Some exact results for the statistical physics problem of high-dimensional linear regression

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Abstract

High-dimensional linear regression have become recently a subject of many investigations which use statistical physics. The main bulk of this work relies on powerful approximation techniques but also a more rigorous approaches are becoming a more prominent. Considering Bayesian setting, we derive a number of exact results for the inference and related statistical physics problems of the linear regression.

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The statistical physics connection between the information theory and statistical inference has been established a while ago by Jaynes [1] and more recently in the studies of information processing [2] and machine learning [3] systems. Here the parameters of statistical model are the degrees of freedom and the data sample is the quenched disorder [4]. The free energy in this framework, akin to cumulant generating function in statistics, encodes statistical properties of inference but its direct computation, which involves high-dimensional integrals, is often difficult and non-rigorous methods such as mean-field approximation, replica trick and cavity method were developed in statistical physics [4].

The advent of modern high-dimensional data, where its dimension is growing with the sample size, poses a significant challenges to statistical inference. The latter is largely well understood in the low-dimensional regime of constant dimension and growing sample size but for high-dimensional data inference methods of even simplest linear regression [5] have to be revised [6]. The problem of linear regression (LR) in high-dimensional regime have attracted a significant attention of researchers in the mathematics [7–9] and statistical physics communities [10–12]. Furthermore, the message passing, which can be seen as algorithmic implementation of the cavity method [13], emerged as a very efficient inference and analysis framework for this model [14–16].

For high-dimensional regime most of rigorous results available for LR either assume uncorrelated data [8, 11, 14, 16] or uncorrelated data and sparsity in parameters [7, 9]. Also parameters of noise in the data are assumed to be known unlike the statistical setting where they are usually inferred [5]. Recently, correlations in sampling were modelled in [15] but inferring parameters of noise is still not considered in the latter. In this article, we report a number of exact results for high-dimensional regime of the Bayesian LR and the related statistical physics problem which complement the aforementioned studies of LR.

Let us assume that we observe a data sample of ‘input-output’ pairs \( \{(z_1, t_1), \ldots, (z_N, t_N)\} \), where \((z_i, t_i) \in \mathbb{R}^{d+1}\), generated randomly and independently from the distribution

\[
P(t, z | \theta) = P(t | z, \theta) P(z)
\]

with some unknown to us parameters \( \theta \). If we assume the distribution \( P(\theta) \), then the distribution of \( \theta \) given the data follows from the Bayes formula

\[
P(\theta | \mathcal{D}) = \frac{P(\theta) \prod_{i=1}^{N} P(t_i | z_i, \theta)}{\int P(\tilde{\theta}) \left\{ \prod_{i=1}^{N} P(t_i | z_i, \tilde{\theta}) \right\} d\theta}.
\]
where $\mathcal{D} = \{ \mathbf{t}, \mathbf{Z} \}$ with $\mathbf{t} = (t_1, \ldots, t_N)$ and $\mathbf{Z} = (z_1, \ldots, z_N)$ is the $N \times d$ matrix. The above is the posterior distribution of $\boldsymbol{\theta}$ given the prior distribution $P(\boldsymbol{\theta})$ and observed data $\mathcal{D}$.

The simplest way to use (2) for inference is to compute the maximum a posteriori (MAP) estimator

$$\hat{\boldsymbol{\theta}}[\mathcal{D}] = \arg\min_{\boldsymbol{\theta}} E(\boldsymbol{\theta}|\mathcal{D}),$$

(3)

where the Bayesian likelihood function

$$E(\boldsymbol{\theta}|\mathcal{D}) = -\sum_{i=1}^{N} \log P(t_i|z_i, \boldsymbol{\theta}) - \log P(\boldsymbol{\theta})$$

(4)

has the likelihood, used in maximum likelihood (ML) inference, for the first term and the second term in above can be seen as a regulariser for the latter. Thus Bayesian inference framework can be seen as a generalisation of ML one.

To quantify the quality of inference in (3) the square error $\frac{1}{d} ||\boldsymbol{\theta}_0 - \hat{\boldsymbol{\theta}}[\mathcal{D}]||^2$, where $||\cdots||$ is Euclidean norm and $\boldsymbol{\theta}_0$ are true parameters of the data $\mathcal{D}$, is usually used. The first moment of the latter is the mean square error (MSE) $\frac{1}{d} \langle\langle||\boldsymbol{\theta}_0 - \hat{\boldsymbol{\theta}}[\mathcal{D}]||^2\rangle\rangle_{\boldsymbol{\theta}_0}$. Furthermore, the posterior mean

$$\hat{\boldsymbol{\theta}}[\mathcal{D}] = \int P(\boldsymbol{\theta}|\mathcal{D}) \, d\boldsymbol{\theta}$$

(5)

is a minimiser of MSE for any estimator function of $\boldsymbol{\theta}$, so it is the minimum MSE (MMSE) estimator.

Both of discussed above types of Bayesian inference can be unified in one statistical physics (SP) framework via the Gibbs-Boltzmann distribution

$$P_\beta(\boldsymbol{\theta}|\mathcal{D}) = \frac{e^{-\beta E(\boldsymbol{\theta}|\mathcal{D})}}{Z_\beta[\mathcal{D}]},$$

(6)

where

$$Z_\beta[\mathcal{D}] = \int e^{-\beta E(\boldsymbol{\theta}|\mathcal{D})} \, d\boldsymbol{\theta}$$

(7)

is the normalisation constant or partition function (for $\beta = 1$ this is the evidence term of Bayesian statistics). The Bayesian likelihood function (4) plays the role of ‘energy’ in (6) and $\beta = T^{-1}$ is the (fictional) inverse temperature. The latter can be interpreted as a noise parameter in the stochastic gradient descent minimising $E(\boldsymbol{\theta}|\mathcal{D})$. 3
The estimators (3) and (5) are recovered from the average \( \int P_\beta (\theta | D) \theta d \theta \) by, respectively, taking the zero ‘temperature’ limit \( \beta \to \infty \) and setting \( \beta = 1 \). This follows by observing that for \( \beta = 1 \) the distribution (6) and the posterior (2) are exactly the same and
\[
\hat{\theta}[D] = \lim_{\beta \to \infty} \int P_\beta (\theta | D) \theta d \theta
\]
by the Laplace argument [17]. We note that interpretation of the MAP estimator (3) in the SP framework (6) is that \( \hat{\theta}[D] \) is the ground state of the latter, i.e. the state \( \theta \) which minimises the energy \( E(\theta | D) \).

Properties of the system described by (6) are usually studied by considering the ‘free energy’
\[
F_\beta [D] = -\frac{1}{\beta} \log Z_\beta [D]
\]
which is from a statistical point of view is a ‘moment generating function’. The derivatives of \( F_\beta [D] \) with respect to \( \beta \) generate averages of the energy \( E(\theta | D) \) and if we replace the energy with \( E(\theta | D) + h.\theta \) in (9) we can use the latter to compute moments of (6).

The Kullback-Leibler (KL) ‘distance’ [18] (or relative entropy)
\[
D(\hat{P}[D] || P_\theta) = \int dt \, dz \, \hat{P}(t, z | D) \log \frac{\hat{P}(t, z | D)}{P(t, z | \theta)}
\]
between the distribution \( P(t, z | \theta) \) and its empirical version \( \hat{P}(t, z | D) \) can be also used to obtain the ML estimator by the optimisation \( \hat{\theta}[D] = \arg\min_\theta D(\hat{P}||P_\theta) \). Furthermore, we note that

\[
ND(\hat{P}[D] || P_\theta) = E(\theta | D) + \log P(\theta) - NS(\hat{P}[D])
\]
and hence MAP estimator can be obtained by the optimisation
\[
\hat{\theta}[D] = \arg\min_\theta \left\{ ND(\hat{P}||P_\theta) - \log P(\theta) \right\}.
\]

Finally, the KL distance [11] can be used to define the difference \( \Delta D(\theta, \theta_0 | D) = D(\hat{P}[D] || P_{\theta_0}) - D(\hat{P}[D] || P_\theta) \), where \( \theta_0 \) are true parameters, which gives rise to the ‘measures’ of over-fitting \( \min_\theta \Delta D(\theta, \theta_0 | D) \) in ML inference [19] which was recently extended to MAP inference in generalised linear models [12]. Both of these studies used SP framework, equivalent to (9), to study typical properties of inference in the high-dimensional regime of \( N \to \infty, d \to \infty \) and \( d/N \) finite via the average free energy \( \langle F_\beta [D] \rangle_D / N \). The latter was computed by non-rigorous replica method [4] which uses the identity \( \langle \log Z_\beta [D] \rangle_D = \lim_{n \to 0} \frac{1}{n} \log \langle Z_\beta^n [D] \rangle_D \).
In Bayesian linear regression (LR) with Gaussian prior, i.e. the ridge regression of statistics, it is assumed that data is sampled from the distribution $\mathcal{N}(t|\theta, \sigma^2)P(z)$ and the energy function is given by

$$E(\theta, \sigma^2|\mathcal{D}) = \frac{1}{2\sigma^2} \|t - Z\theta\|^2 + \frac{1}{2} \|\theta\|^2 + \frac{1}{2} N \log(2\pi\sigma^2) - \log P(\sigma^2),$$

(12)

where $t = Z\theta_0 + \epsilon$. The noise vector $\epsilon$ is sampled from some distribution, e.g. the multivariate Gaussian $\mathcal{N}(0, \sigma^2 I_N)$, with the mean 0 and covariance $\sigma^2 I_N$. Here $\theta_0$, $\sigma^2_0$ are the true parameters of $\mathcal{D}$ and $\eta \geq 0$ is the hyper-parameter. The distribution $P(\sigma^2)$ is the prior for the noise parameter $\sigma^2$. \[20\]

The energy function can be also represented as

$$2\sigma^2 E(\theta, \sigma^2|\mathcal{D}) = \left( \theta - J^{-1}_\sigma Z^T t \right)^T J_{\sigma^2} \left( \theta - J^{-1}_\sigma Z^T t \right) + t^T \left( I_N - Z J^{-1}_\sigma Z^T \right) t + \sigma^2 \left( N \log(2\pi\sigma^2) - 2 \log P(\sigma^2) \right),$$

(13)

where in above we have defined the sample covariance matrix $J = Z^T Z$ with its element $[J]_{k\ell} = \sum_{i=1}^N z_i(k)z_i(\ell)$ and introduced its ‘reguralised’ version $J_\eta = J + \eta I_d$. From above follows that the distribution (14) is given by

$$P_\beta(\theta, \sigma^2|\mathcal{D}) = \frac{P_\beta(\theta|\sigma^2, \mathcal{D})e^{-\beta F_{\beta, \sigma^2}[\mathcal{D}] + \frac{1}{2} N \log(2\pi\sigma^2) - \log P(\sigma^2)}}{\int_0^\infty \! \! d\tilde{\sigma}^2 e^{-\beta F_{\beta, \tilde{\sigma}^2}[\mathcal{D}] + \frac{1}{2} N \log \tilde{\sigma}^2 - \log P(\tilde{\sigma}^2)}},$$

(14)

where in above $P_\beta(\theta|\sigma^2, \mathcal{D})$ is the Gaussian distribution

$$P_\beta(\theta|\sigma^2, \mathcal{D}) = \mathcal{N} \left( \theta \middle| J^{-1}_\sigma Z^T t, \sigma^2 \beta^{-1} J^{-1}_\sigma \right),$$

(15)

with the mean $J^{-1}_\sigma Z^T t$ and covariance $\sigma^2 \beta^{-1} J^{-1}_\sigma$. Also we have defined the conditional free energy

$$F_{\beta, \sigma^2}[\mathcal{D}] = \frac{d}{2\beta} + \frac{1}{2\sigma^2} t^T \left( I_N - Z J^{-1}_\sigma Z^T \right) t - \frac{1}{2\beta} \log |2\pi \sigma^2 \beta^{-1} J^{-1}_\sigma|,$$
but the free energy, associated with (14), is given by

\[
F_\beta[\mathcal{D}] = -\frac{1}{\beta} \log \int d\sigma^2 e^{-\beta E(\theta, \sigma^2|\mathcal{D})}
\]

\[
= -\frac{1}{\beta} \log \int_0^\infty d\sigma^2 e^{-\beta N \left[ F_{\beta, \sigma^2}[^{\mathcal{D}}] + \frac{1}{2} \log(2\pi\sigma^2) - \frac{1}{N} \log P(\sigma^2) \right]}.
\] (17)

We note that if the noise parameter \( \sigma^2 \) is known, i.e. \( \sigma^2 = \sigma_0^2 \), then \( F_\beta[\mathcal{D}] = F_{\beta, \sigma^2}[\mathcal{D}] \) and \( P_\beta(\theta, \sigma^2|\mathcal{D}) = P_\beta(\theta|\sigma^2, \mathcal{D}) \). For \( \beta \to \infty \) the free energy is given by

\[
F_\infty[\mathcal{D}] = \min_{\theta, \sigma^2} E(\theta, \sigma^2|\mathcal{D}).
\] (18)

by the Laplace method, i.e. \( F_\infty[\mathcal{D}] \) is the ground state energy of (14). Furthermore, the ground state \( \{ \hat{\theta}[\mathcal{D}], \hat{\sigma}^2[\mathcal{D}] \} = \arg\min_{\theta, \sigma^2} E(\theta, \sigma^2|\mathcal{D}) \), given by

\[
\hat{\theta}[\mathcal{D}] = J^{-1} \sigma^2_0 Z^T t,
\] (19)

i.e. the mean of the distribution (15), and the solution of the equation

\[
\sigma^2 = \frac{1}{N} \left[ t - Z \hat{\theta}[\mathcal{D}] \right]^2 + \frac{2\sigma^4}{N} \frac{\partial}{\partial \sigma^2} \log P(\sigma^2),
\] (20)

is the MAP estimator of parameters \( \{ \theta, \sigma^2 \} \). Also, by the second second line in (17), we have that

\[
F_\infty[\mathcal{D}] = \min_{\sigma^2} \left[ F_{\infty, \sigma^2}[\mathcal{D}] + \frac{N \log(2\pi\sigma^2)}{2} - \log P(\sigma^2) \right].
\] (21)

Furthermore, as \( N \to \infty \) from (17) follows the free energy density \( f_\beta[\mathcal{D}] = \frac{1}{N} F_\beta[\mathcal{D}] \):

\[
f_\beta[\mathcal{D}] = \min_{\sigma^2} \left[ \frac{F_{\beta, \sigma^2}[\mathcal{D}]}{N} + \frac{\log(2\pi\sigma^2)}{2} - \frac{\log P(\sigma^2)}{N} \right]
\] (22)

by the Laplace argument.

For \( \beta = 1 \) the distribution (14) can be used to compute the MMSE estimators of \( \theta \) and \( \sigma^2 \) given by the averages

\[
\int_0^\infty P_\beta(\theta, \sigma^2|\mathcal{D}) \theta d\theta d\sigma^2 = \langle J_{\sigma^2_0}^{-1} Z^T t \rangle_{\sigma^2}
\] (23)

\[
\int_0^\infty P_\beta(\theta, \sigma^2|\mathcal{D}) \sigma^2 d\theta d\sigma^2 = \langle \sigma^2 \rangle_{\sigma^2},
\]

where in above the \( \langle \cdots \rangle_{\sigma^2} \) average is generated by the marginal

\[
P_\beta(\sigma^2|\mathcal{D}) = \frac{e^{-\beta N \left[ F_{\beta, \sigma^2}[\mathcal{D}] + \frac{1}{2} \log(2\pi\sigma^2) - \frac{1}{N} \log P(\sigma^2) \right]}}{\int_0^\infty d\tilde{\sigma}^2 e^{-\beta N \left[ F_{\beta, \tilde{\sigma}^2}[\mathcal{D}] + \frac{1}{2} \log(2\pi\tilde{\sigma}^2) - \frac{1}{N} \log P(\tilde{\sigma}^2) \right]}}.
\] (24)

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of the distribution (14). For \( N \to \infty \) above is dominated by (22) and the Bayesian estimator of \( \theta \) in (23) is given by (19), where \( \sigma^2 \) is the solution of the equation

\[
\sigma^2 = \frac{\beta}{(\beta - \zeta)} \frac{1}{N} \left| t - Z \tilde{\theta} \right|^2 - \frac{\sigma^4 \eta}{(\beta - \zeta)} \frac{1}{N} \text{Tr} \left[ J^{-1}_{\sigma^2}\eta \right] \\
+ \frac{2\sigma^4 \beta}{(\beta - \zeta)N} \frac{\partial}{\partial \sigma^2} \log P(\sigma^2),
\]

which recovers the MAP estimators (19) and (20) when \( \beta \to \infty \).

The conditional (16) and full (17) free energies satisfy standard Helmholtz free energy relations. In particular for the latter, if we define

\[
E(\theta|D) = E(\theta, \sigma^2|D) - \frac{1}{2} N \log(2\pi \sigma^2) + \log P(\sigma^2),
\]

we have

\[
F_{\beta,\sigma^2}[D] = E_{\beta}[D] - TS_{\beta}[D],
\]

where \( T = 1/\beta \), with the average energy

\[
E_{\beta}[D] = \int P_{\beta}(\theta|\sigma^2, D) E(\theta|D) \, d\theta
\]

and differential entropy

\[
S_{\beta}[D] = - \int P_{\beta}(\theta|\sigma^2, D) \log P_{\beta}(\theta|\sigma^2, D) \, d\theta.
\]

In the free energy (16) we have

\[
E_{\beta}[D] = \frac{d}{2\beta} \frac{1}{2\sigma^2} t^T \left( I_N - Z J^{-1}_{\sigma^2}\eta Z^T \right) t
\]

and

\[
S_{\beta}[D] = \frac{1}{2} \log |2\pi e \sigma^2 \beta^{-1} J^{-1}_{\sigma^2}\eta|.
\]

Furthermore, from above follows that the average energy

\[
E_{\beta}[D] = \frac{d}{2\beta} + \min_{\theta} E(\theta|D).
\]

We consider Bayesian linear regression in the high-dimensional regime: \( (N, d) \to (\infty, \infty) \) and \( \zeta = d/N \in (0, \infty) \) or from now just \( (N, d) \to \infty \) to simplify notation. For the latter we derive the following results, with details of derivations provided in the Appendix, for the inference and related statistical physics problems.
**Distribution of \( \hat{\theta} \) estimator in MAP inference**—Assuming that the noise parameter \( \sigma^2 \) is independent from the data \( \mathcal{D} \), e.g. \( \sigma^2 \) is known or expected to be self-averaging in \( (N, d) \to \infty \) regime, and the distribution of noise \( \epsilon \) is the Gaussian \( \mathcal{N}(0, \sigma^2_0 I_N) \), the distribution

\[
P(\hat{\theta}) = \left\langle \delta \left( \hat{\theta} - J^{-1}_{\sigma^2_\eta} Z^T t \right) \right\rangle_{\mathcal{D}}
\]

is distribution of MAP estimator \( \hat{\theta} \). We note that for \( \eta = 0 \), i.e. ML inference, and without averaging over \( Z \) recovers the Theorem 7.6b in [5]. To consider the \( (N, d) \to \infty \) regime, we assume that \( z_i(\mu) = z_i(\mu)/\sqrt{d} \) then \( J = J/\zeta \), where \( [J]_{kt} = \frac{1}{N} \sum_{i=1}^{N} z_i(k) z_i(\ell) \) is (sample) covariance, and \( J^{-1}_{\sigma^2_\eta} = \zeta J^{-1}_{\sigma^2_\eta} \) giving us

\[
P(\hat{\theta}) = \left\langle \mathcal{N}\left( \hat{\theta} \mid J^{-1}_{\sigma^2_\eta} [J] \theta_0, \zeta \sigma^2_0 J^{-2}_{\sigma^2_\eta} [J] J \right) \right\rangle_{Z}
\]

(33)

Furthermore, for a Gaussian sample with the true covariance \( \Sigma \), i.e. each \( z_i \) in \( Z \) is from the distribution \( \mathcal{N}(0, \Sigma) \), the distribution of \( \hat{\theta} \) for finite \( (N, d) \) is the Gaussian mixture

\[
P(\hat{\theta}) = \int dJ \mathcal{W}(J|\Sigma/N, d, N)
\]

\[
\times \mathcal{N}\left( \hat{\theta} \mid J^{-1}_{\zeta \sigma^2_\eta} [J] \theta_0, \zeta \sigma^2_0 J^{-2}_{\zeta \sigma^2_\eta} [J] J \right),
\]

(34)

where in above \( \mathcal{W}(J|\Sigma/N, d, N) \) is the Wishart distribution non-singular when \( d \leq N \). We note that above is also the distribution of ‘ground states’ of [15].

**Distribution of \( \hat{\theta} \) estimator in ML inference**—For \( \eta = 0 \) the distribution is the multivariate Student’s t distribution

\[
P(\hat{\theta}) = \frac{\Gamma \left( \frac{N+1}{2} \right)}{\Gamma \left( \frac{N}{2} \right)} \left| \frac{(1 - \zeta + 1/N) \Sigma}{\pi N + 1 - d} \right|^{rac{1}{2}}
\]

\[
\times \left[ 1 + \frac{1}{N + 1 - d} \frac{1}{\zeta \sigma^2_0} \left( \hat{\theta} - \theta_0 \right)^T \left( \hat{\theta} - \theta_0 \right) \right]^{-\frac{N+1}{2}}
\]

(35)

with \( N + 1 - d \) degrees of freedom. Here the vector of true parameters \( \theta_0 \) is the mode and \( \frac{\zeta \sigma^2_0 \Sigma^{-1}}{1 - \zeta - 1/N} \) is the covariance of the above. The latter, in the \( (N, d) \to \infty \) regime, recovers parameters of the multivariate Gaussian suggested by replica method [12]. We note that any finite subset of components of \( \hat{\theta} \) variables is governed by the Gaussian in this regime [22] [23].

