Wigner matrix normalized as in the previous example and $\mathbf{X} \in \mathbb{C}^{N \times M}$ is drawn from $P_{X,M}(\mathbf{X}) \propto \exp \operatorname{Tr}[-M\mathbf{X}\mathbf{X}^{\dagger}]$. Let $\varphi := N/M$. For $\varphi \leq 1$ the eigenvalue j.p.d.f. is well defined, and corresponds to the potential $V(x) = 2(1 - 1/\varphi) \ln |x| + 2x/\varphi$ in (4) (see, e.g., [91]). When $\varphi > 1$ the matrix is rank deficient and there is no well defined j.p.d.f. for the eigenvalues but the model can be regularized as explained in Section 2 and the final conjectures apply. In particular the Marcenko-Pastur distribution for the eigenvalues of $\mathbf{S} = \mathbf{X}\mathbf{X}^{\dagger}$ is well defined for all $\varphi > 0$:

(31)
$$\rho_{\rm MP}(x) = \max(1 - 1/\varphi, 0)\delta(x) + \frac{\mathbf{1}(c \le x \le d)}{2\pi\varphi x}\sqrt{(x - c)(d - x)}$$

where $c := (\sqrt{\varphi} - 1)^2$ and $d := (\sqrt{\varphi} + 1)^2$. The spectral moments are deduced by standard integration methods and we find

$$\lim_{N \to +\infty} \frac{1}{N} \operatorname{Tr}(\boldsymbol{X} \boldsymbol{X}^{\dagger})^{p} = \lim_{N \to +\infty} \frac{1}{N} \mathbb{E} \operatorname{Tr}(\boldsymbol{X} \boldsymbol{X}^{\dagger})^{p} = \frac{1}{p} \sum_{k \leq p} \varphi^{k-1} {p \choose k} {p \choose k-1}.$$

In particular for the first moment $\lim_{N\to+\infty} N^{-1}\mathbb{E}\operatorname{Tr} X X^{\dagger} = 1$.

Now, as explained before, in order to compute the mutual information it is convenient to center the signal so that it becomes trace-less. In other words we replace $\boldsymbol{X}\boldsymbol{X}^{\dagger}$ by $\boldsymbol{S} = \boldsymbol{X}\boldsymbol{X}^{\dagger} - I_{d,N}$ so that $N^{-1}\text{Tr}\boldsymbol{S} \rightarrow 0$. This also implies $\boldsymbol{Y} = \sqrt{\lambda}(\boldsymbol{X}\boldsymbol{X}^{\dagger} - I_{d,N}) + \boldsymbol{\xi}$ and $N^{-1}\text{Tr}\boldsymbol{Y} \rightarrow 0$. The first moments of the spectral density of this \boldsymbol{S} are in the asymptotic limit $\theta_2 = \varphi, \theta_3 = \varphi^2, \theta_4 = \varphi^3 + 2\varphi^2, \theta_5 = \varphi^4 + 5\varphi^3,$ $\theta_6 = 5\varphi^3 + 9\varphi^4 + \varphi^5$ and those of \boldsymbol{Y} are $\bar{\theta}_1 = 0, \bar{\theta}_2 = 1 + \lambda\varphi, \bar{\theta}_3 = \lambda^{3/2}\varphi^2, \bar{\theta}_4 = \lambda^2(\varphi^3 + 2\varphi^2) + 4\lambda\varphi + 2,$ $\bar{\theta}_5 = O(\lambda^{3/2}), \bar{\theta}_6 = 5 + O(\lambda)$. This yields

(32)
$$\begin{cases} F_2 = \frac{\varphi}{2} + \lambda \frac{\varphi^2}{2}, \\ F_3 = \lambda^{3/2} \frac{\varphi^4}{3}, \\ F_4 = -\frac{\varphi^4}{4} - \lambda \frac{\varphi^3}{2} + \lambda^2 \frac{1}{4} (\varphi^6 - \varphi^4), \\ F_5 = O(\lambda^{3/2}), \\ F_6 = \frac{\varphi^3}{3} - \frac{\varphi^4}{6} + O(\lambda). \end{cases}$$

For the mutual information we find

(33)
$$\lim_{N \to +\infty} \frac{1}{N^2} I(\boldsymbol{Y}; \boldsymbol{S}) = \lambda \frac{\varphi}{2} - \lambda^2 \frac{\varphi^2}{4} + \lambda^3 \frac{\varphi^3 - \varphi^4}{6} + O(\lambda^4)$$

We note that the contribution of the order $O(\lambda^3)$ only comes from the order $O(\lambda)$ in F_4 and the constant term in F_6 . We also remark that for $\varphi = 1$ the first two orders are the same than the pure Wigner case of Example 1. It is possible to show that this is a universal feature for all matrices S such that $N^{-1}\text{Tr} S \to 0$ and $N^{-1}\text{Tr} S^2 \to 1$, see the next example.

Example 3 (general case): As before $(\theta_p)_{p\geq 1}$ correspond to the asymptotic spectral moments of the signal S. It easy to skim through the above calculations and obtain the first terms of an expansion for general signals with even spectral density such that $\theta_2 = 1$ and $\theta_{2p+1} = 0$, $p \geq 0$ (note that for the trace-less Marchenko-Pastur distribution this is true only if p = 0). At third order the resulting expansion can be read off by removing the contribution of F_3 and the term $-\varphi^4/6$ from F_6 and we find

(34)
$$\lim_{N \to +\infty} \frac{1}{N^2} I(\boldsymbol{Y}; \boldsymbol{S}) = \frac{\lambda}{2} - \frac{\lambda^2}{4} + \frac{\lambda^3}{6} + O(\lambda^4).$$

The generic case until fourth order is heavy to handle by hand. We provide in Appendix D a MATHEMATICA code to get the following expansions. Let $(k_p)_{p\geq 2}$ be the free cumulants associated with the asymptotic spectral density ρ_S of S (see, e.g., [4,81] to know about free cumulants). For $N \to +\infty$ followed by $\lambda \to 0_+$ and a ρ_S such that $\theta_1 = k_1 = 0$ and $\theta_2 = k_2 = 1$,

(35)
$$\lim_{N \to +\infty} \frac{1}{N^2} I(\boldsymbol{Y}; \boldsymbol{S}) = \frac{\lambda}{2} - \frac{\lambda^2}{4} + \lambda^3 \frac{1 - k_3^2}{6} - \lambda^4 \frac{1 + 4k_3^2 + k_4^2}{8} + o(\lambda^4).$$

Or expressed in terms of the moments (the mapping between moments and free cumulants can be obtained using the routines in Appendix D),

(36)
$$\lim_{N \to +\infty} \frac{1}{N^2} I(\boldsymbol{Y}; \boldsymbol{S}) = \frac{\lambda}{2} - \frac{\lambda^2}{4} + \lambda^3 \frac{1 - \theta_3^2}{6} - \lambda^4 \frac{5 + 4\theta_3^2 + \theta_4^2 - 4\theta_4}{8} + o(\lambda^4).$$

Interestingly, for any even spectral density this matches the pure Wigner case of Example 1 up to third order. However this breaks down at fourth order as soon as the fourth moment θ_4 of ρ_S is different from 2. This is another indication that the curves for the uniform spectrum and Wigner cases of Figure 2 are different. Indeed, it can be checked that the (F_n) in the expansion (28) for these two cases are very close but different. Or that their respective expansions (36) are the same up to order three, but the order four for the Wigner case is $-\frac{1}{8}\lambda^4$ while it is $-\frac{1}{8}\frac{26}{25}\lambda^4$ for the case of uniform spectrum in $[-\sqrt{3}, \sqrt{3})$, and is thus very close.

3.2. Large signal-to-noise regime. For this regime we can use a result of [89]. We briefly indicate here the main steps of this application for the ease of the reader. Let ρ_Z and its asymptotic cumulative density of eigenvalues $F_Z(x) \coloneqq \int_{-\infty}^x d\rho_Z(u)$. It is monotone increasing and has a inverse $F_Z^{-1}(p)$ which solves $p = F_Z(x)$. Then $(\rho_{\sqrt{\lambda}S})$ is the asymptotic spectral density of $\sqrt{\lambda}S$

$$I^{(2)}[\rho_{S},\rho_{Y},\sqrt{\lambda}] = \int_{0}^{1} dp \, F_{\sqrt{\lambda}S}^{-1}(p) F_{Y}^{-1}(p) - \frac{1}{2} \int d\rho_{\sqrt{\lambda}S}(x) \, d\rho_{\sqrt{\lambda}S}(y) \ln|x-y| - \frac{1}{2} \int d\rho_{Y}(x) \, d\rho_{Y}(y) \ln|x-y| - \frac{3}{4} - \frac{\pi^{2}}{6} \int_{0}^{1} dp \, \rho_{\sqrt{\lambda}S}(F_{\sqrt{\lambda}S}^{-1}(p)) \, \rho_{Y}(F_{Y}^{-1}(p)) + O(\lambda^{-3/2}).$$

Now we notice the scaling properties

$$\rho_{aZ}(u) = \frac{1}{a}\rho_Z(u), \quad F_{aZ}^{-1}(p) = aF_Z^{-1}(p), \quad \rho_{aZ}(F_{aZ}^{-1}(p)) = \frac{1}{a}\rho_Z(F^{-1}(p)).$$

These imply

(38)

$$I^{(2)}[\rho_{S},\rho_{Y},\sqrt{\lambda}] = \sqrt{\lambda} \int_{0}^{1} dp \, F_{S}^{-1}(p) \, F_{Y}^{-1}(p) - \frac{3 + \ln \lambda}{4} - \frac{1}{2} \int d\rho_{S}(x) \, d\rho_{S}(y) \ln |x - y| - \frac{1}{2} \int d\rho_{Y}(x) \, d\rho_{Y}(y) \ln |x - y| - \frac{\pi^{2}}{6\sqrt{\lambda}} \int_{0}^{1} dp \, \rho_{S}(F_{S}^{-1}(p)) \, \rho_{Y}(F_{Y}^{-1}(p)) + O(\lambda^{-3/2}).$$

Example: Consider as before $\mathbf{S} = \mathbf{X}\mathbf{X}^{\dagger}$ and $\mathbf{Y} = \sqrt{\lambda}\mathbf{X}\mathbf{X}^{\dagger} + \boldsymbol{\xi}$ constructed as in the Wishart case of Example 2 from the previous section. The density of eigenvalues of \mathbf{Y} can be computed by R-transform techniques [93,94]. It does not appear to be easy to analytically compute the terms of the expansion (and will not be done here) but the integrals can be computed numerically.

4. Denoising of a rotationally invariant matrix: non-Hermitian case

4.1. The model. We consider again a model of the form (2) but we now relax the hypothesis that \boldsymbol{S} is Hermitian. This time we consider that $\boldsymbol{\xi}$ is a standard (non-Hermitian) Ginibre matrix with law

$$dP_{\boldsymbol{\xi},N}(\boldsymbol{\xi}) = C_N d\boldsymbol{\xi} \exp \operatorname{Tr} \Big[-\frac{\beta N}{2} \boldsymbol{\xi} \boldsymbol{\xi}^{\dagger} \Big].$$

Its entries are typically of order $O(1/\sqrt{N})$ and singular values O(1). The planted full-rank matrix signal $\mathbf{S} \in \mathbb{K}^{N \times N}$ is no longer Hermitian but is still rotationally invariant in the sense that

$$dP_{S,N}(S) = dP_{S,N}(OSO)$$

for any orthogonal/unitary O, \tilde{O} . It has $O(1/\sqrt{N})$ entries and O(1) singular values. Its singular values decomposition (SVD) reads $S = \tilde{U}\sigma^S \tilde{V}$. Its singular values σ^S have a generic empirical distribution converging as $N \to +\infty$ to ρ_S with finite support. Left and right rotational invariance implies that its measure can be decomposed as

$$dP_{S,N}(\boldsymbol{S}) \propto d\mu_N^{(\beta)}(\tilde{\boldsymbol{U}}) \, d\mu_N^{(\beta)}(\tilde{\boldsymbol{V}}) \, dp_{S,N}(\boldsymbol{\sigma}^S),$$

where the Vandermonde determinant and other terms inherent to the change of variable are included in the generic symmetric j.p.d.f. $p_{S,N}(\boldsymbol{\sigma}^S)$ of the singular values. For example, in the case of a measure defined by a rotationally invariant potential it reads [95]

(39)
$$dP_{S,N}(\boldsymbol{S}) \propto d\mu_N^{(\beta)}(\tilde{\boldsymbol{U}}) d\mu_N^{(\beta)}(\tilde{\boldsymbol{V}}) d\boldsymbol{\sigma}^S \exp \operatorname{Tr} \left[-\frac{\beta N}{2} V(\boldsymbol{\sigma}^S) \right] |\Delta_N(\boldsymbol{\sigma}_S^2)|^{\beta} \left(\prod_{i \leq N} \sigma_i^S \right)^{\beta-1}$$

4.2. Free entropy through random matrix analysis. Using the SVD $s = U\sigma^s V$ the free entropy reads

$$\begin{split} f_{N} &\coloneqq \frac{1}{N^{2}} \ln \int dP_{S,N}(\boldsymbol{s}) \exp \frac{\beta N}{2} \operatorname{Tr} \Big[\sqrt{\lambda} \boldsymbol{Y}^{\dagger} \boldsymbol{s} + \sqrt{\lambda} \boldsymbol{Y} \boldsymbol{s}^{\dagger} - \lambda \boldsymbol{s}^{\dagger} \boldsymbol{s} \Big] \\ &\propto \frac{1}{N^{2}} \ln \int dp_{S,N}(\boldsymbol{\sigma}^{s}) \exp \Big(-\frac{\beta \lambda N}{2} \operatorname{Tr} \boldsymbol{\sigma}_{s}^{2} + (\beta - 1) \sum_{i \leq N} \ln \sigma_{i}^{s} \Big) \\ &\qquad \times \int d\mu_{N}^{(\beta)}(\boldsymbol{U}) d\mu_{N}^{(\beta)}(\boldsymbol{V}) \exp \beta \sqrt{\lambda} N \Re \operatorname{Tr} \Big[\boldsymbol{Y}^{\dagger} \boldsymbol{U} \boldsymbol{\sigma}^{s} \boldsymbol{V} \Big] \\ &= \frac{1}{N^{2}} \ln \int d\boldsymbol{\sigma}^{s} \exp N^{2} \Big(\frac{1}{N^{2}} \ln p_{S,N}(\boldsymbol{\sigma}^{s}) - \frac{\beta \lambda}{2N} \operatorname{Tr} \boldsymbol{\sigma}_{s}^{2} + J_{N}^{(\beta)} \big(\boldsymbol{\sigma}^{s}, \boldsymbol{\sigma}^{Y}, 2\sqrt{\lambda} \big) \Big) + O(1/N). \end{split}$$

Here and everywhere integrals over indivudual singular values are restricted to $\mathbb{R}_{\geq 0}$. The expression of the rectangular log-spherical integral density is [96, 97]

(40)
$$J_N^{(\beta)}(\boldsymbol{A}, \boldsymbol{B}, \gamma) = J_N^{(\beta)}(\boldsymbol{\sigma}^A, \boldsymbol{\sigma}^B, \gamma) \coloneqq \frac{1}{N^2} \ln \int d\mu_N^{(\beta)}(\boldsymbol{U}) \, d\mu_N^{(\beta)}(\boldsymbol{V}) \exp \frac{\beta \gamma}{2} N \Re \operatorname{Tr} \left[\boldsymbol{\sigma}^A \boldsymbol{U} \boldsymbol{\sigma}^B \boldsymbol{V} \right]$$

for generic $N \times N$ matrices A, B with respective singular values σ^A and σ^B . It has a well-defined limit [98,99]:

$$J^{(\beta)}[\rho_A,\rho_B,\gamma] \coloneqq \lim_{N \to +\infty} J^{(\beta)}_N(\boldsymbol{\sigma}^A,\boldsymbol{\sigma}^B,\gamma),$$

where ρ_A, ρ_B are the asymptotic normalized densities of singular values associated with A and B, respectively. Let ρ_Y be the the asymptotic singular values density associated with the data Y; again both σ^Y and ρ_Y are obtainable. In the large size limit $N \to +\infty$ we obtain by saddle-point the following conjecture for $f_N(Y)$:

$$f_N = \sup_{\boldsymbol{\sigma}^s \in \mathbb{R}^N_{\geq 0}} \left\{ \frac{1}{N^2} \ln p_{S,N}(\boldsymbol{\sigma}^s) - \frac{\beta \lambda}{2N} \operatorname{Tr} \boldsymbol{\sigma}_s^2 + J_N^{(\beta)}(\boldsymbol{\sigma}^s, \boldsymbol{\sigma}^Y, 2\sqrt{\lambda}) \right\} + \tau_N$$

Focusing on the case of a prior of the form (39),

$$f_N = \sup_{\boldsymbol{\sigma}^s \in \mathbb{R}_{\geq 0}^N} \left\{ \frac{\beta}{2} \sum_{i \neq j}^{1,N} \frac{\ln \left| (\boldsymbol{\sigma}_i^s)^2 - (\boldsymbol{\sigma}_j^s)^2 \right|}{N^2} - \frac{\beta}{2} \sum_{i \leq N} \frac{\lambda(\boldsymbol{\sigma}_i^s)^2 + V(\boldsymbol{\sigma}_i^s)}{N} + J_N^{(\beta)}(\boldsymbol{\sigma}^s, \boldsymbol{\sigma}^Y, 2\sqrt{\lambda}) \right\} + \tau_N.$$

Introducing asymptotic densities of singular values it reads

$$f_N \to \sup_{\rho_s \in \mathcal{P}_{\geq 0}} \left\{ \frac{\beta}{2} \int d\rho_s(x) \, d\rho_s(y) \ln |x^2 - y^2| - \frac{\beta}{2} \int d\rho_s(x) \big(\lambda x^2 + V(x)\big) + J^{(\beta)}[\rho_s, \rho_Y, 2\sqrt{\lambda}] \right\} + \tau.$$

The optimization is over a p.d.f. with bounded non-negative support. The constants τ_N and τ are fixed by the constraint $f_N(\lambda = 0) = 0$:

$$\begin{aligned} \tau_{N} &\coloneqq -\sup_{\sigma^{s} \in \mathbb{R}_{\geq 0}^{N}} \left\{ \frac{\beta}{2} \sum_{i \neq j}^{1,N} \frac{\ln |(\sigma_{i}^{s})^{2} - (\sigma_{j}^{s})^{2}|}{N^{2}} - \frac{\beta}{2} \sum_{i \leq N} \frac{V(\sigma_{i}^{s})}{N} \right\} + o_{N}(1), \\ \tau &\coloneqq -\sup_{\rho_{s} \in \mathcal{P}_{\geq 0}} \left\{ \frac{\beta}{2} \int d\rho_{s}(x) \, d\rho_{s}(y) \ln |x^{2} - y^{2}| - \frac{\beta}{2} \int d\rho_{s}(x) \, V(x) \right\} \end{aligned}$$

Again, as f_N ends up being solely a function of the singular values of the data matrix, it is expected to be self-averaging with respect to \mathbf{Y} : $\mathbb{E}f_N = f_N + o_N(1)$.

