Supplementary Material:
Information bottleneck theory of high-dimensional regression: relevancy, efficiency and optimality

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A Information content of maximally efficient algorithms

Consider an IB problem where we are interested in an information efficient representation of Y that is predictive of W (Fig 1a). When Y and W are Gaussian correlated, the central object in constructing an IB solution is the normalized regression matrix $\Sigma_{Y|W}\Sigma_Y^{-1}$; in particular, its eigenvalues $\nu_i[\Sigma_{Y|W}\Sigma_Y^{-1}]$ completely characterize the information content of the IB optimal representation $\tilde{T}$ via (see Ref [1] for a derivation)

$$I(\tilde{T};W) = \frac{1}{2}\sum_{i=1}^{N} \max\left(0,\ \ln\frac{1-\gamma^{-1}}{\nu_i[\Sigma_{Y|W}\Sigma_Y^{-1}]}\right) \tag{1}$$

$$I(\tilde{T};Y\mid W) = \frac{1}{2}\sum_{i=1}^{N} \max(0,\ \ln(\gamma(1-\nu_i[\Sigma_{Y|W}\Sigma_Y^{-1}]))), \tag{2}$$

where N is the dimension of Y and γ parametrizes the IB trade-off [Eq (1)].

Our work focuses on the following generative model for W and Y (see Sec 1.1)

$$W\sim N(0,\tfrac{\omega^2}{P}I_P) \quad\text{and}\quad Y\mid W\sim N(X^\top W,\sigma^2 I_N). \tag{3}$$

Marginalizing out W yields

$$Y\sim N(0,\sigma^2 I_N+\tfrac{1}{P}X^\top X). \tag{4}$$

As a result, the normalized regression matrix reads

$$\Sigma_{Y|W}\Sigma_Y^{-1} = \sigma^2 I_N\frac{1}{\sigma^2 I_N+\frac{1}{P}X^\top X} = \left(I_N+\frac{1}{\lambda^*}\frac{X^\top X}{N}\right)^{-1} \quad\text{where}\quad \lambda^*\equiv\frac{P}{N}\frac{\sigma^2}{\omega^2}. \tag{5}$$

Substituting Eq (5) into Eqs (1-2) gives

$$I(\tilde{T};W) = \frac{1}{2}\sum_{i=1}^{N} \max\left(0,\ \ln\left((1-\gamma^{-1})(1+\phi_i[X^\top X/N]/\lambda^*)\right)\right) \tag{6}$$

$$I(\tilde{T};Y\mid W) = \frac{1}{2}\sum_{i=1}^{N} \max\left(0,\ \ln\frac{\gamma\phi_i[X^\top X/N]}{\lambda^*+\phi_i[X^\top X/N]}\right), \tag{7}$$

where $\phi_i[X^\top X/N]$ denote the eigenvalues of $X^\top X/N$. Since the eigenvalues of $X^\top X/N$ and the sample covariance $\Psi = XX^\top/N$ are identical except for the zero modes which do not contribute to information, we can recast the above equations as

$$I(\tilde{T};W) = \frac{1}{2}\sum_{i=1}^{P} \max\left(0,\ \ln(1-\gamma^{-1})(1+\psi_i/\lambda^*)\right) \tag{8}$$

$$I(\tilde{T};Y\mid W) = \frac{1}{2}\sum_{i=1}^{P} \max\left(0,\ \ln\frac{\gamma\psi_i}{\lambda^*+\psi_i}\right), \tag{9}$$

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where ψ_i are the eigenvalues of Ψ and the summation limits change to P, the number of eigenvalues of Ψ. Introducing the cumulative spectral distribution F^{Ψ} and replacing the summations with integrals results in

$$I(\tilde{T};W) = \frac{P}{2}\int dF^{\Psi}(\psi)\max\left(0,\ \ln\left((1-\gamma^{-1})(1+\psi/\lambda^*)\right)\right) \tag{10}$$

$$I(\tilde{T};Y\mid W) = \frac{P}{2}\int dF^{\Psi}(\psi)\max\left(0,\ \ln\frac{\gamma\psi}{\lambda^*+\psi}\right). \tag{11}$$

We see that the contributions to the integrals come from the logarithms but only when they are positive. This condition can be recast into integration limits (note that $\gamma > 0$ and $\lambda^* > 0$)

$$\ln\left((1-\gamma^{-1})(1+\psi/\lambda^*)\right) > 0 \implies \psi > \lambda^*/(\gamma-1) \tag{12}$$

$$\ln\frac{\gamma\psi}{\lambda^*+\psi} > 0 \implies \psi > \lambda^*/(\gamma-1). \tag{13}$$