**Statistical properties of \( \hat{\sigma}^2 \) estimator in ML and MAP inference**—For \( \eta = 0 \) the estimator simplifies considerably

\[
\hat{\sigma}^2[\mathcal{D}] = (Z^T Z)^{-1} Z^T t
\]

(36)
giving us, via (20), the noise estimator

$$\hat{\sigma}^2 = \frac{1}{N} \left\| t - Z\hat{\theta} \right\|^2 = \frac{1}{N} \epsilon^T \left( I_N - Z (Z^T Z)^{-1} Z^T \right) \epsilon.$$  \hspace{1cm} (37)

For the noise $\epsilon$ coming from a distribution with mean $0$ and covariance $\sigma_0^2 I_N$ the mean is

$$\langle \hat{\sigma}^2 \rangle_{\epsilon} = \sigma_0^2 (1 - \zeta)$$  \hspace{1cm} (38)

and the variance is

$$\left\langle (\hat{\sigma}^2)^2 \right\rangle_{\epsilon} - \langle \hat{\sigma}^2 \rangle_{\epsilon}^2 = \frac{2\sigma_0^4}{N} (1 - \zeta),$$  \hspace{1cm} (39)

i.e. the noise estimator (37) is independent from $Z$ and self-averaging in the $(N, d) \to \infty$ regime.

Furthermore, for finite $(N, d)$ the probability of event $\hat{\sigma}^2 \notin (\sigma_0^2(1 - \zeta) - \delta, \sigma_0^2(1 - \zeta) + \delta)$, where $\delta > 0$, is given by

$$\text{Prob} \left[ \hat{\sigma}^2 \notin (\sigma_0^2(1 - \zeta) - \delta, \sigma_0^2(1 - \zeta) + \delta) \right] = \text{Prob} \left[ N\hat{\sigma}^2 \leq N (\sigma_0^2(1 - \zeta) - \delta) \right] + \text{Prob} \left[ N\hat{\sigma}^2 \geq N (\sigma_0^2(1 - \zeta) + \delta) \right] \leq \left\langle e^{-\frac{1}{2}a||t - Z\hat{\theta}||^2} \right\rangle_{\epsilon} e^{\frac{1}{2}aN(\sigma_0^2(1 - \zeta) - \delta)} + \left\langle e^{\frac{1}{2}a||t - Z\hat{\theta}||^2} \right\rangle_{\epsilon} e^{-\frac{1}{2}aN(\sigma_0^2(1 - \zeta) + \delta)}. \hspace{1cm} (40)$$

Assuming that the noise $\epsilon$ is Gaussian $\mathcal{N}(0, \sigma_0^2 I_N)$ the moment-generating function (MGF)

$$\left\langle e^{\frac{1}{2a}||t - Z\hat{\theta}||^2} \right\rangle_{\epsilon} = e^{-\frac{1}{2a}(1 - \zeta)\log(1 - a\sigma_0^2)}$$  \hspace{1cm} (41)

is independent from $Z$ allowing us to estimate the fluctuations of $\hat{\sigma}^2$ via the inequality

$$\text{Prob} \left[ \hat{\sigma}^2 \notin (\sigma_0^2(1 - \zeta) - \delta, \sigma_0^2(1 - \zeta) + \delta) \right] \leq e^{-\frac{1}{2}N \left[ (1 - \zeta) \log \left( \frac{(1 - \zeta) - \delta}{\sigma_0^2} \right) \right] - \delta/\sigma_0^2} + e^{-\frac{1}{2}N \left[ (1 - \zeta) \log \left( \frac{(1 - \zeta) + \delta}{\sigma_0^2} \right) \right] + \delta/\sigma_0^2} \hspace{1cm} (42)$$

for $\delta \in (0, \sigma_0^2(1 - \zeta))$. We note that an argument similar to the one that leads to (42) could be also constructed for a more general scenario of sub-gaussian noise by employing techniques used in [24].
For $\alpha = 2i\alpha$ the MGF (41) is the characteristic function (CF)

$$\left\langle e^{i\alpha ||t - Z\hat{\theta}[G]||^2} \right\rangle_G = \left(1 - i\alpha 2\sigma_0^2\right)^{-1/2 N(1-\zeta)}$$

of the random variable $||t - Z\hat{\theta}[G]||^2$. We note that above is CF of gamma distribution (see Theorem 7.6b in [5]) with the mean $N\sigma_0^2 (1 - \zeta)$ and variance $N2\sigma_0^4 (1 - \zeta)$. The mean and variance of $\hat{\sigma}^2$ is, respectively, $\sigma_0^2 (1 - \zeta)$ and $2\sigma_0^4 (1 - \zeta)/N$. Finally, because of (38), (39) and (25) the finite temperature ML estimator of noise is given by

$$\hat{\sigma}^2 = \frac{\beta}{\beta - \zeta} \sigma_0^2 (1 - \zeta)$$

in high-dimensional regime. We note that above can be also derived from the average free energy computed by replica method [12]. Finally, we note that self-averageness of the MAP (20) and Bayesian, which is a solution of (25) with $\beta = 1$, estimators in the high-dimensional $(N,d) \to \infty$ regime is conditional on self-averageness of eigenvalue spectrum of the covariance matrix $Z^T Z$ (see Appendix G).

**Statistical properties of MSE in ML inference**—Using the distribution (35) and $\lambda_i(\Sigma) \leq \lambda_2(\Sigma) \leq \cdots \leq \lambda_d(\Sigma)$ for the eigenvalues of true covariance matrix $\Sigma$, the CF of the MSE $\frac{1}{d}||\theta - \hat{\theta}[G]||^2$, for a finite $(N,d)$, is given by

$$\left\langle e^{i\alpha ||\theta_0 - \hat{\theta}[G]||^2} \right\rangle_G = \int_0^{\infty} \Gamma_{N+1-d}(\omega) d\omega \times \prod_{\ell=1}^d \left(1 - \frac{i\alpha 2\zeta \sigma_0^2}{\omega(1 - \zeta + 1/N)\lambda_\ell(\Sigma)}\right)^{-1/2},$$

where for $\nu > 0$

$$\Gamma_{\nu}(\omega) = \frac{\nu^{\nu/2}}{2^{\nu/2} \Gamma(\nu/2)} \omega^{\nu-2} e^{-\frac{1}{2} \nu \omega}$$

is the gamma distribution. We note that the last term in above is the product of CFs of gamma distributions with the same ‘shape’ parameter 1/2 but different ‘scale’ parameters $\frac{2\zeta \sigma_0^2}{\omega(1 - \zeta + 1/N)\lambda_\ell(\Sigma)}$.

The CF (45) can be used to obtain the mean

$$\frac{1}{d} \left\langle ||\theta_0 - \hat{\theta}[G]||^2 \right\rangle_G = \frac{\zeta \sigma_0^2}{1 - \zeta - 1/N} \frac{\text{Tr}[\Sigma^{-1}]}{d}$$

and variance

$$\text{Var}\left(\frac{1}{d} ||\theta_0 - \hat{\theta}[G]||^2\right) = \frac{2\zeta^2 \sigma_0^4}{(1 - \zeta)^2} \frac{\text{Tr}[\Sigma^{-2}]}{d^2}.$$
\[ \text{The latter gives us the condition for the self-averaging } \text{Var} \left( \frac{1}{d} \| \bar{\theta}_0 - \hat{\theta}[\mathcal{G}] \|^2 \right) \to 0 \text{ as } (N, d) \to \infty. \]

Finally, we consider deviations of \( \frac{1}{d} \| \bar{\theta}_0 - \hat{\theta}[\mathcal{G}] \|^2 \) from the mean \( \mu(\Sigma) = \frac{\xi \sigma^2}{1 - \xi - 1/N} \text{ Tr}[\Sigma^{-1}] \).

The probability of event \( \frac{1}{d} \| \bar{\theta}_0 - \hat{\theta}[\mathcal{G}] \|^2 \notin (\mu(\Sigma) - \delta, \mu(\Sigma) + \delta) \) for \( \delta > 0 \), some sufficiently small \( \alpha > 0 \) and some positive constants \( C_{\pm} \) is bounded from above as follows

\[
\text{Prob} \left[ \frac{1}{d} \| \bar{\theta}_0 - \hat{\theta}[\mathcal{G}] \|^2 \notin (\mu(\Sigma) - \delta, \mu(\Sigma) + \delta) \right] = \text{Prob} \left[ \| \bar{\theta}_0 - \hat{\theta}[\mathcal{G}] \|^2 \leq d(\mu(\Sigma) - \delta) \right] \\
+ \text{Prob} \left[ \| \bar{\theta}_0 - \hat{\theta}[\mathcal{G}] \|^2 \geq d(\mu(\Sigma) + \delta) \right] \\
\leq C_{-}e^{-N\Phi_{-}[\alpha, \mu(\lambda_d), \delta]} + C_{+}e^{-N\Phi_{+}[\alpha, \mu(\lambda_1), \delta]}, \quad (49)
\]

In above for the rate function \( \Phi_{-}[\alpha, \mu(\lambda_d), \delta] \) to be positive for arbitrary small \( \delta \) it is sufficient that \( \mu(\lambda_d) \geq 1 \), where \( \mu(\lambda) = \frac{\xi \sigma^2}{1 - \xi \lambda} \), but for \( \mu(\lambda_d) < 1 \) for this to happen the \( \delta \) must be such that \( \delta > 1 - \mu(\lambda_d) \). The rate function \( \Phi_{+}[\alpha, \mu(\lambda_1), \delta] \) is positive for any \( \delta \in (0, \mu(\lambda_1)) \).

**Statistical properties of free energy**—We consider the free energy \( (16) \) for the finite inverse temperature \( \beta \) and finite \( (N, d) \). Assuming that the noise \( \epsilon \) has mean \( 0 \) and covariance \( \sigma^2 \mathbf{I}_N \), and the noise parameter \( \sigma^2 \) is independent from \( \mathcal{G} \), the average free energy is given by

\[
\langle F_{\beta, \sigma^2} [\mathcal{G}] \rangle_{\mathcal{G}} = \frac{d}{2\beta} + \frac{1}{2\sigma^2} \theta_0^T \left( \mathbf{J} - \mathbf{J} \left[ \mathbf{J} \sigma^2 \eta \right] \right) \theta_0 \\
+ \frac{\sigma^2}{2\sigma^2} \left( N - \mathbf{J} \left[ \mathbf{J} \sigma^2 \eta \right] \right) \\
- \frac{1}{2\beta} \left( \log |2\pi \epsilon \sigma^2 \beta^{-1} \mathbf{J}^{-1} \sigma^2 | \right), \quad (50)
\]

for any distribution of \( \mathbf{Z} \). Also under the same assumption the variance of \( F_{\beta, \sigma^2} [\mathcal{G}] \) can be obtained by exploiting the Helmholtz free energy representation \( F_{\beta, \sigma^2} [\mathcal{G}] = E_\beta[\mathcal{G}] - T S_\beta[\mathcal{G}] \), giving us the variance

\[
\text{Var} \left( F_{\beta, \sigma^2} [\mathcal{G}] \right) = \text{Var} \left( E_\beta[\mathcal{G}] \right) + T^2 \text{Var} \left( S_\beta[\mathcal{G}] \right) \\
- 2T \text{Cov} \left( E_\beta[\mathcal{G}], S_\beta[\mathcal{G}] \right), \quad (51)
\]

where details of each term in above are provided in the Appendix.

**Free energy of ML inference**—For \( \eta = 0 \) and \( \mathbf{Z} = \mathbf{Z}/\sqrt{d} \) the density of the average free
energy (50) is given by
\[ \left\langle \frac{F_{\beta,\sigma^2} [\mathcal{D}]}{N} \right\rangle = \frac{1}{2} \sigma_0^2 + \frac{\zeta}{2\beta} \log \left( \frac{\beta}{2\pi \sigma_0^2} \right) + \frac{\zeta}{2\beta} \int \rho_d(\lambda) \log(\lambda) \, d\lambda \tag{52} \]
where in above we defined the average \( \rho_d(\lambda) = \langle \rho_d(\lambda|Z) \rangle_Z \) of the eigenvalue density
\[ \rho_d(\lambda|Z) = \frac{1}{d} \sum_{\ell=1}^d \delta(\lambda - \lambda_{\ell} (Z^T Z/N)). \tag{53} \]
Furthermore, the variance of free energy is given by
\[ \text{Var} \left( \frac{F_{\beta,\sigma^2} [\mathcal{D}]}{N} \right) = \text{Var} \left( \frac{E[\mathcal{D}]}{N} \right) + T^2 \text{Var} \left( \frac{S(P[Z])}{N} \right) \]
\[ = \frac{\sigma_0^4}{2\sigma^4 N} (1 - \zeta) + \frac{\zeta^2}{4\beta^2} \int \int C_d(\lambda, \tilde{\lambda}) \times \log(\lambda) \log(\tilde{\lambda}) \, d\lambda \, d\tilde{\lambda}, \tag{54} \]
where in above we have defined the correlation function
\[ C_d(\lambda, \tilde{\lambda}) = \langle \rho_d(\lambda|Z) \rho_d(\tilde{\lambda}|Z) \rangle_Z \]
\[ - \langle \rho_d(\lambda|Z) \rangle_Z \langle \rho_d(\tilde{\lambda}|Z) \rangle_Z. \tag{55} \]
We note that if \( \int \int C_d(\lambda, \tilde{\lambda}) f(\lambda, \tilde{\lambda}) \, d\lambda \, d\tilde{\lambda} \to 0 \), for any smooth function \( f(\lambda, \tilde{\lambda}) \), as \( (N, d) \to \infty \), then the free energy \( F_{\beta} [\mathcal{D}] / N \) is self-averaging.

Finally, using (52) in the free energy (22) for \( \eta = 0 \) and Gaussian data with the true covariance \( \Sigma = I_d \) gives us
\[ \lim_{N \to \infty} f_{\beta} [\mathcal{D}] = \frac{\beta - \zeta}{2\beta} \log \left( \frac{2\pi \sigma_0^2 (1 - \zeta)}{\beta - \zeta} \right) + \frac{\log(\beta) + 1}{2} \]
\[ - \frac{1}{2\beta} \left( \zeta \log(\zeta) + (1 - \zeta) \log(1 - \zeta) + 2\zeta \right) \tag{56} \]
for \( \beta \in [\zeta, \infty) \), with the convention \( 0 \log 0 = 0 \), and
\[ \lim_{N \to \infty} f_{\beta} [\mathcal{D}] = -\infty \tag{57} \]
for \( \beta \in (0, \zeta) \). Since the eigenvalue spectrum \( \rho_d(\lambda|Z) \to \frac{1}{2\pi \zeta \sqrt{\lambda}} \sqrt{(\lambda - a_-)(a_+ - \lambda)} \) for \( \lambda \in [a_-, a_+] \), where \( a_\pm = (1 \pm \sqrt{\zeta})^2 \), in probability [25] as \( (N, d) \to \infty \) with \( 0 < \zeta < 1 \), the free energy density is self-averaging. Furthermore, the average density (56) is exactly equal to
FIG. 1. Free energy of ML inference as a function of temperature $1/\beta$ plotted for $\zeta \in \{1/10, 1/5, \ldots, 9/10\}$ (from right to left) in the high-dimensional regime of $N \to \infty$ and $\zeta = d/N$. For $\beta \to \infty$ we approach $\frac{1}{2} \log (2\pi e \sigma_0^2 (1 - \zeta))$. For $\beta \to 0$ we approach $\frac{1}{2N} (\zeta \log (1 - \zeta) - \log (1 - \zeta) - \zeta)$ and for $\beta \in (0, \zeta)$ the free energy is $-\infty$. The true noise parameter is $\sigma_0^2 = 1$ and the true covariance of data is $I_d$.

replica symmetric free energy [12]. We note that (56) is $-\infty$ for $\beta < \zeta$, so the system has zero-order phase transition [26].

**Free energy of MAP inference**—Let us assume that the true parameters $\theta_0$ are random, with the mean 0 and covariance $S^2 I_d$, and $Z = Z/\sqrt{d}$, so that $J = J/\zeta$ and $J^{-1} = \zeta J^{-1}$, where $J = Z^T Z/N$, then the average of (50) over the $\theta_0$ is given by

$$
\left\langle \frac{F_{\beta, \sigma^2} [\theta]}{N} \right\rangle_{\theta_0} = \frac{\zeta}{2\beta} + \frac{S^2 \zeta \eta}{2} \int \frac{\rho_d(\lambda) \lambda d\lambda}{\lambda + \zeta \sigma^2 \eta} + \frac{\sigma_0^2}{2\sigma^2} \left( 1 - \zeta \int \frac{\rho_d(\lambda) \lambda d\lambda}{\lambda + \zeta \sigma^2 \eta} \right)
- \frac{\zeta}{2\beta} \log \left( 2\pi e \sigma^2 \beta^{-1} \zeta \right)
+ \frac{\zeta}{2\beta} \int \rho_d(\lambda) \log (\lambda + \zeta \sigma^2 \eta) d\lambda.
$$

(58)
Furthermore, using (51), we obtain, under the same assumptions, the variance

\[
\text{Var}\left(\frac{F_{\beta,\sigma^2}[\mathcal{D}]}{N}\right) = \frac{1}{2} \int \int \left\{ \frac{\zeta^2 (S^4 \sigma^4 \eta^2 + \sigma_0^2 - 2\sigma_0^2 S^2 \sigma^2 \eta)}{2\sigma^4} \times \frac{\lambda \hat{\lambda}}{(\lambda + \zeta \sigma^2 \eta) (\hat{\lambda} + \zeta \sigma^2 \eta)} + \frac{T^2 \zeta^2 \log (\lambda + \zeta \sigma^2 \eta) \log (\hat{\lambda} + \zeta \sigma^2 \eta)}{2} \right. \\
- \frac{T \zeta}{\sigma^2} \left[ S^2 \frac{\lambda \zeta \sigma^2 \eta}{\lambda + \zeta \sigma^2 \eta} + \sigma_0^2 \left(1 - \frac{\lambda \zeta}{\lambda + \zeta \sigma^2 \eta}\right) \right] \\
\times \log (\hat{\lambda} + \zeta \sigma^2 \eta) \right\} C_d(\lambda, \hat{\lambda}) \, d\lambda \, d\hat{\lambda} + O\left(\frac{1}{N}\right)
\]

(59)

From above follows that for \(\eta > 0\) the free energy is self-averaging if the noise estimator \(\hat{\sigma}^2\) and eigenvalue spectrum \(\rho_d(\lambda|Z)\) are self-averaging. The latter is true for the Gaussian data with covariance \(\Sigma = I_d\).

Summary—We mapped the Bayesian model (2) of the linear regression \(t = Z\theta + \sigma^2 \epsilon\), where the pair \(t \in \mathbb{R}^N, Z \in \mathbb{R}^{N \times d}\) is observed and the parameters \(\theta \in \mathbb{R}^d, \sigma^2 \rightarrow \mathbb{R}^+\) are not observed, onto the Gibbs-Boltzmann distribution (14), with inverse ‘temperature’ \(\beta\), of statistical physics which allows us to investigate properties of different statistical inferences. We assumed the Gaussian prior \(\mathcal{N}(0, \eta^{-1} I_d)\) for \(\theta\) and some prior \(P(\sigma^2)\) for the noise parameter \(\sigma^2\). Also we assumed that the rows in \(Z\) are sampled independently and the noise vector \(\epsilon \in \mathbb{R}^N\) has mean \(0\) and covariance \(I_N\). In the high-dimensional regime of \((N, d) \rightarrow \infty\) with \(\zeta = \frac{d}{N} \in (0, \infty)\), we derive the following results for the inference and related statistical physics problems.

Assuming that \(\sigma^2\) is known and that the distributions of \(Z\) and \(\epsilon\) are Gaussian the distribution of the MAP estimator of \(\theta\), \(\hat{\theta}\), is the Gaussian mixture (34) for the finite pair \((N, d)\). The latter is also the distribution of ground states. We used (34) to show that the distribution of ML estimator \(\hat{\theta}\) is the Student’s t-distribution (35). However, any (finite) marginal of the latter is a Gaussian when \((N, d) \rightarrow \infty\). Also, independently from the distributions of \(Z\) and \(\epsilon\), the ML estimator of the noise parameter \(\hat{\sigma}^2\), \(\hat{\sigma}^2\), is self-averaging. Furthermore, we estimated deviations of \(\hat{\sigma}^2\) from its mean for Gaussian \(\epsilon\), given by the bound in (42), for finite \((N, d)\). This result is independent from \(Z\). We used the distribution of ML estimator (35) to derive characteristic function of the MSE \(\frac{1}{N}||\theta_0 - \hat{\theta}[\mathcal{D}]||^2\), where \(\theta_0\)
are the true parameters, for finite \((N,d)\). The latter was used to derive the condition (18) for self-averageness of MSE when \((N,d) \to \infty\) and to estimate deviations from its mean, given by the bound (19), for finite \((N,d)\).