The free entropy is linked to the mutual information through

$$I(\boldsymbol{Y};\boldsymbol{S}) = -\mathbb{E}f_N + \frac{\beta\lambda N}{2}\mathbb{E}\mathrm{Tr}\boldsymbol{S}\boldsymbol{S}^{\dagger}.$$

With the Ginibre noise instead of Wigner and for a non-Hermitian signal \boldsymbol{S} the I-MMSE relation reads

(41)
$$\frac{1}{N^2} \mathbb{E} \| \boldsymbol{S} - \mathbb{E} [\boldsymbol{S} \mid \boldsymbol{Y}] \|^2 = \frac{2}{\beta N^2} \frac{d}{d\lambda} I(\boldsymbol{Y}; \boldsymbol{S}).$$

Like in the Hermitian case, the Nishimori identities combined with the concentration of the moments of the density of singular values of the posterior samples imply together that the supremum is attained for the density of singular values of the planted signal S.

Conjecture 3 (Mutual information of rotationally invariant matrix denoising). Let the singular values $\sigma^s \sim p_{S,N}$ of a random matrix drawn according to the prior $P_{S,N}$. The mutual information of model (2) in the case where S is not necessarily Hermitian and the noise ξ is a standard Ginibre matrix verifies

$$\frac{1}{N^2}I(\boldsymbol{Y};\boldsymbol{S}) = \frac{\beta\lambda}{N} \operatorname{Tr} \boldsymbol{\sigma}_s^2 - J_N^{(\beta)}(\boldsymbol{\sigma}^s, \boldsymbol{\sigma}^Y, 2\sqrt{\lambda}) + o_N(1).$$

Introducing asymptotic densities of singular values it reads as $N \to +\infty$

$$\frac{1}{N^2}I(\boldsymbol{Y};\boldsymbol{S}) \to \beta\lambda \int d\rho_s(x) x^2 - J^{(\beta)}[\rho_s,\rho_Y,2\sqrt{\lambda}]$$

where ρ_s is the asymptotic density of singular values of $s \sim P_{S,N}$.

We deduce from (41) that the minimum mean-square error verifies

$$\frac{1}{N^2} \mathbb{E} \|\boldsymbol{S} - \mathbb{E} [\boldsymbol{S} \mid \boldsymbol{Y}] \|^2 = \frac{2}{N} \mathbb{E} \operatorname{Tr} \boldsymbol{\sigma}_s^2 - \frac{2}{\beta} \frac{d}{d\lambda} J_N^{(\beta)}(\boldsymbol{\sigma}^s, \boldsymbol{\sigma}^Y, \sqrt{\lambda}) + o_N(1),$$

or, working with the asymptotic densities of singular values,

$$\frac{1}{N^2} \mathbb{E} \|\boldsymbol{S} - \mathbb{E} [\boldsymbol{S} \mid \boldsymbol{Y}] \|^2 \to 2 \int d\rho_s(x) \, x^2 - \frac{2}{\beta} \frac{d}{d\lambda} J^{(\beta)} [\rho_s, \rho_Y, \sqrt{\lambda}].$$

5. Hermitian positive definite dictionary learning

We now move to the more challenging problem of dictionary learning, first in the positive-definite case. Its analysis will require the introduction of the main methodological novelty of this paper: the spectral replica method.

5.1. The model. Consider a ground-truth matrix signal $\boldsymbol{X} = [X_{ik}] \in \mathbb{K}^{N \times M}$, with

$$M = \alpha N + o(N)$$

with fixed $\alpha > 0$, and with prior distribution $\mathbf{X} \sim P_{X,N}$ which is centered $\mathbb{E}X_{ik} = 0$ and such that typically $X_{ik} = O(1)$. This prior is *not* necessarily rotationally invariant nor factorized over the matrix entries, but we require that it induces a symmetric j.p.d.f. over the singular values of \mathbf{X} . Let $\mathbf{Z} = \mathbf{Z}^{\dagger} \in \mathbb{K}^{N \times N}$ a noise Wigner matrix with p.d.f.

$$P_{Z,N}(\boldsymbol{Z}) \propto \exp \operatorname{Tr} \left[-\frac{\beta}{4} \boldsymbol{Z}^2 \right]$$

With this scaling the eigenvalues of \mathbf{Z} are $O(\sqrt{N})$. Consider having access to an Hermitian data matrix $\mathbf{Y} = [Y_{ij}] \in \mathbb{K}^{N \times N}$ with entries generated through the following observation channel:

(42)
$$\boldsymbol{Y} = \sqrt{\frac{\lambda}{N}} \boldsymbol{X} \boldsymbol{X}^{\dagger} + \boldsymbol{Z}$$

Matrix $\sqrt{\lambda/N} \mathbf{X} \mathbf{X}^{\dagger}$ has O(1) entries and $O(\sqrt{N})$ eigenvalues like the noise, thus the correct scaling of the signal-to-noise $\sqrt{\lambda/N}$. The Bayesian posterior reads

$$dP_{X|Y,N}(\boldsymbol{x} \mid \boldsymbol{Y}) = \frac{1}{\mathcal{Z}(\boldsymbol{Y})} dP_{X,N}(\boldsymbol{x}) \exp \frac{\beta}{2} \operatorname{Tr} \Big[\sqrt{\frac{\lambda}{N}} \boldsymbol{Y} \boldsymbol{x} \boldsymbol{x}^{\dagger} - \frac{\lambda}{2N} (\boldsymbol{x} \boldsymbol{x}^{\dagger})^{2} \Big].$$

Note the invariance of the model under $X \to XU$ for any $M \times M$ orthogonal/unitary U such that $P_{X,N}(XU) = P_{X,N}(X)$.

The mutual information I(Y; X), which we aim at computing, is obtained by similar manipulations as in the previous sections:

$$\frac{I(\boldsymbol{Y};\boldsymbol{X})}{MN} = -\frac{1}{MN} \mathbb{E}_{\boldsymbol{Y}} \ln \int dP_{X,N}(\boldsymbol{x}) \exp \frac{\beta}{2} \operatorname{Tr} \left[\sqrt{\frac{\lambda}{N}} \boldsymbol{Y} \boldsymbol{x} \boldsymbol{x}^{\dagger} - \frac{\lambda}{2N} (\boldsymbol{x} \boldsymbol{x}^{\dagger})^{2} \right] + \frac{\beta \lambda}{4MN^{2}} \mathbb{E} \operatorname{Tr} (\boldsymbol{X} \boldsymbol{X}^{\dagger})^{2}$$

where the first term is minus the expected free entropy

$$\mathbb{E}f_N \coloneqq \frac{1}{MN} \mathbb{E}_{\boldsymbol{Y}} \ln \mathcal{Z}(\boldsymbol{Y})$$

Note that compared with our analysis on matrix denoising, we now do consider the expectation over the data in the free entropy.

In the case where the matrix X is rotationally invariant, and therefore XX^{\dagger} too, the results of the previous section on denoising can be applied. But it is important to notice right away that even in this case, the previous conjectures do not give any information about the main quantity of interest, namely, the overlap between the ground-truth X and a sample x from the posterior $P_{X|Y,N}$:

(43)
$$q \coloneqq \lim_{N \to +\infty} \frac{1}{N^2} \mathbb{E} \langle | \mathrm{Tr} \boldsymbol{x} \boldsymbol{X}^{\dagger} | \rangle.$$

The absolute value is needed because Y contains no information about the sign of X, so x and -x have same posterior weight. Only the MMSE on the product XX^{\dagger} is obtainable through this approach, through the I-MMSE identity. But this quantity is much less interesting than q as it does not carry information about the reconstruction of the internal structure of XX^{\dagger} . In particular, as noted in [53], in the present linear-rank regime of Hermitian dictionary learning with a factorized prior $P_{X,N} = g^{\otimes N(N+1)/2}$ over the matrix entries, the MMSE on XX^{\dagger} is expected to be a universal quantity independent of the specific distribution g of the individual entries of X

(as long as the first few moments exist). This is because the entries of XX^{\dagger} are sums of many independent random contributions and thus the resulting matrix should behave at the level of the mutual information and MMSE on XX^{\dagger} as a random matrix from the Wishart ensemble (i.e., as if X had i.i.d. standard normal entries) due to strong universality properties [100]. Therefore, it is crucial to:

- access the non-universal $P_{X,N}$ -dependent scalar overlap q, both in rotationally invariant and non rotationally invariant models;
- go beyond models with factorized distributions over the components of the hidden matrices.

Concerning the second point: as it will become clear, the spectral replica method presented below does not *a-priori* require the hidden matrix X (or S, T in the non-symmetric case) to have independent entries. But the possibility to concretely evaluate expressions in the ensuing conjectures depends on the solution of a classical (but in general highly non-trivial) RMT sub-problem, namely that of evaluating the j.p.d.f. of the matrix product between two i.i.d. samples from the prior $P_{X,N}$. As a consequence, in situations where this task can be solved (despite the lack of independence of the signal matrix entries) then quantitative predictions may be reachable. Advancing on the above two points is the main role of the spectral replica method as compared with the pure RMT approaches.

To fix ideas let us consider at the moment the complex case $\beta = 2$. Model (42) is equivalent to three coupled real models:

$$\begin{cases} \Re Y_{ij} \sim \mathcal{N}\left(\sqrt{\frac{\lambda}{N}} \frac{\langle \mathbf{X}_i, \bar{\mathbf{X}}_j \rangle + \langle \bar{\mathbf{X}}_i, \mathbf{X}_j \rangle}{2}, \frac{1}{2}\right) & \text{for } i < j \in [N]^2, \\ \Im Y_{ij} \sim \mathcal{N}\left(\sqrt{\frac{\lambda}{N}} \frac{\langle \mathbf{X}_i, \bar{\mathbf{X}}_j \rangle - \langle \bar{\mathbf{X}}_i, \mathbf{X}_j \rangle}{2\mathrm{i}}, \frac{1}{2}\right) & \text{for } i < j \in [N]^2, \\ Y_{ii} \sim \mathcal{N}\left(\sqrt{\frac{\lambda}{N}} \|\mathbf{X}_i\|^2, 1\right) & \text{for } i \in [N]. \end{cases}$$

The average free entropy then concretely reads

$$\mathbb{E}f_{N} = \frac{1}{NM} \mathbb{E}\ln\int dP_{X,N}(\boldsymbol{x}) \exp\sum_{i\leq N} \left(\sqrt{\frac{\lambda}{N}}Y_{ii}\|\boldsymbol{x}_{i}\|^{2} - \frac{\lambda}{2N}\|\boldsymbol{x}_{i}\|^{4}\right)$$

$$\times \exp 2\sum_{i< j}^{1,N} \left(\sqrt{\frac{\lambda}{N}}\Re Y_{ij}\frac{\langle\boldsymbol{x}_{i},\bar{\boldsymbol{x}}_{j}\rangle + \langle\bar{\boldsymbol{x}}_{i},\boldsymbol{x}_{j}\rangle}{2} - \frac{\lambda}{2N}\left(\frac{\langle\boldsymbol{x}_{i},\bar{\boldsymbol{x}}_{j}\rangle + \langle\bar{\boldsymbol{x}}_{i},\boldsymbol{x}_{j}\rangle}{2}\right)^{2}\right)$$

$$\times \exp 2\sum_{i< j}^{1,N} \left(\sqrt{\frac{\lambda}{N}}\Im Y_{ij}\frac{\langle\boldsymbol{x}_{i},\bar{\boldsymbol{x}}_{j}\rangle - \langle\bar{\boldsymbol{x}}_{i},\boldsymbol{x}_{j}\rangle}{2\mathrm{i}} - \frac{\lambda}{2N}\left(\frac{\langle\boldsymbol{x}_{i},\bar{\boldsymbol{x}}_{j}\rangle - \langle\bar{\boldsymbol{x}}_{i},\boldsymbol{x}_{j}\rangle}{2\mathrm{i}}\right)^{2}\right).$$

$$(44)$$

5.2. Replica trick. The new important difficulty is that the lack of rotational invriance of X and therefore of $S = XX^{\dagger}$ prevents the direct use of spherical integration of the rotational degrees of freedom. But combining random matrix theory with the replica method will allow to face this difficulty. The approach starts from the replica trick:

(45)
$$\lim_{N \to +\infty} \mathbb{E} f_N = \lim_{N \to +\infty} \lim_{u \to 0_+} \frac{1}{NMu} \ln \mathbb{E} \mathcal{Z}(\boldsymbol{Y})^u = \lim_{u \to 0_+} \lim_{N \to +\infty} \frac{1}{NMu} \ln \mathbb{E} \mathcal{Z}(\boldsymbol{Y})^u,$$

where we assumed commutation of limits in u and N in the second equality. We therefore need to evaluate the expectation of the replicated partition function. We directly integrate the quenched

gaussian observations in (44) using the following useful formula:

(46) if
$$Y \sim \mathcal{N}\left(\sqrt{\frac{\lambda}{N}}f_0, \gamma\right)$$
 then $\mathbb{E}_{Y|f_0} \prod_{a \le u} \exp \gamma\left(\sqrt{\frac{\lambda}{N}}Yf_a - \frac{\lambda}{2N}f_a^2\right) = \prod_{a < b}^{0, u} \exp \frac{\gamma\lambda}{N}f_a f_b.$

In the Bayes-optimal setting the ground-truth X plays a totally similar role as one additional replica, so we rename it $x^0 := X$. We set $x_i^a = (x_{ik}^a)_{k \leq M}$ and introduce the notation

$$\int dP_{X,N}(\{\boldsymbol{x}\}_0^u) \cdots = \int_{\mathbb{R}^{MNu}} \prod_{a=0}^u dP_{X,N}(\boldsymbol{x}^a) \cdots$$

The above formula (46) applied thrice yields

$$\mathbb{E}\mathcal{Z}(\boldsymbol{Y})^{u} = \int dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) \prod_{a

$$\times \exp \frac{2\lambda}{N} \sum_{i

$$\times \exp \frac{2\lambda}{N} \sum_{i

$$= \int dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) \prod_{a

$$= \int dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) \prod_{a

$$= \int dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) \prod_{a

$$= \int dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) \prod_{a$$$$$$$$$$$$$$

Define the complex-valued $M \times M$ overlap matrix

(48)
$$\boldsymbol{Q}^{ab} \coloneqq \left(\frac{1}{N}\sum_{i\leq N} x^a_{ik} \bar{x}^b_{i\ell}\right)_{k,\ell\leq M} = \frac{(\boldsymbol{x}^a)^{\mathsf{T}} \bar{\boldsymbol{x}}^b}{N} = (\boldsymbol{Q}^{ba})^{\dagger}.$$

Keep in mind that Q^{ab} has same singular values as $N^{-1}(x^b)^{\dagger}x^a$. To simplify the expression we use the gaussian identity

$$\int_{\mathbb{R}} dz \exp(-\gamma z^2 + \kappa z) = \sqrt{\frac{\pi}{\gamma}} \exp\frac{\kappa^2}{4\gamma}$$

with $\gamma = N, \kappa = \sqrt{\lambda} \sum_{i} (x_{ik}^{a} \bar{x}_{i\ell}^{b} + \bar{x}_{ik}^{a} x_{i\ell}^{b})$ for the real part and $\gamma = N, \kappa = -i\sqrt{\lambda} \sum_{i} (x_{ik}^{a} \bar{x}_{i\ell}^{b} - \bar{x}_{ik}^{a} x_{i\ell}^{b})$ for the imaginary one. It introduces $M \times M$ real-valued gaussian fields

$$\boldsymbol{q}^{ab} = (q^{ab}_{k\ell})_{k,\ell \leq M}$$
 and $\boldsymbol{r}^{ab} = (r^{ab}_{k\ell})_{k,\ell \leq M}$,

(which play the role of new spins/variables that are going to interact with the replicas) and yields

$$\begin{split} \mathbb{E}\mathcal{Z}^{u} &\propto \int dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) \int_{\mathbb{R}^{M^{2}u(u+1)}} \prod_{a < b}^{0,u} d\boldsymbol{r}^{ab} d\boldsymbol{q}^{ab} \\ &\times \exp \sum_{k,\ell \leq M} \left(\sqrt{\lambda} r_{k\ell}^{ab} \sum_{i \leq N} (x_{ik}^{a} \bar{x}_{i\ell}^{b} + \bar{x}_{ik}^{a} x_{i\ell}^{b}) - \mathrm{i}\sqrt{\lambda} q_{k\ell}^{ab} \sum_{i \leq N} (x_{ik}^{a} \bar{x}_{i\ell}^{b} - \bar{x}_{ik}^{a} x_{i\ell}^{b}) - N(r_{k\ell}^{ab})^{2} - N(q_{k\ell}^{ab})^{2} \right) \\ &= \int dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) \int_{\mathbb{R}^{M^{2}u(u+1)}} \prod_{a < b}^{0,u} d\boldsymbol{r}^{ab} d\boldsymbol{q}^{ab} \\ &\times \exp N \mathrm{Tr} \Big[\sqrt{\lambda} (\boldsymbol{r}^{ab} - \mathrm{i}\boldsymbol{q}^{ab})^{\mathsf{T}} \boldsymbol{Q}^{ab} + \sqrt{\lambda} (\boldsymbol{r}^{ab} + \mathrm{i}\boldsymbol{q}^{ab}) (\bar{\boldsymbol{Q}}^{ab})^{\mathsf{T}} - (\boldsymbol{r}^{ab})^{\mathsf{T}} \boldsymbol{r}^{ab} - (\boldsymbol{q}^{ab})^{\mathsf{T}} \boldsymbol{q}^{ab} \Big] \\ &= \int dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) \int_{\mathbb{C}^{M^{2}u(u+1)}} \prod_{a < b}^{0,u} d\boldsymbol{z}^{ab} \exp N \mathrm{Tr} \Big[\sqrt{\lambda} (\boldsymbol{z}^{ab})^{\dagger} \boldsymbol{Q}^{ab} + \sqrt{\lambda} ((\boldsymbol{z}^{ab})^{\dagger} \boldsymbol{q}^{ab})^{\dagger} - (\boldsymbol{z}^{ab})^{\dagger} \boldsymbol{z}^{ab} \Big] \\ &= \int dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) \int_{\mathbb{C}^{M^{2}u(u+1)}} \prod_{a < b}^{0,u} d\boldsymbol{z}^{ab} \exp N \Re \mathrm{Tr} \Big[2\sqrt{\lambda} (\boldsymbol{z}^{ab})^{\dagger} \boldsymbol{Q}^{ab} - (\boldsymbol{z}^{ab})^{\dagger} \boldsymbol{z}^{ab} \Big] \end{split}$$

where we define the complex-valued matrix $z^{ab} \coloneqq r^{ab} + iq^{ab}$ (note the integration over \mathbb{C}). The same computations can be carried out in the real case. The generic formula then reads

(49)
$$\mathbb{E}\mathcal{Z}^{u} \propto \int dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) \int_{\mathbb{K}^{M^{2}u(u+1)}} \prod_{a$$

with $\boldsymbol{Q}^{ab}, \boldsymbol{z}^{ab} \in \mathbb{K}^{M \times M}$.