Finally we define the lower cutoff $\psi_c \equiv \lambda^*/(\gamma-1)$ and use the above limits to rewrite the expressions for relevant and residual informations,

$$I(\tilde{T};W) = \frac{P}{2}\int_{\psi>\psi_c} dF^{\Psi}(\psi)\ln\frac{\psi+\lambda^*}{\psi_c+\lambda^*} = \frac{P}{2}\int_{\psi>\psi_c} dF^{\Psi}(\psi)\ln\left(1+\frac{\psi-\psi_c}{\psi_c+\lambda^*}\right) \tag{14}$$

$$I(\tilde{T};Y\mid W) = \frac{P}{2}\int_{\psi>\psi_c} dF^{\Psi}(\psi)\ln\frac{\psi}{\psi_c}\frac{\psi_c+\lambda^*}{\psi+\lambda^*} = \frac{P}{2}\int_{\psi>\psi_c} dF^{\Psi}(\psi)\ln\frac{\psi}{\psi_c} - I(\tilde{T};W). \tag{15}$$

These equations are identical to Eqs (8-9) in the main text.

B Information content of Gibbs-posterior regression

To compute the information content of Gibbs regression [Eq (14)], we first recall that the mutual information between two Gaussian correlated variables, A and B, is given by

$$I(A;B) = \frac{1}{2}\ln\det\Sigma_A\Sigma_{A|B}^{-1}, \tag{16}$$

where Σ_A is the covariance of A, and $\Sigma_{A|B}$ of $A\mid B$.

We now write down the relevant information, using the covariances $\Sigma_{T|W}$ and Σ_T from Eqs (17-18),

$$\begin{aligned}
I(T;W) &= \frac{1}{2}\ln\det\left(\Sigma_T\Sigma_{T|W}^{-1}\right) && (17)\\
&= \frac{1}{2}\ln\det\frac{\frac{1}{2\beta}\frac{1}{\Psi+\lambda I_P}+\frac{\sigma^2}{N}\frac{\Psi}{(\Psi+\lambda I_P)^2}+\frac{\omega^2}{P}\frac{\Psi^2}{(\Psi+\lambda I_P)^2}}{\frac{1}{2\beta}\frac{1}{\Psi+\lambda I_P}+\frac{\sigma^2}{N}\frac{\Psi}{(\Psi+\lambda I_P)^2}} && (18)\\
&= \frac{1}{2}\ln\det\left(I_P+\frac{\Psi^2/\lambda^*}{\Psi+\frac{N}{2\beta\sigma^2}(\Psi+\lambda I_P)}\right) && (19)\\
&= \frac{1}{2}\operatorname{tr}\ln\left(I_P+\frac{\Psi^2/\lambda^*}{\Psi+\frac{N}{2\beta\sigma^2}(\Psi+\lambda I_P)}\right) && (20)\\
&= \frac{1}{2}\sum_{i=1}^{P}\ln\left(1+\frac{\psi_i^2/\lambda^*}{\psi_i+\frac{N}{2\beta\sigma^2}(\psi_i+\lambda)}\right) && (21)\\
&= \frac{P}{2}\int_{\psi>0} dF^{\Psi}(\psi)\ln\left(1+\frac{\psi^2/\lambda^*}{\psi+\frac{N}{2\beta\sigma^2}(\psi+\lambda)}\right), && (22)
\end{aligned}$$

where $\lambda^* = P\sigma^2/N\omega^2$. In the above, we use the identity $\ln\det H = \operatorname{tr}\ln H$ which holds for any positive-definite Hermitian matrix H, let ψ_i denote the eigenvalues of the sample covariance Ψ and introduce F^{Ψ}, the cumulative distribution of eigenvalues. We also assume that λ and β are finite and positive. Note that the integral is limited to positive real numbers because the eigenvalues of a covariance matrix is non-negative and the integrand vanishes for $\psi = 0$.

Following the same logical steps as above and noting that the Markov constraint $W \leftrightarrow Y \leftrightarrow T$ implies $\Sigma_{T|Y,W} = \Sigma_{T|Y}$, we write down the residual information,

$$\begin{aligned} I(T;Y \mid W) &= \frac{1}{2} \ln \det \left(\Sigma_{T|W} \Sigma_{T|Y,W}^{-1} \right) && (23) \\ &= \frac{1}{2} \ln \det \left(\Sigma_{T|W} \Sigma_{T|Y}^{-1} \right) && (24) \\ &= \frac{1}{2} \ln \det \left(\frac{\frac{1}{2\beta} \frac{1}{\Psi + \lambda I_P} + \frac{\sigma^2}{N} \frac{\Psi}{(\Psi + \lambda I_P)^2}}{\frac{1}{2\beta} \frac{1}{\Psi + \lambda I_P}} \right) && (25) \\ &= \frac{P}{2} \int_{\psi > 0} dF^{\Psi}(\psi) \ln \left(1 + \frac{2\beta\sigma^2}{N} \frac{\psi}{\psi + \lambda} \right) && (26) \end{aligned}$$

where we use the covariance matrices $\Sigma_{T|W}$ and $\Sigma_{T|Y}$ from Eqs (17) & (14).