Assuming that \(\sigma^2\) is known we derived the average (52) and variance (54) of the conditional free energy (16) of ML inference with finite temperature \(T = 1/\beta\) for finite \((N,d)\). This result is independent from the distribution of the data \(Z\) and noise \(\epsilon\). In the finite \(T\) ML inference the noise estimator \(\hat{\sigma}^2\), given by (25) with \(\eta > 0\), is self-averaging when \((N,d) \to \infty\) and the latter is also true for the free energy density (22) if the spectrum of the covariance matrix \(Z^T Z / N\) is also self-averaging. The ML estimator \(\hat{\sigma}^2\) diverges at \(\beta = \zeta\) and the free energy (22) is discontinuous at this value of \(\beta\). With an additional assumption that the true parameters \(\theta_0\) are random with mean \(0\) and covariance \(S^2 I_d\), we derived the average (58) and variance (59) of the conditional free energy (16) of MAP inference with finite \(T\) for finite \((N,d)\). This result is independent from the distribution of the data \(Z\) and noise \(\epsilon\). The free energy (22) is self-averaging if \(\hat{\sigma}^2\) and the spectrum of \(Z^T Z / N\) is self-averaging as \((N,d) \to \infty\). The spectrum is known to be self-averaging if the true covariance of a Gaussian data is \(\Sigma = I_d\). In this case, and with Gaussian assumption on noise \(\epsilon\), the free energy (22) recovers recent result obtained by the replica method in [12].

As one can see much can be learned about high-dimensional inference of the Bayesian linear regression by exact calculations, but this work also leaves many open questions. Some of the latter, such as properties of MAP inference (34) for \((N,d) \to \infty\), we envisage to be within our reach but some, such as the mismatch in the model and data, can be quite challenging.

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Appendix A: Ingredients

We write \(I_N\) for \(N \times N\) identity matrix. The data \(\mathcal{D} = \{t, Z\}\), where \(t \in \mathbb{R}^N\) and \(Z = (z_1, \ldots, z_N)\) is the \(N \times d\) matrix, is a set of observed ‘input-output’ pairs.
\[
\{(z_1, t_1), \ldots, (z_N, t_N)\}
\] generated by the process

\[
t = Z\theta_0 + \epsilon,
\]

where the true parameter vector \( \theta_0 \in \mathbb{R}^d \) is unknown and the vector \( \epsilon \in \mathbb{R}^N \) represents noise with mean 0 and covariance \( \sigma_0^2 I_N \) with the true noise parameter \( \sigma_0^2 \) also unknown to us. The (empirical) covariance matrix of the input data is given by

\[
J[Z] = Z^T Z,
\]

where \([J[Z]]_{k\ell} = \sum_{i=1}^N z_i(k)z_i(\ell)\). To simplify notation we will sometimes omit dependence on \( Z \) and use instead \( J \equiv J[Z] \). The maximum a posteriori estimator (MAP) of \( \theta_0 \) in the linear regression with Gaussian prior \( \mathcal{N}(0, \eta^{-1}I_d) \) is given by

\[
\hat{\theta}[D] = J^{-1} \sigma_2^2 \eta Z^T t,
\]

where \( J_\eta = J + \eta I_d \). For \( \eta = 0 \) above gives us the maximum likelihood (ML) estimator

\[
\hat{\theta}[D] = J^{-1} Z^T t
\]

We are interested in the high-dimensional regime: \((N, d) \to (\infty, \infty)\) and \( \zeta = d/N \in (0, \infty) \), or just \((N, d) \to \infty\) to simplify notation.

Appendix B: Distribution of \( \hat{\theta} \) estimator in MAP inference

Let us assume that noise parameter \( \sigma^2 \) is independent from data \( D \) and that the noise \( \epsilon \) is sampled from the Gaussian \( \mathcal{N}(0, \sigma_0^2 I_N) \) then the distribution of MAP estimator \([A3]\) can
be computed as follows

\[
P(\hat{\theta}) = \left\langle \delta \left( \hat{\theta} - J^{-1}_{\sigma^2 \eta} Z^T t \right) \right\rangle_Z
\]

\[
= \left\langle \delta \left( \hat{\theta} - J^{-1}_{\sigma^2 \eta} Z^T (Z\theta_0 + \epsilon) \right) \right\rangle_Z
\]

\[
= \left\langle \left\langle \delta \left( \hat{\theta} - J^{-1}_{\sigma^2 \eta} J\theta_0 - J^{-1}_{\sigma^2 \eta} Z^T \epsilon \right) \right\rangle_{\epsilon} \right\rangle_Z
\]

\[
= \int \frac{dx}{(2\pi)^d} e^{ix^T \hat{\theta}} \left\langle e^{-ix^T J^{-1}_{\sigma^2 \eta} J\theta_0} e^{-ix^T J^{-1}_{\sigma^2 \eta} Z^T \epsilon} \right\rangle_{\epsilon} Z
\]

\[
= \int \frac{dx}{(2\pi)^d} \left\langle \frac{1}{(2\pi)^d} \left| \left( \sigma^2_0 J^{-2}_{\sigma^2 \eta} \right)^{-1} \right| \right\rangle_x Z
\]

\[
\times \int dx N \left( x | 0, \left( \sigma^2_0 J^{-2}_{\sigma^2 \eta} \right)^{-1} \right) e^{ix^T \left( \theta - J^{-1}_{\sigma^2 \eta} \theta_0 \right)} Z
\]

\[
= \left\langle N \left( \hat{\theta} | J^{-1}_{\sigma^2 \eta} J\theta_0, \sigma^2_0 J^{-2}_{\sigma^2 \eta} J \right) \right\rangle_Z
\]

In order to take the \((N, d) \to \infty\) limit, we assume that \(z_i(\mu) = z_i(\mu)/\sqrt{d}\) then the covariance matrix \(J = J/\zeta\), where \(\zeta = d/N\), and \(J^{-1}_{\sigma^2 \eta} = \zeta J^{-1}_{\sigma^2 \eta}\) giving us the distribution

\[
P(\hat{\theta}) = \left\langle N \left( \hat{\theta} | J^{-1}_{\zeta \sigma^2 \eta} J\theta_0, \zeta \sigma^2_0 J^{-2}_{\zeta \sigma^2 \eta} J \right) \right\rangle_Z
\]

Furthermore, since \(J \equiv J[Z]\) and \(J^{-1}_{\zeta \sigma^2 \eta} \equiv J^{-1}_{\zeta \sigma^2 \eta} [J[Z]]\) we have that

\[
P(\hat{\theta}) = \left\langle N \left( \hat{\theta} | J^{-1}_{\zeta \sigma^2 \eta} [J[Z]] J[Z] \theta_0, \zeta \sigma^2_0 J^{-2}_{\zeta \sigma^2 \eta} [J[Z]] J[Z] \right) \right\rangle_Z
\]

\[
= \int dJ \left\{ \prod_{i=1}^N \int P(z_i) dz_i \right\} \delta (J - J[Z]) \times \cdots
\]

\[
\times N \left( \hat{\theta} | J^{-1}_{\zeta \sigma^2 \eta} [J[Z]] J[Z] \theta_0, \zeta \sigma^2_0 J^{-2}_{\zeta \sigma^2 \eta} [J[Z]] J[Z] \right)
\]

\[
= \int dJ \int \frac{dC}{(2\pi)^d} \left\{ \prod_{i=1}^N \int P(z_i) dz_i \right\} \times \cdots
\]

\[
\times \exp \left[ i \text{Tr} \left\{ C(J - J[Z]) \right\} \right] \times \cdots
\]

\[
\times N \left( \hat{\theta} | J^{-1}_{\zeta \sigma^2 \eta} [J] J[Z] \theta_0, \zeta \sigma^2_0 J^{-2}_{\zeta \sigma^2 \eta} [J] J[Z] \right)
\]

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Let us now consider the average

\[
\left\{ \prod_{i=1}^{N} \int P(z_i)dz_i \right\} \exp \left[ -i \text{Tr} \left\{ \hat{C} J [Z] \right\} \right] \quad (B4)
\]

\[
= \left\{ \prod_{i=1}^{N} \int P(z_i)dz_i \right\} \exp \left[ -i \frac{1}{N} \text{Tr} \left\{ \hat{C} \sum_{i=1}^{N} z_i z_i^T \right\} \right]
\]

\[
= \left[ \int P(z)dz e^{-\frac{i}{N} \text{Tr} \left\{ \hat{C} z z^T \right\}} \right]^N
\]

Assuming that \( z \) is sampled from the Gaussian distribution \( \mathcal{N}(0, \Sigma) \) above is given by

\[
\left| I + \frac{2}{N} \Sigma \hat{C} \right|^{-\frac{N}{2}},
\]

which is characteristic function of the Wishart distribution \[27\] with the density

\[
\mathcal{W}(J | \Sigma/N, d, N) = \frac{|\Sigma/N|^{-\frac{N}{2}} |J|^{\frac{N-d-1}{2}}}{2^{\frac{Nd}{2}} \pi^{\frac{d(d-1)}{4}}} \prod_{\ell=1}^{d} \Gamma \left( \frac{N+1-\ell}{2} \right) e^{-\frac{1}{2} \text{Tr}(J \Sigma^{-1}) \left( J \sigma_0^2 \right)^{-1}}.
\]

We note that Wishart distribution is singular when \( d > N \). Thus for Gaussian \( z \) the distribution \[B1\] is the Gaussian mixture

\[
P(\hat{\theta}) = \int dJ \mathcal{W}(J | \Sigma/N, d, N) \mathcal{N}\left( \hat{\theta} | J^{-1} \sigma_0^2 \sigma_0^T \left[ J \right] J \theta_0, \sigma_0^2 \sigma_0^T \left[ J \right] J \theta_0 \right)
\]

\[
= \int dJ \frac{|\Sigma/N|^{-\frac{N}{2}} |J|^{\frac{N-d-1}{2}}}{2^{\frac{Nd}{2}} \pi^{\frac{d(d-1)}{4}}} \prod_{\ell=1}^{d} \Gamma \left( \frac{N+1-\ell}{2} \right) e^{-\frac{1}{2} \text{Tr}(J \Sigma^{-1}) \left( J \sigma_0^2 \sigma_0^T \left[ J \right] J \theta_0 \right)} \times \ldots
\]

\[
\ldots \times e^{-\frac{1}{2\sigma_0^2} \left( \hat{\theta} - J^{-1} \sigma_0^2 \sigma_0^T \left[ J \right] J \theta_0 \right)^T \left( J^{-2} \sigma_0^2 \sigma_0^T \left[ J \right] J \right)^{-1} \left[ J \right] \left( \hat{\theta} - J^{-1} \sigma_0^2 \sigma_0^T \left[ J \right] J \theta_0 \right) \times \left[ 2\pi \sigma_0^2 \sigma_0^T \left[ J \right] J \right]^\frac{1}{2}}.
\]

We note that alternative derivation of above result is provided in \[12\].
Appendix C: Distribution of $\hat{\theta}$ estimator in ML inference

Let us consider the integral

$$
\int dJ \left| J \right|^{N-d-1} e^{-\frac{1}{2} Tr(J\Sigma^{-1})} \times \ldots
$$

$$
\ldots \times e^{-\frac{1}{2\sigma_0^2} \left( \hat{\theta} - J_{\sigma_0^2} \right)^T \left( J_{\sigma_0^2} \hat{\theta} - J \right)^{-1} \left( \hat{\theta} - J_{\sigma_0^2} \right)}
$$

$$
\left| 2\pi \sigma_0^2 J_{\sigma_0^2} \right|^{\frac{1}{2}}
$$

\(= \int dJ \left| J \right|^{N-d-1} \times \ldots \times e^{-\frac{1}{2} Tr\left\{ J \left[ N\Sigma^{-1} + \frac{1}{\sigma_0^2} \left( \hat{\theta} - \theta_0 \right) \left( \hat{\theta} - \theta_0 \right)^T \right] \right\} \left| 2\pi \sigma_0^2 J_{\sigma_0^2} \right|^{\frac{1}{2}}
$$

appearing in the distribution of MAP estimator (B7). For $\eta = 0$, i.e. ML inference, the integral

$$
\int dJ \left| J \right|^{N-d-1} e^{-\frac{1}{2} Tr\left\{ J \left[ N\Sigma^{-1} + \frac{1}{\sigma_0^2} \left( \hat{\theta} - \theta_0 \right) \left( \hat{\theta} - \theta_0 \right)^T \right] \right\} \left| 2\pi \sigma_0^2 J_{\sigma_0^2} \right|^{\frac{1}{2}}
$$

\(= \left( \frac{1}{2\pi \sigma_0^2} \right)^{\frac{N-d}{2}} \int dJ \left| J \right|^{N-d-1} e^{-\frac{1}{2} Tr\left\{ J \left[ N\Sigma^{-1} + \frac{1}{\sigma_0^2} \left( \hat{\theta} - \theta_0 \right) \left( \hat{\theta} - \theta_0 \right)^T \right] \right\}}
$$

can be computed by using the normalisation identity

$$
\int dJ W(J|\Sigma, d, N) = \int dJ \left| J \right|^{N-d-1} e^{-\frac{1}{2} Tr(J\Sigma^{-1})} = 1
$$

\(= \int dJ \left| J \right|^{N-d-1} e^{-\frac{1}{2} Tr(J\Sigma^{-1})} \left| \Sigma \right|^{-\frac{N}{2}} \left| J \right|^{N-d-1} \frac{2\pi^{\frac{d(d-1)}{4}} \prod_{\ell=1}^{d} \Gamma \left( \frac{N+1-\ell}{2} \right)}{N^{\frac{d(d-1)}{2}}} e^{-\frac{1}{2} Tr(J\Sigma^{-1})} = 1,
$$

(C2)

from which follows

$$
\int dJ \left| J \right|^{N-d-1} e^{-\frac{1}{2} Tr(J\Sigma^{-1})}
$$

$$
= \left| \Sigma \right|^{\frac{N}{2}} \frac{2\pi^{\frac{d(d-1)}{4}} \prod_{\ell=1}^{d} \Gamma \left( \frac{N+1-\ell}{2} \right)}{N^{\frac{d(d-1)}{2}}}
$$

(C3)

which applied for $N + 1$

$$
\int dJ \left| J \right|^{N-d-1} e^{-\frac{1}{2} Tr(J\Sigma^{-1})}
$$

$$
= \left| \Sigma \right|^{\frac{N+1}{2}} \frac{2\pi^{\frac{d(d-1)}{4}} \prod_{\ell=1}^{d} \Gamma \left( \frac{N+2-\ell}{2} \right)}{N^{\frac{d(d-1)}{2}}}
$$

(C4)
gives us the result

\[
\int dJ \left| J \right|^{\frac{N-d}{2}} e^{-\frac{1}{2} \text{Tr} \left\{ J \left( N\Sigma^{-1} + \frac{1}{\zeta\sigma_0^2} (\hat{\theta} - \theta_0) (\hat{\theta} - \theta_0)^T \right) \right\}} = \left| N\Sigma^{-1} + \frac{1}{\zeta\sigma_0^2} (\hat{\theta} - \theta_0) (\hat{\theta} - \theta_0)^T \right|^{\frac{N+1}{2}} \times 2^{\frac{(N+1)d}{2}} \pi^{\frac{d(d-1)}{4}} \prod_{\ell=1}^{d} \Gamma \left( \frac{N + 2 - \ell}{2} \right). \quad \text{(C5)}
\]

Let us now consider the distribution \([37]\) for \(\eta = 0\):

\[
P(\hat{\theta}) = \int dJ \mathcal{W}(J|\Sigma/N, d, N) \mathcal{N} \left( \hat{\theta} | \theta_0, \zeta\sigma_0^2 J^{-1} \right)
= \int dJ \left| \Sigma/N \right|^{\frac{N-d}{2}} \left| J \right|^{\frac{N-d-1}{2}} e^{-\frac{1}{2} \text{Tr} \left\{ J N\Sigma^{-1} \right\}} \times \ldots \times e^{-\frac{1}{2} \zeta\sigma_0^2 (\hat{\theta} - \theta_0)^T J (\hat{\theta} - \theta_0)} \left| 2\pi \zeta\sigma_0^2 J^{-1} \right|^{\frac{N}{2}}.
\]

\[
= \frac{\pi^{\frac{d}{2}}}{\Gamma \left( \frac{N+1-d}{2} \right)} \prod_{\ell=1}^{d} \Gamma \left( \frac{N + 2 - \ell}{2} \right) \mathcal{N} \left( \hat{\theta} | \theta_0, \zeta\sigma_0^2 \Sigma/N \right) \left| N\Sigma^{-1} + \frac{1}{\zeta\sigma_0^2} (\hat{\theta} - \theta_0) (\hat{\theta} - \theta_0)^T \right|^{-\frac{N+1}{2}}.
\]

The last line in above was obtained using the ‘matrix determinant lemma’. Thus, after slight rearrangement of the above, we obtain

\[
P(\hat{\theta}) = (\pi (N + 1 - d))^{-\frac{d}{2}} \Gamma \left( \frac{N+1}{2} \right) \left| (1 - \zeta + N/\Sigma) \zeta\sigma_0^2 \right|^{\frac{N}{2}} \times \ldots \times \left( 1 + (\hat{\theta} - \theta_0)^T \frac{1}{N + 1 - d} (1 - \zeta + N/\Sigma) \zeta\sigma_0^2 (\hat{\theta} - \theta_0) \right)^{-\frac{N+1}{2}} \quad \text{(C7)}
\]

which is the multivariate Student’s t distribution with \(N+1-d\) degrees of freedom, ‘location’ vector \(\theta_0\) and ‘shape’ matrix \(\frac{\zeta\sigma_0^2 \Sigma^{-1}}{(1-\zeta+1/N)}\).
Appendix D: Statistical properties of $\hat{\sigma}^2$ estimator in ML inference

In ML inference the estimator of $\theta$ is given by (A4) and the estimator of noise parameter $\sigma^2$ is given by the density

$$\hat{\sigma}^2[\mathcal{D}] = \frac{1}{N} \left\| t - Z\hat{\theta}[\mathcal{D}] \right\|^2$$

$$= \frac{1}{N} \left\| t - Z (Z^T Z)^{-1} Z^T t \right\|^2 = \frac{1}{N} \left\| \left( I_N - Z (Z^T Z)^{-1} Z^T \right) Z\theta_0 + \epsilon \right\|^2$$

$$= \frac{1}{N} \left\| \left( I_N - Z (Z^T Z)^{-1} Z^T \right) Z\theta_0 + (I_N - Z J^{-1} Z) \epsilon \right\|^2$$

$$= \frac{1}{N} \left\| \left( I_N - Z (Z^T Z)^{-1} Z^T \right) \epsilon \right\|^2$$

$$= \frac{1}{N} \epsilon^T \left( I_N - Z (Z^T Z)^{-1} Z^T \right) \epsilon$$

(D1)

In above we used $\left( I_N - Z (Z^T Z)^{-1} Z^T \right) Z\theta_0 = \left( Z\theta_0 - Z (Z^T Z)^{-1} Z^T Z\theta_0 \right) = 0$ and $\left( I_N - Z (Z^T Z)^{-1} Z^T \right)^2 = \left( I_N - Z (Z^T Z)^{-1} Z^T \right)$, i.e. $\left( I_N - Z (Z^T Z)^{-1} Z^T \right)$ is idempotent matrix. For $\epsilon$ sampled from any distribution with mean 0 and covariance $\sigma_0^2 I_N$ the average

$$\langle \hat{\sigma}^2[\mathcal{D}] \rangle_\epsilon = \frac{1}{N} \left\langle \epsilon^T \left( I_N - Z (Z^T Z)^{-1} Z^T \right) \epsilon \right\rangle_\epsilon = \frac{\sigma_0^2}{N} \text{Tr} \left( I_N - Z (Z^T Z)^{-1} Z^T \right) = \sigma_0^2 (1 - \zeta)$$

(D2)

and the variance

$$\langle \hat{\sigma}^4[\mathcal{D}] \rangle_\epsilon - \langle \hat{\sigma}^2[\mathcal{D}] \rangle^2_\epsilon = \frac{2\sigma_0^4}{N} (1 - \zeta)$$

(D3)

by Wick’s theorem.

