## Random Matrix Methods for Machine Learning

Romain Couillet University Grenoble Alpes, France romain.couillet@gipsa-lab.grenoble-inp.fr

Zhenyu Liao Huazhong University of Science and Technology, China zhenyu\_liao@hust.edu.cn<sup>1</sup>

April 17, 2023

<sup>1</sup>Disclaimer: This material will be published by Cambridge University Press under the title of "Random Matrix Methods for Machine Learning." This pre-publication version is free to view and download for personal use only, and is not for redistribution, re-sale or use in derivative works. 

## Erratum

**Theorem 2.11** (Inspired by Mestre [2008]). Under the setting of Theorem 6 with  $\mathbb{E}[|\mathbf{Z}_{ij}|^4] < \infty$  and  $\max_{1 \leq i \leq p} \operatorname{dist}(\lambda_i(\mathbf{C}), \operatorname{supp}(\nu)) \to 0$ , let  $f : \mathbb{C} \to \mathbb{C}$  be a complex function analytic on the complement of  $\gamma(\mathbb{C} \setminus \operatorname{supp}(\mu))$  in  $\mathbb{C}$  with  $\gamma$ defined in (2.39). Then,

$$\frac{1}{p}\sum_{i=1}^{p}f(\lambda_{i}(\mathbf{C})) - \frac{1}{2c\pi\imath}\oint_{\Gamma_{\mu}}f\left(\frac{-1}{m_{\frac{1}{n}\mathbf{X}^{\mathsf{T}}\mathbf{X}}(\omega)}\right)\omega m'_{\frac{1}{n}\mathbf{X}^{\mathsf{T}}\mathbf{X}}(\omega)d\omega \xrightarrow{a.s.} 0,$$

for some complex positively oriented contour  $\Gamma_{\mu} \subset \mathbb{C}$  surrounding  $\operatorname{supp}(\mu) \setminus \{0\}$ . In particular, if c < 1, the result holds for any f analytic on  $\{z \in \mathbb{C}, \Re[z] > 0\}$ with  $\Gamma_{\mu}$  chosen as any such contour within  $\{z \in \mathbb{C}, \Re[z] > 0\}$ .

Section Equation (2.43).

$$\ell_a - \hat{\ell}_a \xrightarrow{a.s.} 0, \quad \hat{\ell}_a = -\frac{n}{p_a} \frac{1}{2\pi \imath} \oint_{\Gamma_\mu^{(a)}} \omega \frac{m'_{\frac{1}{n} \mathbf{X}^{\mathsf{T}} \mathbf{X}}(\omega)}{m_{\frac{1}{n} \mathbf{X}^{\mathsf{T}} \mathbf{X}}(\omega)} d\omega.$$
(2.43)

Section 3.1.1 "GLRT asymptotics" around Equation (3.2). As a consequence, in order to set a maximum false alarm rate (or false positive, or Type I error) of r > 0 in the limit of large n, p, one must choose a threshold  $f(\alpha)$  for  $T_p$  such that

$$\mathbb{P}(T_p \ge f(\alpha)) = r,$$

that is, such that

$$\mu_{\text{TW}_1}([A_p, +\infty)) = r, \quad A_p = (f(\alpha) - (1 + \sqrt{c})^2)(1 + \sqrt{c})^{-\frac{4}{3}}c^{\frac{1}{6}}n^{\frac{2}{3}}$$
(3.2)

with  $\mu_{TW_1}$  the Tracy-Widom measure in Theorem 2.15.

Section 3.1.2 "Linear and Quadratic Discriminant Analysis" before Remark 3.1 Plugging this result into the expression of  $T_{\text{LDA}}^{(\gamma)}(\mathbf{x})$ , we find that



Figure 1: Comparison between empirical false alarm rates and  $1 - \text{TW}_1(A_p)$  for  $A_p$  of the form in (3.2), as a function of the threshold  $f(\alpha) \in [(1 + \sqrt{c})^2 - 5n^{-2/3}, (1 + \sqrt{c})^2 + 5n^{-2/3}]$ , for p = 256, n = 1024 and  $\sigma = 1$ . Results obtained from 500 runs. Link to code: Matlab and Python.