5.3. Spectral replica symmetric ansatz. Until now the computation is standard. The novelty starts here. We introduce the singular value decompositions

$$\boldsymbol{z}^{ab} = \boldsymbol{U}^{ab} \boldsymbol{\sigma}_z^{ab} \boldsymbol{V}^{ab}$$
 and $\boldsymbol{Q}^{ab} = \boldsymbol{A}^{ab} \boldsymbol{\sigma}_Q^{ab} \boldsymbol{B}^{ab}$

All matrices are of size $M \times M$; note that the overlaps $(\mathbf{Q}^{ab})_{a < b}$ have rank equal to $\min(N, M)$, so $(\boldsymbol{\sigma}_Q^{ab})_{a < b}$ have $\min(N, M)$ non-zero entries on their diagonal. Matrices $(\boldsymbol{z}^{ab})_{a < b}$ are instead full-rank. We have the change of variable

$$d\boldsymbol{z}^{ab} = d\mu_M^{(\beta)}(\boldsymbol{U}^{ab}) d\mu_M^{(\beta)}(\boldsymbol{V}^{ab}) d\boldsymbol{\sigma}_z^{ab} |\Delta_M((\boldsymbol{\sigma}_z^{ab})^2)|^{\beta} (\prod_{k \le M} \sigma_k^{z,ab})^{\beta-1}.$$

The dependence of the replicated system in the spins $(\boldsymbol{x}^a)_a$ is through the overlap matrices $(\boldsymbol{Q}^{ab})_{a < b}$. Changing variables for $(\boldsymbol{Q}^{ab})_{a < b}$ we have the completely generic change of density

$$dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) = dP_{(Q),M}((\boldsymbol{Q}^{ab})_{a < b})$$

= $dP_{(A,B)|(\sigma_{Q}),M}((\boldsymbol{A}^{ab}, \boldsymbol{B}^{ab})_{a < b} | (\boldsymbol{\sigma}_{Q}^{ab})_{a < b}) dP_{(\sigma_{Q}),M}((\boldsymbol{\sigma}_{Q}^{ab})_{a < b})$

for a generic conditional j.p.d.f. $P_{(A,B)|(\sigma_Q),M}$ of the singular vectors and j.p.d.f. of singular values $P_{(\sigma_Q),M}$. This measure couples all matrices of singular vectors and singular values. It thus seems hopeless to go further without assuming some sort of simplification. We are now in position to move forward thanks to a novel type of decoupling assumption, which we think is the weakest (and most natural) possible assumption allowing to carry on computations from there.

The spectral replica symmetric ansatz states that the replicated partition function is dominated by configurations such that the joint law $P_{(\sigma_Q),M}((\boldsymbol{\sigma}_Q^{ab})_{a < b})$ factorizes as $N, M \to +\infty$ into a product of same laws:

(50) Assumption (spectral replica symmetry):
$$P_{(\sigma_Q),M}((\sigma_Q^{ab})_{a < b}) \rightarrow \prod_{a < b}^{0,u} p_M(\sigma_Q^{ab})$$

The convergence \rightarrow means that both the left and right hand sides weakly converge to the same asymptotic distribution as $N \rightarrow +\infty$. The j.p.d.f. $p_M(\sigma_Q^{ab})$, which is shared by assumption by the different overlap matrices/pairs of replica indices a < b, may be obtained using random matrix theory from the knowledge of $P_{X,N}$. We will discuss further this point in the next section. Note that we do *not* assume anything at the level of singular vectors which is an important feature. The decoupling is only assumed at the spectral level. So we have now that at leading exponential order

$$\mathbb{E}\mathcal{Z}^{u} \propto \int \prod_{a < b}^{0,u} d\boldsymbol{\sigma}_{z}^{ab} d\boldsymbol{\sigma}_{Q}^{ab} |\Delta_{M}((\boldsymbol{\sigma}_{z}^{ab})^{2})|^{\beta} (\prod_{k \leq M} \sigma_{k}^{z,ab})^{\beta-1} \exp \operatorname{Tr} \left[-\frac{\beta N}{2} (\boldsymbol{\sigma}_{z}^{ab})^{2} \right] p_{M}(\boldsymbol{\sigma}_{Q}^{ab}) \times \int dP_{(A,B)|(\sigma_{Q}),M}((\boldsymbol{A}^{ab}, \boldsymbol{B}^{ab})_{a < b} | (\boldsymbol{\sigma}_{Q}^{ab})_{a < b}) \times \int \prod_{a < b}^{0,u} d\mu_{M}^{(\beta)}(\boldsymbol{U}^{ab}) d\mu_{M}^{(\beta)}(\boldsymbol{V}^{ab}) \exp \beta \sqrt{\lambda} N \Re \operatorname{Tr} \left[(\boldsymbol{V}^{ab})^{\dagger} \boldsymbol{\sigma}_{z}^{ab} (\boldsymbol{U}^{ab})^{\dagger} \boldsymbol{A}^{ab} \boldsymbol{\sigma}_{Q}^{ab} \boldsymbol{B}^{ab} \right].$$
(51)

We change variables as $(U^{ab})^{\dagger} A^{ab} \rightarrow U^{ab}$ and $B^{ab}(V^{ab})^{\dagger} \rightarrow V^{ab}$; this change has unit Jacobian determinant. These new matrices are still independent and Haar distributed, and this for arbitrary dependency between the unitary A^{ab} and B^{ab} . Therefore the conditional law $P_{(A,B)|(\sigma_Q),M}$ does not matter as it can directly be integrated to one even if the singular vectors depend on each others. The last term then becomes

$$\int \prod_{a$$

which is a rectangular log-spherical integral as (40). All these manipulations allow us to factorize the integrals over different pairs (a, b) with a < b of replica indices (two pairs sharing one replica index are different and decouple too). To sum up: the i.i.d. Haar matrices coming from the gaussian fields $(\boldsymbol{z}^{ab})_{a < b}$ destroyed the dependence between the singular vectors of the overlaps (without the need of any kind of assumption), while the spectral replica symmetric ansatz formalizes the idea that the dependence between the singular values of different overlaps are weak. We end up with

$$\mathbb{E}\mathcal{Z}^{u} \propto \left(\int d\boldsymbol{\sigma}_{z} \, d\boldsymbol{\sigma}_{Q} \exp \frac{\beta MN}{2} \left[\sum_{k\neq\ell}^{1,M} \frac{\ln |(\sigma_{k}^{z})^{2} - (\sigma_{\ell}^{z})^{2}|}{MN} - \frac{\operatorname{Tr}\boldsymbol{\sigma}_{z}^{2}}{M} + \frac{2\ln p_{M}(\boldsymbol{\sigma}_{Q})}{\beta MN} + \frac{2M}{\beta N} J_{M}^{(\beta)} \left(\boldsymbol{\sigma}_{z}, \boldsymbol{\sigma}_{Q}, \frac{2\sqrt{\lambda}N}{M}\right) + \frac{2(\beta-1)}{\beta} \sum_{k\leq M} \frac{\ln \sigma_{k}^{z}}{MN} \right]\right)^{u(u+1)/2}$$
(52)

Therefore the replica computation gives, using formula (45) and after evaluation of the above integral by saddle-point as $N \to +\infty$ followed by the analytic continuation $u \to 0_+$, the Conjecture 4 below.

Our computation shows that one of the order parameters is the matrix $\boldsymbol{\sigma}_Q$ of singular values of the overlap matrix $\boldsymbol{Q} \coloneqq N^{-1}\boldsymbol{x}^{\dagger}\tilde{\boldsymbol{x}}$ between i.i.d. samples $\boldsymbol{x}, \tilde{\boldsymbol{x}}$ from the posterior distribution $P_{X|Y,N}$ (i.e., two conditionally independent replicas). Let us see how the scalar overlap q defined by (43) can be deduced from it. A general Nishimori identity reads (see [67])

(53)
$$\mathbb{E}\langle g(\boldsymbol{x}, \tilde{\boldsymbol{x}}) \rangle = \mathbb{E}\langle g(\boldsymbol{x}, \boldsymbol{X}) \rangle.$$

When two or more replicas appear inside a Gibbs bracket $\langle \cdot \rangle$ it has to be understood as the expectation with respect to the product Gibbs measure. From it, one can deduce the non-universal scalar overlap q. Indeed, the latter is equal to

(54)
$$q \coloneqq \lim_{N \to +\infty} \frac{1}{N} \mathbb{E} \langle |\mathrm{Tr} \boldsymbol{x} \boldsymbol{X}^{\dagger}| \rangle = \lim_{N \to +\infty} \frac{1}{N} \mathbb{E} \langle |\mathrm{Tr} \boldsymbol{Q}| \rangle = \lim_{N \to +\infty} \frac{1}{N} |\mathrm{Tr} \mathbb{E} \langle \boldsymbol{Q} \rangle| = \frac{1}{N} |\mathrm{Tr} \boldsymbol{Q}| + o_N(1).$$

The second equality follows from (53), while the third and last by concentration of the spectral moments of \mathbf{Q} ; this does not mean that \mathbf{Q} concentrates elementwise, only the moments $N^{-1}\text{Tr}\mathbf{Q}^k = N^{-1}\text{Tr}\mathbb{E}\langle\mathbf{Q}\rangle^k + o_N(1)$ do. Finally, because $\mathbb{E}\langle\mathbf{Q}\rangle = \mathbb{E}[\langle\mathbf{x}\rangle\langle\mathbf{x}\rangle^\dagger]$ is positive definite, its trace is also the sum of its singular values which, by the assumed self-averaging of the (moments of the) distribution of singular values, must be relatively close to $\text{Tr}\sigma_Q$ of singular values of \mathbf{Q} (which is not symmetric). Therefore, the mean of the singular values of the overlap matrix yield the scalar overlap q.

Conjecture 4 (Replica symmetric formula for Hermitian dictionary learning). Let the j.p.d.f. of the M singular values of O(1) of the matrix $N^{-1}\boldsymbol{x}_{0}^{\dagger}\boldsymbol{\tilde{x}}_{0}$, where $\boldsymbol{x}_{0}, \boldsymbol{\tilde{x}}_{0}$ are i.i.d. $N \times M$ random matrices drawn from the prior $P_{X,N}$, be p_{M} .

The mutual information of model (42) verifies

(55)
$$\frac{1}{MN}I\left(\boldsymbol{X}; \sqrt{\frac{\lambda}{N}}\boldsymbol{X}\boldsymbol{X}^{\dagger} + \boldsymbol{Z}\right) = -\frac{\beta}{4} \sup_{(\boldsymbol{\sigma}_{z},\boldsymbol{\sigma}_{Q})\in\mathcal{S}_{M}(\lambda)} \left\{ \sum_{k\neq\ell}^{1,M} \frac{\ln|(\boldsymbol{\sigma}_{z}^{z})^{2} - (\boldsymbol{\sigma}_{\ell}^{z})^{2}|}{MN} - \frac{\operatorname{Tr}\boldsymbol{\sigma}_{z}^{2}}{M} + \frac{2\ln p_{M}(\boldsymbol{\sigma}_{Q})}{\beta MN} + \frac{2M}{\beta N} J_{M}^{(\beta)} \left(\boldsymbol{\sigma}_{z}, \boldsymbol{\sigma}_{Q}, \frac{2\sqrt{\lambda}N}{M}\right) \right\} + \frac{\beta\lambda}{4} \frac{\operatorname{ETr}(\boldsymbol{X}\boldsymbol{X}^{\dagger})^{2}}{MN^{2}} + \tau_{N}.$$

The set of extrema $\mathcal{S}_M(\lambda)$ is defined as

$$\mathcal{S}_{M}(\lambda) \coloneqq \{(\boldsymbol{\sigma}_{z}, \boldsymbol{\sigma}_{Q}) \in \mathbb{R}_{\geq 0}^{M} \times \mathbb{R}_{\geq 0}^{M} : \boldsymbol{\sigma}_{Q} \text{ is of rank } \min(M, N), \\ \nabla_{\boldsymbol{\sigma}_{z}} g_{M}^{\mathrm{RS}}(\boldsymbol{\sigma}_{z}, \boldsymbol{\sigma}_{Q}, \lambda) = \nabla_{\boldsymbol{\sigma}_{Q}} g_{M}^{\mathrm{RS}}(\boldsymbol{\sigma}_{z}, \boldsymbol{\sigma}_{Q}, \lambda) = \mathbf{0} \},$$

where $g_M^{\text{RS}} : \mathbb{R}_{\geq 0}^M \times \mathbb{R}_{\geq 0} \to \mathbb{R}$ is the replica symmetric potential function defined by the curly brackets in the variational problem (55). Constant τ_N fixes $I(\mathbf{X}; \mathbf{Z}) = 0$, i.e.,

$$\tau_N \coloneqq \frac{\beta}{4} \sup_{(\boldsymbol{\sigma}_z, \boldsymbol{\sigma}_Q) \in \mathcal{S}_M(0)} g_M^{\mathrm{RS}}(\boldsymbol{\sigma}_z, \boldsymbol{\sigma}_Q, \lambda = 0) + o_N(1).$$

Denote σ_Q^* the overlap singular values achieving the supremum in (55). The overlap (54) is then

(56)
$$q = \frac{1}{N} \operatorname{Tr} \boldsymbol{\sigma}_Q^* + o_N(1)$$

Introducing asymptotic singular values densities ρ_z and ρ_Q associated to σ_z and σ_Q , respectively, and assuming it exists a functional Γ depending only on the asymptotic density ρ_Q and such that

(57)
$$\Gamma[\rho_Q] \coloneqq \lim_{M \to +\infty} \frac{1}{M^2} \ln p_M(\boldsymbol{\sigma}_Q)$$

the conjecture can be re-expressed in the limit $N \to +\infty$ and $M/N \to \alpha$ as

$$\frac{1}{MN}I\left(\boldsymbol{X}; \sqrt{\frac{\lambda}{N}}\boldsymbol{X}\boldsymbol{X}^{\dagger} + \boldsymbol{Z}\right) \rightarrow -\frac{\beta}{4} \sup_{(\rho_{z},\rho_{Q})\in\mathcal{S}(\lambda)} \left\{\alpha \int d\rho_{z}(x) \, d\rho_{z}(y) \ln|x^{2} - y^{2}| - \int d\rho_{z}(x) \, x^{2} + \frac{2\alpha}{\beta}\Gamma[\rho_{Q}] + \frac{2\alpha}{\beta}J^{(\beta)}\left[\rho_{z},\rho_{Q},\frac{2\sqrt{\lambda}}{\alpha}\right]\right\} + \frac{\beta\lambda}{4\alpha} \lim_{N \to +\infty} \frac{\mathbb{E}\mathrm{Tr}(\boldsymbol{X}\boldsymbol{X}^{\dagger})^{2}}{N^{3}} + \tau.$$
(58)

The optimization is over probability densities with finite non-negative support belonging to the extremal set

$$\begin{aligned} \mathcal{S}(\lambda) &\coloneqq \left\{ (\rho_z, \rho_Q) = (\rho_z, (1 - \min(1, \alpha))\delta_0 + \min(1, \alpha)\tilde{\rho}_Q) \text{ with } (\rho_z, \tilde{\rho}_Q) \in \mathcal{P}_{\geq 0} \times \mathcal{P}_{\geq 0} : \\ \delta_{\rho_z} g^{\mathrm{RS}}[\rho_z, \rho_Q, \lambda] = \delta_{\tilde{\rho}_Q} g^{\mathrm{RS}}[\rho_z, \rho_Q, \lambda] = 0 \right\}, \end{aligned}$$

where $\delta_{\rho_z} g^{\text{RS}}[\rho_z, \rho_Q, \lambda]$ and $\delta_{\tilde{\rho}_Q} g^{\text{RS}}[\rho_z, \rho_Q, \lambda]$ are the functional derivatives of the replica symmetric potential functional $g^{\text{RS}} : \mathcal{P}_{\geq 0} \times \mathcal{P}_{\geq 0} \times \mathbb{R}_{\geq 0} \mapsto \mathbb{R}$ defined by the curly brackets in (64). Constant τ fixes the contraint $I(\mathbf{X}; \mathbf{Z}) = 0$:

$$\tau \coloneqq \frac{\beta}{4} \sup_{(\rho_z, \rho_Q) \in \mathcal{S}(0)} g^{\mathrm{RS}}[\rho_z, \rho_Q, \lambda = 0].$$

Denoting by $\rho_Q^* = (1 - \min(1, \alpha))\delta_0 + \min(1, \alpha)\tilde{\rho}_Q^*$ the density of singular values of the overlap that achieves the supremum in (64), the overlap reads

(59)
$$q = \int d\rho_Q^*(x) x$$

Let us say few words about the interpretation of the role of the three contributions entering this conjecture. i) Both terms depending only on a single density ρ_z or ρ_Q (or σ_z, σ_Q in the finite system size case) play a symmetric role, and can be thought as "prior terms". They tend to give to their respective arguments the shape they would have in the case of no interation between them, which happens only if $\lambda = 0$. The functional $\Gamma[\rho_Q]$ (or the j.p.d.f. $p_M(\sigma_Q)$) shapes the density ρ_Q towards the one of a large random matrix $N^{-1}\boldsymbol{x}_0^{\dagger}\boldsymbol{\tilde{x}}_0$, where $\boldsymbol{x}_0, \boldsymbol{\tilde{x}}_0$ are i.i.d. $N \times M$ random matrices drawn from $P_{X,N}$. In the non-interacting case $\lambda = 0$, this would correctly yield a scalar overlap associated with a dumb estimator $\boldsymbol{\hat{x}}$ purely drawn from the prior $P_{X,N}$ (i.e., not having access to data). The term associated with the spectral density ρ_z of the "conjugate spins/variables" tends to shape it as a semicircle. *ii*) In contrast, the interaction term given by the spherical integral $J^{(\beta)}[\rho_z, \rho_Q, f(\lambda, \alpha)]$ depending on both densities is the "informative term", in the sense that it is the one conveying the information extracted from the data. The competition between these two types of terms is controlled by the signal-to-noise ratio λ .

