

Detection problems in spiked Wigner matrices

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Spiked Wigner matrix

- Spike: $\mathbf{x} = (x_1, x_2, \dots, x_N) \in \mathbb{R}^N$
- Noise: H is an $N \times N$ real symmetric random matrix
- Data: Signal-plus-noise

$$M = \sqrt{\lambda} \mathbf{x} \mathbf{x}^T + H$$

(λ : Signal-to-Noise Ratio (SNR))

- Prior: distribution of \mathbf{x} ($\|\mathbf{x}\| = 1$)
 - Spherical prior: \mathbf{x} is uniformly distributed on the unit sphere.
 - Rademacher prior: $\mathbb{P}(\sqrt{N}x_i = 1) = \mathbb{P}(\sqrt{N}x_i = -1) = \frac{1}{2}$.
- Wigner matrix: i.i.d. upper-diagonal entries with $\mathbb{E}[H_{ij}] = 0$, $\mathbb{E}[H_{ij}^2] = N^{-1}$.
 ($\|H\| \rightarrow 2$ as $N \rightarrow \infty$)

Detection

$$M = \sqrt{\lambda} \mathbf{x} \mathbf{x}^T + H \quad (\|\mathbf{x}\|_2 = 1, \quad \|H\| \rightarrow 2)$$

- Hypothesis testing

$$H_0 : \lambda = 0, \quad H_1 : \lambda = \omega > 0$$

- Error: $\text{err}(\omega) = \mathbb{P}(\hat{H} = H_1 | H_0) + \mathbb{P}(\hat{H} = H_0 | H_1)$
- Strong (reliable) detection: $\text{err}(\omega) \rightarrow 0$ as $N \rightarrow \infty$
- Weak detection: $\text{err}(\omega) \rightarrow \alpha \in (0, 1)$ as $N \rightarrow \infty$

Main questions

- Threshold for the strong detection
- Fundamental limit of the weak detection
- Efficient algorithm for the weak detection that achieves the optimal error

Mathematical objects

- Largest eigenvalue
- (Log) likelihood ratio
- Linear spectral statistics

Edge universality

- For a large class of random matrices, the fluctuation of the largest eigenvalues are given by Tracy–Widom distribution.
(Dyson, Mehta, Tracy-Widom, Forrester, Soshnikov, Tao-Vu, Erdős-Yau-Yin, L.-Yin)

- For $M = \sqrt{\lambda} \mathbf{x} \mathbf{x}^T + H$, if $\lambda = 0$, then

$$N^{2/3}(\mu_1 - 2) \Rightarrow TW_1$$

Baik-Ben Arous-Péché (BBP) transition

$$M = \sqrt{\lambda} \mathbf{x} \mathbf{x}^T + H \quad (\|\mathbf{x}\|_2 = 1, \quad \|H\| \rightarrow 2)$$

- If $\lambda = \omega > 1$,

$$\mu_1 \rightarrow \sqrt{\omega} + \frac{1}{\sqrt{\omega}} > 2$$

- If $\lambda = \omega < 1$,

$$\mu_1 \rightarrow 2$$

If $\lambda = \omega > 1$, strong detection is possible via principal component analysis (PCA).

Entrywise transformation

$$M = \sqrt{\lambda} \mathbf{x} \mathbf{x}^T + H \quad (\|\mathbf{x}\|_2 = 1, \quad \|H\| \rightarrow 2)$$

- If we transform M entrywise by $\tilde{M}_{ij} = h(\sqrt{N}M_{ij})/\sqrt{N}$,

$$\begin{aligned} \tilde{M}_{ij} &\approx \frac{h(\sqrt{N}H_{ij})}{\sqrt{N}} + \sqrt{\lambda} h'(\sqrt{N}H_{ij}) x_i x_j \\ &\approx \frac{h(\sqrt{N}H_{ij})}{\sqrt{N}} + \sqrt{\lambda} \mathbb{E}[h'(\sqrt{N}H_{ij})] x_i x_j. \end{aligned}$$

- The transformed matrix is approximately a spiked Wigner matrix.