We are interested in the probability of event $\hat{\sigma}^2[\mathcal{D}] \notin (\sigma_0^2 (1 - \zeta) - \delta, \sigma_0^2 (1 - \zeta) + \delta)$. The
latter is given by

$$\Prob \left[ \frac{1}{N} \sum_{i=1}^{N} (t_i - \hat{\theta}[\mathcal{D}]_i)^2 \leq \sigma_0^2 (1 - \zeta) - \delta, \sigma_0^2 (1 - \zeta) + \delta \right]$$

First, we consider the probability

$$\Prob \left[ \sum_{i=1}^{N} (t_i - \hat{\theta}[\mathcal{D}]_i)^2 \leq N \left( \sigma_0^2 (1 - \zeta) - \delta \right) \right]$$

where in above $\alpha > 0$ and we used Markov inequality to derive the upper bound. Let

$$\Prob \left[ \sum_{i=1}^{N} (t_i - \hat{\theta}[\mathcal{D}]_i)^2 \geq N \left( \sigma_0^2 (1 - \zeta) + \delta \right) \right].$$

where in above $\alpha > 0$ and we used Markov inequality to derive the upper bound. Let us assume that the distribution of noise is Gaussian and consider the moment-generating function

$$\left\langle e^{\frac{\alpha}{N} \sum_{i=1}^{N} (t_i - \hat{\theta}[\mathcal{D}]_i)^2} \right\rangle$$

$$= \left\langle e^{\frac{\alpha}{2} \epsilon^2} (\mathbf{I}_N - \mathbf{Z}(\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T) \epsilon \right\rangle$$

$$= \int \mathcal{D} \mathcal{N}(0, \sigma_0^2 \mathbf{I}_N) \left\langle e^{\frac{\alpha}{2} \epsilon^2} (\mathbf{I}_N - \mathbf{Z}(\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T) \epsilon \right\rangle$$

$$= \frac{1}{(2\pi\sigma_0^2)^N/2} \left\langle \int \mathcal{D} \mathcal{N}(0, \sigma_0^2 \mathbf{I}_N) e^{-\frac{\epsilon^2}{2\sigma_0^2} + \frac{\alpha}{2} \epsilon^2} \mathbf{Z}^{-1} \mathbf{Z}^T \right\rangle$$

$$= \frac{1}{(2\pi\sigma_0^2)^N/2} \left\langle \int \mathcal{D} \mathcal{N}(0, \sigma_0^2 \mathbf{I}_N) e^{-\frac{\epsilon^2}{2\sigma_0^2} + \frac{\alpha}{2} \epsilon^2} \mathbf{I}_N - \mathbf{Z}(\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \right\rangle$$

$$= \frac{1}{(2\pi\sigma_0^2)^N/2} \left\langle 2\pi \left[ \mathbf{I}_N / \sigma_0^2 - \alpha \left( \mathbf{I}_N - \mathbf{Z}(\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \right) \right]^{-\frac{1}{2}} \right\rangle$$

$$= \left\langle \mathbf{I}_N - \alpha \sigma_0^2 \left( \mathbf{I}_N - \mathbf{Z}(\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \right) \right\rangle^{\frac{1}{2}}$$

$$= \left\langle \mathbf{I}_N (1 - \alpha \sigma_0^2) + \alpha \sigma_0^2 \mathbf{Z}(\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \right\rangle^{\frac{1}{2}}$$

$$= (1 - \alpha \sigma_0^2)^{-N/2} \left\langle \frac{\alpha \sigma_0^2}{\mathbf{I}_N + \sigma_0^2 \mathbf{Z}(\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T} \right\rangle (D6)\right.$$
Now $\mathbf{Z} (\mathbf{Z}^\top \mathbf{Z})^{-1} \mathbf{Z}^\top$ is a projection matrix and its eigenvalue are $\lambda_i \in \{0, 1\}$ giving us

$$
\left< \frac{1}{2} \alpha \sum_{i=1}^N (t_i - \hat{\theta} [\mathcal{D}], \mathbf{z}_i)^2 \right> \geq (1 - \alpha \sigma_0^2)^{-N/2} \left< \frac{1}{\mathbf{I}_N + \frac{\alpha \sigma_0^2}{1 - \alpha \sigma_0^2} \mathbf{Z} (\mathbf{Z}^\top \mathbf{Z})^{-1} \mathbf{Z}^\top} \right>^2 Z
$$

$$
= (1 - \alpha \sigma_0^2)^{-N/2} \left< \frac{1}{\prod_{i=1}^N \left[ 1 + \frac{\alpha \sigma_0^2}{1 - \alpha \sigma_0^2} \lambda_i (\mathbf{Z} (\mathbf{Z}^\top \mathbf{Z})^{-1} \mathbf{Z}^\top) \right]^{1/2}} \right> Z
$$

$$
= (1 - \alpha \sigma_0^2)^{-N/2} \left< e^{-\frac{N}{2} \sum_{\lambda \sigma} \frac{1}{N} \sum_{i=1}^N \delta_{\lambda \lambda_i} (\mathbf{z} (\mathbf{z}^\top)^{-1} \mathbf{z}^\top)^{1/2}} \right> Z
$$

$$
= (1 - \alpha \sigma_0^2)^{-N/2} \left< e^{-\frac{1}{2} \log \left[ 1 + \frac{\alpha \sigma_0^2}{1 - \alpha \sigma_0^2} \right] \mathbf{Tr} \{ \mathbf{Z} (\mathbf{Z}^\top \mathbf{Z})^{-1} \} \} \right> Z
$$

$$
= (1 - \alpha \sigma_0^2)^{-N/2} \left< e^{-\frac{1}{2} \log \left[ 1 + \frac{\alpha \sigma_0^2}{1 - \alpha \sigma_0^2} \right]} \right> Z
$$

$$
= e^{\frac{N}{2} \left[ \log \left( 1 + \frac{\alpha \sigma_0^2}{1 - \alpha \sigma_0^2} \right) + \log (1 - \alpha \sigma_0^2) \right]} = e^{-\frac{N}{2} (1 - \zeta) \log (1 - \alpha \sigma_0^2)}
$$

and hence

$$
\text{Prob} \left[ \sum_{i=1}^N (t_i - \hat{\theta} [\mathcal{D}], \mathbf{z}_i)^2 \geq N \left( \sigma_0^2 (1 - \zeta) + \delta \right) \right] 
\leq e^{\frac{1}{2} \alpha \sum_{i=1}^N (t_i - \hat{\theta} [\mathcal{D}], \mathbf{z}_i)^2} \cdot e^{-\frac{1}{2} \alpha N (\sigma_0^2 (1 - \zeta) + \delta)}
\leq e^{-\frac{1}{2} N (1 - \zeta) \log (1 - \alpha \sigma_0^2)} e^{-\frac{1}{2} \alpha N (\sigma_0^2 (1 - \zeta) + \delta)}
\leq e^{-\frac{1}{2} N \left[ (1 - \zeta) \log (1 - \alpha \sigma_0^2) + \alpha (\sigma_0^2 (1 - \zeta) + \delta) \right]} = e^{-\frac{1}{2} N \Phi(\alpha)}. 
$$

The rate function

$$
\Phi(\alpha) = (1 - \zeta) \log (1 - \alpha \sigma_0^2) + \alpha (\sigma_0^2 (1 - \zeta) + \delta)
$$

has a maximum at

$$
\alpha = \frac{\delta}{\sigma_0^2 ((1 - \zeta) \sigma_0^2 + \delta)},
$$

such that $\Phi = (1 - \zeta) \log \left( \frac{(1 - \zeta) \sigma_0^2}{(1 - \zeta) \sigma_0^2 + \delta} \right) + \delta / \sigma_0^2$, and hence

$$
\text{Prob} \left[ \sum_{i=1}^N (t_i - \hat{\theta} [\mathcal{D}], \mathbf{z}_i)^2 \geq N \left( \sigma_0^2 (1 - \zeta) + \delta \right) \right] 
\leq e^{-\frac{1}{2} N \left( (1 - \zeta) \log \left( \frac{(1 - \zeta) \sigma_0^2}{(1 - \zeta) \sigma_0^2 + \delta} \right) + \delta / \sigma_0^2 \right)}.
$$
We note that in above the rate function \((1 - \zeta) \log \left( \frac{(1 - \zeta)}{(1 - \zeta) + \delta / \sigma_0^2} \right) + \delta / \sigma_0^2 \) is 0 for \(\delta / \sigma_0^2 = 0\) and monotonic increasing function of \(\delta / \sigma_0^2\).

Second, for \(\alpha > 0\) we consider the probability
\[
\begin{align*}
\text{Prob} \left[ \sum_{i=1}^{N} (t_i - \hat{\theta}([\mathcal{D}], z_i))^2 \leq N \left( \sigma_0^2 (1 - \zeta) - \delta \right) \right] &= \text{Prob} \left[ e^{-\frac{1}{2}N \sum_{i=1}^{N} (t_i - \hat{\theta}([\mathcal{D}], z_i))^2} \geq e^{-\frac{1}{2}N (\sigma_0^2 (1 - \zeta) - \delta)} \right] \\
&\leq e^{-\frac{1}{2}N (1 - \zeta) \log \left( \frac{(1 - \zeta)}{(1 - \zeta) + \delta / \sigma_0^2} \right) - \delta / \sigma_0^2} = e^{-\frac{N}{2} \phi(\alpha)},
\end{align*}
\]
where
\[
\phi(\alpha) = (1 - \zeta) \log \left( 1 + \alpha \sigma_0^2 \right) - \alpha \left( \sigma_0^2 (1 - \zeta) - \delta \right),
\]
and in above we used Markov inequality and the result (D7) with \(\alpha \to -\alpha\). The rate function \(\phi(\alpha)\) has a maximum at \(\alpha = \frac{\delta}{\sigma_0^2 (1 - \zeta) - \delta}\), such that \(\phi = (1 - \zeta) \log \left( \frac{(1 - \zeta)}{(1 - \zeta) - \delta / \sigma_0^2} \right) - \delta / \sigma_0^2\), and hence
\[
\begin{align*}
\text{Prob} \left[ \sum_{i=1}^{N} (t_i - \hat{\theta}([\mathcal{D}], z_i))^2 \leq N \left( \sigma_0^2 (1 - \zeta) - \delta \right) \right] &\leq e^{-\frac{N}{2} (1 - \zeta) \log \left( \frac{(1 - \zeta)}{(1 - \zeta) - \delta / \sigma_0^2} \right) - \delta / \sigma_0^2}.
\end{align*}
\]
We note that in above the rate function \((1 - \zeta) \log \left( \frac{(1 - \zeta)}{(1 - \zeta) - \delta / \sigma_0^2} \right) - \delta / \sigma_0^2\) is 0 for \(\delta / \sigma_0^2 = 0\) and monotonic increasing function of \(\delta / \sigma_0^2\) when \(\sigma_0^2 (1 - \zeta) > \delta\).

Finally, combining the inequalities (D11) and (D14) we obtain the inequality
\[
\begin{align*}
\text{Prob} \left[ \hat{\sigma}^2([\mathcal{D}]) \notin \left( \sigma_0^2 (1 - \zeta) - \delta, \sigma_0^2 (1 - \zeta) + \delta \right) \right] &\leq e^{-\frac{1}{2}N \left[ (1 - \zeta) \log \left( \frac{(1 - \zeta)}{(1 - \zeta) - \delta / \sigma_0^2} \right) - \delta / \sigma_0^2 \right]} \\
&+ e^{-\frac{1}{2}N \left[ (1 - \zeta) \log \left( \frac{(1 - \zeta)}{(1 - \zeta) + \delta / \sigma_0^2} \right) + \delta / \sigma_0^2 \right]},
\end{align*}
\]
which is valid for \(\delta \in (0, \sigma_0^2 (1 - \zeta))\).

**Appendix E: Statistical properties of MSE in ML inference**

In this section we consider statistical properties of the *minimum square error* (MSE)\(\frac{1}{2}||\theta_0 - \hat{\theta}([\mathcal{D}]||)^2\), where \(\theta_0\) is the vector of *true* parameters and \(\hat{\theta}([\mathcal{D}]\) is the ML estimator (A4).
1. Moment generating function

Let us consider the moment generating function

\[
\left\langle e^{\frac{1}{2} \alpha |\theta - \hat{\theta}|^2} \right\rangle = \int P(\hat{\theta}) e^{\frac{1}{2} \alpha |\theta - \hat{\theta}|^2} d\hat{\theta} = (\pi (N + 1 - d))^{-\frac{d}{2}} \frac{\Gamma\left(\frac{N+1}{2}\right)}{\Gamma\left(\frac{N+1}{2} - d\right)} \left|\frac{(1 - \frac{\zeta}{1/N})\Sigma}{\zeta_0^2}\right|^\frac{1}{2} \times \int \left(1 + (\hat{\theta} - \theta_0)^T \frac{1}{N + 1 - d} (1 - \frac{\zeta}{1/N})\Sigma (\hat{\theta} - \theta_0)\right)^{-\frac{N+1}{2}} d\hat{\theta} \tag{E1}
\]

\[
= (\pi (N + 1 - d))^{-\frac{d}{2}} \frac{\Gamma\left(\frac{N+1}{2}\right)}{\Gamma\left(\frac{N+1}{2} - d\right)} \left|\frac{(1 - \frac{\zeta}{1/N})\Sigma}{\zeta_0^2}\right|^\frac{1}{2} \times \int \left(1 + \hat{\theta}^T \frac{1}{N + 1 - d} (1 - \frac{\zeta}{1/N})\Sigma \hat{\theta}\right)^{-\frac{N+1}{2}} d\hat{\theta}
\]

\[
= \int \int \int \int \int \int N(\hat{\theta} | 0, \omega(1 - \zeta + 1/N)\Sigma^{-1}) \Gamma_{N+1-d}(\omega) \ d\omega \times e^{\frac{1}{2} \alpha |\theta_0|^2} d\theta
\]

\[
= \int \int e^{-\frac{1}{2} \hat{\theta}^T \left(\frac{\omega(1 - \zeta + 1/N)\Sigma}{\zeta_0^2} - \alpha I_d\right) \hat{\theta}} \left|2\pi \frac{\zeta_0^2}{\omega(1 - \zeta + 1/N)\Sigma^{-1}}\right|^\frac{1}{2} d\hat{\theta} \Gamma_{N+1-d}(\omega) d\omega
\]

\[
= \int \left(\frac{\Gamma_{N+1-d}(\omega)}{\omega(1 - \zeta + 1/N)\Sigma^{-1}}\right)^\frac{1}{2} \left|\frac{\omega(1 - \zeta + 1/N)\Sigma}{\zeta_0^2} - \alpha I_d\right| d\omega
\]

\[
= \int \left(\Gamma_{N+1-d}(\omega)\right)^{\frac{1}{2}} \left|I_d - \alpha \frac{\zeta_0^2}{\omega(1 - \zeta + 1/N)\Sigma^{-1}}\right| d\omega
\]

\[
= \int e^{-\frac{1}{2} \log |I_d - \alpha \frac{\zeta_0^2}{\omega(1 - \zeta + 1/N)\Sigma^{-1}}|} \Gamma_{N+1-d}(\omega) d\omega
\]

\[
= \int e^{-\frac{1}{2} \frac{\alpha \zeta_0^2}{\omega(1 - \zeta + 1/N)\Sigma}} \Gamma_{N+1-d}(\omega) d\omega \tag{E2}
\]

where for \(\nu > 0\)

\[
\Gamma_{\nu}(\omega) = \frac{\nu^{\nu/2}}{2^{\nu/2} \Gamma(\nu/2)} \omega^{\nu-2} e^{-\frac{1}{2} \nu \omega} \tag{E3}
\]

is the gamma distribution. We note that line five in above was obtained using the mixture of Gaussians representation of multivariate Student t distribution [28]. Thus the moment
generating function is given by

\[
\left\langle e^{\frac{1}{2}\alpha||\hat{\theta} - \theta||^2} \right\rangle = \int_{0}^{\infty} \frac{\Gamma_{N+1-d}(\omega)}{|\mathbf{I}_d - \frac{\alpha}{\omega(1 - \zeta + 1/N)} \Sigma^{-1}|^{\frac{1}{2}}} d\omega
\]

\[= \int_{0}^{\infty} \Gamma_{N+1-d}(\omega) d\omega \prod_{\ell=1}^{d} \left(1 - \frac{\alpha}{\omega(1 - \zeta + 1/N)} \lambda_{\ell}(\Sigma) \right)^{-\frac{1}{2}}
\]

and, by the transformation \(\alpha = 2i\alpha\) in above, we also obtain the characteristic function

\[
\left\langle e^{i\alpha||\hat{\theta} - \theta||^2} \right\rangle = \int_{0}^{\infty} \Gamma_{N+1-d}(\omega) d\omega \prod_{\ell=1}^{d} \left(1 - i\alpha \frac{2\zeta \sigma_0^2}{\omega(1 - \zeta + 1/N)\lambda_{\ell}(\Sigma)} \right)^{-\frac{1}{2}}.
\]

We note that the last term in above is the product of characteristic functions of gamma distributions. Each gamma distribution has the same ‘shape’ parameter \(1/2\) and different scale parameter \(\frac{2\zeta \sigma_0^2}{\omega(1 - \zeta + 1/N)\lambda_{\ell}(\Sigma)}\).

a. The first two moments of MSE

Let us now consider derivatives of the moment generating function (E4) with \(\alpha = \alpha/d\). The derivative with respect to \(\alpha\) gives us

\[
2 \frac{\partial}{\partial \alpha} \left\langle e^{\frac{1}{2}\alpha||\hat{\theta} - \theta||^2} \right\rangle = 2 \int_{0}^{\infty} \Gamma_{N+1-d}(\omega) d\omega \prod_{\ell=1}^{d} \left(1 - \frac{\alpha}{\omega(1 - \zeta + 1/N)} \lambda_{\ell}(\Sigma) \right)^{-\frac{1}{2}}
\]

\[
= \int_{0}^{\infty} \Gamma_{N+1-d}(\omega) d\omega \prod_{\ell=1}^{d} \left(1 - \frac{\alpha}{\omega(1 - \zeta + 1/N)} \lambda_{\ell}(\Sigma) \right)^{-\frac{1}{2}}
\]

\[
\times \frac{1}{d} \sum_{\ell=1}^{d} \left(1 - \frac{\alpha}{\omega(1 - \zeta + 1/N)} \lambda_{\ell}(\Sigma) \right)^{-1} \frac{\zeta \sigma_0^2}{\omega(1 - \zeta + 1/N)\lambda_{\ell}(\Sigma)} (E6)
\]

Above for \(\alpha = 0\) gives us the average

\[
\frac{1}{d} \left\langle ||\hat{\theta} - \theta||^2 \right\rangle = \frac{\zeta \sigma_0^2}{1 - \zeta + 1/N} \frac{1}{d} \text{Tr} \left\{ \Sigma^{-1} \right\} \int_{0}^{\infty} \Gamma_{N+1-d}(\omega) \omega^{-1} d\omega
\]

\[= \frac{\zeta \sigma_0^2}{1 - \zeta + 1/N} \frac{1}{d} \text{Tr} \left[ \Sigma^{-1} \right] \]

\[= \frac{\zeta \sigma_0^2}{1 - \zeta - 1/N} \frac{1}{d} \text{Tr} \left[ \Sigma^{-1} \right]. \quad (E7)
\]
Now consider the second derivative with respect to $\alpha$:

\[
\frac{4}{\partial \alpha^2} \left\langle e^{\frac{1}{2} \alpha \| \hat{\theta}_0 - \hat{\theta}[\varphi] \|^2} \right\rangle_{\mathcal{F}}
\]

\[
= 4 \int_0^\infty \Gamma_{N+1-d} (\omega) d\omega \left( 1 - \alpha \frac{\zeta \sigma_0^2}{\omega d(1 - \zeta + 1/N) \lambda(\Sigma)} \right) - \frac{1}{2}
\]\n
\[
= 2 \int_0^\infty \Gamma_{N+1-d} (\omega) d\omega \left( 1 - \alpha \frac{\zeta \sigma_0^2}{\omega d(1 - \zeta + 1/N) \lambda(\Sigma)} \right) - \frac{1}{2}
\]

\[
\times \frac{1}{d} \sum_{\ell=1}^d \left( 1 - \alpha \frac{\zeta \sigma_0^2}{\omega d(1 - \zeta + 1/N) \lambda(\Sigma)} \right) \frac{\zeta \sigma_0^2}{\omega (1 - \zeta + 1/N) \lambda(\Sigma)}
\]

\[
= \int_0^\infty \Gamma_{N+1-d} (\omega) d\omega \left\{ 2 \frac{\partial}{\partial \alpha} \prod_{\ell=1}^d \left( 1 - \alpha \frac{\zeta \sigma_0^2}{\omega d(1 - \zeta + 1/N) \lambda(\Sigma)} \right) - \frac{1}{2}
\]

\[
\times \frac{1}{d} \sum_{\ell=1}^d \left( 1 - \alpha \frac{\zeta \sigma_0^2}{\omega d(1 - \zeta + 1/N) \lambda(\Sigma)} \right) \frac{\zeta \sigma_0^2}{\omega (1 - \zeta + 1/N) \lambda(\Sigma)}
\]

\[
+ 2 \prod_{\ell=1}^d \left( 1 - \alpha \frac{\zeta \sigma_0^2}{\omega d(1 - \zeta + 1/N) \lambda(\Sigma)} \right) - \frac{1}{2}
\]

\[
\times \frac{\partial}{\partial \alpha} \frac{1}{d} \sum_{\ell=1}^d \left( 1 - \alpha \frac{\zeta \sigma_0^2}{\omega d(1 - \zeta + 1/N) \lambda(\Sigma)} \right) \frac{\zeta \sigma_0^2}{\omega (1 - \zeta + 1/N) \lambda(\Sigma)}
\]

\[
= \int_0^\infty \Gamma_{N+1-d} (\omega) d\omega \prod_{\ell=1}^d \left( 1 - \alpha \frac{\zeta \sigma_0^2}{\omega d(1 - \zeta + 1/N) \lambda(\Sigma)} \right) - \frac{1}{2}
\]

\[
\times \left\{ \left[ \frac{1}{d} \sum_{\ell=1}^d \left( 1 - \alpha \frac{\zeta \sigma_0^2}{\omega d(1 - \zeta + 1/N) \lambda(\Sigma)} \right) \frac{\zeta \sigma_0^2}{\omega (1 - \zeta + 1/N) \lambda(\Sigma)} \right]^2
\]

\[
+ \frac{2}{d^2} \sum_{\ell=1}^d \left( 1 - \alpha \frac{\zeta \sigma_0^2}{\omega d(1 - \zeta + 1/N) \lambda(\Sigma)} \right) \frac{\zeta \sigma_0^2}{\omega (1 - \zeta + 1/N) \lambda(\Sigma)} \right]^2 \right\}
\]