Evaluating the j.p.d.f. p_M of singular values of the overlaps (48) translates in the presence of the functional $\Gamma[\rho_Q]$ assumed to depend solely on the density of singular values. Indeed, we expect that the variational formula for the mutual information and scalar overlap are expressible in terms of *densities* of singular values instead of the whole populations σ_z, σ_Q . In the Appendix C we argue that the functional Γ exists in general. In the next section we provide its explicit form in the special case of a Ginibre signal.

5.4. A more explicit special case: the Ginibre signal. The j.p.d.f. p_M of singular values entering the conjecture may be highly non-trivial to obtain from the knowledge of $P_{X,N}$, but it has the merit of being a well defined "standard" random matrix theory problem. In certain cases it is known. E.g., for products of i.i.d. gaussian (Ginibre) matrices (or with an additional source [101]). In this case the law p_M is given by a determinantal point process defined in terms of the Meijer G-function, see [85,102–106]. Products of finitely but arbitrarily many matrices are considered in these references, but for us only the case of a product between two matrices is needed. There also exist results for products of truncated unitary matrices [107, 108] and for more general product ensembles (but with less explicit formulas) [86]. We refer to [109] for a review on the subject. See also [110, 111] for information about fluctuations and universality properties in such matrix product ensembles, or [112–116] for results concerning their asymptotic density of eigenvalues and singular values (instead of the j.p.d.f.). Using this body of work we can go further in explicitating Conjecture 4 in these known cases. Here we restrict ourselves to the special case where the signal \boldsymbol{X} is a Ginibre matrix, so that $\boldsymbol{X}\boldsymbol{X}^{\dagger}$ is Wishart. We want to find the j.p.d.f. of the matrix $N^{-1}\boldsymbol{x}_{0}^{\dagger}\boldsymbol{\tilde{x}}_{0}$ where $\boldsymbol{x}_{0}, \boldsymbol{\tilde{x}}_{0}$ are i.i.d. $N \times M$ Ginibre matrices with O(1) entries, which is equivalent to find the j.p.d.f. of the matrix $\boldsymbol{y}_{0}^{\dagger}\boldsymbol{\tilde{y}}_{0}$ where $\boldsymbol{y}_{0}, \boldsymbol{\tilde{y}}_{0}$ are i.i.d. $N \times M$ standard Ginibre matrices with law

$$P_{Y_{0},N}(\boldsymbol{y}_{0}) \propto \exp \operatorname{Tr} \left[-\frac{\beta N}{2} \boldsymbol{y}_{0} \boldsymbol{y}_{0}^{\dagger}
ight]$$

Let

 $n \coloneqq \min(N, M).$

The steps leading to equation (2.7) of [106] for the square case M = N, or those leading to (13) of [85] for the general rectangular case (where M and N do not necessarily match), imply that the j.p.d.f. p_n of the *n* non-zero singular values $\boldsymbol{\sigma}$ of the matrix $\boldsymbol{y}_0^{\dagger} \tilde{\boldsymbol{y}}_0$ can be expressed in terms of a two-matrix model:

(60)
$$p_{n}(\boldsymbol{\sigma}) \propto |\Delta_{n}(\boldsymbol{\sigma}^{2})|^{\beta} \Big(\prod_{k \leq n} \sigma_{k}\Big)^{\beta(M-n+1)-1} L(\boldsymbol{\sigma})$$
$$\propto \exp n^{2} \Big(\frac{\beta}{n^{2}} \sum_{i < j}^{1, n} \ln |\sigma_{i}^{2} - \sigma_{j}^{2}| + \beta \frac{M-n}{n^{2}} \operatorname{Tr} \ln \boldsymbol{\sigma} + \frac{1}{n^{2}} \ln L_{n}(\boldsymbol{\sigma}) + o_{n}(1)\Big),$$

where the function

(61)

$$L_{n}(\boldsymbol{\sigma}) \coloneqq \int_{\mathbb{R}^{n}_{\geq 0}} d\boldsymbol{r} \, |\Delta_{n}(\boldsymbol{r}^{2})|^{\beta} \exp \operatorname{Tr} \left[-\frac{\beta N}{2} \boldsymbol{r}^{2} \right] \left(\prod_{k \leq n} r_{k} \right)^{\beta(N-M-n+1)-1} \times \int d\mu_{n}^{(\beta)}(\boldsymbol{U}) \exp \operatorname{Tr} \left[-\frac{\beta N}{2} \boldsymbol{U}^{\dagger} \boldsymbol{\sigma}^{2} \boldsymbol{U} \boldsymbol{r}^{-2} \right].$$

The spherical integral appears in the function $L_n(\boldsymbol{\sigma})$, that we re-express in a form appropriate for a saddle-point evaluation:

$$\int d\boldsymbol{r} \exp n^2 \Big(\frac{\beta}{n^2} \sum_{i < j}^{1,n} \ln |r_i^2 - r_j^2| - \frac{\beta N}{2n^2} \operatorname{Tr} \boldsymbol{r}^2 + \beta \frac{N - M - n}{n^2} \operatorname{Tr} \ln \boldsymbol{r} + I_n^{(\beta)} \Big(\boldsymbol{\sigma}^2, \boldsymbol{r}^{-2}, -\frac{N}{n} \Big) + o_n(1) \Big).$$

Therefore we reach

$$\frac{\ln L_n(\boldsymbol{\sigma})}{n^2} = \sup_{\boldsymbol{r} \in \mathbb{R}^n_{\geq 0}} \left\{ \frac{\beta}{n^2} \sum_{i < j}^{1, n} \ln |r_i^2 - r_j^2| - \frac{\beta N}{2n^2} \operatorname{Tr} \boldsymbol{r}^2 + \beta \frac{N - M - n}{n^2} \operatorname{Tr} \ln \boldsymbol{r} + I_n^{(\beta)} \left(\boldsymbol{\sigma}^2, \boldsymbol{r}^{-2}, -\frac{N}{n}\right) \right\} + o_n(1).$$

Thus we end up with

(62)

$$\frac{2\ln p_{M}(\boldsymbol{\sigma})}{\beta M N} = \sup_{\boldsymbol{r} \in \mathbb{R}_{\geq 0}^{n}} \left\{ \sum_{i \neq j}^{1,n} \frac{\ln |\sigma_{i}^{2} - \sigma_{j}^{2}|}{M N} + 2 \frac{M - n}{M N} \operatorname{Tr} \ln \boldsymbol{\sigma} + \sum_{i \neq j}^{1,n} \frac{\ln |r_{i}^{2} - r_{j}^{2}|}{M N} - \frac{\operatorname{Tr} \boldsymbol{r}^{2}}{M} + 2 \frac{N - M - n}{M N} \operatorname{Tr} \ln \boldsymbol{r} + \frac{2n^{2}}{\beta M N} I_{n}^{(\beta)} \left(\boldsymbol{\sigma}^{2}, \boldsymbol{r}^{-2}, -\frac{N}{n}\right) \right\} + o_{n}(1).$$

With this expression in hand we can write down a refined conjecture when the signal is Ginibre.

Conjecture 5 (Replica symmetric formula for Hermitian dictionary learning with a Ginibre signal). Let $n := \min(N, M)$. In the case where the prior $P_{X,N}(\mathbf{X}) \propto \exp \operatorname{Tr}[-(\beta/2)\mathbf{X}\mathbf{X}^{\dagger}]$, the mutual information of model (42) verifies

$$\frac{1}{MN}I\left(\boldsymbol{X};\sqrt{\frac{\lambda}{N}}\boldsymbol{X}\boldsymbol{X}^{\dagger}+\boldsymbol{Z}\right) = -\frac{\beta}{4}\sup_{(\boldsymbol{\sigma}_{z},\boldsymbol{\sigma}_{Q},\boldsymbol{r})\in\mathcal{S}_{M}(\lambda)}\left\{\sum_{k\neq\ell}^{1,M}\frac{\ln\left|(\boldsymbol{\sigma}_{k}^{z})^{2}-(\boldsymbol{\sigma}_{\ell}^{z})^{2}\right|}{MN} - \frac{\mathrm{Tr}\boldsymbol{\sigma}_{z}^{2}}{M}\right. \\
\left. + \sum_{i\neq j}^{1,n}\frac{\ln\left|(\boldsymbol{\sigma}_{i}^{Q})^{2}-(\boldsymbol{\sigma}_{j}^{Q})^{2}\right|}{MN} + 2\frac{M-n}{MN}\sum_{i\leq n}\ln\boldsymbol{\sigma}_{i}^{Q} + \sum_{i\neq j}^{1,n}\frac{\ln\left|r_{i}^{2}-r_{j}^{2}\right|}{MN} - \frac{\mathrm{Tr}\,\boldsymbol{r}^{2}}{M} + 2\frac{N-M-n}{MN}\sum_{i\leq n}\ln\boldsymbol{r}_{i}\right. \\
\left. + \frac{2n^{2}}{\beta MN}I_{n}^{(\beta)}\left(\mathrm{diag}\left(\left((\boldsymbol{\sigma}_{i}^{Q})^{2}\right)_{i\leq n}\right), \boldsymbol{r}^{-2}, -\frac{N}{n}\right) + \frac{2M}{\beta N}J_{M}^{(\beta)}\left(\boldsymbol{\sigma}_{z}, \boldsymbol{\sigma}_{Q}, \frac{2\sqrt{\lambda}N}{M}\right)\right\} \\
\left. + \frac{\beta\lambda}{4}\frac{\mathbb{E}\mathrm{Tr}(\boldsymbol{X}\boldsymbol{X}^{\dagger})^{2}}{MN^{2}} + \tau_{N}. \right\}$$
(63)

The above sums over $(\sigma_i^Q)_{i\leq n}$ in the logarithmic and Vandermonde terms and the spherical integral $I_n^{(\beta)}$ only include the *n* non-zero diagonal elements of $\boldsymbol{\sigma}^Q$ (which can be taken ordered as $\sigma_1^Q > \sigma_2^Q > \cdots > \sigma_n^Q > \sigma_{n+1}^Q = \cdots = \sigma_M^Q = 0$). The $n \times n$ matrix diag $(((\sigma_i^Q)^2)_{i\leq n})$ is diagonal with $((\sigma_i^Q)^2)_{i\leq n}$ as entries on its diagonal. The set of extrema $\mathcal{S}_M(\lambda)$ is

$$\mathcal{S}_{M}(\lambda) \coloneqq \left\{ (\boldsymbol{\sigma}_{z}, \boldsymbol{\sigma}_{Q}, \boldsymbol{r}) \in \mathbb{R}_{\geq 0}^{M} \times \mathbb{R}_{\geq 0}^{M} \times \mathbb{R}_{\geq 0}^{n} : \boldsymbol{\sigma}_{Q} \text{ is of rank } n, \\ \nabla_{\boldsymbol{\sigma}_{z}} g_{M}^{\mathrm{RS}}(\boldsymbol{\sigma}_{z}, \boldsymbol{\sigma}_{Q}, \boldsymbol{r}, \lambda) = \nabla_{\boldsymbol{\sigma}_{Q}} g_{M}^{\mathrm{RS}}(\boldsymbol{\sigma}_{z}, \boldsymbol{\sigma}_{Q}, \boldsymbol{r}, \lambda) = \boldsymbol{0}, \ \nabla_{\boldsymbol{r}} g_{M}^{\mathrm{RS}}(\boldsymbol{\sigma}_{z}, \boldsymbol{\sigma}_{Q}, \boldsymbol{r}, \lambda) = \boldsymbol{0} \right\},$$

for the replica symmetric potential function $g_M^{\text{RS}} : \mathbb{R}^M_{\geq 0} \times \mathbb{R}^M_{\geq 0} \times \mathbb{R}^n_{\geq 0} \times \mathbb{R}_{\geq 0} \mapsto \mathbb{R}$ defined by the curly bracket $\{\cdots\}$ in the variational problem (63). Constant τ_N fixes $I(\boldsymbol{X}; \boldsymbol{Z}) = 0$, i.e.,

$$\tau_N \coloneqq \frac{\beta}{4} \sup_{(\boldsymbol{\sigma}_z, \boldsymbol{\sigma}_Q, \boldsymbol{r}) \in \mathcal{S}_M(0)} g_M^{\mathrm{RS}}(\boldsymbol{\sigma}_z, \boldsymbol{\sigma}_Q, \boldsymbol{r}, \lambda = 0) + o_N(1).$$

Denote σ_Q^* the overlap singular values achieving the supremum in (63). The overlap (54) is then given by $q = N^{-1} \text{Tr} \sigma_Q^* + o_N(1)$.

Introducing asymptotic singular values densities ρ_z , ρ_Q and ρ_r associated to σ_z , σ_Q and r, respectively, the conjecture can be re-expressed in the limit $N \to +\infty$ and $M/N \to \alpha$ as

$$\frac{1}{MN}I\left(\boldsymbol{X};\sqrt{\frac{\lambda}{N}}\boldsymbol{X}\boldsymbol{X}^{\dagger}+\boldsymbol{Z}\right) \rightarrow -\frac{\beta}{4}\sup_{(\rho_{z},\rho_{Q},\rho_{r})\in\mathcal{S}(\lambda)}\left\{\alpha\int d\rho_{z}(x)\,d\rho_{z}(y)\ln|x^{2}-y^{2}| - \int d\rho_{z}(x)\,x^{2}\right.
\left.+\min(1,\alpha)\min(1,\alpha^{-1})\int d\tilde{\rho}_{Q}(x)\,d\tilde{\rho}_{Q}(y)\ln|x^{2}-y^{2}|\right.
\left.+2\min(1,\alpha)\left(1-\min(1,\alpha^{-1})\right)\int d\tilde{\rho}_{Q}(x)\ln x\right.
\left.+\min(1,\alpha)\min(1,\alpha^{-1})\int d\rho_{r}(x)d\rho_{r}(y)\ln|x^{2}-y^{2}|-\min(1,\alpha^{-1})\int d\rho_{r}(x)x^{2}\right.
\left.+2\left(\min(1,\alpha^{-1})-\min(1,\alpha)-\min(1,\alpha)\min(1,\alpha^{-1})\right)\int d\rho_{r}(x)\ln x\right.
\left.+\frac{2}{\beta}\min(1,\alpha)\min(1,\alpha^{-1})I^{(\beta)}\left[\tilde{\rho}_{Q^{2}},\rho_{r^{-2}},\frac{-1}{\min(1,\alpha)}\right] + \frac{2\alpha}{\beta}J^{(\beta)}\left[\rho_{z},\rho_{Q},\frac{2\sqrt{\lambda}}{\alpha}\right]\right\}$$
(64)
$$\left.+\frac{\beta\lambda}{4\alpha}\lim_{N\to+\infty}\frac{\mathbb{E}\mathrm{Tr}(\boldsymbol{X}\boldsymbol{X}^{\dagger})^{2}}{N^{3}} + \tau.$$

The optimization is over probability densities with finite non-negative support belonging to the extremal set

$$\mathcal{S}(\lambda) \coloneqq \{ (\rho_z, \rho_Q, \rho_r) = (\rho_z, (1 - \min(1, \alpha))\delta_0 + \min(1, \alpha)\tilde{\rho}_Q, \rho_r) \text{ with } (\rho_z, \tilde{\rho}_Q, \rho_r) \in \mathcal{P}_{\geq 0} \times \mathcal{P}_{\geq 0} \times \in \mathcal{P}_{\geq 0} : \delta_{\rho_z} g^{\mathrm{RS}}[\rho_z, \rho_Q, \rho_r, \lambda] = \delta_{\tilde{\rho}_Q} g^{\mathrm{RS}}[\rho_z, \rho_Q, \rho_r, \lambda] = \delta_{\rho_r} g^{\mathrm{RS}}[\rho_z, \rho_Q, \rho_r, \lambda] = 0 \},$$

where the three terms of the form $\delta_{\rho}g^{\mathrm{RS}}[\cdots]$ are the functional derivatives of the replica symmetric potential functional $g^{\mathrm{RS}}: \mathcal{P}_{\geq 0} \times \mathcal{P}_{\geq 0} \times \mathcal{P}_{\geq 0} \times \mathbb{R}_{\geq 0} \mapsto \mathbb{R}$ defined by the curly brackets in (64). Using a standard change of density the following two densities belonging to $\mathcal{P}_{\geq 0}$ can be expressed in terms of $\tilde{\rho}_Q$ and ρ_r over which the optimization takes place:

(65)
$$\tilde{\rho}_{Q^2}(x) = \frac{\tilde{\rho}_Q(\sqrt{x})}{2\sqrt{x}} \quad and \quad \rho_{r^{-2}}(x) = \frac{\rho_r(1/\sqrt{x})}{2x^{3/2}}$$

Constant τ fixes the contraint $I(\mathbf{X}; \mathbf{Z}) = 0$:

$$\tau \coloneqq \frac{\beta}{4} \sup_{(\rho_z, \rho_Q, \rho_r) \in \mathcal{S}(0)} g^{\mathrm{RS}}[\rho_z, \rho_Q, \rho_r, \lambda = 0].$$

Denoting by $\rho_Q^* = (1 - \min(1, \alpha))\delta_0 + \min(1, \alpha)\tilde{\rho}_Q^*$ the density of singular values of the overlap that achieves the supremum in (64), the overlap reads $q = \int d\rho_Q^*(x) x$.

5.5. Alternative "symmetric" method. In the case of the Hermitian model (42) it is possible to derive another variational formula for the mutual information, conjectured equivalent. We consider the real case $\beta = 1$ as the additional new assumption (just below) will be more transparent in this case. The symmetry $\mathbf{A}_{sy} = \mathbf{A}_{sy}^{T} \coloneqq (\mathbf{A} + \mathbf{A}^{T})/2$ will be emphasized by the subscript "sy".