in the large  $n_0, n_1, p$  limit,

$$T_{\text{LDA}}^{(\gamma)}(\mathbf{x}) = \frac{(-1)^{\ell}}{2} (\boldsymbol{\mu}_0 - \boldsymbol{\mu}_1)^{\mathsf{T}} \bar{\mathbf{Q}}^{\circ} (\boldsymbol{\mu}_0 - \boldsymbol{\mu}_1) - \frac{g_0(-\gamma)}{2c_0} + \frac{g_1(-\gamma)}{2c_1} + \mathbf{z}^{\mathsf{T}} \mathbf{C}_{\ell}^{\frac{1}{2}} \mathbf{Q}^{\circ} \mathbf{U} \begin{bmatrix} 1 \\ -1 \\ \frac{1}{\gamma \tilde{g}_0(-\gamma)} \\ -\frac{\gamma \tilde{g}_1(-\gamma)}{\gamma \tilde{g}_1(-\gamma)} \end{bmatrix} + o(1)$$

where we used in particular the fact that  $\frac{1-\gamma \tilde{g}_0(-\gamma)}{\gamma \tilde{g}_0(-\gamma)} = g_0(-\gamma).$ 

**Theorem 2.11** (Optimal decision threshold). Since  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_p)$ , it is clear that the expectation  $\mathbb{E}[T_{\text{LDA}}^{(\gamma)}(\mathbf{x})]$  is dominated by  $\pm \frac{1}{2}(\boldsymbol{\mu}_0 - \boldsymbol{\mu}_1)^{\mathsf{T}} \bar{\mathbf{Q}}^{\circ}(\boldsymbol{\mu}_0 - \boldsymbol{\mu}_1)$  which is positive when  $\ell = 0$  and negative when  $\ell = 1$ , as expected. Yet, the term  $\frac{g_1(-\gamma)}{2c_0} - \frac{g_0(-\gamma)}{2c_0}$  intervenes as a bias. If  $\mathbf{C}_0 = \mathbf{C}_1$  (which is indeed the assumption of LDA) and the training set is "balanced" with  $c_0 = c_1$ , then  $g_0 = g_1$  and this bias disappears; however, for  $\mathbf{C}_0, \mathbf{C}_1$  distinct, this bias in general remains and must be accounted for in the decision threshold which, therefore, should not be zero.

Section 5.1.1 "Regression with random neural network" after Equation (5.12). The fact that this denominator scales like  $\|\gamma \bar{\mathbf{Q}}\|$  as  $\gamma \to 0$  explains the major difference between the training and test error behavior in Figure 5.5. Due to the  $\gamma^2$  prefactor in  $\bar{E}_{\text{train}}$ , the training error is guaranteed to be finite (even possibly to vanish) as  $\gamma \to 0$ . But for the test error, since  $\gamma \bar{\mathbf{Q}} \to 0$  as N approaches n from each side, if the numerator term  $\frac{1}{\hat{n}} \operatorname{tr} \bar{\mathbf{K}}_{\hat{\mathbf{X}}\hat{\mathbf{X}}} - \frac{1}{\hat{n}} \operatorname{tr}(\mathbf{I}_n + \gamma \bar{\mathbf{Q}})(\bar{\mathbf{K}}_{\mathbf{X}\hat{\mathbf{X}}} \bar{\mathbf{K}}_{\mathbf{X}\hat{\mathbf{X}}}^{\mathsf{T}} \bar{\mathbf{Q}})$  does not scale like  $\gamma \bar{\mathbf{Q}}$ , then  $\bar{E}_{\text{test}}$  diverges to infinity at N = n. A first counterexample is of course when  $\hat{\mathbf{X}} = \mathbf{X}$ , for which the numerator term of  $\bar{E}_{\text{test}}$  is now

$$\frac{1}{\hat{n}}\operatorname{tr}\bar{\mathbf{K}}_{\hat{\mathbf{X}}\hat{\mathbf{X}}} - \frac{1}{\hat{n}}\operatorname{tr}(\mathbf{I}_n + \gamma \bar{\mathbf{Q}})(\bar{\mathbf{K}}_{\mathbf{X}\hat{\mathbf{X}}}\bar{\mathbf{K}}_{\mathbf{X}\hat{\mathbf{X}}}^{\mathsf{T}}\bar{\mathbf{Q}}) = \frac{\gamma^2}{n}\operatorname{tr}\bar{\mathbf{Q}}\bar{\mathbf{K}}\bar{\mathbf{Q}}$$

## Bibliography

Xavier Mestre. Improved Estimation of Eigenvalues and Eigenvectors of Covariance Matrices Using Their Sample Estimates. *IEEE Transactions* on Information Theory, 54(11):5113–5129, 2008. ISSN 0018-9448. doi: 10.1109/tit.2008.929938.