(E8)
Evaluated at $\alpha = 0$ above gives us the second moment

$$
\left\langle \frac{1}{d^2} ||\theta_0 - \hat{\theta}||^4 \right\rangle = \left( \frac{\zeta \sigma_0^2}{(1 - \zeta + 1/N)} \right)^2 \int_0^\infty \Gamma_{N+1-d}(\omega) \omega^{-2} d\omega
\times \left[ \left( \frac{1}{d} \sum_{\ell=1}^d \frac{1}{\lambda_{\ell}(\Sigma)} \right)^2 + \frac{2}{d^2} \sum_{\ell=1}^d \left( \frac{1}{\lambda_{\ell}(\Sigma)} \right)^2 \right]
= \left( \frac{\zeta \sigma_0^2}{(1 - \zeta + 1/N)} \right)^2 \int_0^\infty \Gamma_{N+1-d}(\omega) \omega^{-2} d\omega
\times \left[ \left( \frac{1}{d} \text{Tr} [\Sigma^{-1}] \right)^2 + \frac{2}{d^2} \text{Tr} [\Sigma^{-2}] \right]
= \left( \frac{\zeta \sigma_0^2}{(1 - \zeta + 1/N)} \right)^2 \frac{(1 - \zeta + 1/N)^2}{(1 - \zeta - 1/N)(1 - \zeta - 3/N)}
\times \left[ \left( \frac{1}{d} \text{Tr} [\Sigma^{-1}] \right)^2 + \frac{2}{d^2} \text{Tr} [\Sigma^{-2}] \right]
= \frac{\zeta^2 \sigma_0^4}{(1 - \zeta - 1/N)(1 - \zeta - 3/N)} \left[ \left( \frac{1}{d} \text{Tr} [\Sigma^{-1}] \right)^2 + \frac{2}{d^2} \text{Tr} [\Sigma^{-2}] \right] \quad (\text{E9})
$$

Now combining the mean (E7) and second moment (E9) we obtain the variance

$$
\left\langle \frac{1}{d^2} ||\theta_0 - \hat{\theta}||^4 \right\rangle - \frac{1}{d^2} \left\langle ||\theta_0 - \hat{\theta}||^2 \right\rangle^2
= \frac{\zeta^2 \sigma_0^4}{(1 - \zeta - 1/N)(1 - \zeta - 3/N)}
\times \left[ \left( \frac{1}{d} \text{Tr} [\Sigma^{-1}] \right)^2 + \frac{2}{d^2} \text{Tr} [\Sigma^{-2}] \right]
\times \left[ \frac{\zeta^2 \sigma_0^4}{(1 - \zeta - 1/N)(1 - \zeta - 3/N)} \right]
\times \left[ \frac{\zeta^2 \sigma_0^4}{(1 - \zeta - 1/N)^2} \right]
\times \frac{1}{d^2} \text{Tr}^2 [\Sigma^{-1}]
+ \frac{\zeta^2 \sigma_0^4}{(1 - \zeta - 1/N)(1 - \zeta - 3/N)} \cdot \frac{2}{d^2} \text{Tr} [\Sigma^{-2}]
= 2 \left( \frac{\zeta \sigma_0^2}{1 - \zeta} \right)^2 \frac{1}{d^2} \text{Tr} [\Sigma^{-2}] \quad (\text{E10})
$$

of the random variable $\frac{1}{d} ||\theta_0 - \hat{\theta}||^2$ for $(N, d) \to \infty$. 

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b. Properties of MGF for large \((N,d)\)

Let us consider the moment generating function \((E4)\) for the covariance matrix \(\Sigma = \lambda I_d\). For the latter the mean \(\left\langle \frac{1}{2}||\theta_0 - \hat{\theta}[\mathcal{G}]||^2 \right\rangle_{\mathcal{G}}\), using the equation \((E7)\) for large \((N,d)\), is given by

\[
\mu(\lambda) = \frac{\zeta \sigma_0^2}{(1 - \zeta)\lambda}
\]  

(E11)

and the MGF is given by

\[
\left\langle e^{\frac{1}{2}||\theta_0 - \hat{\theta}[\mathcal{G}]||^2} \right\rangle_{\mathcal{G}} = \int_0^{\infty} \Gamma_{N+1-d}(\omega) \frac{1}{\left(1 - \alpha \frac{\zeta \sigma_0^2}{\omega(1 - \zeta + 1/N)\lambda}\right)^{\frac{d}{2}}} d\omega
\]

\[
= \int_0^{\infty} \Gamma_{N+1-d}(\omega) d\omega \left(\frac{\omega(1 - \zeta + 1/N)\lambda}{\omega(1 - \zeta + 1/N)\lambda - \alpha \zeta \sigma_0^2}\right)^{\frac{d}{2}}
\]

\[
= \int_0^{\infty} \Gamma_{N+1-d}(\omega) \left(\frac{\omega}{\omega - \alpha \mu(\lambda)}\right)^{\frac{d}{2}} d\omega,
\]  

(E12)

where the last line in above was obtained by assuming \((N,d)\) large. Let us now consider the integral

\[
\frac{1}{N} \log \int_0^{\infty} \Gamma_{N+1-d}(\omega) \left(\frac{\omega}{\omega - \alpha}\right)^{\frac{d}{2}} d\omega
\]

\[
= \frac{1}{N} \log \frac{(N + 1 - d)(N+1-d)/2}{2^{(N+1-d)/2} \Gamma((N + 1 - d)/2)} + \frac{1}{N} \log \int_0^{\infty} \omega^{\frac{N-d-1}{2}} e^{-\frac{1}{2}(N-d+1)\omega} \left(\frac{\omega}{\omega - \alpha}\right)^{\frac{d}{2}} d\omega
\]

\[
= \frac{1}{N} \log \left(\frac{1 - \zeta}{2N}\right)^{\frac{1-\zeta}{2}} / \Gamma\left(\frac{1 - \zeta}{2}\right) + \frac{1}{N} \log \int_0^{\infty} e^{\frac{\zeta}{2} (1-\zeta) \log \omega - \frac{\zeta}{2} (1-\zeta) \omega + \frac{\zeta}{2} \log(\omega - \alpha)} d\omega
\]

\[
= \frac{1 - \zeta}{2} + \frac{1}{2N} \log \left(\frac{1 - \zeta}{4\pi N}\right) + O\left(N^{-2}\right) + \frac{1}{2} \phi(-\omega_0) + \frac{1}{2N} \log \left(\frac{4\pi}{N(-\phi''(\omega_0))}\right) + O\left(N^{-2}\right)
\]

\[
= \frac{1 - \zeta}{2} + \frac{1}{2} \phi(-\omega_0) + \frac{1}{2N} \log \left(\frac{\zeta - 1}{\phi''(\omega_0)}\right) + O\left(N^{-2}\right),
\]  

(E13)
where \( \omega_0 = \arg\max_{\omega \in [0, \infty)} \phi_-(\omega) \) of the function

\[
\phi_-(\omega) = \left[ (1 - \zeta) \log \omega - (1 - \zeta) \omega + \zeta \log \left( \frac{\omega}{\omega - \alpha} \right) \right]
\]  

(E14)

We note \( \phi_-(\omega) \) has a maximum when the solution of

\[
\phi'_-(\omega) = \frac{(1 - \zeta) \omega^2 - (\alpha + 1) (1 - \zeta) \omega + \alpha}{(\alpha - \omega) \omega} = 0
\]

(E15)
satisfies the condition \( \phi''_-(\omega) > 0 \) given by the inequality \( \omega^2 \zeta - (\omega - \alpha)^2 < 0 \). The latter is satisfied when \( \omega \in \left( 0, \frac{(1 - \sqrt{\zeta})\alpha}{1 - \zeta} \right) \cup \left( \frac{(1 + \sqrt{\zeta})\alpha}{1 - \zeta}, \infty \right) \) for \( \zeta \in (0, 1) \) and when \( \omega \in (0, \alpha/2) \) for \( \zeta = 1 \). However, the difference \( \omega - \alpha \) on the interval \( \left( 0, \frac{(1 - \sqrt{\zeta})\alpha}{1 - \zeta} \right) \) for \( \zeta \in [0, 1) \) is negative, so \( \phi_-(\omega) \) is undefined. The latter is also true for \( (0, \alpha/2) \) at \( \zeta = 1 \) thus leaving us only with the interval \( \left( \frac{(1 + \sqrt{\zeta})\alpha}{1 - \zeta}, \infty \right) \) with \( \zeta \in (0, 1) \).

The equation (E15) has real solutions \( \frac{1 + \alpha}{2} \pm \sqrt{\left( \frac{1 + \alpha}{2} \right)^2 - \frac{\alpha}{(1 - \zeta)}} \) when the inequality \( \left( \frac{\alpha + 1}{2} \right)^2 / \alpha \geq 1 / (1 - \zeta) \) is satisfied. The latter is true when \( \alpha \in \left( 0, \frac{1 + \zeta - 2\sqrt{\zeta}}{1 - \zeta} \right) \cup \left( \frac{1 + \zeta + 2\sqrt{\zeta}}{1 - \zeta}, \infty \right) \), but only one solution \( \omega_0 = \frac{1 + \alpha}{2} + \sqrt{\left( \frac{1 + \alpha}{2} \right)^2 - \frac{\alpha}{(1 - \zeta)}} \) belongs to the interval \( \left( \frac{(1 + \sqrt{\zeta})\alpha}{1 - \zeta}, \infty \right) \), where \( \zeta \in (0, 1) \), when \( \alpha \in \left( 0, \frac{1 + \zeta - 2\sqrt{\zeta}}{1 - \zeta} \right) \), i.e. it corresponds to the maximum of \( \phi_-(\omega) \).

We note that for \( \alpha = \alpha \mu(\lambda) \), appearing in the integral (E12), we obtain

\[
\omega_0 = \frac{1 + \alpha \mu(\lambda)}{2} + \sqrt{\left( \frac{1 + \alpha \mu(\lambda)}{2} \right)^2 - \frac{\alpha \mu(\lambda)}{(1 - \zeta)}}
\]

(E16)

for \( \alpha \in \left( 0, \frac{1 + \zeta - 2\sqrt{\zeta}}{\zeta \sigma_0} \right) \) and \( \zeta \in (0, 1) \). Now the moment generating function (E12), using the result (E13), for large \( N \) is given by

\[
\left\langle e^{\frac{1}{d} \| \hat{\theta}_0 - \hat{\theta}[\mathcal{D}] \|^2} \right\rangle \cong \sqrt{\frac{\zeta - 1}{\phi''_-(\omega_0)}} e^{\frac{1}{d} N \left( 1 - \zeta + \phi_-(\omega_0) \right)} + O(1/N).
\]  

(E17)

2. Deviations from the mean

We are interested in the probability of event \( \frac{1}{d} \| \hat{\theta}_0 - \hat{\theta}[\mathcal{D}] \|^2 \notin (\mu(\lambda) - \delta, \mu(\lambda) + \delta) \). The latter is given by

\[
\text{Prob} \left[ \frac{1}{d} \| \hat{\theta}_0 - \hat{\theta}[\mathcal{D}] \|^2 \notin (\mu(\lambda) - \delta, \mu(\lambda) + \delta) \right] = \text{Prob} \left[ \| \hat{\theta}_0 - \hat{\theta}[\mathcal{D}] \|^2 \leq d (\mu(\lambda) - \delta) \right] + \text{Prob} \left[ \| \hat{\theta}_0 - \hat{\theta}[\mathcal{D}] \|^2 \geq d (\mu(\lambda) + \delta) \right].
\]  

(E18)
First, for $\alpha > 0$ we consider the probability

$$\text{Prob} \left[ ||\theta_0 - \hat{\theta} ||^2 \geq d (\mu (\lambda) + \delta) \right]$$

$$= \text{Prob} \left[ e^{\frac{1}{2} \alpha ||\theta_0 - \hat{\theta} ||^2} \geq e^{\frac{1}{2} \alpha d (\mu (\lambda) + \delta)} \right]$$

$$\leq \left( e^{\frac{1}{2} \alpha ||\theta_0 - \hat{\theta} ||^2} \right) \leq e^{-\frac{1}{2} \alpha d (\mu (\lambda) + \delta)}$$

$$= \sqrt{\frac{\zeta - 1}{\phi''(\omega_0^+)} e^{\frac{1}{2} N (1 - \zeta + \phi_+ (\omega_0^+)) + O(1/N)} e^{-\frac{1}{2} \alpha \zeta N (\mu (\lambda) + \delta)}}$$

$$= \sqrt{\frac{\zeta - 1}{\phi''(\omega_0^+)} e^{-\frac{1}{2} N (\zeta - 1 + \phi_+ (\omega_0^+)) + \alpha \zeta (\mu (\lambda) + \delta) + O(1/N)}} \quad \text{(E19)}$$

From above follows that for $N \to \infty$ we have that

$$-\frac{2}{N} \log \text{Prob} \left[ ||\theta_0 - \hat{\theta} ||^2 \geq d (\mu (\lambda) + \delta) \right] \geq \zeta - 1 - \phi_+ (\omega_0^+) + \alpha \zeta (\mu (\lambda) + \delta) + O (1/N) \quad \text{(E20)}$$

We would like to optimise above bound with respect to $\alpha$, but it is not clear how to implement this analytically for any $\alpha$. However, for small $\alpha$ the function (divided by $\zeta$) appearing in lower bound of the above has the following Taylor expansion

$$(\mu (\lambda) - 1 + \delta) \alpha + \frac{\zeta (\mu (\lambda) - 1)^2 - 1}{2(1 - \zeta)} \alpha^2$$

$$+ \frac{(\mu - 1)^3 \zeta^2 + (3 \mu^3 - 3 \mu^2 - 3 \mu + 2) \zeta - 1}{3 (1 - \zeta)^2} \alpha^3 + O (\alpha^4), \quad \text{(E21)}$$

so if $\mu (\lambda) + \delta > 1$ then first term in above is positive and hence if $\alpha > 0$ is sufficiently small then the RHS of (E20) is positive. We note that for $\mu (\lambda) \geq 1$, where $\mu (\lambda) = \frac{\zeta \sigma_d^2}{(1 - \zeta) \lambda}$, the $\delta > 0$ can be made arbitrary small, but for $\mu < 1$ positivity of first term in above is dependent on $\delta$.

Second, for $\alpha > 0$ we consider the probability

$$\text{Prob} \left[ ||\theta_0 - \hat{\theta} ||^2 \leq d (\mu (\lambda) - \delta) \right]$$

$$= \text{Prob} \left[ e^{-\frac{1}{2} \alpha ||\theta_0 - \hat{\theta} ||^2} \geq e^{-\frac{1}{2} \alpha d (\mu (\lambda) - \delta)} \right]$$

$$\leq \left( e^{-\frac{1}{2} \alpha ||\theta_0 - \hat{\theta} ||^2} \right) \leq e^{\frac{1}{2} \alpha d (\mu (\lambda) - \delta)}$$

$$= \sqrt{\frac{\zeta - 1}{\phi''(\omega_0^+)} e^{\frac{1}{2} N (1 - \zeta + \phi_+ (\omega_0^+)) + O(1/N)} e^{\frac{1}{2} \alpha \zeta N (\mu (\lambda) - \delta)}}$$

$$= \sqrt{\frac{\zeta - 1}{\phi''(\omega_0^+)} e^{-\frac{1}{2} N (\zeta - 1 + \phi_+ (\omega_0^+)) - \alpha \zeta (\mu (\lambda) - \delta) + O(1/N)}, \quad \text{(E22)}}$$

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where the function $\phi_+$, is defined by
\[
\phi_+(\omega) = \left( (1 - \zeta) \log \omega - (1 - \zeta) \omega + \zeta \log \left( \frac{\omega}{\omega + \alpha} \right) \right),
\]
has a maximum at
\[
\omega_0^+ = (1 - \alpha + \sqrt{(\alpha - 1)^2 + 4\alpha/(1 - \zeta)})/2.
\]
Now for $\alpha = \alpha \mu(\lambda)$ the function
\[
(\zeta - 1 - \phi_+(\omega_0^+)) = \delta \zeta \alpha - \frac{\mu^2(\lambda) \zeta}{2 (1 - \zeta)} \alpha^2 + \frac{\mu^3(\lambda) \zeta}{3 (1 - \zeta)^2} \alpha^3
\]
\[
- \frac{\mu^4(\lambda) \zeta}{4 (1 - \zeta)^3} \alpha^4 + O(\alpha^5),
\]
appearing in exponential of (E22), is positive for some small $\alpha$ and hence the lower bound in the inequality
\[
-\frac{2}{N} \log \text{Prob} \left[ ||\Theta_0 - \hat{\Theta}[\mathcal{D}]||^2 \leq d (\mu(\lambda) - \delta) \right]
\]
\[
\geq (\zeta - 1 - \phi_+(\omega_0^+)) = \alpha \zeta (\mu(\lambda) - \delta) + O(1/N),
\]
is positive for any $\delta \in (0, \mu(\lambda))$ and sufficiently small $\alpha$ when $N \to \infty$.

Now combining (E20) with (E26) allows us bound the probability (E18) as follows
\[
\text{Prob} \left[ \left| \frac{1}{d} ||\Theta_0 - \hat{\Theta}[\mathcal{D}]||^2 \right| \notin (\mu(\lambda) - \delta, (\mu(\lambda) + \delta) \right]
\]
\[
\leq C_- e^{-\frac{N}{2} |\mu - \mu(\lambda)|} + C_+ e^{-\frac{N}{2} |\mu - \mu(\lambda)| - \alpha \zeta (\mu(\lambda) - \delta) |},
\]
for some constants $C_\pm$ and some sufficiently small $\alpha > 0$. We note that for the first term in the above upper bound to vanish, as $N \to \infty$, for arbitrary small $\delta$ it is sufficient that $\mu(\lambda) \geq 1$, where $\mu(\lambda) = \varsigma \sigma^2 / (1 - \zeta) \lambda$, but for $\mu(\lambda) < 1$ for this to happen the $\delta$ must be such that $\delta > 1 - \mu(\lambda)$. The second term in the upper bound is vanishing for any $\delta \in (0, \mu(\lambda))$.