We start again from identity (49). Our additional assumption is that the replicated partition function is dominated by configurations such that

Assumption (trace symmetry): $\operatorname{Tr}(\boldsymbol{z}^{ab})^{\mathsf{T}}\boldsymbol{Q}^{ab} \approx \operatorname{Tr}\boldsymbol{z}^{ab}\boldsymbol{Q}^{ab} \approx \operatorname{Tr}(\boldsymbol{z}^{ab})^{\mathsf{T}}\boldsymbol{Q}^{ba}$.

The symbol \approx means that the ratio of the left and right-hand sides tend to 1 as $N \to +\infty$. This assumption is not the same as assuming that z^{ab} is symmetric. It implies a fully symmetric expression

$$\mathbb{E}\mathcal{Z}(\boldsymbol{Y})^{u} \propto \int dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) \prod_{a < b}^{0,u} d\boldsymbol{z}^{ab} \exp N \operatorname{Tr}\left[\sqrt{\lambda} \boldsymbol{Q}_{\mathrm{sy}}^{ab} \boldsymbol{z}_{\mathrm{sy}}^{ab} - \frac{1}{2} (\boldsymbol{z}^{ab})^{\mathsf{T}} \boldsymbol{z}^{ab}\right].$$

where the matrices have been symmetrized using basic properties of the trace. We now average a function of the symmetric $(\boldsymbol{z}_{sy}^{ab})_{a < b}$ only, and therefore the densities over $(\boldsymbol{z}^{ab})_{a < b}$ can be simplified. Indeed, for any function of a symmetrized \boldsymbol{z}_{sy} we have that the expectation $\mathbb{E}_{\boldsymbol{z}} g(\boldsymbol{z}_{sy})$ verifies

$$\mathbb{E}_{\boldsymbol{z}} g(\boldsymbol{z}_{\mathrm{sy}}) \propto \int_{\mathbb{R}^{M^2}} d\boldsymbol{z} \exp \operatorname{Tr} \left[-\frac{N}{2} \boldsymbol{z}^{\mathsf{T}} \boldsymbol{z} \right] g(\boldsymbol{z}_{\mathrm{sy}}) \\ \propto \int_{\mathbb{R}^{M(M+1)/2}} \prod_{k<\ell}^{1,M} dz_{\mathrm{sy},k\ell} \exp \left(-N z_{\mathrm{sy},k\ell}^2 \right) \prod_{k\leq M} dz_{\mathrm{sy},kk} \exp \left(-\frac{N}{2} z_{\mathrm{sy},kk}^2 \right) g(\boldsymbol{z}_{\mathrm{sy}}) \\ \propto \int_{\mathbb{R}^{M(M+1)/2}} d\boldsymbol{z}_{\mathrm{sy}} \exp \operatorname{Tr} \left[-\frac{N}{2} \boldsymbol{z}_{\mathrm{sy}}^2 \right] g(\boldsymbol{z}_{\mathrm{sy}}).$$

We used that under the expectation \mathbb{E}_{z} the random variables $z_{k\ell}$ and $z_{\ell k}$ are independent and drawn from $\mathcal{N}(0, 1/N)$ so that $z_{sy,k\ell} = z_{sy,\ell k} \coloneqq (z_{k\ell} + z_{\ell k})/2 \sim \mathcal{N}(0, 1/(2N))$ for $k < \ell$ while

 $z_{\text{sy},kk} \sim \mathcal{N}(0, 1/N)$. So at this stage

$$\mathbb{E}\mathcal{Z}(\boldsymbol{Y})^{u} \propto \int dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) \prod_{a < b}^{0,u} d\boldsymbol{z}_{sy}^{ab} \exp N \operatorname{Tr}\left[\sqrt{\lambda} \boldsymbol{Q}_{sy}^{ab} \boldsymbol{z}_{sy}^{ab} - \frac{1}{2} (\boldsymbol{z}_{sy}^{ab})^{2}\right].$$

Both matrices can now be diagonalized with real eigenvalues (instead of using the SVD as before):

$$\boldsymbol{z}_{sy}^{ab} = \boldsymbol{z}_{sy}^{ba} = (\boldsymbol{U}^{ab})^{\top} \boldsymbol{\lambda}_{z}^{ab} \boldsymbol{U}^{ab}$$
 and $\boldsymbol{Q}_{sy}^{ab} = \boldsymbol{Q}_{sy}^{ba} = (\boldsymbol{V}^{ab})^{\top} \boldsymbol{\lambda}_{Q}^{ab} \boldsymbol{V}^{ab}.$

All matrices are $M \times M$ and the overlaps are or rank min(M, N). The measure over the gaussian fields, once expressed in the eigenbasis, becomes

$$d\boldsymbol{z}_{\rm sy}^{ab} \exp \operatorname{Tr} \left[-\frac{N}{2} (\boldsymbol{z}_{\rm sy}^{ab})^2 \right] \propto d\mu_M^{(1)}(\boldsymbol{U}^{ab}) \, d\boldsymbol{\lambda}_z^{ab} \exp \operatorname{Tr} \left[-\frac{N}{2} (\boldsymbol{\lambda}_z^{ab})^2 \right] |\Delta_M(\boldsymbol{\lambda}_z^{ab})|$$

As before, only the overlaps $(\mathbf{Q}_{sy}^{ab})_{a<b}$ depend on the replicas $(\mathbf{x}^a)_a$ so the measure $dP_{X,N}(\{\mathbf{x}\}_0^u)$ induces a joint law $dP((\mathbf{Q}_{sy}^{ab})_{a<b})$ over these matrices. We change variables from matrices $(\mathbf{Q}_{sy}^{ab})_{a<b}$ to eigenvalues and eigenvectors. Using a similar spectral replica symmetric ansatz as (50) but for the j.p.d.f. of overlaps eigenvalues,

Assumption (spectral replica symmetry): $P_{(\lambda_Q),M}((\lambda_Q^{ab})_{a < b}) \rightarrow \prod_{a < b}^{0,u} p_M(\lambda_Q^{ab}),$

we have the change of density

$$dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) = dP_{(Q),M}((\boldsymbol{Q}_{\mathrm{sy}}^{ab})_{a < b}) \rightarrow dP_{(V)|(\lambda_{Q}),M}((\boldsymbol{V}^{ab})_{a < b} \mid (\boldsymbol{\lambda}_{Q}^{ab})_{a < b}) \prod_{a < b}^{0,u} p_{M}(\boldsymbol{\lambda}_{Q}^{ab}) d\boldsymbol{\lambda}_{Q}^{ab}.$$

The replicated partition function is thus at leading order equal to

$$\mathbb{E}\mathcal{Z}(\boldsymbol{Y})^{u} \propto \int \prod_{a < b}^{0,u} d\boldsymbol{\lambda}_{z}^{ab} d\boldsymbol{\lambda}_{Q}^{ab} |\Delta(\boldsymbol{\lambda}_{z}^{ab})| \exp \operatorname{Tr} \Big[-\frac{N}{2} (\boldsymbol{\lambda}_{z}^{ab})^{2} \Big] p_{M}(\boldsymbol{\lambda}_{Q}^{ab}) \times \int dP_{(V)|(\lambda_{Q}),M}((\boldsymbol{V}^{ab})_{a < b} | (\boldsymbol{\lambda}_{Q}^{ab})_{a < b}) \times \int \prod_{a < b}^{0,u} d\mu_{M}^{(1)}(\boldsymbol{U}^{ab}) \exp \frac{1}{2} \frac{2\sqrt{\lambda}N}{M} M \operatorname{Tr} \Big[(\boldsymbol{U}^{ab})^{\mathsf{T}} \boldsymbol{\lambda}_{z}^{ab} \boldsymbol{U}^{ab} (\boldsymbol{V}^{ab})^{\mathsf{T}} \boldsymbol{\lambda}_{Q}^{ab} \boldsymbol{V}^{ab} \Big].$$

Each V^{ab} can be absorbed in an independent Haar distributed U^{ab} by the change of variable $U^{ab}(V^{ab})^{\intercal} \rightarrow U^{ab}$ (of unit Jacobian determinant), and the new matrices remain Haar and independent. So the measure over eigenvectors can be integrated to one. The last term then makes appear the HCIZ integral (9). We thus get

$$\mathbb{E}\mathcal{Z}(\boldsymbol{Y})^{u} \propto \left(\int d\boldsymbol{\lambda}_{z} d\boldsymbol{\lambda}_{Q} \exp \frac{MN}{2} \left[\sum_{k\neq\ell}^{1,M} \frac{\ln|\lambda_{k}^{z} - \lambda_{\ell}^{z}|}{MN} - \frac{\operatorname{Tr}\boldsymbol{\lambda}_{z}^{2}}{M} + \frac{2\ln p_{M}(\boldsymbol{\lambda}_{Q})}{MN} + \frac{2M}{N} I_{M}^{(1)} \left(\boldsymbol{\lambda}_{z}, \boldsymbol{\lambda}_{Q}, \frac{2\sqrt{\lambda}N}{M}\right)\right]\right)^{u(u+1)/2}$$

The replica computation gives, using (45) and after evaluation of the above integral by saddle-point as $N \to +\infty$ followed by the analytic continuation $u \to 0_+$, the following conjecture for the mutual information. From the same arguments as before, we can also obtain the overlap from it.

Conjecture 6 (Replica symmetric formula for symmetric dictionary learning, symmetrized version). Let the j.p.d.f. of the M eigenvalues of O(1) of the matrix $(2N)^{-1}(\boldsymbol{x}_0^{\mathsf{T}} \tilde{\boldsymbol{x}}_0 + \tilde{\boldsymbol{x}}_0^{\mathsf{T}} \boldsymbol{x}_0)$, where $\boldsymbol{x}_0, \tilde{\boldsymbol{x}}_0$ are *i.i.d.* $N \times M$ random matrices drawn from $P_{X,N}$, be p_M . The mutual information of model (42) in the real case $\beta = 1$ verifies

(66)
$$\frac{1}{MN}I\left(\boldsymbol{X}; \sqrt{\frac{\lambda}{N}}\boldsymbol{X}\boldsymbol{X}^{\mathsf{T}} + \boldsymbol{Z}\right) = -\frac{1}{4}\sup_{(\boldsymbol{\lambda}_{z},\boldsymbol{\lambda}_{Q})\in\mathcal{S}_{M}(\lambda)} \left\{\sum_{k\neq\ell}^{1,M} \frac{\ln|\lambda_{k}^{z} - \lambda_{\ell}^{z}|}{MN} - \frac{\mathrm{Tr}\boldsymbol{\lambda}_{z}^{2}}{M} + \frac{2\ln p_{M}(\boldsymbol{\lambda}_{Q})}{MN} + \frac{2M}{N}I_{M}^{(1)}\left(\boldsymbol{\lambda}_{z},\boldsymbol{\lambda}_{Q},\frac{2\sqrt{\lambda}N}{M}\right)\right\} + \frac{\lambda}{4}\frac{\mathbb{E}\mathrm{Tr}(\boldsymbol{X}\boldsymbol{X}^{\mathsf{T}})^{2}}{MN^{2}} + \tau_{N}.$$

The set of extrema $\mathcal{S}_M(\lambda)$ is defined as

$$S_M(\lambda) \coloneqq \{ (\boldsymbol{\lambda}_z, \boldsymbol{\lambda}_Q) \in \mathbb{R}^M \times \mathbb{R}^M : \boldsymbol{\lambda}_Q \text{ is of rank } \min(M, N), \\ \nabla_{\boldsymbol{\lambda}_z} h_M^{\mathrm{RS}}(\boldsymbol{\lambda}_z, \boldsymbol{\lambda}_Q, \lambda) = \nabla_{\boldsymbol{\lambda}_Q} h_M^{\mathrm{RS}}(\boldsymbol{\lambda}_z, \boldsymbol{\lambda}_Q, \lambda) = \mathbf{0} \}$$

where $h_M^{\text{RS}} : \mathbb{R}^M \times \mathbb{R}^M \times \mathbb{R}_{\geq 0} \mapsto \mathbb{R}$ is the replica symmetric potential function defined by the curly brackets in (66). Constant Z_N fixes the contraint $I(\mathbf{X}; \mathbf{Z}) = 0$, i.e.,

$$\tau_N \coloneqq \frac{1}{4} \sup_{(\boldsymbol{\lambda}_z, \boldsymbol{\lambda}_Q) \in \mathcal{S}_M(0)} h_M^{\mathrm{RS}}(\boldsymbol{\lambda}_z, \boldsymbol{\lambda}_Q, \boldsymbol{\lambda} = 0) + o_N(1).$$

Denote λ_Q^* the overlap spectral density achieving the supremum in (66). The overlap (54) is then

(67)
$$q = \frac{1}{N} \operatorname{Tr} \boldsymbol{\lambda}_Q^* + o_N(1).$$

As for Conjecture 4, in case of existence of a functional $\Gamma[\rho_Q] := \lim_{M \to +\infty} M^{-2} \ln p_M(\lambda_Q)$ depending on the *density* ρ_Q of eigenvalues of Q_{sy} , the conjecture can readily be expressed as a variational problem over eigenvalues densities in the limit $N \to +\infty$ and $M/N \to \alpha$. Additionally, by using the results of Section 5.4 this conjecture can be made more explicit in the special case of a Ginibre signal if needed.

5.6. A comparison with previous attempts. The Bayes-optimal setting of linear-rank dictionary learning has been previously studied in the inspiring works [52,53] (in the real case $\beta = 1$). But we think that these approaches provide approximations to the exact asymptotic formulas. In [52] the ansatz is the simplest one: the authors consider constant matrices $\mathbf{z}^{ab} = (\mathbf{z})$ in (49). It is probable that this ansatz cannot capture the important rotational degrees of freedom of the model. In his thesis [53] C. Schmidt proposed instead $\mathbf{z}^{ab} = \mathbf{z}$ and, additionally, that it is symmetric $\mathbf{z} = \mathbf{z}^{\top}$ (while there is no reasons for it to be so): we believe that these weaker assumptions nevertheless remain too strong to yield the correct formulas. By symmetry he could work in eigenbasis $\mathbf{z}^{ab} = \mathbf{z} = \mathbf{U}^{\top} \boldsymbol{\lambda}^{\mathbf{z}} \mathbf{U}$. This assumption that both eigenvalues and eigenvectors are replica independent is physically equivalent to assume that the overlaps $(\mathbf{Q}^{ab})_{a < b}$ concentrate *entrywise* (but not towards a constant matrix as the authors of [52] implicitely assumed). But we expect that only the joint statistics of eigen/singular values can be self-averaging as often in random matrix theory. The same phenomenon happens in large covariances matrices: only the spectral properties become deterministic while the matrix entries fluctuate even in the large size limit.

In the most generic version of the method leading to Conjecture 4, our new ansatz is only at the level of the distribution of singular values of the overlaps $Q^{ab} = A^{ab} \sigma_Q^{ab} B^{ab}$: the matrices σ_Q^{ab} are assumed to decouple and to have identical statistics in the large size limit. Nothing is assumed on the singular vectors, which are naturally absorbed in the rectangular spherical integral $J^{(\beta)}$.

The spectral decoupling assumption (50) allows us to carry on the computation while completely capturing the relevant rotational degrees of freedom and invariances.

The spectral replica method therefore allows us to reduce the challenging task of computing the quenched free entropy (or mutual information), which is an integral over $\Theta(N^2)$ matrix elements (and that additionally should be averaged over the data distribution), into two well defined RMT sub-problems:

- (1) obtaining the j.p.d.f. of the singular values (or eigenvalues) of a product of two i.i.d. random matrices drawn from the prior distribution $P_{X,N}$;
- (2) analyzing a Coulomb gas with multiple interacting populations/densities through spherical integrals, i.e., an optimization problem over $\Theta(N)$ interacting degrees of freedom representing the singular values (or eigenvalues) of certain matrix order parameters entering the analysis (or equivalently, solving a functional optimization problem over the associated asymptotic densities).

As discussed already, the first task does not require a-priori the prior $P_{X,N}$ to be factorized over the entries of the matrix X. So in cases where the j.p.d.f. p_M can be evaluated, the spectral replica method yields concrete asymptoic formulas for the mutual information and MMSE.

In the symmetric version of the replica approach leading to Conjecture 6, we only assume replica symmetry in the sense that for typical realizations of the matrices \boldsymbol{z}^{ab} and \boldsymbol{Q}^{ab} , the "macroscopic quantity" $\operatorname{Tr}(\boldsymbol{z}^{ab})^{\mathsf{T}}\boldsymbol{Q}^{ab}$ is essentially invariant by transposition of \boldsymbol{z}^{ab} . Or equivalently, invariant under swithching of replica indices of the overlap matrix: $\operatorname{Tr}(\boldsymbol{z}^{ab})^{\mathsf{T}}\boldsymbol{Q}^{ab} \approx \operatorname{Tr}(\boldsymbol{z}^{ab})^{\mathsf{T}}\boldsymbol{Q}^{ba}$. This assumption allows to symmetrize the action and work with symmetric matrices. We then assume the same spectral replica symmetric ansatz on the spectra of the symmetrized overlaps $(\boldsymbol{Q}^{ab}_{sv})_{a < b}$ and carry on the computation using the standard spherical integral $I^{(\beta)}$.

We believe that our methodology yields asymptotically exact formulas for the main informationtheoretic quantities. There is a possibility that in special cases our formulas may be further simplified. E.g., by finding simpler terms correctly capturing the interactions induced by the j.p.d.f. $\ln p_M(\lambda_Q)$, or by simplifying the HCIZ integral. But we doubt that this is possible in general because the effective models described by our formulas correspond to strongly interacting eigenvalues/singular values evolving at vanishing temperature. And, to the best of our knowledge, there is no systematic exact simplifications for such Coulomb gas systems.