C Marchenko-Pastur law

Consider $X = \Sigma^{1/2} Z$ where $Z \in \mathbb{R}^{P \times N}$ is a matrix with iid entries drawn from a distribution with zero mean and unit variance, and $\Sigma \in \mathbb{R}^{P \times P}$ is a covariance matrix. In addition we take the asymptotic limit $N \longrightarrow \infty$, $N \longrightarrow \infty$ and $P/N \longrightarrow \alpha \in (0, \infty)$. If the population spectral distribution F^{Σ} converges to a limiting distribution, the spectral distribution of the sample covariance $\Psi = XX^{\mathsf{T}}/N$ becomes deterministic [2]. The density, $f^{\Psi}(\psi) = dF^{\Psi}(\psi)/d\psi$, is related to its Stieltjes transform $m(z)$ via

$$f^{\Psi}(\psi) = \frac{1}{\pi} \operatorname{Im} m(\psi + i\,0^{+}), \quad \psi \in \mathbb{R}. \tag{27}$$

We can obtain f^{Ψ} by solving the Silverstein equation for the companion Stieltjes transform $v(z)$ [3],

$$-\frac{1}{v(z)} = z - \alpha \int_{\mathbb{R}^{+}} dF^{\Sigma}(s) \frac{s}{1 + s v(z)}, \quad z \in \mathbb{C}^{+}, \tag{28}$$

and using the relation

$$m(z) = \alpha^{-1}(v(z) + z^{-1}) - z^{-1}. \tag{29}$$

Here $\mathbb{C}^{+}$ denotes the upper half of the complex plane.

D Supplementary figure

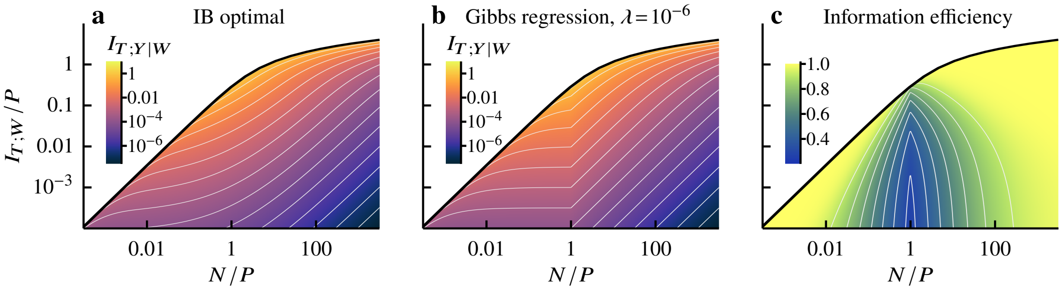

Figure 1: Gibbs ridge regression is least information efficient around $N/P = 1$. **a** Residual information $I(T;Y\mid W)$ of the IB optimal algorithm over a range of sample densities N/P (horizontal axis) and given extracted relevant bits $I(T;W)$ (vertical axis). The extracted relevant bits are bounded by the available relevant bits in the data (black curve), i.e., the data processing inequality implies $I(T;W) \le I(Y;W)$. **b** Same as (a) but for Gibbs regression with $\lambda = 10^{-6}$. Holding other things equal, Gibbs regression estimators encode more residual bits than optimal representations. **c** Information efficiency, the ratio between residual bits in optimal representations (a) and Gibbs estimator (b), is minimum around $N/P = 1$. Here we set $\omega^2/\sigma^2 = 1$ and let $P, N \to \infty$ at the same rate such that the ratio N/P remains fixed and finite. The eigenvalues of the sample covariance follow the standard Marchenko-Pastur law (see Sec 4).

References

[1] G. Chechik, A. Globerson, N. Tishby, and Y. Weiss, Information bottleneck for Gaussian variables, Journal of Machine Learning Research **6**, 165 (2005).

[2] V. A. Marčenko and L. A. Pastur, Distribution of eigenvalues for some sets of random matrices, Mathematics of the USSR–Sbornik **1**, 457 (1967).

[3] J. Silverstein and S. Choi, Analysis of the Limiting Spectral Distribution of Large Dimensional Random Matrices, Journal of Multivariate Analysis **54**, 295 (1995).