Finally we consider deviations of $\frac{1}{d} ||\Theta_0 - \hat{\Theta}[\mathcal{D}]||^2$ from its mean $\mu(\Sigma) = \varsigma \sigma^2 / (1 - \zeta - 1/N) \text{ Tr } [\Sigma^{-1}]$, derived in (E7). To this end we consider the probability of event $\frac{1}{d} ||\Theta_0 - \hat{\Theta}[\mathcal{D}]||^2 \notin$
$(\mu(\Sigma) - \delta, \mu(\Sigma) + \delta)$ given by the sum

$$
\text{Prob} \left[ \left| \mathbf{\theta}_0 - \hat{\mathbf{\theta}}[\mathcal{G}] \right|^2 \leq d(\mu(\Sigma) - \delta) \right] 
+ \text{Prob} \left[ \left| \mathbf{\theta}_0 - \hat{\mathbf{\theta}}[\mathcal{G}] \right|^2 \geq d(\mu(\Sigma) + \delta) \right] 
\leq \left\langle e^{-\frac{1}{2}a|\mathbf{\theta}_0 - \hat{\mathbf{\theta}}[\mathcal{G}]|^2} \right\rangle_{\mathcal{G}} e^{\frac{1}{2}ad(\mu(\Sigma) - \delta)} 
+ \left\langle e^{\frac{1}{2}a|\mathbf{\theta}_0 - \hat{\mathbf{\theta}}[\mathcal{G}]|^2} \right\rangle_{\mathcal{G}} e^{-\frac{1}{2}ad(\mu(\Sigma) + \delta)}
$$

(E28)

for $\alpha > 0$. Let us order the eigenvalues of $\Sigma$ in a such a way that $\lambda_1(\Sigma) \leq \lambda_2(\Sigma) \leq \cdots \leq \lambda_d(\Sigma)$ then, using (E4), for the moment generating functions in above we obtain

$$
\left\langle e^{-\frac{1}{2}a|\mathbf{\theta}_0 - \hat{\mathbf{\theta}}[\mathcal{G}]|^2} \right\rangle_{\mathcal{G}} = \int_0^\infty \Gamma_{N+1-d}(\omega) \, d\omega
\times \prod_{\ell=1}^d \left( 1 + \frac{\zeta \sigma_0^2}{\omega(1 - \zeta + 1/N)\lambda_\ell(\Sigma)} \right)^{-\frac{1}{2}}
\leq \int_0^\infty \Gamma_{N+1-d}(\omega) \, d\omega \left( 1 + \frac{\zeta \sigma_0^2}{\omega(1 - \zeta + 1/N)\lambda_1(\Sigma)} \right)^{-\frac{1}{2}}
$$

(E29)

and

$$
\left\langle e^{\frac{1}{2}a|\mathbf{\theta}_0 - \hat{\mathbf{\theta}}[\mathcal{G}]|^2} \right\rangle_{\mathcal{G}} = \int_0^\infty \Gamma_{N+1-d}(\omega) \, d\omega
\times \prod_{\ell=1}^d \left( 1 - \frac{\zeta \sigma_0^2}{\omega(1 - \zeta + 1/N)\lambda_\ell(\Sigma)} \right)^{-\frac{1}{2}}
\leq \int_0^\infty \Gamma_{N+1-d}(\omega) \, d\omega \left( 1 - \frac{\zeta \sigma_0^2}{\omega(1 - \zeta + 1/N)\lambda_d(\Sigma)} \right)^{-\frac{1}{2}}
$$

(E30)

Furthermore, by the inequalities $1/\lambda_d(\Sigma) \leq \frac{1}{2} \text{Tr} \left[ \Sigma^{-1} \right] \leq 1/\lambda_1(\Sigma)$ the mean $\mu(\lambda_d(\Sigma)) \leq \mu(\lambda) = \frac{\zeta \sigma_0^2}{(1 - \zeta - 1/N)a}$. The latter combined with the upper bounds in (E29) and (E30) gives us

$$
\text{Prob} \left[ \left| \mathbf{\theta}_0 - \hat{\mathbf{\theta}}[\mathcal{G}] \right|^2 \not\in (\mu(\Sigma) - \delta, \mu(\Sigma) + \delta) \right]
\leq \int_0^\infty \Gamma_{N+1-d}(\omega) \, d\omega \left( 1 + \frac{\zeta \sigma_0^2}{\omega(1 - \zeta + 1/N)\lambda_1(\Sigma)} \right)^{-\frac{1}{2}} e^{\frac{1}{2}ad(\mu(\lambda_1(\Sigma)) - \delta)}
+ \int_0^\infty \Gamma_{N+1-d}(\omega) \, d\omega \left( 1 - \frac{\zeta \sigma_0^2}{\omega(1 - \zeta + 1/N)\lambda_d(\Sigma)} \right)^{-\frac{1}{2}} e^{-\frac{1}{2}ad(\mu(\lambda_d(\Sigma)) + \delta)}
$$

(E31)

Finally, using similar steps leading us up to (E27) in above gives us

$$
\text{Prob} \left[ \left| \mathbf{\theta}_0 - \hat{\mathbf{\theta}}[\mathcal{G}] \right|^2 \not\in (\mu(\Sigma) - \delta, \mu(\Sigma) + \delta) \right]
\leq C_- e^{-N\Phi_-[a,\mu(\lambda_d),\delta]} + C_+ e^{-N\Phi_+[a,\mu(\lambda_1),\delta]},
$$

(E32)
for some constants $C_±$ and some sufficiently small $α > 0$. In above we have defined the (rate) functions

$$\Phi_−[α, μ(λ_1), δ] = \frac{ζ − 1 − ϕ_−(ω_0^−)}{2} + α ζ (μ(λ_d(Σ))) + δ,$$  \hspace{1cm} (E33)

where the function $ϕ_−(ω_0^−)$ is defined by (E14) and (E16) with $μ(λ)$ replaced by $μ(λ_d)$, and

$$\Phi_+[α, μ(λ_1), δ] = \frac{ζ − 1 − ϕ_+(ω_0^+)}{2} − α ζ (μ(λ_1(Σ)) − δ),$$  \hspace{1cm} (E34)

where the function $ϕ_+(ω_0^+)$ is defined by (E23) and (E24) with $α$ replaced by $αμ(λ_1)$. We note that for the first term in the above upper bound to vanish, as $(N, d) → ∞$, for arbitrary small $δ$ it is sufficient that $μ(λ_d) ≥ 1$, where $μ(λ) = \frac{ζσ_0^2(1 − ζ)}{α}$, but for $μ(λ_d) < 1$ for this to happen the $δ$ must be such that $δ > 1 − μ(λ_d)$. The second term in the upper bound is vanishing for any $δ ∈ (0, μ(λ))$.

Appendix F: Statistical properties of free energy

In this section we consider statistical properties of the (conditional) free energy

$$F_{β, σ^2} [D] = \frac{d}{2β} + \frac{1}{2σ^2} t^T (I_N − ZJ_{σ^2}^{-1}Z^T) t − \frac{1}{2β} \log \frac{2πσ^2}{J_{σ^2}^{-1}}.$$  \hspace{1cm} (F1)

assuming that $σ^2$ is independent from data $D$.

1. The average of free energy

Let us consider the average free energy

$$⟨F_{β, σ^2} [D]⟩_D = \frac{d}{2β} + \frac{1}{2σ^2} ⟨t^T (I_N − ZJ_{σ^2}^{-1}Z^T) t⟩_D − \frac{1}{2β} ⟨\log |2πσ^2 J_{σ^2}^{-1}|⟩_D$$

$$= \frac{d}{2β} + \frac{1}{2σ^2} ⟨t^T (I_N − ZJ_{σ^2}^{-1}Z^T) t⟩_Z − \frac{1}{2β} ⟨\log |2πσ^2 J_{σ^2}^{-1}|⟩_Z.$$  \hspace{1cm} (F2)
Now, assuming that the noise vector $\epsilon$ has mean 0 and covariance $\sigma_0^2 I_N$, the average

$$\langle t^T (I_N - ZJ_{\sigma^2_0} Z^T) t \rangle_{\epsilon}$$

$$= \langle \text{Tr} \left[ \left( I_N - ZJ_{\sigma^2_0} Z^T \right) tt^T \right] \rangle_{\epsilon}$$

$$= \text{Tr} \left[ \left( I_N - ZJ_{\sigma^2_0} Z^T \right) \langle (Z\theta_0 + \epsilon)(Z\theta_0 + \epsilon)^T \rangle_{\epsilon} \right]$$

$$= \text{Tr} \left[ \left( I_N - ZJ_{\sigma^2_0} Z^T \right) (Z\theta_0 \theta_0^T Z^T + 2Z\theta_0 \langle \epsilon \rangle_{\epsilon} + \langle \epsilon \epsilon^T \rangle_{\epsilon}) \right]$$

$$= \text{Tr} \left[ \left( I_N - ZJ_{\sigma^2_0} Z^T \right) (Z\theta_0 \theta_0^T Z^T + \sigma_0^2 I_N) \right]$$

$$= \theta_0^T Z^T \left( I_N - ZJ_{\sigma^2_0} Z^T \right) Z\theta_0 + \sigma_0^2 \text{Tr} \left[ I_N - ZJ_{\sigma^2_0} Z^T \right]$$

$$= \theta_0^T \left( J - J_{\sigma^2_0} J \right) \theta_0 + \sigma_0^2 \left( N - \text{Tr} \left[ J J_{\sigma^2_0} J \right] \right), \tag{F3}$$

and hence the average free energy is given by

$$\langle F_{\beta,\sigma^2} [\mathcal{D}] \rangle_\theta = \frac{d}{2\beta} + \frac{1}{2\sigma^2} \theta_0^T \left( J - J_{\sigma^2_0} J \right) \theta_0 + \frac{\sigma_0^2}{2\sigma^2} \left( N - \text{Tr} \left[ J J_{\sigma^2_0} J \right] \right)$$

$$- \frac{1}{2\beta} \langle \log \left| 2\pi \sigma^2 \beta^{-1} J_{\sigma^2_0} J \right| \rangle_Z. \tag{F4}$$

2. The variance of free energy

We also want to know the variance of (random) free energy $F_{\beta,\sigma^2} [\mathcal{D}]$. To this end we exploit the free energy equality $F = U - TS$ giving us the variance $\text{Var}(F) = \text{Var}(U - TS) = \text{Var}(U) - 2T \text{Cov}(U, S) + T^2 \text{Var}(S)$. The latter applied to (F1) gives us the variance

$$\text{Var} \left( F_{\beta,\sigma^2} [\mathcal{D}] \right) = \text{Var} \left( E[\mathcal{D}] \right) + T^2 \text{Var} \left( S[\mathcal{D}] \right) - 2T \text{Cov} \left( E[\mathcal{D}], S[\mathcal{D}] \right) \tag{F5}$$

Let us consider the energy variance

$$\text{Var} \left( E[\mathcal{D}] \right) = \text{Var} \left( \frac{d}{2\beta} + \frac{1}{2\sigma^2} \theta_0^T \left( J - J_{\sigma^2_0} J \right) \theta_0 \right) \tag{F6}$$

$$= \frac{1}{4\sigma^4} \text{Var} \left( (Z\theta_0 + \epsilon)^T \left( I_N - ZJ_{\sigma^2_0} Z^T \right) (Z\theta_0 + \epsilon) \right)$$

If we define $v = Z\theta_0$ and $A = \left( I_N - ZJ_{\sigma^2_0} Z^T \right)$ then above is of the form

$$\text{Var} \left( (v + \epsilon)^T A (v + \epsilon) \right)$$

$$= \text{Var} \left( v^T A v + 2 \epsilon^T A v + \epsilon^T A \epsilon \right)$$

$$= \text{Var} \left( v^T A v \right) + 4 \text{Var} \left( \epsilon^T A v \right) + \text{Var} \left( \epsilon^T A \epsilon \right)$$

$$+ 2 \left[ 2 \text{Cov} \left( v^T A v, \epsilon^T A \epsilon \right) + \text{Cov} \left( v^T A v, \epsilon^T A \epsilon \right) + 2 \text{Cov} \left( \epsilon^T A v, \epsilon^T A \epsilon \right) \right]. \tag{F7}$$

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In the following we will use that for
\( A = \left( I_N - ZJ^{-1}_{\sigma^2 \eta} Z^T \right) \) we have that \( \text{Tr}[A] = N - \text{Tr} \left[ JJ^{-1}_{\sigma^2 \eta} \right] \),
for \( A^2 = \left( I_N - 2ZJ^{-1}_{\sigma^2 \eta} Z^T + ZJ^{-1}_{\sigma^2 \eta} JJ^{-1}_{\sigma^2 \eta} Z^T \right) \) we have \( \text{Tr} [A^2] = \left( N - 2\text{Tr} \left[ JJ^{-1}_{\sigma^2 \eta} \right] + \text{Tr} \left[ \left( JJ^{-1}_{\sigma^2 \eta} \right)^2 \right] \right) \),
\( Z^T A Z = J - J J^{-1}_{\sigma^2 \eta} J \)
and \( Z^T A^2 Z = J \left( I_d - J^{-1}_{\sigma^2 \eta} J \right)^2 \). Now we compute each term in (E.Z) as follows:

1. \( \text{Var} (v^T A v) = \text{Var} \left( \theta_0^T Z^T \left( I_N - ZJ^{-1}_{\sigma^2 \eta} Z^T \right) Z \theta_0 \right) = \text{Var} \left( \theta_0^T \left( J - J J^{-1}_{\sigma^2 \eta} J \right) \theta_0 \right) = \left( \theta_0^T \left( J - J J^{-1}_{\sigma^2 \eta} J \right) \theta_0 \right)^2 \)
2. \( \text{Var} (e^T A v) = \langle \langle (e^T A v)^2 \rangle_e \rangle_z - \langle \langle e^T A v \rangle_e \rangle_z^2 = \langle \langle e^T A v \rangle^2 \rangle_e \rangle_z = \langle v^T A^T e e^T A v \rangle_z = \sigma_0^2 \langle v^T A^2 v \rangle_z = \sigma_0^2 \left( \theta_0^T Z^T \left( I_N - ZJ^{-1}_{\sigma^2 \eta} Z^T \right)^2 Z \theta_0 \right) \)
3. \( \text{Var} (e^T A e) = \langle \langle (e^T A e)^2 \rangle_e \rangle_z - \langle \langle e^T A e \rangle_e \rangle_z^2 = \sigma_0^2 \left( \langle \text{Tr}^2 [A] \rangle_z + 2 \langle \text{Tr}[A^2] \rangle_z - \langle \text{Tr}[A] \rangle_z^2 \right) = \sigma_0^2 \left[ \langle N - \text{Tr} \left[ JJ^{-1}_{\sigma^2 \eta} \right] \rangle_z^2 + 2 \langle N - 2\text{Tr} \left[ JJ^{-1}_{\sigma^2 \eta} \right] + \text{Tr} \left[ \left( JJ^{-1}_{\sigma^2 \eta} \right)^2 \right] \rangle_z \right] - \langle \left( N - \text{Tr} \left[ JJ^{-1}_{\sigma^2 \eta} \right] \right) \rangle_z^2 \)
4. \( \text{Cov} (v^T A v, e^T A v) = \langle \langle v^T A v e^T A v \rangle_e \rangle_z - \langle \langle v^T A v \rangle_e \rangle_z \langle \langle e^T A v \rangle_e \rangle_z = 0 \)
5. \( \text{Cov} (v^T A v, e^T A e) = \langle \langle v^T A v e^T A e \rangle_e \rangle_z - \langle \langle v^T A v \rangle_e \rangle_z \langle \langle e^T A e \rangle_e \rangle_z = \langle v^T A v \text{Tr} [A] e^T e \rangle_e \rangle_z - \langle v^T A v \rangle_z \langle \langle e^T A e \rangle_e \rangle_z = \sigma_0^2 \left( \langle \theta_0^T \left( J - J J^{-1}_{\sigma^2 \eta} J \right) \theta_0 \left( N - \text{Tr} [J J^{-1}_{\sigma^2 \eta}] \right) \rangle_z \right) - \langle \theta_0^T \left( J - J J^{-1}_{\sigma^2 \eta} J \right) \theta_0 \rangle_z \langle \left( N - \text{Tr} [J J^{-1}_{\sigma^2 \eta}] \right) \rangle_z \right) \)
6. \( \text{Cov} (\epsilon^T A v, \epsilon^T A \epsilon) = \langle \langle \epsilon^T A v \epsilon^T A \epsilon \rangle \rangle Z - \langle \langle \epsilon^T A v \rangle \rangle Z \langle \langle \epsilon^T A \epsilon \rangle \rangle Z = 0 \)

where in above we also used the following result

\[
\langle (\epsilon^T A \epsilon)^2 \rangle_{\epsilon} = \sum_{i_1,\ldots,i_4} \langle \epsilon_{i_1} \epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4} \rangle_{\epsilon} A_{i_1i_2} A_{i_3i_4} \\
= \sigma_0^4 \sum_{i_1,\ldots,i_4} \{ \delta_{i_1;i_2} \delta_{i_3;i_4} + \delta_{i_1;i_3} \delta_{i_2;i_4} + \delta_{i_1;i_4} \delta_{i_2;i_3} \} A_{i_1i_2} A_{i_3i_4} \\
= \sigma_0^4 \sum_{i_1,i_2} \{ A_{i_1i_1} A_{i_2i_2} + 2A^2_{i_1i_2} \} \\
= \sigma_0^4 \left( \text{Tr}^2[A] + 2\text{Tr}[A^2] \right). \\
\text{(F8)}
\]

Using all of the above results in \( \text{(F6)} \) we obtain

\[
4\sigma^4 \text{Var} (E[\mathcal{D}]) = \left( \langle \theta_0^T (J - J J^{-1}_{\sigma^2 \eta}) \theta_0 \rangle^2 \right)_Z - \left( \langle \theta_0^T (J - J J^{-1}_{\sigma^2 \eta}) \theta_0 \rangle \right)_Z^2 \\
+ 4\sigma_0^2 \theta_0^T \left( J \left( I_d - J J^{-1}_{\sigma^2 \eta} \right) \right)_Z^2 \theta_0 \\
+ \sigma_0^4 \left[ \left( N - \text{Tr} \left[ J J^{-1}_{\sigma^2 \eta} \right] \right)_Z^2 \\
+ 2 \left( \left( N - 2\text{Tr} \left[ J J^{-1}_{\sigma^2 \eta} \right] + \text{Tr} \left[ \left( J J^{-1}_{\sigma^2 \eta} \right)_Z^2 \right] \right)_Z \\
- \left( \left( N - \text{Tr} \left[ J J^{-1}_{\sigma^2 \eta} \right] \right)_Z^2 \right) \right] \\
+ 2\sigma_0^2 \left( \langle \theta_0^T (J - J J^{-1}_{\sigma^2 \eta}) \theta_0 \left( N - \text{Tr}[J J^{-1}_{\sigma^2 \eta}] \right)_Z \langle \langle \left( N - \text{Tr}[J J^{-1}_{\sigma^2 \eta}] \right)_Z \rangle \right) \right)_Z, \\
\text{(F9)}
\]

the entropy variance is given by

\[
\text{Var} (S[\mathcal{D}]) = \text{Var} \left( \frac{1}{2} \log |2\pi \sigma^2 \beta^{-1} J^{-1}_{\sigma^2 \eta}| \right) \\
= \frac{1}{4} \langle \log^2 |J^{-1}_{\sigma^2 \eta}| \rangle_Z - \frac{1}{4} \langle \log |J^{-1}_{\sigma^2 \eta}| \rangle_Z^2 \\
\text{(F10)}
\]
and the covariance

\[
\text{Cov} (E[\mathcal{D}], S[\mathcal{D}]) = \text{Cov} \left( \frac{d}{2\beta} + \frac{1}{2\sigma^2} t^T \left( I_N - Z J\sigma^2 \epsilon^T Z^T \right) t, \frac{d}{2} \log(2\pi e \sigma^2 \beta^{-1}) + \frac{1}{2} \log |J^{-1}| \right)
\]

\[
= \frac{1}{4\sigma^2} \text{Cov} \left( t^T \left( I_N - Z J\sigma^2 \epsilon^T Z^T \right) t, \log |J^{-1}| \right)
\]

\[
= \frac{1}{4\sigma^2} \left\langle t^T \left( I_N - Z J\sigma^2 \epsilon^T Z^T \right) t, \log |J^{-1}| \right\rangle_Z - \frac{1}{4\sigma^2} \left\langle t^T \left( I_N - Z J\sigma^2 \epsilon^T Z^T \right) t, \log |J^{-1}| \right\rangle_Z
\]

\[
= \frac{1}{4\sigma^2} \left\langle \theta_0^T \left( J - J J\sigma^2 \epsilon^T J \right) \theta_0 + \sigma_0^2 \left( N - \text{Tr} \left[ J J\sigma^2 \epsilon^T J \right] \right), \log |J^{-1}| \right\rangle_Z
\]

\[
= \frac{1}{4\sigma^2} \left\langle \theta_0^T \left( J - J J\sigma^2 \epsilon^T J \right) \theta_0 + \sigma_0^2 \left( N - \text{Tr} \left[ J J\sigma^2 \epsilon^T J \right] \right), \log |J^{-1}| \right\rangle_Z
\]

Finally, using the results (F9), (F10) and (F11) the variance of free energy follows from the equation (F15).