6. Dictionary learning

6.1. The model. Let the ground-truth dictionary $\boldsymbol{S} = [S_{ik}] \in \mathbb{K}^{N \times K}$ be drawn from a centered distribution $\boldsymbol{S} \sim P_{S,K}$, and the coefficients $\boldsymbol{T} = [T_{jk}] \in \mathbb{K}^{M \times K}$ from $\boldsymbol{T} \sim P_{T,K}$ centered also, where the entries of both \boldsymbol{S} and \boldsymbol{T} are typically O(1). These two priors should induce symmetric j.p.d.f. of singular values for \boldsymbol{S} and \boldsymbol{T} . We set

$$N = \alpha K + o(K)$$
 and $M = \gamma K + o(K)$

with fixed $\alpha, \gamma > 0$ as $K \to +\infty$. Consider having access to a data matrix $\mathbf{Y} = [Y_{ij}] \in \mathbb{K}^{N \times M}$ with entries generated according to

(68)
$$\boldsymbol{Y} = \sqrt{\frac{\lambda}{N}} \boldsymbol{S} \boldsymbol{T}^{\dagger} + \boldsymbol{Z},$$

with a Ginibre noise matrix $\boldsymbol{Z} \in \mathbb{K}^{N \times M}$ with law

$$P_{Z,N}(\mathbf{Z}) \propto \exp \operatorname{Tr} \left[-\frac{\beta}{2} \mathbf{Z} \mathbf{Z}^{\dagger} \right]$$

The scaling in N of the matrix entries and eigenvalues are the same as in the positive definite case (42). We assume this time that both priors are bi-orthogonal/unitary rotationally invariant, i.e.,

(69)
$$dP_{S,K}(\boldsymbol{S}) = dP_{S,K}(\boldsymbol{O}\boldsymbol{S}\boldsymbol{\tilde{O}}) \text{ and } dP_{T,K}(\boldsymbol{T}) = dP_{T,K}(\boldsymbol{O}\boldsymbol{T}\boldsymbol{\tilde{O}})$$

for any orthogonal ($\beta = 1$) or unitary ($\beta = 2$) matrices O and O. Rotational invariance of the prior was not needed in the Hermitian case of dictionary learning, but it seems required in the less symmetric present setting. We jointly denote X := (S, T) and $x := (s, t) \in \mathbb{K}^{N \times K} \times \mathbb{K}^{M \times K}$. Let $dP_{X,K}(x) := dP_{S,K}(s) dP_{T,K}(t)$. The joint posterior reads

(70)
$$dP_{X|Y,K}(\boldsymbol{x} \mid \boldsymbol{Y}) = \frac{1}{\mathcal{Z}(\boldsymbol{Y})} dP_{X,K}(\boldsymbol{x}) \exp \frac{\beta}{2} \operatorname{Tr} \Big[\sqrt{\frac{\lambda}{N}} \boldsymbol{Y}^{\dagger} \boldsymbol{s} \boldsymbol{t}^{\dagger} + \sqrt{\frac{\lambda}{N}} \boldsymbol{Y} \boldsymbol{t} \boldsymbol{s}^{\dagger} - \frac{\lambda}{N} \boldsymbol{s}^{\dagger} \boldsymbol{s} \boldsymbol{t}^{\dagger} \boldsymbol{t} \Big].$$

Note the invariance of the model under $(S,T) \rightarrow (SU,TU)$ for any orthogonal/unitary U.

The object of interest is the average free entropy

$$\mathbb{E}f_N \coloneqq \frac{1}{NM} \mathbb{E} \ln \mathcal{Z}(\boldsymbol{Y}).$$

It is linked to the mutual information by

$$\frac{1}{MN}I(\boldsymbol{Y};(\boldsymbol{S},\boldsymbol{T})) = -\mathbb{E}f_N + \frac{\beta\lambda}{2MN^2}\mathbb{E}\mathrm{Tr}\boldsymbol{S}^{\dagger}\boldsymbol{S}\boldsymbol{T}^{\dagger}\boldsymbol{T}.$$

6.2. Replica trick and freeness assumption. As before, working in the Bayes-optimal setting allows us to simply rename the ground truth $x^0 = X$ which will play the same role as all other replicas $x^a = (s^a, t^a) \in \mathbb{K}^{N \times K} \times \mathbb{K}^{M \times K}$ of x. We set

$$\int dP_{X,K}(\{\boldsymbol{x}\}_0^u) \cdots = \int_{\mathbb{K}^{NK(u+1)}} \prod_{a=0}^u dP_{S,K}(\boldsymbol{s}^a) \int_{\mathbb{K}^{MK(u+1)}} \prod_{a=0}^u dP_{T,K}(\boldsymbol{t}^a) \cdots$$

The replica trick (45) requires computing the moments of the partition function. As in Section 5 we consider first the more cumbersome complex case $\beta = 2$. Model (68) is then equivalent to

$$\begin{cases} \Re Y_{ij} \sim \mathcal{N}\left(\sqrt{\frac{\lambda}{N}} \frac{\langle \boldsymbol{S}_i, \bar{\boldsymbol{T}}_j \rangle + \langle \bar{\boldsymbol{S}}_i, \boldsymbol{T}_j \rangle}{2}, \frac{1}{2}\right) \\ \Im Y_{ij} \sim \mathcal{N}\left(\sqrt{\frac{\lambda}{N}} \frac{\langle \boldsymbol{S}_i, \bar{\boldsymbol{T}}_j \rangle - \langle \bar{\boldsymbol{S}}_i, \boldsymbol{T}_j \rangle}{2\mathrm{i}}, \frac{1}{2}\right) & \text{for} \quad (i, j) \in [N] \times [M]. \end{cases}$$

We integrate Y which is, conditionally on (S, T), a complex gaussian multivariate random variable, by using formula (46) and obtain that $\mathbb{E}\mathcal{Z}(Y)^u$ equals

$$\int dP_{X,K}(\{\boldsymbol{x}\}_{0}^{u}) \mathbb{E}_{\boldsymbol{Y}|\boldsymbol{x}^{0}} \prod_{a \leq u} \exp 2 \sum_{i,j}^{N,M} \left(\sqrt{\frac{\lambda}{N}} \Re Y_{ij} \frac{\langle \boldsymbol{s}_{i}^{a}, \bar{\boldsymbol{t}}_{j}^{a} \rangle + \langle \bar{\boldsymbol{s}}_{i}^{a}, \boldsymbol{t}_{j}^{a} \rangle}{2} - \frac{\lambda}{2N} \left(\frac{\langle \boldsymbol{s}_{i}^{a}, \bar{\boldsymbol{t}}_{j}^{a} \rangle + \langle \bar{\boldsymbol{s}}_{i}^{a}, \boldsymbol{t}_{j}^{a} \rangle}{2} \right)^{2} \right) \\ \times \exp 2 \sum_{i,j}^{N,M} \left(\sqrt{\frac{\lambda}{N}} \Im Y_{ij} \frac{\langle \boldsymbol{s}_{i}^{a}, \bar{\boldsymbol{t}}_{j}^{a} \rangle - \langle \bar{\boldsymbol{s}}_{i}^{a}, \boldsymbol{t}_{j}^{a} \rangle}{2\mathrm{i}} - \frac{\lambda}{2N} \left(\frac{\langle \boldsymbol{s}_{i}^{a}, \bar{\boldsymbol{t}}_{j}^{a} \rangle - \langle \bar{\boldsymbol{s}}_{i}^{a}, \boldsymbol{t}_{j}^{a} \rangle}{2\mathrm{i}} \right)^{2} \right)$$

We introduced the $K \times K$ (a-priori non-Hermitian) overlap matrices and their SVD decompositions:

$$\boldsymbol{Q}_{s}^{ab} \coloneqq \left(\frac{1}{N}\sum_{i\leq N}s_{ik}^{a}\bar{s}_{i\ell}^{b}\right)_{k,\ell\leq K} = \frac{(\boldsymbol{s}^{a})^{\top}\bar{\boldsymbol{s}}^{b}}{N} = \boldsymbol{A}_{s}^{ab}\boldsymbol{\sigma}_{s}^{ab}\boldsymbol{B}_{s}^{ab},$$
$$\boldsymbol{Q}_{t}^{ab} \coloneqq \left(\frac{1}{N}\sum_{j\leq M}\bar{t}_{jk}^{a}t_{j\ell}^{b}\right)_{k,\ell\leq K} = \frac{(\boldsymbol{t}^{a})^{\dagger}\boldsymbol{t}^{b}}{N} = \boldsymbol{A}_{t}^{ab}\boldsymbol{\sigma}_{t}^{ab}\boldsymbol{B}_{t}^{ab}.$$

The overlaps $(\boldsymbol{Q}_s^{ab})_{a < b}$ are of rank min(N, K), and thus $(\boldsymbol{\sigma}_s^{ab})_{a < b}$ have min(N, K) non-zero entries on their diagonal, while $(\boldsymbol{Q}_t^{ab})_{a < b}$ have rank min(M, K) implying that $(\boldsymbol{\sigma}_t^{ab})_{a < b}$ have min(M, K)non-zero entries on their diagonal. The following product form of the prior measure $dP_{X,K}(\{\boldsymbol{x}\}_0^u) = \prod_{a=0}^u dP_{S,K}(\boldsymbol{s}^a) dP_{T,K}(\boldsymbol{t}^a)$ induces a j.p.d.f. of the overlaps factorized over the two types of overlaps: (71) $dP_{(Q_s,Q_t),K}((\boldsymbol{Q}_s^{ab}, \boldsymbol{Q}_t^{ab})_{a < b}) = dP_{(Q_s),K}((\boldsymbol{Q}_s^{ab})_{a < b}) dP_{(Q_t),K}((\boldsymbol{Q}_t^{ab})_{a < b}).$

At this stage we need one additional assumption when compared with the Hermitian case of Section 5. For each pair a < b of replica indices let i.i.d. Haar matrices U^{ab} , $V^{ab} \sim \mu_K^{(\beta)}$ independent of everything else. We assume the following equality in distribution in the large size limit³, which is suggested by the combination of the independence (71) between the two types of overlaps together with the rotational invariance (69) of both priors (from which the overlap matrices Q_s^{ab} and Q_t^{ab} must inherit).

Assumption (equality in law): For any pair a < b: $\operatorname{Tr} \boldsymbol{Q}_s^{ab} (\boldsymbol{Q}_t^{ab})^{\dagger} \sim \operatorname{Tr} \left[\boldsymbol{U}^{ab} \boldsymbol{Q}_s^{ab} \boldsymbol{V}^{ab} (\boldsymbol{Q}_t^{ab})^{\dagger} \right]$ as $M, N, K \to +\infty$.

As a consequence,

$$\mathbb{E}\mathcal{Z}(\boldsymbol{Y})^{u} \propto \int dP_{(Q_{s},Q_{t}),K}((\boldsymbol{Q}_{s}^{ab},\boldsymbol{Q}_{t}^{ab})_{a
$$= \int dP_{(Q_{s}),K}((\boldsymbol{Q}_{s}^{ab})_{a
$$\times \prod_{a$$$$$$

³We note that this assumption is reminiscent of results in [117] (see also [118]) for the addition of two large random matrices with at least one being bi-unitary invariant.

We now change variables for the SVD decompositions of the overlaps:

$$dP_{(Q_s),K}((\boldsymbol{Q}_s^{ab})_{a < b}) = dP_{(A_s,B_s)|(\sigma_s),K}((\boldsymbol{A}_s^{ab}, \boldsymbol{B}_s^{ab})_{a < b} | (\boldsymbol{\sigma}_s^{ab})_{a < b}) dP_{(\sigma_s),K}((\boldsymbol{\sigma}_s^{ab})_{a < b}),$$

and similarly for $dP_{(Q_t),K}((Q_t^{ab})_{a < b})$. The spectral replica symmetric ansatz reads in this case:

(72) Assumption (spectral replica symmetry):
$$\begin{cases} P_{(\sigma_s),K}((\sigma_s^{ab})_{a < b}) \to \prod_{a < b}^{0,u} p_{S,K}(\sigma_s^{ab}), \\ P_{(\sigma_t),K}((\sigma_t^{ab})_{a < b}) \to \prod_{a < b}^{0,u} p_{T,K}(\sigma_t^{ab}), \end{cases}$$

for certain j.p.d.f. $p_{S,K}$ and $p_{T,K}$ to be determined using RMT. As before, symbol \rightarrow means that both sides weakly converge to the same asymptotic distribution as $N, M, K \rightarrow +\infty$ together. Thus

$$\mathbb{E}\mathcal{Z}(\boldsymbol{Y})^{u} \propto \int \prod_{a < b}^{0, u} dp_{S,K}(\boldsymbol{\sigma}_{s}^{ab}) dp_{T,K}(\boldsymbol{\sigma}_{t}^{ab})$$

$$\times \int dP_{(A_{s},B_{s})|(\boldsymbol{\sigma}_{s}),K}((\boldsymbol{A}_{s}^{ab},\boldsymbol{B}_{s}^{ab})_{a < b} | (\boldsymbol{\sigma}_{s}^{ab})_{a < b}) dP_{(A_{t},B_{t})|(\boldsymbol{\sigma}_{t}),K}((\boldsymbol{A}_{t}^{ab},\boldsymbol{B}_{t}^{ab})_{a < b} | (\boldsymbol{\sigma}_{t}^{ab})_{a < b})$$

$$\times \int \prod_{a < b}^{0, u} d\mu_{K}^{(\beta)}(\boldsymbol{U}^{ab}) d\mu_{K}^{(\beta)}(\boldsymbol{V}^{ab}) \exp \beta \lambda N \Re \operatorname{Tr} [\boldsymbol{U}^{ab} \boldsymbol{A}_{s}^{ab} \boldsymbol{\sigma}_{s}^{ab} \boldsymbol{B}_{s}^{ab} \boldsymbol{V}^{ab} (\boldsymbol{B}_{t}^{ab})^{\dagger} \boldsymbol{\sigma}_{t}^{ab} (\boldsymbol{A}_{t}^{ab})^{\dagger}].$$

As before, the mechanism here is to absorb the left and right singular vectors into the Haar distributed matrices: we redefine $(A_t^{ab})^{\dagger}U^{ab}A_s^{ab} \rightarrow U^{ab}$ and $B_s^{ab}V^{ab}(B_t^{ab})^{\dagger} \rightarrow V^{ab}$ which remain independent and Haar distributed; these changes have unit Jacobian determinant. Thus, the distributions of singular vectors, which a-priori couple the different pairs of replicas, are integrated and decoupling of the integrals over the pairs of indices a < b takes place. This yields

$$\mathbb{E}\mathcal{Z}(\boldsymbol{Y})^{u} \propto \left(\int dp_{S,K}(\boldsymbol{\sigma}_{s}) dp_{T,K}(\boldsymbol{\sigma}_{t}) d\mu_{K}^{(\beta)}(\boldsymbol{U}) d\mu_{K}^{(\beta)}(\boldsymbol{V}) \exp\beta\lambda N \Re \mathrm{Tr}\left[\boldsymbol{U}\boldsymbol{\sigma}_{s}\boldsymbol{V}\boldsymbol{\sigma}_{t}\right]\right)^{u(u+1)/2} \\ = \left(\int d\boldsymbol{\sigma}_{s} d\boldsymbol{\sigma}_{t} \exp MN \left[\frac{\ln p_{S,K}(\boldsymbol{\sigma}_{s})}{MN} + \frac{\ln p_{T,K}(\boldsymbol{\sigma}_{t})}{MN} + \frac{K^{2}}{MN} J_{K}^{(\beta)}(\boldsymbol{\sigma}_{s}, \boldsymbol{\sigma}_{t}, 2\lambda)\right]\right)^{u(u+1)/2}$$

Saddle-point estimation and taking $u \to 0_+$ yields the following conjecture for the mutual information and, thus, the non-universal scalar overlaps (see the justifications below (54)):

(73)
$$q_s \coloneqq \lim_{N \to +\infty} \frac{1}{N} \mathbb{E} \langle |\operatorname{Tr} \boldsymbol{s} \boldsymbol{S}^{\dagger}| \rangle = \lim_{N \to +\infty} \frac{1}{N} \mathbb{E} \langle |\operatorname{Tr} \boldsymbol{Q}_s| \rangle = \lim_{N \to +\infty} \frac{1}{N} |\operatorname{Tr} \mathbb{E} \langle \boldsymbol{Q}_s \rangle| = \frac{1}{N} |\operatorname{Tr} \boldsymbol{Q}_s| + o_K(1),$$

and q_t defined similarly when replacing (s, S, Q_s) by (t, T, Q_t) . Here the overlaps $Q_s := N^{-1} s^{\dagger} \tilde{s}$ and $Q_t := N^{-1} t^{\dagger} \tilde{t}$ for two i.i.d. samples $\boldsymbol{x} = (s, t)$ and $\tilde{\boldsymbol{x}} = (\tilde{s}, \tilde{t})$ from the joint posterior distribution $P_{X|Y,N}$ given by (70).

Conjecture 7 (Replica symmetric formula for dictionary learning). Let the j.p.d.f. of the K singular values of O(1) of the matrix $N^{-1}\mathbf{s}_0^{\dagger}\tilde{\mathbf{s}}_0$, where $\mathbf{s}_0, \tilde{\mathbf{s}}_0$ are i.i.d. $N \times K$ random matrices drawn from $P_{S,K}$, be $p_{S,K}$. Similarly, let the j.p.d.f. of the K singular values of O(1) of $N^{-1}\mathbf{t}_0^{\dagger}\tilde{\mathbf{t}}_0$, where $\mathbf{t}_0, \tilde{\mathbf{t}}_0$ are i.i.d. $M \times K$ random matrices drawn from $P_{T,K}$, be $p_{T,K}$.