3. Free energy of ML inference

For \( \eta = 0 \) the matrix \( J\sigma^2 = J \) and the average free energy (F4) is given by

\[
\langle F_{\beta, \sigma^2} [\mathcal{D}] \rangle_Z = \frac{d}{2\beta} + \frac{1}{2\sigma^2} \theta_0^T \left( J - J J\sigma^2 \epsilon^T J \right) \theta_0 + \sigma_0^2 \left( N - \text{Tr} \left[ J J\sigma^2 \epsilon^T J \right] \right) \left\langle \log |J^{-1}| \right\rangle_Z
\]

\[
= \frac{d}{2\beta} + \frac{\sigma_0^2}{2\sigma^2} (N - d) - \frac{d}{2\beta} \log(2\pi e \sigma^2) + \frac{d}{2\beta} \log(\beta) + \frac{1}{2\beta} \left\langle \log |J| \right\rangle_Z \quad (F12)
\]

Let us assume that \( Z = Z/\sqrt{d} \) then from above follows the average free energy density

\[
\frac{1}{N} \langle F_{\beta, \sigma^2} [\mathcal{D}] \rangle_Z = \frac{1}{2\sigma^2} \left( 1 - \zeta \right) + \frac{\zeta}{2\beta} \log \left( \frac{\beta}{2\pi \sigma^2 \zeta^2} \right) + \frac{\zeta}{2\beta} \int d\lambda \left\langle \rho_d(\lambda|Z) \right\rangle_Z \log \lambda \quad (F13)
\]

where in above we defined the density of eigenvalues

\[
\rho_d(\lambda|Z) = \frac{1}{d} \sum_{\ell=1}^d \delta \left( \lambda - \lambda_\ell \left( \frac{1}{N} Z^T Z \right) \right). \quad (F14)
\]

Let us now consider the free energy variance (F3) for \( \eta = 0 \) and \( Z = Z/\sqrt{d} \). Firstly, we consider the energy variance (F9) which is given by

\[
\text{Var} (E[\mathcal{D}]) = \frac{\sigma_0^4}{2\sigma^4} (N - d) \quad (F15)
\]
and from above follows that

$$\text{Var} \left( \frac{E[\mathcal{D}]}{N} \right) = \frac{\sigma_0^4}{2\sigma^4} \frac{(1 - \zeta)}{N}. \quad (F16)$$

Secondly, the entropy variance \((F10)\) is given by

$$\text{Var} \left( S[\mathcal{D}] \right) = \frac{1}{4} \langle \log^2 |J| \rangle_\mathcal{Z} - \frac{1}{4} \langle \log |J| \rangle_\mathcal{Z}^2 \nonumber$$

$$= \frac{d^2}{4} \left[ \left\langle \left( \frac{1}{d} \sum_{\ell=1}^d \log \lambda_\ell \right)^2 \right\rangle_\mathcal{Z} - \left\langle \frac{1}{d} \sum_{\ell=1}^d \log \lambda_\ell \right\rangle_\mathcal{Z}^2 \right] \nonumber$$

$$= \frac{d^2}{4} \left[ \left\langle \left( \int d\lambda \rho_d(\lambda|\mathcal{Z}) \log \lambda \right)^2 \right\rangle_\mathcal{Z} - \left\langle \int d\lambda \rho_d(\lambda|\mathcal{Z}) \log \lambda \right\rangle_\mathcal{Z}^2 \right] \quad (F17)$$

and from above follows

$$\text{Var} \left( \frac{S[\mathcal{D}]}{N} \right) = \frac{\zeta^2}{4} \left[ \left\langle \left( \int d\lambda \rho_d(\lambda|\mathcal{Z}) \log \lambda \right)^2 \right\rangle_\mathcal{Z} - \left\langle \int d\lambda \rho_d(\lambda|\mathcal{Z}) \log \lambda \right\rangle_\mathcal{Z}^2 \right] \quad (F18)$$

Finally, we consider the covariance \((F11)\) which gives us

$$\text{Cov} \left( E[\mathcal{D}], S[\mathcal{D}] \right) = \frac{\sigma_0^2}{4\sigma^2} (N - d) \left\langle \log \left| J^{-1}_{\sigma^2,\eta} \right| \right\rangle_\mathcal{Z} - \frac{\sigma_0^2}{4\sigma^2} (N - d) \left\langle \log \left| J^{-1}_{\sigma^2,\eta} \right| \right\rangle_\mathcal{Z} = 0 \quad (F19)$$

Now using above results in the identity \((F5)\) we obtain the variance of free energy

$$\text{Var} \left( \frac{F_{\beta,\sigma^2}[\mathcal{D}]}{N} \right) = \text{Var} \left( \frac{E[\mathcal{D}]}{N} \right) + T^2 \text{Var} \left( \frac{S[\mathcal{D}]}{N} \right) \nonumber$$

$$= \frac{\sigma_0^4}{2\sigma^4} \frac{(1 - \zeta)}{N} + \frac{\zeta^2}{4\beta^2} \int \int \left[ \left\langle \rho_d(\lambda|\mathcal{Z}) \rho_d(\tilde{\lambda}|\mathcal{Z}) \right\rangle_\mathcal{Z} - \left\langle \rho_d(\lambda|\mathcal{Z}) \right\rangle_\mathcal{Z} \left\langle \rho_d(\tilde{\lambda}|\mathcal{Z}) \right\rangle_\mathcal{Z} \right] \times \log(\lambda) \log(\tilde{\lambda}) \, d\lambda \, d\tilde{\lambda} \quad (F20)$$
a. Free energy of MAP inference

Let us assume that the true parameters $\theta_0$ are random with the mean $0$ and covariance $S^2 I_d$ and consider the average of $\langle F_4 \rangle$ as follows

$$\langle F_4 \rangle \approx \frac{d}{2 \beta} + \frac{1}{2 \sigma^2} \left( \langle \theta_0^T (J - JJ_{\sigma^2 \eta}) \theta_0 \rangle \right)_{\theta_0} + \frac{\sigma_0^2}{2 \sigma^2} \left( N - \langle \text{Tr} \left[ JJ_{\sigma^2 \eta}^{-1} \right] \rangle \right)_{\theta_0} \langle \log |2 \pi e \sigma^2 \beta^{-1} JJ_{\sigma^2 \eta}^{-1}| \rangle_{\theta_0}$$

$$= \frac{d}{2 \beta} + \frac{1}{2 \sigma^2} \left( \langle \text{Tr} \left[ (J - JJ_{\sigma^2 \eta}) (\theta_0 \theta_0^T) \theta_0 \right] \right)_{\theta_0} + \frac{\sigma_0^2}{2 \sigma^2} \left( N - \langle \text{Tr} \left[ JJ_{\sigma^2 \eta}^{-1} \right] \rangle \right) \langle \log |2 \pi e \sigma^2 \beta^{-1} JJ_{\sigma^2 \eta}^{-1}| \rangle_{\theta_0}$$

$$= \frac{d}{2 \beta} + \frac{S^2}{2 \sigma^2} \left( \langle \text{Tr} \left[ (J - JJ_{\sigma^2 \eta}) \right] \rangle \right)_{\theta_0} + \frac{\sigma_0^2}{2 \sigma^2} \left( N - \langle \text{Tr} \left[ JJ_{\sigma^2 \eta}^{-1} \right] \rangle \right) \langle \log |2 \pi e \sigma^2 \beta^{-1} JJ_{\sigma^2 \eta}^{-1}| \rangle_{\theta_0}$$

$$= \frac{d}{2 \beta} + \frac{S^2}{2 \sigma^2} \left( \langle \text{Tr} \left[ (J - JJ_{\sigma^2 \eta}) \right] \rangle \right)_{\theta_0} + \frac{\sigma_0^2}{2 \sigma^2} \left( N - \langle \text{Tr} \left[ JJ_{\sigma^2 \eta}^{-1} \right] \rangle \right) \langle \log |2 \pi e \sigma^2 \beta^{-1} JJ_{\sigma^2 \eta}^{-1}| \rangle_{\theta_0} \rangle \langle \log |2 \pi e \sigma^2 \beta^{-1} JJ_{\sigma^2 \eta}^{-1}| \rangle_{\theta_0}.$$

In above we assumed $Z = Z/\sqrt{d}$ and used that $J = J/\zeta$ and $J_{\sigma^2 \eta}^{-1} = \zeta J_{\sigma^2 \eta}^{-1}$, where $J = Z^T Z/N$, for this scaling of $Z$.

Let us consider the product of matrices $JJ_{\eta}^{-1} = J (J + \eta I_d)^{-1} = ((J + \eta I_d) J^{-1})^{-1} = (I_d + \eta J^{-1})^{-1}$ and hence

$$\text{Tr} \left[ JJ_{\eta}^{-1} \right] = \text{Tr} \left[ (I_d + \eta J^{-1})^{-1} \right] = \sum_{\ell=1}^d \frac{1}{\lambda_\ell} (I_d + \eta J^{-1}) = \sum_{\ell=1}^d \frac{1}{(1 + \eta \lambda_\ell) J^{-1})}$$

$$= \sum_{\ell=1}^d \frac{1}{(1 + \eta \lambda_\ell^{-1}) (J)} = \sum_{\ell=1}^d \lambda_\ell (J) / (\lambda_\ell (J) + \eta).$$

Also for

$$J^2 J_{\eta}^{-1} = J^2 (J + \eta I_d)^{-1} = J (I_d + \eta J^{-1})^{-1} = ((I_d + \eta J^{-1}) J^{-1})^{-1} = (J^{-1} + \eta J^{-2})$$

and

$$J_{\eta}^{-1} J^2 = (J + \eta I_d)^{-1} J^2 = (I_d + \eta J^{-1})^{-1} J = (J^{-1} + \eta J^{-2})^{-1},$$

i.e. the matrices $J^2$ and $(J + \eta I_d)^{-1}$ commute, so

$$\text{Tr} \left[ JJ_{\eta}^{-1} \right] = \text{Tr} \left[ J^2 J_{\eta}^{-1} \right] = \sum_{\ell=1}^d \lambda_\ell (J^2) / \lambda_\ell (J) = \sum_{\ell=1}^d \frac{\lambda_\ell^2 (J)}{\lambda_\ell (J)}.$$

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Now

\[ J_\eta = (J + \eta I_d) = J (I_d + \eta J^{-1}) = (I_d + \eta J^{-1}) J \]  

(F26)

and hence

\[ \lambda_\ell (J_\eta) = \lambda_\ell (J) \lambda_\ell (I_d + \eta J^{-1}) = \lambda_\ell (J) \left( 1 + \eta \lambda_\ell (J^{-1}) \right) = \lambda_\ell (J) + \eta. \]  

(F27)

Thus \( \text{Tr} \left[ JJ_\eta^{-1} J \right] = \sum_{\ell=1}^d \lambda_\ell^2 (J) / (\lambda_\ell (J) + \eta) \). Finally, we consider the inverse

\[ J_\eta^{-1} = (J + \eta I_d)^{-1} = (I_d + \eta J^{-1})^{-1} = J^{-1} (I_d + \eta J^{-1})^{-1}, \]  

(F28)

i.e. the matrices \( J^{-1} \) and \( (I_d + \eta J^{-1})^{-1} \) commute, and hence the \( \ell \)-th eigenvalue

\[
\lambda_\ell (J_\eta^{-1}) = \lambda_\ell \left( J^{-1} (I_d + \eta J^{-1})^{-1} \right) = \lambda_\ell (J^{-1}) \lambda_\ell \left( (I_d + \eta J^{-1})^{-1} \right) \\
= \lambda_\ell^{-1} (J) \lambda_\ell^{-1} (I_d + \eta J^{-1}) = \lambda_\ell^{-1} (J) \lambda_\ell^{-1} (I_d + \eta J^{-1}) \\
= \lambda_\ell^{-1} (J) (1 + \eta \lambda_\ell^{-1} (J))^{-1} = 1 / (\lambda_\ell (J) + \eta).
\]  

(F29)

Now using above results for matrices in (F21) allows to compute average free energy as follows

\[
\left\langle \left\langle \frac{1}{N} F_{\beta, \sigma^2} [\rho] \right\rangle_{\mathcal{B}_c} \right\rangle = \frac{\zeta}{2\beta} + \frac{S^2}{2\zeta \sigma^2} \frac{1}{N} \left\langle \text{Tr} \left[ (J - JJ_{\zeta \sigma^2}^{-1} J) \right] \right\rangle_Z \\
+ \frac{\sigma_0^2}{2\sigma^2} \left( 1 - \frac{1}{N} \left\langle \text{Tr} \left[ JJ_{\zeta \sigma^2}^{-1} \right] \right\rangle_Z \right) \\
- \frac{1}{2\beta} \frac{1}{N} \left\langle \log \left| 2\pi \sigma^2 \beta^{-1} \zeta J_{\zeta \sigma^2}^{-1} \right| \right\rangle_Z \\
= \frac{\zeta}{2\beta} + \frac{S^2}{2\zeta \sigma^2} \frac{d}{Nd} \sum_{\ell=1}^d \left\langle \lambda_\ell (J) - \frac{\lambda_\ell^2 (J)}{\lambda_\ell (J) + \zeta \sigma^2} \right\rangle_Z \\
+ \frac{\sigma_0^2}{2\sigma^2} \left( 1 - \frac{d}{Nd} \left\langle \sum_{\ell=1}^d \frac{\lambda_\ell (J)}{\lambda_\ell (J) + \zeta \sigma^2} \right\rangle_Z \right) \\
- \frac{\zeta}{2\beta} \log \left( 2\pi \sigma^2 \beta^{-1} \zeta \right) \\
+ \frac{\zeta}{2\beta} \frac{1}{d} \left( \sum_{\ell=1}^d \log \left( \lambda_\ell (J) + \zeta \sigma^2 \right) \right)_Z \\
= \frac{\zeta}{2\beta} + \frac{S^2 \zeta \eta}{2} \int \langle \rho_d (\lambda | Z) \rangle_Z \frac{\lambda}{\lambda + \zeta \sigma^2} \lambda d\lambda \\
+ \frac{\sigma_0^2}{2\sigma^2} \left( 1 - \zeta \int \langle \rho_d (\lambda | Z) \rangle_Z \frac{\lambda}{\lambda + \zeta \sigma^2} \lambda d\lambda \right) \\
- \frac{\zeta}{2\beta} \log \left( 2\pi \sigma^2 \beta^{-1} \zeta \right) \\
+ \frac{\zeta}{2\beta} \int \langle \rho_d (\lambda | Z) \rangle_Z \log \left( \lambda + \zeta \sigma^2 \right) \lambda d\lambda \quad \text{ (F30)}
\]
and hence the average free energy density is given by

\[
\left\langle \left\langle \frac{1}{N} F_{\beta,\sigma^2}[\mathcal{G}] \right\rangle \right\rangle_{\Theta_0} = \frac{\zeta}{2\beta} + \frac{S^2\zeta\eta}{2} \int \langle \rho_d(\lambda|Z) \rangle_z \frac{\lambda}{\lambda + \zeta\sigma^2\eta} d\lambda \\
+ \frac{\sigma_0^2}{2\sigma^2} \left( 1 - \zeta \int \langle \rho_d(\lambda|Z) \rangle_z \frac{\lambda}{\lambda + \zeta\sigma^2\eta} d\lambda \right) \\
- \frac{\zeta}{2\beta} \log (2\pi\sigma^2\beta^{-1}\zeta) \\
+ \frac{\zeta}{2\beta} \int \langle \rho_d(\lambda|Z) \rangle_z \log (\lambda + \zeta\sigma^2\eta) d\lambda
\]  

(F31)

We note that in derivation of above results the following eigenvalue identities

\[
\lambda_\ell (J^{-1}_\eta) = \frac{1}{\lambda_\ell (J) + \eta} \\
\lambda_\ell (JJ^{-1}_\eta) = \frac{\lambda_\ell (J)}{\lambda_\ell (J) + \eta} \\
\lambda_\ell (J - JJ^{-1}_\eta J) = \lambda_\ell ((I_d - JJ^{-1}_\eta) J) = \lambda_\ell (J (I_d - JJ^{-1}_\eta)) \\
= \lambda_\ell (J) \lambda_\ell (I_d - JJ^{-1}_\eta) = \frac{\eta\lambda_\ell (J)}{\lambda_\ell (J) + \eta}.
\]  

(F32)

where in above we used \( JJ^{-1}_\eta = J^{-1}_\eta J \), from which follow the identities

\[
\text{Tr} [J - JJ^{-1}_\eta] = d\eta \int \rho_d(\lambda|Z) \frac{\lambda}{\lambda + \eta} d\lambda \\
\text{Tr} [JJ^{-1}_\eta] = d \int \rho_d(\lambda|Z) \frac{\lambda}{\lambda + \eta} d\lambda
\]  

(F33)

were useful.

Finally, we compute variance of the free energy (F1). First, we consider the energy
variance (F9) which is given by

\[
4\sigma^4 \text{Var}(E[\mathcal{Q}]) = \left\langle \left( \theta_0^T \left( J - JJ_{\sigma^2\eta}^{-1} J \right) \theta_0 \right)^2 \right\rangle_{\mathcal{Q}} - \left\langle \left( \theta_0^T \left( J - JJ_{\sigma^2\eta}^{-1} J \right) \theta_0 \right)^2 \right\rangle_{\mathcal{Q}}
\]

\[
+ 4 \left\langle \sigma_0^2 \theta_0^T \left( J \left( \mathbf{I}_d - J_{\sigma^2\eta}^{-1} J \right) \right)^2 \theta_0 \right\rangle_{\mathcal{Q}}
\]

\[
+ \sigma_0^4 \left\langle \left( N - \text{Tr} \left[ JJ_{\sigma^2\eta}^{-1} \right] \right)^2 \right\rangle_{\mathcal{Q}}
\]

\[
\langle \langle \left( \left( J - JJ_{\sigma^2\eta}^{-1} J \right)^2 \right) \theta_0 \rangle_{\mathcal{Q}} \rangle_{\mathcal{Q}}
\]

\[
+ 2 \left\langle \left( N - 2 \text{Tr} \left[ JJ_{\sigma^2\eta}^{-1} \right] + \text{Tr} \left[ \left( JJ_{\sigma^2\eta}^{-1} \right)^2 \right] \right) \theta_0 \right\rangle_{\mathcal{Q}} \left\langle \left( N - \text{Tr} \left[ JJ_{\sigma^2\eta}^{-1} \right] \right) \right\rangle_{\mathcal{Q}}
\]

\[
= S^4 \left\langle \text{Tr}^2 \left[ \left( J - JJ_{\sigma^2\eta}^{-1} J \right) \right] + 2 \text{Tr} \left[ \left( J - JJ_{\sigma^2\eta}^{-1} J \right)^2 \right] \right\rangle_{\mathcal{Q}}
\]

\[
- S^4 \left\langle \text{Tr} \left[ J - JJ_{\sigma^2\eta}^{-1} J \right] \right\rangle_{\mathcal{Q}}
\]

\[
+ 4 \sigma_0^2 S^2 \left\langle \text{Tr} \left[ J \left( \mathbf{I}_d - J_{\sigma^2\eta}^{-1} J \right)^2 \right] \right\rangle_{\mathcal{Q}}
\]

\[
+ \sigma_0^4 \left\langle \left( N - \text{Tr} \left[ JJ_{\sigma^2\eta}^{-1} \right] \right)^2 \right\rangle_{\mathcal{Q}}
\]

\[
+ 2 \left\langle \left( N - 2 \text{Tr} \left[ JJ_{\sigma^2\eta}^{-1} \right] + \text{Tr} \left[ \left( JJ_{\sigma^2\eta}^{-1} \right)^2 \right] \right) \right\rangle_{\mathcal{Q}}
\]

\[
- \left\langle \left( N - \text{Tr} \left[ JJ_{\sigma^2\eta}^{-1} \right] \right)^2 \right\rangle_{\mathcal{Q}}
\]

\[
+ 2 \sigma_0^2 S^2 \left\langle \text{Tr} \left[ J - JJ_{\sigma^2\eta}^{-1} J \right] \left( N - \text{Tr} \left[ JJ_{\sigma^2\eta}^{-1} \right] \right) \right\rangle_{\mathcal{Q}}
\]

\[
- \left\langle \text{Tr} \left[ J - JJ_{\sigma^2\eta}^{-1} J \right] \right\rangle_{\mathcal{Q}} \left\langle \left( N - \text{Tr} \left[ JJ_{\sigma^2\eta}^{-1} \right] \right) \right\rangle_{\mathcal{Q}}
\]

\[\text{(F34)}\]
where we have used (F8), and hence for $Z = Z/\sqrt{d}$ we have

$$
4\sigma^4 \text{Var} \left( \frac{E[\mathcal{D}]}{N} \right)
= \frac{S^4}{\zeta^2 N^2} \left\langle \text{Tr}^2 \left[ \left( J - JJ^{-1}_{\zeta \sigma^2 \eta} J \right) \right] + 2 \text{Tr} \left[ \left( J - JJ^{-1}_{\zeta \sigma^2 \eta} J \right)^2 \right] \right\rangle_Z - \frac{S^4}{\zeta^2 N^2} \left\langle \text{Tr} \left[ J - JJ^{-1}_{\zeta \sigma^2 \eta} J \right]^2 \right\rangle_Z
+ \frac{4\sigma_0^2 S^2}{\zeta N^2} \left\langle \text{Tr} \left[ J \left( I_d - JJ^{-1}_{\zeta \sigma^2 \eta} J \right)^2 \right] \right\rangle_Z
+ \frac{\sigma_0^4}{N^2} \left\langle \left( N - \text{Tr} \left[ JJ^{-1}_{\zeta \sigma^2 \eta} J \right] \right)^2 \right\rangle_Z
+ 2 \left\langle \left( N - 2 \text{Tr} \left[ JJ^{-1}_{\zeta \sigma^2 \eta} J \right] + \text{Tr} \left[ \left( JJ^{-1}_{\zeta \sigma^2 \eta} J \right)^2 \right] \right) \right\rangle_Z
- \left\langle \left( N - \text{Tr} \left[ JJ^{-1}_{\zeta \sigma^2 \eta} J \right] \right)^2 \right\rangle_Z

+ 2\sigma_0^2 S^2 \frac{1}{\zeta N^2} \left\langle \text{Tr} \left[ J - JJ^{-1}_{\zeta \sigma^2 \eta} J \right] \left( N - \text{Tr} \left[ JJ^{-1}_{\zeta \sigma^2 \eta} J \right] \right) \right\rangle_Z
- \left\langle \text{Tr} \left[ J - JJ^{-1}_{\zeta \sigma^2 \eta} J \right] \left( N - \text{Tr} \left[ JJ^{-1}_{\zeta \sigma^2 \eta} J \right] \right) \right\rangle_Z

= \frac{S^4}{\zeta^2 N^2} \left\langle \left[ d\zeta \sigma^2 \eta \int \rho_d(\lambda|Z) \frac{\lambda}{\lambda + \zeta \sigma^2 \eta} d\lambda \right]^2 + 2d(\zeta \sigma^2 \eta)^2 \int \rho_d(\lambda|Z) \left( \frac{\lambda}{\lambda + \zeta \sigma^2 \eta} \right)^2 d\lambda \right\rangle_Z
- \frac{S^4}{\zeta^2 N^2} \left\langle d\zeta \sigma^2 \eta \int \rho_d(\lambda|Z) \frac{\lambda}{\lambda + \zeta \sigma^2 \eta} d\lambda \right\rangle_Z^2
+ \frac{4\sigma_0^2 S^2}{\zeta N^2} \left\langle d(\zeta \sigma^2 \eta)^2 \int \rho_d(\lambda|Z) \frac{\lambda}{(\lambda + \zeta \sigma^2 \eta)^2} d\lambda \right\rangle_Z
+ \frac{\sigma_0^4}{N^2} \left\langle \left( 1 - \frac{d}{N} \int \rho_d(\lambda|Z) \frac{\lambda}{\lambda + \zeta \sigma^2 \eta} d\lambda \right)^2 \right\rangle_Z
+ 2\frac{1}{N^2} \left\langle \left( N - 2d \int \rho_d(\lambda|Z) \frac{\lambda}{\lambda + \zeta \sigma^2 \eta} d\lambda + d \int \rho_d(\lambda|Z) \left( \frac{\lambda}{\lambda + \zeta \sigma^2 \eta} \right)^2 d\lambda \right) \right\rangle_Z
- \left\langle \left( 1 - \frac{d}{N} \int \rho_d(\lambda|Z) \frac{\lambda}{\lambda + \zeta \sigma^2 \eta} d\lambda \right)^2 \right\rangle_Z
+ 2\sigma_0^2 S^2 \frac{1}{\zeta} \left\langle \left[ d\zeta \sigma^2 \eta \int \rho_d(\lambda|Z) \frac{\lambda}{\lambda + \zeta \sigma^2 \eta} d\lambda \left( 1 - \frac{d}{N} \int \rho_d(\lambda|Z) \frac{\lambda}{\lambda + \zeta \sigma^2 \eta} d\lambda \right) \right] \right\rangle_Z
- \left\langle \left[ \frac{d}{N} \zeta \sigma^2 \eta \int \rho_d(\lambda|Z) \frac{\lambda}{\lambda + \zeta \sigma^2 \eta} d\lambda \right] \left( 1 - \frac{d}{N} \int \rho_d(\lambda|Z) \frac{\lambda}{\lambda + \zeta \sigma^2 \eta} d\lambda \right) \right\rangle_Z

= \zeta^2 \left( S^4 \sigma^4 \eta^2 + \sigma_0^4 - 2\sigma_0^2 S^2 \sigma^2 \eta \right) \left\langle \left( \int \rho_d(\lambda|Z) \frac{\lambda}{\lambda + \zeta \sigma^2 \eta} d\lambda \right)^2 \right\rangle_Z
- \left\langle \int \rho_d(\lambda|Z) \frac{\lambda}{\lambda + \zeta \sigma^2 \eta} d\lambda \right\rangle_Z^2 + O(1/N)
$$

(F35)
From above follows that

\[
\text{Var} \left( \frac{E[\mathcal{D}]}{N} \right) = \frac{\zeta^2}{4\sigma^4} \left( S^4\sigma^4\eta^2 + \sigma_0^4 - 2\sigma_0^2S^2\sigma^2\eta \right)
\]

\[
\times \left[ \left\langle \left( \int \rho_d(\lambda|Z) \frac{\lambda}{\lambda + \zeta\sigma^2\eta} \lambda \right)^2 \right\rangle_Z - \left\langle \left( \int \rho_d(\lambda|Z) \frac{\lambda}{\lambda + \zeta\sigma^2\eta} \lambda \right)^2 \right\rangle_Z \right] + O(1/N). \quad (F36)
\]

Furthermore, the covariance (F11) can be computed as follows

\[
4\sigma^2 \text{Cov} \left( E[\mathcal{D}], S[\mathcal{D}] \right) = \text{Cov} \left( t^T \left( I_N - ZJJ^{-1}_{\sigma^2\eta} Z^T \right) t, \log \left| J^{-1}_{\sigma^2\eta} \right| \right)
\]

\[
= \left\langle \left[ \left\langle \theta_0^T \left( J - JJ^{-1}_{\sigma^2\eta} J \right) \theta_0 \right\rangle_{\theta_0} + \cdots \right. \right. \\
\cdots + \sigma_0^2 \left( N - \text{Tr} \left[ JJ^{-1}_{\sigma^2\eta} \right] \right) \log \left| J^{-1}_{\sigma^2\eta} \right| \right\rangle_Z \\
- \left\langle \left[ \left\langle \theta_0^T \left( J - JJ^{-1}_{\sigma^2\eta} J \right) \theta_0 \right\rangle_{\theta_0} + \cdots \right. \right. \\
\cdots + \sigma_0^2 \left( N - \text{Tr} \left[ JJ^{-1}_{\sigma^2\eta} \right] \right) \left\rangle \log \left| J^{-1}_{\sigma^2\eta} \right| \right\rangle_Z \\
= \left\langle \left[ S^2 \text{Tr} \left[ J - JJ^{-1}_{\sigma^2\eta} J \right] + \cdots \right. \right. \\
\cdots + \sigma_0^2 \left( N - \text{Tr} \left[ JJ^{-1}_{\sigma^2\eta} \right] \right) \log \left| J^{-1}_{\sigma^2\eta} \right| \right\rangle_Z \\
- \left\langle \left[ S^2 \text{Tr} \left[ J - JJ^{-1}_{\sigma^2\eta} J \right] + \cdots \right. \right. \\
\cdots + \sigma_0^2 \left( N - \text{Tr} \left[ JJ^{-1}_{\sigma^2\eta} \right] \right) \left\rangle \log \left| J^{-1}_{\sigma^2\eta} \right| \right\rangle_Z \quad (F37)
\]
From above for \( Z = Z/\sqrt{d} \) follows the result

\[
4 \sigma^2 \text{Cov} \left( E[\mathscr{D}] / N, S[\mathscr{D}] / N \right)
= \left\langle \left[ S^2 \frac{1}{ \zeta N } \text{Tr} \left[ J - J J^{-1}_{\zeta \sigma^2} J \right] + \ldots \right. \right.
\left. \ldots + \sigma_0^2 \left( 1 - \frac{1}{N} \text{Tr} \left[ J J^{-1}_{\zeta \sigma^2} \right] \right) \right\rangle \frac{1}{N} \log \left| J J^{-1}_{\zeta \sigma^2} \right|_Z
- \left\langle \left[ S^2 \frac{1}{ \zeta N } \text{Tr} \left[ J - J J^{-1}_{\zeta \sigma^2} J \right] + \ldots \right. \right.
\left. \ldots + \sigma_0^2 \left( 1 - \frac{1}{N} \text{Tr} \left[ J J^{-1}_{\zeta \sigma^2} \right] \right) \right\rangle \frac{1}{N} \left\langle \log \left| J J^{-1}_{\zeta \sigma^2} \right|_Z \right\rangle
\]

\[
= \zeta \int \int \left[ \langle \rho_d(\lambda | Z) \rangle_Z \langle \rho_d(\tilde{\lambda} | Z) \rangle_Z - \langle \rho_d(\lambda | Z) \rangle_Z \langle \rho_d(\tilde{\lambda} | Z) \rangle_Z \right]
\times \left[ S^2 \frac{\lambda \zeta \sigma^2 \eta}{\lambda + \zeta \sigma^2 \eta} + \sigma_0^2 \left( 1 - \frac{\lambda \zeta}{\lambda + \zeta \sigma^2 \eta} \right) \right]
\times \log \left( \tilde{\lambda} + \zeta \sigma^2 \eta \right) d\lambda d\tilde{\lambda}.
\] (F38)

Finally, the entropy variance (F10) for \( Z = Z/\sqrt{d} \) is given by

\[
\text{Var} \left( \frac{S[\mathscr{D}]}{N} \right) = \frac{\epsilon^2}{4} \int \int \left[ \langle \rho_d(\lambda | Z) \rangle_Z \langle \rho_d(\tilde{\lambda} | Z) \rangle_Z - \langle \rho_d(\lambda | Z) \rangle_Z \langle \rho_d(\tilde{\lambda} | Z) \rangle_Z \right]
\times \log \left( \lambda + \zeta \sigma^2 \eta \right) \log \left( \tilde{\lambda} + \zeta \sigma^2 \eta \right) d\lambda d\tilde{\lambda}.
\] (F39)

Using all of the above results in (F5) we obtain the free energy variance

\[
\text{Var} \left( \frac{F_{\beta, \sigma^2} [\mathscr{D}]}{N} \right) = \int \int \left[ \langle \rho_d(\lambda | Z) \rangle_Z \langle \rho_d(\tilde{\lambda} | Z) \rangle_Z - \langle \rho_d(\lambda | Z) \rangle_Z \langle \rho_d(\tilde{\lambda} | Z) \rangle_Z \right]
\times \left\{ \frac{\zeta^2}{4\sigma^4} \left( S^4 \sigma^4 \eta^2 + \sigma_0^4 - 2\sigma_0^2 S^2 \sigma^2 \eta \right) \right.
\frac{\lambda}{\lambda + \zeta \sigma^2 \eta} \frac{\tilde{\lambda}}{\tilde{\lambda} + \zeta \sigma^2 \eta}
+ \frac{T^2 \zeta^2}{4} \log \left( \lambda + \zeta \sigma^2 \eta \right) \log \left( \tilde{\lambda} + \zeta \sigma^2 \eta \right)
- \frac{T \zeta}{2\sigma^2} \left[ S^2 \frac{\lambda \zeta \sigma^2 \eta}{\lambda + \zeta \sigma^2 \eta} + \sigma_0^2 \left( 1 - \frac{\lambda \zeta}{\lambda + \zeta \sigma^2 \eta} \right) \right]
\times \log \left( \tilde{\lambda} + \zeta \sigma^2 \eta \right) \right\} d\lambda d\tilde{\lambda} + O(1/N).
\] (F40)
Appendix G: Self-averageness of \( \hat{\sigma}^2 \) estimator

Let us consider the equation

\[
\sigma^2 = \frac{\beta}{(\beta - \zeta)} \frac{1}{N} \left\| t - Z\hat{\theta} \right\|^2 - \frac{\sigma^4 \eta}{(\beta - \zeta)} \frac{1}{N} \text{Tr} \left[ J_{\sigma^2 \eta} \right] + \frac{2\sigma^4 \beta}{(\beta - \zeta) N} \frac{\partial}{\partial \sigma^2} \log P(\sigma^2). \tag{G1}
\]

Using in above the MAP estimator \( (A3) \) and the definition \( \sigma^2 = v \) we obtain

\[
v = \frac{\beta}{(\beta - \zeta)} \frac{1}{N} t^T \left( I_N - ZJ^{-1} v \eta Z^T \right)^2 t - \frac{v^2 \eta}{(\beta - \zeta)} \frac{1}{N} \text{Tr} \left[ J_{v \eta}^{-1} \right] + \frac{2v^2 \beta}{(\beta - \zeta) N} \frac{\partial}{\partial v} \log P(v). \tag{G2}
\]

To solve above equation for \( v \) we define the recursion

\[
v_{t+1} = \frac{\beta}{(\beta - \zeta)} \frac{1}{N} t^T \left( I_N - ZJ^{-1} v \eta Z^T \right)^2 t - \frac{v_{t}^2 \eta}{(\beta - \zeta)} \frac{1}{N} \text{Tr} \left[ J_{v \eta}^{-1} \right] + \frac{2v_{t}^2 \beta}{(\beta - \zeta) N} \frac{\partial}{\partial v} \log P(v) \bigg|_{v=v_{t}}. \tag{G3}
\]

where in above we have defined \( \frac{\partial}{\partial v} \equiv \frac{\partial}{\partial v} \). We note that above, because of \( t = Z\theta_0 + \epsilon \), is of the form

\[
v_{t+1} = \Psi \left[ v_t | Z, \theta_0, \epsilon \right]. \tag{G4}
\]

Thus for a random trio \( \{Z, \theta_0, \epsilon\} \), i.e. the ‘disorder’, the function \( \Psi \) is a random non-linear operator acting on \( v_t \). If the initial value \( v_0 \) is independent from the disorder then the next value \( v_1 \) is independent from a particular realisation of disorder, i.e. \( v_1 \) is self-averaging, if the operator \( \Psi \) is self-averaging, i.e. if

\[
\lim_{(N,d) \to \infty} \left\langle \Psi^2 \left[ v_0 | Z, \theta_0, \epsilon \right] \right\rangle_{Z,\theta_0,\epsilon} - \left\langle \Psi^2 \left[ v_0 | Z, \theta_0, \epsilon \right] \right\rangle_{Z,\theta_0,\epsilon} = 0. \tag{G5}
\]

Furthermore, by induction the \( v_t \) is also self-averaging for all \( t \geq 2 \), so the equation \( \text{[G4]} \) can be replaced by

\[
v_{t+1} = \left\langle \Psi \left[ v_t | Z, \theta_0, \epsilon \right] \right\rangle_{Z,\theta_0,\epsilon} \tag{G6}
\]

when \( (N,d) \to \infty \).

From the above argument follows that if \( \text{[G1]} \) is solved for \( \sigma^2 \) recursively then the solution of this recursion, \( \hat{\sigma}^2 \), is self-averaging.

To prove self-averaging of \( \Psi \) we assume that the true parameters \( \theta_0 \) and noise \( \epsilon \) have
mean $0$ and, respectively, the covariances $S^2 I_d$ and $\sigma_0^2 I_N$. Let us first consider the average

$$
\langle \Psi [v_0 | Z, \theta_0, \epsilon] \rangle_{Z, \theta_0, \epsilon} = \frac{\beta}{(\beta - \zeta)} \frac{1}{N} \langle t^T (I_N - ZJ_{v_0}^{-1}Z^T)^2 t \rangle_{Z, \theta_0, \epsilon} - \frac{\nu_0^2 \eta}{(\beta - \zeta)} \frac{1}{N} \langle \text{Tr} [J_{v_0}^{-1}] \rangle Z + \frac{2
u_0^2 \beta}{(\beta - \zeta) N} \partial_v \log P(v) |_{v = v_0}
$$

$$
= \frac{\beta}{(\beta - \zeta)} \frac{1}{N} \sigma_0^2 \langle \text{Tr} \left[ (I_N - ZJ_{v_0}^{-1}Z^T)^2 \right] \rangle Z + \frac{\beta}{(\beta - \zeta)} \frac{1}{N} \langle \text{Tr} [J_{v_0}^{-1}] \rangle Z + \frac{2
u_0^2 \beta}{(\beta - \zeta) N} \partial_v \log P(v) |_{v = v_0}
$$

$$
= \beta \frac{\sigma_0^2}{(\beta - \zeta)} \left( 1 - \frac{1}{N} \langle \text{Tr} \left[ (I_d - J^{-1}J)^2 \right] \rangle Z \right) + \frac{\beta S^2}{(\beta - \zeta)} \frac{1}{N} \langle \text{Tr} [J (I_d - J_{v_0}^{-1}J)^2] \rangle Z
$$

where in above we assumed that $Z = Z/\sqrt{d}$ and defined the average $\rho_d(\lambda) = \langle \rho_d(\lambda | Z) \rangle_{Z}$ of the eigenvalue density $\rho_d(\lambda | Z) = \frac{1}{d} \sum_{l=1}^{d} \delta (\lambda - \lambda_l (Z^TZ/N))$. Thus the average is given by

$$
\langle \Psi [v_0 | Z, \theta_0, \epsilon] \rangle_{Z, \theta_0, \epsilon} = \frac{\beta \sigma_0^2}{(\beta - \zeta)} \left( 1 - \zeta + \zeta \int \rho_d(\lambda) \left( \frac{\zeta v_0 \eta}{\lambda + \zeta v_0 \eta} \right)^2 d\lambda \right) + \frac{\beta S^2}{(\beta - \zeta)} \int \rho_d(\lambda) \left( \frac{\zeta v_0 \eta}{\lambda + \zeta v_0 \eta} \right)^2 \lambda d\lambda
$$

$$
- \frac{\nu_0^2 \zeta^2}{(\beta - \zeta)} \int \rho_d(\lambda) \frac{\lambda + \zeta v_0 \eta}{\lambda + \zeta v_0 \eta} d\lambda + \frac{2
u_0^2 \beta}{(\beta - \zeta) N} \partial_v \log P(v) |_{v = v_0} \tag{G7}
$$

Now consider the variance

$$
\text{Var}(\Psi [v_0 | Z, \theta_0, \epsilon]) = \left( \frac{\beta}{(\beta - \zeta)} \right)^2 \frac{1}{N^2} \text{Var} \left( t^T (I_N - ZJ_{v_0}^{-1}Z^T)^2 t \right) + \frac{\nu_0^2 \eta^2}{(\beta - \zeta)^2} \frac{1}{N^2} \text{Var} \left( \text{Tr} [J_{v_0}^{-1}] \right)
$$

$$
- \frac{2\beta v_0^2 \eta^2}{(\beta - \zeta)^2 N^2} \text{Cov} \left( t^T (I_N - ZJ_{v_0}^{-1}Z^T)^2 t, \text{Tr} [J_{v_0}^{-1}] \right) \tag{G9}
$$
Computing in above averages over the random variables $Z$, $\theta_0$ and $\epsilon$ gives us the result

\[
\text{Var}(\Psi [v_0|Z, \theta_0, \epsilon]) = \int \int C_d(\lambda, \tilde{\lambda}) \left\{ \left( \frac{\beta}{\beta - \zeta} \right)^2 \left( \frac{\zeta v_0 \eta}{\lambda + \zeta v_0 \eta} \right)^2 \left( \frac{\zeta v_0 \eta}{\lambda + \zeta v_0 \eta} \right)^2 \left[ \sigma_0^4 \zeta^2 + S^4 \lambda \tilde{\lambda} + 2\sigma_0^2 S^2 \zeta \lambda \right] \\
+ \left( \frac{\beta^2 \zeta^2 \eta}{(\beta - \zeta)^2} \right)^2 \left( \frac{1}{(\lambda + \zeta v_0 \eta)} \right)^2 \left( \frac{1}{(\lambda + \zeta v_0 \eta)} \right)^2 \left[ \sigma_0^2 \zeta + S^2 \lambda \right] \right\} d\lambda d\tilde{\lambda} \\
+ \frac{2}{N} \left( \frac{\beta}{\beta - \zeta} \right)^2 \int \rho_d(\lambda) \left\{ \sigma_0^4 \left[ 1 - \zeta + \zeta \left( \frac{\zeta v_0 \eta}{\lambda + \zeta v_0 \eta} \right)^4 \right] + S^4 \left( \frac{\zeta v_0 \eta}{\lambda + \zeta v_0 \eta} \right)^4 \lambda^2 \right\} d(\lambda) \tag{G10}
\]

where in above we have defined the correlation function $C_d(\lambda, \tilde{\lambda}) = \langle \rho_d(\lambda|Z) \rho_d(\tilde{\lambda}|Z) \rangle_Z - \langle \rho_d(\lambda|Z) \rangle_Z \langle \rho_d(\tilde{\lambda}|Z) \rangle_Z$. Thus if the latter is self-averaging when $(N, d) \to \infty$ then $\Psi [v_0|Z, \theta_0, \epsilon]$ is also self-averaging in this limit.

[1] E. T. Jaynes, Physical review 106, 620 (1957).

[2] H. Nishimori, Statistical physics of spin glasses and information processing: an introduction (Clarendon Press, 2001).

[3] C. M. Bishop, Pattern recognition and machine learning (Springer, 2006).

[4] M. Mézard, G. Parisi, and M. Virasoro, Spin glass theory and beyond: An Introduction to the Replica Method and Its Applications (World Scientific Publishing Co Inc, 1987).

[5] A. C. Rencher and G. B. Schaalje, Linear models in statistics (John Wiley & Sons, 2008).

[6] P. J. Huber and E. M. Ronchetti, Robust statistics (John Wiley & Sons, 2009).

[7] M. Bayati and A. Montanari, IEEE Transactions on Information Theory 58, 1997 (2011).

[8] N. El Karoui, D. Bean, P. J. Bickel, C. Lim, and B. Yu, Proceedings of the National Academy of Sciences 110, 14557 (2013).

[9] M. J. Wainwright, High-dimensional statistics: A non-asymptotic viewpoint (Cambridge University Press, 2019).

[10] M. Advani and S. Ganguli, Physical Review X 6, 031034 (2016).

[11] J. Barbier, F. Krzakala, N. Macris, L. Miolane, and L. Zdeborová, P. Natl. Acad. Sci. USA 116, 5451 (2019).
Perhaps the simplest conjugate prior is given by the inverse-$\chi^2$ distribution $P(\sigma^2) = 2^{-\nu/2}(\sigma^2)^{-\nu/2-1}e^{-1/2\sigma^2}/\Gamma(\nu/2)$ with $\nu$ degrees of freedom.

If inverse-$\chi^2$ distribution is used as a prior for $\sigma^2$ then the MAP estimator for the latter is given by $\sigma^2 = \frac{1}{N+\nu+2} + \frac{1}{N+\nu+2} \left\| t - Z\hat{\theta}(\mathcal{D}) \right\|^2$ which suggests that the hyper-parameter $\nu$ has to be extensive in order to be relevant for large $N$. 

S. Nadarajah and S. Kotz, Acta Applicandae Mathematica 89, 53 (2005).

B. G. Kibria and A. H. Joarder, Journal of Statistical research 40, 59 (2006).

M. Rudelson and R. Vershynin, Electronic Communications in Probability 18 (2013).

F. Götze and A. Tikhomirov, Bernoulli 10, 503 (2004).

P.-H. Chavanis, Phys. Rev. E. 65, 056123 (2002).

M. L. Eaton, Multivariate statistics: a vector space approach. (JOHN WILEY & SONS, 1983).

M. Taboga, Lectures on probability theory and mathematical statistics (Independent Publishing Platform, 2017).