The mutual information of model (68) verifies

$$\frac{1}{MN}I((\boldsymbol{S},\boldsymbol{T});\sqrt{\frac{\lambda}{N}}\boldsymbol{S}\boldsymbol{T}^{\dagger}+\boldsymbol{Z}) = -\frac{K^2}{2MN}\sup_{(\boldsymbol{\sigma}_s,\boldsymbol{\sigma}_t)\in\mathcal{S}_K(\lambda)}\left\{\frac{\ln p_{S,K}(\boldsymbol{\sigma}_s)}{K^2} + \frac{\ln p_{T,K}(\boldsymbol{\sigma}_t)}{K^2} + J_K^{(\beta)}(\boldsymbol{\sigma}_s,\boldsymbol{\sigma}_t,2\lambda)\right\} + \frac{\beta\lambda}{2MN^2}\mathbb{E}\mathrm{Tr}\boldsymbol{S}^{\dagger}\boldsymbol{S}\boldsymbol{T}^{\dagger}\boldsymbol{T} + \tau_K.$$
(74)

The set of extrema $\mathcal{S}_K(\lambda)$ is defined as

$$\mathcal{S}_{K}(\lambda) \coloneqq \{ (\boldsymbol{\sigma}_{s}, \boldsymbol{\sigma}_{t}) \in \mathbb{R}_{\geq 0}^{K} \times \mathbb{R}_{\geq 0}^{K} : \boldsymbol{\sigma}_{s} \text{ is of rank } \min(N, K), \ \boldsymbol{\sigma}_{t} \text{ is of rank } \min(M, K), \\ \nabla_{\boldsymbol{\sigma}_{s}} g_{K}^{\mathrm{RS}}(\boldsymbol{\sigma}_{s}, \boldsymbol{\sigma}_{t}, \lambda) = \nabla_{\boldsymbol{\sigma}_{t}} g_{K}^{\mathrm{RS}}(\boldsymbol{\sigma}_{s}, \boldsymbol{\sigma}_{t}, \lambda) = \mathbf{0} \},$$

where $g_K^{\text{RS}} : \mathbb{R}_{\geq 0}^K \times \mathbb{R}_{\geq 0}^K \times \mathbb{R}_{\geq 0} \mapsto \mathbb{R}$ is the replica symmetric potential function defined by the curly brackets $\{\cdots\}$ in the variational problem (74). Constant τ_K fixes $I((\boldsymbol{S}, \boldsymbol{T}); \boldsymbol{Z}) = 0$, i.e.,

$$\tau_{K} \coloneqq \frac{1}{2} \sup_{(\boldsymbol{\sigma}_{s}, \boldsymbol{\sigma}_{t}) \in \mathcal{S}_{K}(0)} g_{K}^{\mathrm{RS}}(\boldsymbol{\sigma}_{s}, \boldsymbol{\sigma}_{t}, \lambda = 0) + o_{K}(1).$$

Denote (σ_s^*, σ_t^*) the overlaps singular values achieving the supremum in (74). The scalar overlaps are

(75)
$$q_s = \frac{1}{N} \operatorname{Tr} \boldsymbol{\sigma}_s^* + o_K(1), \qquad q_t = \frac{1}{N} \operatorname{Tr} \boldsymbol{\sigma}_t^* + o_K(1)$$

Introducing asymptotic singular values densities ρ_s and ρ_t associated to $\boldsymbol{\sigma}_s$ and $\boldsymbol{\sigma}_t$, respectively, and assuming it exist functionals Γ_s and Γ_t depending only on the asymptotic singular values densities ρ_s and ρ_t , respectively, and such that

$$\Gamma_s[\rho_s] \coloneqq \lim_{K \to +\infty} \frac{1}{K^2} \ln p_{S,K}(\boldsymbol{\sigma}_s) \quad and \quad \Gamma_t[\rho_t] \coloneqq \lim_{K \to +\infty} \frac{1}{K^2} \ln p_{T,K}(\boldsymbol{\sigma}_t)$$

the conjecture can be re-expressed in the limit $K \to +\infty$ with $N/K \to \alpha$ and $M/K \to \gamma$ as

(76)
$$\frac{1}{MN}I((\boldsymbol{S},\boldsymbol{T});\sqrt{\frac{\lambda}{N}}\boldsymbol{S}\boldsymbol{T}^{\dagger}+\boldsymbol{Z}) \rightarrow -\frac{1}{2\alpha\gamma}\sup_{(\rho_{s},\rho_{t})\in\mathcal{S}(\lambda)}\left\{\Gamma_{s}[\rho_{s}]+\Gamma_{t}[\rho_{t}]+J^{(\beta)}[\rho_{s},\rho_{t},2\lambda]\right\} +\frac{\beta\lambda}{2}\lim_{K\to+\infty}\frac{\mathbb{E}\mathrm{Tr}\boldsymbol{S}^{\dagger}\boldsymbol{S}\boldsymbol{T}^{\dagger}\boldsymbol{T}}{MN^{2}}+\tau.$$

The optimization is over probability densities with finite non-negative support, and possibly a point mass in δ_0 , belonging to the extremal set

$$\mathcal{S}(\lambda) \coloneqq \{ (\rho_s, \rho_t) = ((1 - \min(1, \alpha))\delta_0 + \min(1, \alpha)\tilde{\rho}_s, (1 - \min(1, \gamma))\delta_0 + \min(1, \gamma)\tilde{\rho}_t) \\ with \ (\tilde{\rho}_s, \tilde{\rho}_t) \in \mathcal{P}_{\geq 0} \times \mathcal{P}_{\geq 0} \colon \ \delta_{\tilde{\rho}_s}g^{\mathrm{RS}}[\rho_s, \rho_t, \lambda] = \delta_{\tilde{\rho}_s}g^{\mathrm{RS}}[\rho_s, \rho_t, \lambda] = 0 \},$$

where $\delta_{\tilde{\rho}_{s/t}}g^{\mathrm{RS}}[\rho_s, \rho_t, \lambda]$ are the functional derivatives of the replica symmetric potential functional $g^{\mathrm{RS}} : \mathcal{P}_{\geq 0} \times \mathcal{P}_{\geq 0} \times \mathbb{R}_{\geq 0} \mapsto \mathbb{R}$ defined by the curly brackets in (76). Constant τ fixes the contraint $I((\boldsymbol{S}, \boldsymbol{T}); \boldsymbol{Z}) = 0$, i.e.,

$$\tau \coloneqq \frac{1}{2\alpha\gamma} \sup_{(\rho_s,\rho_t)\in\mathcal{S}(0)} g^{\mathrm{RS}}[\rho_s,\rho_t,\lambda=0].$$

Denote $(\rho_s^*, \rho_t^*) = ((1 - \min(1, \alpha))\delta_0 + \min(1, \alpha)\tilde{\rho}_s^*, (1 - \min(1, \gamma))\delta_0 + \min(1, \gamma)\tilde{\rho}_t^*)$ the densities achieving the supremum in (76). The overlaps are

(77)
$$q_s = \int d\rho_s^*(x) x, \qquad q_t = \int d\rho_t^*(x) x.$$

Note that in the more symmetric special case of M = N and $P_{S,K} = P_{T,K}$ (which does not correspond to the Hermitian dictionary learning problem (42) as S and T remain i.i.d.), by symmetry the replica symmetric formula can be simplified as

$$\frac{1}{MN}I((\boldsymbol{S},\boldsymbol{T});\sqrt{\frac{\lambda}{N}}\boldsymbol{S}\boldsymbol{T}^{\dagger}+\boldsymbol{Z}) \rightarrow -\sup_{\boldsymbol{\rho}\in\mathcal{S}_{\mathrm{diag}}(\lambda)}\left\{\frac{\Gamma[\boldsymbol{\rho}]}{\alpha^{2}}+\frac{J^{(\boldsymbol{\beta})}[\boldsymbol{\rho},\boldsymbol{\rho},2\lambda]}{2\alpha^{2}}\right\}+\frac{\beta\lambda}{2}\lim_{K\to+\infty}\frac{\mathbb{E}\mathrm{Tr}\boldsymbol{S}^{\dagger}\boldsymbol{S}\boldsymbol{T}^{\dagger}\boldsymbol{T}}{N^{3}}+\tau_{\mathrm{diag}}$$

where $S_{\text{diag}}(\lambda)$ is the "diagonal subset" of $S(\lambda)$ where additionally $\rho_s = \rho_t$ (and the definition of τ_{diag} is modified from τ accordingly), and $\Gamma = \Gamma_s = \Gamma_t$. The unique scalar overlap is in this case $q_s = q_t = \int d\rho^*(x) x$ where ρ^* achieves the supremum in the variational problem for the mutual information.

Appendix A. Spherical integrals

In this appendix we present the HCIZ formula in the Hermitian and general non-Hermitian matrix cases used in this work. For the derivations we refer to the very readable original papers by Itzykson and Zuber [70], and Mehta [57].

A.1. Hermitian case. Consider Hermitian $M \times M$ matrices A, B. These are diagonalized by unitary matrices and have real eigenvalues. Recall the notation $A = U^A \lambda^A (U^A)^{\dagger}$, $B = U^B \lambda^B (U^B)^{\dagger}$. Recall the definition of the Vandermonde (5). The HCIZ formula reads

$$\int_{\mathcal{U}(M)} d\mu_M^{(2)}(\boldsymbol{U}) \exp \gamma M \operatorname{Tr}[\boldsymbol{A} \boldsymbol{U}^{\dagger} \boldsymbol{B} \boldsymbol{U}] = \frac{\prod_{k \le M-1} k!}{(\gamma M)^{M(M-1)/2}} \frac{\operatorname{det}[\exp \gamma M \lambda_i^A \lambda_j^B]}{\Delta_M(\boldsymbol{\lambda}^A) \Delta_M(\boldsymbol{\lambda}^B)},$$

where $\mu_M^{(2)}$ is the normalized Haar measure over the group of unitary $M \times M$ matrices and $[\exp \gamma M \lambda_i^A \lambda_j^B]$ is the matrix $(\exp(\gamma M \lambda_i^A \lambda_j^B))_{i,j \leq M}$. Note that on the left hand side we can replace A, B by λ^A, λ^B since U_A, U_B leave the Haar measure invariant. Note also that by permutation symmetry the ratio of determinants is positive and independent of the ordering of eigenvalues. In the limit $M \to +\infty$ the spherical integral can be described in terms of an hydrodynamical system (the complex Burgers equation) thanks to the work of Matytsin [80] and proven in [79]. See also [89,119]. This is not used in this paper but may be useful for future analyses.

A.2. General non-Hermitian case. Let A, B be two general $M \times M$ matrices. Their singular value decomposition is $A = U^A \sigma^A V^A$ and $B = U^B \sigma^B V^B$ where σ^A , σ^B are the diagonal matrices of non-negative singular values and U^A , V^A , U^B and V^B are unitary matrices. The spherical integral involves the modified Bessel function of first kind:

$$I_0(x) \coloneqq \int_0^\pi \frac{d\theta}{\pi} \exp(x\cos\theta).$$

This function is positive, monotone increasing, $I_0(0) = 1$, and grows as exp x at infinity. We have

$$\int_{\mathcal{U}(M)\times\mathcal{U}(M)} d\mu_M^{(2)}(\boldsymbol{U}) \, d\mu_M^{(2)}(\boldsymbol{V}) \exp\gamma M \Re \operatorname{Tr}[\boldsymbol{A}\boldsymbol{U}\boldsymbol{B}\boldsymbol{V}]$$
$$= \frac{2^{M(M-1)} (\prod_{k \le M-1} k!)^2}{M! (M\gamma)^{M(M-1)}} \frac{\det[I_0(M\gamma \sigma_i^A \sigma_j^B)]}{\Delta_M((\boldsymbol{\sigma}^A)^2) \Delta_M((\boldsymbol{\sigma}^B)^2)}.$$

As before, on the left hand side we can replace A, B by σ^A , σ^B , and the ratio of determinants is positive and invariant under permutations of singular values. This formula first obtained in [96] and proven in [97] can be derived by the same methods used for the classical HCIZ formula based

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on the solution of the heat equation. Like for the standard spherical integral, there also exists an asymptotic $M \to +\infty$ representation of the rectangular spherical integral in terms of a complex hydrodynamical system [98, 99].

Appendix B. Minimum mean-square error: a more explicit formula

By the I-MMSE relation (11), we obtained in Conjecture 2 that the MMSE is directly proportional to the derivative with respect to the signal-to-noise ratio λ of the HCIZ integral. Its dependence in λ is through the data-matrix eigenvalues λ^{Y} . From the HCIZ formula (see Appendix A) we get in the complex case $\beta = 2$, using the Jacobi formula

$$\frac{\partial}{\partial X_{ij}} \ln \det \boldsymbol{X} = (\boldsymbol{X}^{-1})_{ji},$$

that the HCIZ derivative verifies

$$N^{2} \frac{d}{d\lambda} I_{N}^{(2)}(\boldsymbol{\lambda}^{S}, \boldsymbol{\lambda}^{Y}, \sqrt{\lambda}) = \frac{N^{2}}{2\sqrt{\lambda}} \frac{d}{d\sqrt{\lambda}} I_{N}^{(2)}(\boldsymbol{\lambda}, \sqrt{\lambda}\boldsymbol{\lambda}^{Y}, 1)$$

$$= \frac{1}{2\sqrt{\lambda}} \frac{d}{d\sqrt{\lambda}} \ln \det[\exp N\lambda_{c}^{S}(\sqrt{\lambda}\lambda_{d}^{Y})] - \frac{1}{2\sqrt{\lambda}} \frac{d}{d\sqrt{\lambda}} \ln \det[(\sqrt{\lambda}\lambda_{c}^{Y})^{d-1}]$$

$$= \frac{1}{2\sqrt{\lambda}} \sum_{i,j \leq N} \frac{d \ln \det[\exp N\lambda_{c}^{S}(\sqrt{\lambda}\lambda_{d}^{Y})]}{d \exp N\lambda_{i}^{S}(\sqrt{\lambda}\lambda_{j}^{Y})} \frac{d \exp N\lambda_{i}^{S}(\sqrt{\lambda}\lambda_{j}^{Y})}{d\sqrt{\lambda}}$$

$$- \frac{1}{2\sqrt{\lambda}} \sum_{i,j \leq N} \frac{d \ln \det[(\sqrt{\lambda}\lambda_{c}^{Y})^{d-1}]}{d(\sqrt{\lambda}\lambda_{i}^{Y})^{j-1}} \frac{d(\sqrt{\lambda}\lambda_{i}^{Y})^{j-1}}{d\sqrt{\lambda}}$$

$$= \frac{1}{2\sqrt{\lambda}} \sum_{i,j \leq N} ([\exp N\lambda_{c}^{S}(\sqrt{\lambda}\lambda_{d}^{Y})]^{-1})_{ji} N\lambda_{i}^{S}(\exp N\lambda_{i}^{S}(\sqrt{\lambda}\lambda_{j}^{Y})) \frac{d\sqrt{\lambda}\lambda_{j}^{Y}}{d\sqrt{\lambda}}$$

$$- \frac{1}{2\sqrt{\lambda}} \sum_{i,j \leq N} ([(\sqrt{\lambda}\lambda_{c}^{Y})^{d-1}]^{-1})_{ji} (j-1)(\sqrt{\lambda}\lambda_{i}^{Y})^{j-2} \frac{d\sqrt{\lambda}\lambda_{i}^{Y}}{d\sqrt{\lambda}}.$$

Introducing the Y-eigenvectors $Y \psi_i^Y = \lambda_i^Y \psi_i^Y$, the Hellmann-Feynman theorem implies

$$\frac{d\lambda_i^Y}{d\sqrt{\lambda}} = (\boldsymbol{\psi}_i^Y)^{\dagger} \boldsymbol{S} \boldsymbol{\psi}_i^Y.$$

Thus

$$\frac{d\sqrt{\lambda}\lambda_i^Y}{d\sqrt{\lambda}} = (\boldsymbol{\psi}_i^Y)^{\dagger}(\sqrt{\lambda}\boldsymbol{S} + \boldsymbol{\xi})\boldsymbol{\psi}_i^Y + \sqrt{\lambda}(\boldsymbol{\psi}_i^Y)^{\dagger}\boldsymbol{S}\boldsymbol{\psi}_i^Y = (\boldsymbol{\psi}_i^Y)^{\dagger}(2\sqrt{\lambda}\boldsymbol{S} + \boldsymbol{\xi})\boldsymbol{\psi}_i^Y$$

Putting everything together in (15) we find that the MMSE equals (when $\beta = 2$)

$$\frac{1}{N^{2}}\mathbb{E}\|\boldsymbol{S}-\mathbb{E}[\boldsymbol{S}\mid\boldsymbol{Y}]\|^{2} = \frac{4}{N}\mathbb{E}\mathrm{Tr}\boldsymbol{\lambda}_{S}^{2}
- \frac{2}{\sqrt{\lambda}N^{2}}\sum_{i,j\leq N}([\exp N\lambda_{c}^{S}(\sqrt{\lambda}\lambda_{d}^{Y})]^{-1})_{ji}N\lambda_{i}^{S}(\exp N\lambda_{i}^{S}(\sqrt{\lambda}\lambda_{j}^{Y}))(\boldsymbol{\psi}_{j}^{Y})^{\dagger}(2\sqrt{\lambda}\boldsymbol{S}+\boldsymbol{\xi})\boldsymbol{\psi}_{j}^{Y}
+ \frac{2}{\sqrt{\lambda}N^{2}}\sum_{i,j\leq N}([(\sqrt{\lambda}\lambda_{c}^{Y})^{d-1}]^{-1})_{ji}(j-1)(\sqrt{\lambda}\lambda_{i}^{Y})^{j-2}(\boldsymbol{\psi}_{i}^{Y})^{\dagger}(2\sqrt{\lambda}\boldsymbol{S}+\boldsymbol{\xi})\boldsymbol{\psi}_{i}^{Y}+o_{N}(1).$$

Besides the matrix inversions this formula also requires to compute eigenvectors of $\mathbf{Y} = \sqrt{\lambda \mathbf{S}} + \boldsymbol{\xi}$; it may be more practical to use $(\boldsymbol{\psi}_i^Y)^{\dagger} (2\sqrt{\lambda}\mathbf{S} + \boldsymbol{\xi})\boldsymbol{\psi}_i^Y = \lambda_i^Y + \sqrt{\lambda}(\boldsymbol{\psi}_i^Y)^{\dagger}\mathbf{S}\boldsymbol{\psi}_i^Y$.

If one were to start instead from Conjecture 1 the computation would be similar, because at the stationary point, the total λ -derivative is computed by taking a partial derivative only with respect to the explicit λ dependence. Indeed, the terms coming from the implicit dependence in the solution λ^s of the fixed point equations do not contribute.

Appendix C. Free entropy functional in terms of moments and existence of $\Gamma[\rho_Q]$

C.1. Free entropy functional in terms of moments. We briefly explain how the integrand in (8), namely

$$\frac{1}{N^2} \ln p_{S,N}(\boldsymbol{\lambda}^s) - \frac{\beta \lambda}{4N} \operatorname{Tr} \boldsymbol{\lambda}_s^2 + I_N^{(\beta)}(\boldsymbol{\lambda}^s, \boldsymbol{\lambda}^Y, \sqrt{\lambda}),$$

can be expressed entirely in terms of moments $\theta_p := \lim_{N \to +\infty} N^{-1} \operatorname{Tr} \lambda_s^p$ for $p \in \mathbb{N}$, in the special case where the prior has the form (6). This means that the collection of moments can be considered as the order parameters.

For $I^{(2)}[\rho_s, \rho_Y, \sqrt{\lambda}]$ we have the expansion (26) in powers of $\sqrt{\lambda}$ for $\beta = 2$. For $\beta = 1$ we can use this expansion in conjunction with "Zuber's $\frac{1}{2}$ -rule" [90]. The term $\ln p_{S,N}(\lambda^s)$ contains the potential $V(\lambda^s)$ and the contribution of the Coulomb energy $\frac{1}{2}\sum_{i\neq j} \ln |\lambda_i^s - \lambda_j^s|$. For the Coulomb energy we can use the "multipole expansion" of the potential $-\ln |x - y|$. For $x', y' \in [-1, 1]$ we have,

$$-\log|x'-y'| = \ln 2 + \sum_{n\geq 1} \frac{2}{n} T_n(x') T_n(y')$$

where $T_n, n \ge 0$, are orthogonal Chebyshev polynomials of the first kind satisfying

$$\int_{-1}^{1} dx \frac{1}{\sqrt{1-x^2}} T_n(x) T_m(x) = \delta_{nm}.$$

The first few polynomials are

_

$$T_0(x) = 1$$
, $T_1(x) = x$, $T_2(x) = 2x^2 - 1$, $T_3(x) = 4x^3 - 3x$, $T_4(x) = 8x^4 - 8x^2 + 1$.

Since we expect (for small λ) that the density of eigenvalues is supported on an interval [a, b] we use the change of variables x' = (x - m)/d, y' = 2(y - m)/d where m := (a + b)/2, d := (b - a)/2, so that now for $x, y \in [a, b]$ we have the expansion

(78)
$$-\log|x-y| = -\ln\frac{d}{2} + \sum_{n=1}^{+\infty}\frac{2}{n}T_n\left(\frac{x-m}{d}\right)T_n\left(\frac{y-m}{d}\right).$$

Assuming now that for N large enough the eigenvalues are essentially contained in a deterministic interval [a, b] we have⁴

$$-\frac{1}{2N^2}\sum_{i\neq j}^{1,N}\log|\lambda_i^s - \lambda_j^s| \propto -\frac{1}{2}\ln\frac{d}{2} + \frac{1}{N^2}\sum_{i\neq j}^{1,N}\sum_{n\geq 1}\frac{1}{n}\sum_{i\leq N}T_n\left(\frac{\lambda_i^s - m}{d}\right)\sum_{j\leq N}T_n\left(\frac{\lambda_j^s - m}{d}\right) + o_N(1).$$

This is clearly a function of the moments (θ_p) which can be worked out from the expression of the Chebyshev polynomials. Potentials of polynomial form, such as $V(\lambda^s) = \lambda_s^2$, are clearly a function

⁴To properly establish this relation one should regularize the Coulomb potential by introducing a cutoff at the origin in order to remove a subdominant in N correction term from coincident points i = j on the right hand. This is a standard discussion that we omit here, see Section 4.2 of [5].

of moments. In the case of a Wishart potential proportional to $V(\lambda^s) = 2(1 - \varphi^{-1}) \ln \lambda^s + 2\varphi^{-1} \lambda^s$ we can again use the "multipole expansion"

$$-\ln x = -\ln \frac{d}{2} + \sum_{n=1}^{+\infty} \frac{2}{n} T_n \Big(\frac{x-m}{d} \Big) T_n \Big(-\frac{m}{d} \Big).$$

An alternative strategy to see that the integral (8) can be re-expressed in terms of a spectral density as order parameter is the classical approach of introducing a Dirac delta function and integrate over an appropriate space of normalized functions:

$$\int d\boldsymbol{\lambda}^{s} \exp N^{2} \left(\frac{1}{N^{2}} \ln p_{S,N}(\boldsymbol{\lambda}^{s}) - \frac{\beta \lambda}{4N} \operatorname{Tr} \boldsymbol{\lambda}_{s}^{2} + I_{N}^{(\beta)}(\boldsymbol{\lambda}^{s}, \boldsymbol{\lambda}^{Y}, \sqrt{\lambda}) \right)$$

=
$$\int D[\rho] \exp N^{2} \left(\int d\rho(x) \, d\rho(y) \ln |x - y| - \frac{\beta}{4} \int d\rho(x) \left(V(x) + \lambda x^{2} \right) + I_{N}^{(\beta)}(\rho, \hat{\rho}_{Y}, \sqrt{\lambda}) \right)$$

$$\times \int d\boldsymbol{\lambda}^{s} \delta(\rho - \hat{\rho}_{s,N}).$$

Here the spherical integral $I_N^{(\beta)}(\rho, \hat{\rho}_Y, \sqrt{\lambda})$ has to be interpreted as definition (9) for any pair of eigenvalues populations λ^s and λ^Y with empirical densities given by ρ and $\hat{\rho}_Y$, respectively. Now, the entropic contribution $S[\rho] \coloneqq \ln \int d\lambda^s \delta(\rho - \hat{\rho}_{s,N})$ can be evaluated by introducing a Fourier representation of the Dirac delta:

$$\exp S[\rho] = \int d\boldsymbol{\lambda}^s \int D[g] \exp\left(i \int dx \, g(x) \left(N\rho(x) - \sum_{i \le N} \delta(\lambda_i^s - x)\right)\right) \propto \exp NH[\rho],$$

where $H[\rho] \coloneqq -\int d\rho(x) \ln \rho(x)$ is the Shannon entropy of density ρ (see Section 4.2 in Chapter 4, equations (4.14)–(4.18) in [5], or Appendix C of [120]). Therefore, at leading order $\exp(O(N^2))$ in the integrand, this entropic contribution is negligible and thus integral (8) ends up being expressed only as a functional integral over a density.

C.2. A formal remark concerning the existence of $\Gamma[\rho_Q]$. Let us discuss how to identify Γ in the replica symmetric Conjecture 4 (and by extension in the other conjectures too) in cases where the prior is not necessarily of the form (6); in the case where it is of the form (6) it follows by the discussion of the previous section. We start from the replicated partition function (49) that we recall here:

(79)
$$\mathbb{E}\mathcal{Z}^{u} \propto \int dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) \prod_{a < b}^{0,u} d\boldsymbol{z}^{ab} \exp\beta N \Re \operatorname{Tr}\left[\sqrt{\lambda}(\boldsymbol{z}^{ab})^{\dagger} \boldsymbol{Q}^{ab} - \frac{1}{2}(\boldsymbol{z}^{ab})^{\dagger} \boldsymbol{z}^{ab}\right].$$

As seen from the steps leading to (51), by rotational invariance of z^{ab} , the expectation of the above exponential function with respect to the Haar distributed singular vectors (U^{ab}, V^{ab}) of z^{ab} is independent of the singular vectors of the overlaps $(Q^{ab})_{a < b}$: the identity (51) reads, when we do not change variables for the SVD decomposition of the overlaps,

$$\mathbb{E}\mathcal{Z}^{u} \propto \int dP_{X,N}(\{\boldsymbol{x}\}_{0}^{u}) \prod_{a < b}^{0,u} d\boldsymbol{\sigma}_{s}^{ab} \exp\left(\ln|\Delta_{M}((\boldsymbol{\sigma}_{z}^{ab})^{2})|^{\beta} + (\beta - 1) \operatorname{Tr}\boldsymbol{\sigma}_{z}^{ab}\right)$$
$$- \frac{\beta N}{2} \operatorname{Tr}(\boldsymbol{\sigma}_{z}^{ab})^{2} + M^{2} J_{M}^{(\beta)} \left(\boldsymbol{z}^{ab}, \boldsymbol{Q}^{ab}, \frac{2\sqrt{\lambda}N}{M}\right).$$

This independence in the singular vectors is what suggests that the empirical spectral distributions

(80)
$$\hat{\rho}_Q^{ab}(\sigma) \coloneqq \frac{1}{M} \sum_{k \le M} \delta(\sigma_k^{Q,ab} - \sigma) \quad \text{and} \quad \hat{\rho}_z^{ab}(\sigma) \coloneqq \frac{1}{M} \sum_{k \le M} \delta(\sigma_k^{z,ab} - \sigma)$$

or their asymptotic limits are the correct order parameters instead of the whole populations σ_Q^{ab} and σ_z^{ab} (the rectangular spherical integral depends only on these distributions by permutation symmetry): the *density* of singular values must be sufficient to describe the system, no need of the whole j.p.d.f. of singular values. Keep in mind that the density $\hat{\rho}_Q^{ab}(\sigma)$ is a function of the replicas through the definition of the overlaps $Q^{ab} := N^{-1}(\boldsymbol{x}^a)^{\mathsf{T}} \bar{\boldsymbol{x}}^b$.

In order to replace the integrals over the singular values $(\sigma_Q^{ab}, \sigma_z^{ab})_{a < b}$ by integrals over densities we need to introduce entropic contributions by using Delta function similarly as in the previous section. Formally we can write that

$$\mathbb{E}\mathcal{Z}^{u} \propto \int \Big(\prod_{a < b}^{0, u} D[\rho_{z}^{ab}] D[\rho_{Q}^{ab}]\Big) \exp M^{2} \Big(S_{z}[(\rho_{z}^{ab})] + S_{Q}[(\rho_{Q}^{ab})] + \sum_{a < b}^{0, u} J_{M}^{(\beta)} \Big(\rho_{z}^{ab}, \rho_{Q}^{ab}, \frac{2\sqrt{\lambda}N}{M}\Big) - \frac{\beta N}{2M} \sum_{a < b}^{0, u} \int d\rho_{z}^{ab}(x) x^{2} + \frac{\beta}{2} \sum_{a < b}^{0, u} \int d\rho_{z}^{ab}(x) d\rho_{z}^{ab}(y) \ln|x^{2} - y^{2}| + o_{N}(1)\Big),$$
(81)

where the integrations $D[\rho_z^{ab}]$, $D[\rho_Q^{ab}]$ are over all normalized empirical densities with finite support over M singular values (which will tend to continuous non-negative normalized smooth functions in the large size limit), and the entropies

$$S_Q[(\rho_Q^{ab})] \coloneqq \frac{1}{M^2} \ln \int \prod_{a=0}^u dP_{X,N}(\boldsymbol{x}^a) \prod_{a
$$S_z[(\rho_z^{ab})] \coloneqq \frac{1}{M^2} \sum_{a$$$$

In (81) the spherical integral $J_M^{(\beta)}(\rho_z^{ab}, \rho_Q^{ab}, \gamma)$ has to be understood as definition (40) evaluated for any populations of singular values $\boldsymbol{\sigma}_s^{ab}, \boldsymbol{\sigma}_Q^{ab} \in \mathbb{R}^N_{\geq 0}$ whose empirical densities are given by ρ_z^{ab}, ρ_Q^{ab} , respectively. Standard computations discussed in the previous section imply

$$\ln \int d\boldsymbol{\sigma}_z^{ab} \,\delta(\rho_z^{ab} - \hat{\rho}_z^{ab}) \propto MH[\rho_z^{ab}]$$

where $H[\rho_z^{ab}]$ is the Shannon entropy of density ρ_z^{ab} . As we restrict the integral over densities with finite, N-independent support, then $S_z[(\rho_z^{ab})] = O(1/N)$.

The spectral replica symmetric ansatz is then equivalent to assume that

$$S_Q[(\rho_Q^{ab})] \to \frac{u(u+1)}{2} \Gamma_M[\rho_Q] \coloneqq \frac{u(u+1)}{2} \frac{1}{M^2} \ln \int dP_{X,N}(\boldsymbol{x}^0) \, dP_{X,N}(\boldsymbol{x}^1) \, \delta(\rho_Q - \hat{\rho}_Q),$$

where $\hat{\rho}_Q$ is the empirical density of the matrix $N^{-1}(\boldsymbol{x}^0)^{\mathsf{T}} \bar{\boldsymbol{x}}^1$. Thanks to this decoupling assumption we can carry on the computation similarly as before as the integrals are factorized over the pairs of replica indices. It yields in the limit the formula (64), in which we formally have identified the functional Γ as the limit of the entropy contribution Γ_M from above.

APPENDIX D. MATHEMATICA CODES

D.1. Small signal-to-noise expansion. The two first functions provided below allowing to convert moments to free cumulants and vice-versa are taken from [121].

This function gives the free cumulants as function of generic moments (M_i) of a density.

$$\ln[1] := m[z_] := 1 + M1 z + M2 z^2 + M3 z^3 + M4 z^4 + M5 z^5 + M6 z^6 + M7 z^7 + M8 z^8;$$

Simplify[Table[{k,
$$(-(k - 1)^{(-1)/k!})*D[m[z]^{(1 - k)}, \{z, k\}] / . {z -> 0}}, {k, 2, 8}]]$$

The next function gives the moment generating function expressed with the free cumulants and thus allows us to read the expression of the moments in terms of free cumulants. We force the values of the first two free cumulants to $k_1 = 0$ and $k_2 = 1$ (but this is not necessary).

```
Collect[m[z], z]
```

We now express the asymptotic moments $m_i = \theta_i := \lim_{N \to +\infty} N^{-1} \operatorname{Tr} \mathbf{S}^i$ of the signal \mathbf{S} as a function of the free cumulants (k_i) of its asymptotic spectral density thanks to the previous function. We focus on trace-less signals $m_1 = 0 = k_1$ and with normalized variance $m_2 = 1 = k_2$; the first condition does not change anything from the information-theoretic point of view as explained in Remark 1 below Conjecture 2, and the second condition simply amounts to a rescaling of λ if not a-priori verified.

```
ln[3]:= m3 = k3;

m4 = k4 + 2;

m5 = 5 k3 + k5;

m6 = 3 k3^2 + 6 k4 + k6 + 5;

m7 = 7 k3 k4 + 21 k3 + 7 k5 + k7;

m8 = 28 k3^2 + 8 k3 k5 + 4 k4^2 + 28 k4 + 8 k6 + k8 + 14;
```

We express the free cumulants (c_i) of the data \mathbf{Y} as a function of the free cumulants (k_i) of the signal \mathbf{S} . The (c_i) are the $(\bar{\phi}_i)$ in the Zinn-Justin and Zuber expansion [92] (see also [122] for the same expansion in terms of trace-moments, also found in [92]). The Wigner matrix $\boldsymbol{\xi}$ only shifts the second free cumulant of $\sqrt{\lambda}\mathbf{S}$ (which is λ) by 1. Below, variable snr refers to λ .

```
In[4]:= c2 = snr + 1;
c3 = k3 snr^(3/2);
c4 = k4 snr^2;
c5 = k5 snr^(5/2);
c6 = k6 snr^3;
c7 = k7 snr^(7/2);
c8 = k8 snr^4;
```

The terms (F_n) in the Zinn-Justin and Zuber expansion of the spherical integral [92], expressed with the free cumulants (c_i) of the data matrix, and the moments (m_i) of the signal S; the (m_i) are the (θ_i) in the expansion of [92].

$$In[5]:= F2 = c2/2;$$

$$F3 = c3 m3/3;$$

$$F4 = c4 m4/4 - 1/2 (c2^2/2 + c4);$$

$$F5 = c5 m5/5 - m3 (c2 c3 + c5);$$

$$F6 = -1/2 m3^2 (c2^3/3 + c2 c4 + c3^2 + c6)$$

$$+ 1/6 (2 c2^3 + 12 c2 c4 + 5 c3^2 + 7 c6)$$

$$- m4 (c2 c4 + c3^2/2 + c6) + (c6 m6)/6;$$

$$F7 = -m3 m4 (c2^2 c3 + c2 c5 + 2 c3 c4 + c7)$$

$$+ m3 (5 c2^2 c3 + 7 c2 c5 + 8 c3 c4 + 4 c7)$$

$$- m5 (c2 c5 + c3 c4 + c7) + c7 m7/7;$$

$$F8 = -m3 m5 (c2^2 c4 + c2 c3^2 + c2 c6 + 2 c3 c5$$

$$+ c4^2 + c8) + m3^2 (2 c2^4 + 16 c2^2 c4$$

$$+ 20 c2 c3^2 + 16 c2 c6 + 24 c3 c5 + 11 c4^2 + 9 c8)$$

$$- 1/2 m4^2 (c2^4/4 + c2^2 c4 + 2 c2 c3^2)$$

$$+ c2 c6 + 2 c3 c5 + 11 c4^2 + 9 c8)$$

$$+ 1/2 m4 (c2^4 + 11 c2^2 c4 + 14 c2 c3^2)$$

$$+ 16 c2 c6 + 18 c3 c5 + 11 c4^2 + 9 c8)$$

$$- 3/8 (3 c2^4 + 24 c2^2 c4 + 24 c2 c3^2)$$

$$+ 24 c2 c6 + 24 c3 c5 + 15 c4^2 + 10 c8)$$

$$- m6 (c2 c6 + c3 c5 + c4^2/2 + c8) + c8 m8/8;$$

The expansion of the mutual information is, according to our Conjecture 2, given up to $O(\lambda^4)$ by

 $\ln[6] = MI8 = snr - F2 snr - F3 snr^{(3/2)} - F4 snr^{2} - F5 snr^{(5/2)} - F6 snr^{3} - F7 snr^{(7/2)} - F8 snr S^{4};$

```
MutualInfo = Collect[Simplify[MI8], snr];
```

Only the first four order are reliable. This code gives the generic expansions (35) and (36) in the case $m_1 = 0$ and $m_2 = 1$ (but this can be easily adapted using the code).

D.2. Useful code to produce Figures 1 and 2. This parts evaluates the spectral density of the data matrix Y by solving the transcendental equation (24) for its Green function. The spectral density is then extracted from its imaginary part.

```
In[7]:= snr = 1; step = 0.0005; zAndrho = {}; init = I/5; bound = 4;
Do[zAndrho = Append[zAndrho, {z, Abs[Im[g /.
FindRoot[SetAccuracy[z == Sqrt[3 snr] Coth[g Sqrt[3 snr]] + g, 30],
{g, init}, WorkingPrecision -> 20]]]/Pi}], {z, -bound, bound, step}];
```

As there may be multiple solutions depending on the initial point init for the search (that may need to be tuned), a sanity check is to check that the solution found is properly normalized:

```
In[8]:= Print["Normalization = ", Total[zAndrho[[All, 2]]] step];
```

Now we find an interpolating function for the spectral density of Y from the previously equally spaced computed points, using Hermite polynomials. Plotting this interpolating function is what gives the asymptotic red curves in Figure 1:

```
ln[9] = z = zAndrho[[All, 1]]; rho = Chop[zAndrho[[All, 2]]];
```

We can now (approximately) compute the asymptotic mutual information using formula (23), based on the interpolation function, and compare the results to the Wigner case:

```
Print["|Uniform - Wigner mutual info.| = ", Abs[MI - 0.5 Log[1 + snr]]];
```

Using these pieces of code and running them for various λ , one can obtain the pink dots in Figure 2. The finite size curves (blue and orange dots) are instead simply obtained by averaging the associated formulas over many large realizations of the model.

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