Transformed PCA

$$\tilde{M}_{ij} \approx \frac{h(\sqrt{N}H_{ij})}{\sqrt{N}} + \sqrt{\lambda}\mathbb{E}[h'(\sqrt{N}H_{ij})]x_i x_j$$

- If $\sqrt{N}H_{ij}$ has the density p , the optimal transform $h = -p'/p$ (up to a constant factor).
- The effective SNR is λF , where F is the Fisher information defined by

$$F = \int_{-\infty}^{\infty} \frac{p'(x)^2}{p(x)} dx.$$

- Fisher information $F \geq 1$ with equality if and only if p is Gaussian.
- Strong detection is possible via a transformed PCA if $\omega > 1/F$, where one checks the largest eigenvalue of the transformed matrix \tilde{M} .

Reconstruction by the transformed PCA

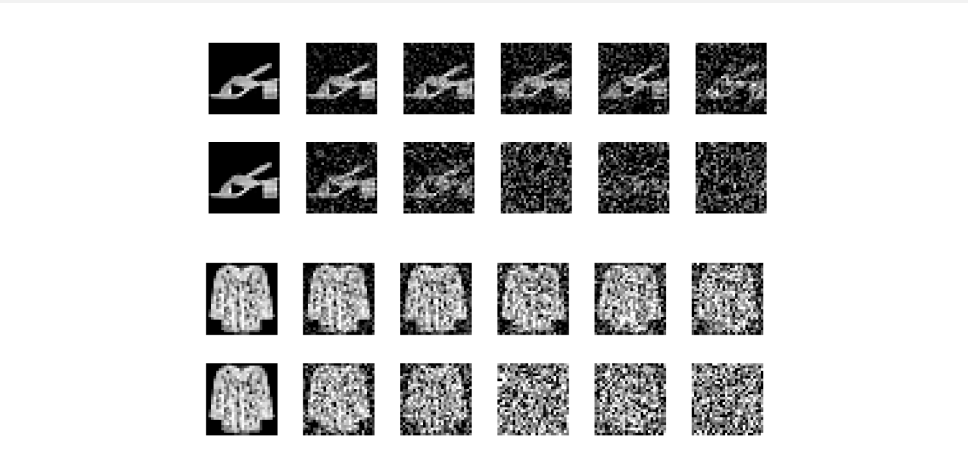


Figure: Reconstruction performance of the transformed PCA (top lines) and the standard PCA (bottom lines) for two FashionMNIST images, with 784 pixels and [3136, 1568, 784, 588, 392] samples.

Likelihood ratio test

$$\mathbf{H}_0 : \lambda = 0, \quad \mathbf{H}_1 : \lambda = \omega > 0$$

- Likelihood ratio (LR)

$$\mathcal{L}(M; \omega) := \left(\int \prod_{i \leq j} p(M_{ij})|_{\mathbf{H}_1} d\mathcal{X}(\mathbf{x}) \right) / \left(\prod_{i \leq j} p(M_{ij})|_{\mathbf{H}_0} \right)$$

- LR test: Accept \mathbf{H}_1 if $\mathcal{L}(M; \omega) > 1$. Reject \mathbf{H}_1 if $\mathcal{L}(M; \omega) \leq 1$.
- LR test minimizes $\text{err}(\omega) = \mathbb{P}(\hat{\mathbf{H}} = \mathbf{H}_1 | \mathbf{H}_0) + \mathbb{P}(\hat{\mathbf{H}} = \mathbf{H}_0 | \mathbf{H}_1)$.
(Neyman–Pearson)

LR with Gaussian noise

Assume that the noise H is GOE.

$$\begin{aligned}
 \mathcal{L}(M; \omega) &= \int \prod_{i < j} \frac{\exp[-\frac{N}{2}(M_{ij} - \sqrt{\omega}x_i x_j)^2]}{\exp[-\frac{N}{2}M_{ij}^2]} \prod_k \frac{\exp[-\frac{N}{4}(M_{kk} - \sqrt{\omega}x_k^2)^2]}{\exp[-\frac{N}{4}M_{kk}^2]} d\mathcal{X}(\mathbf{x}) \\
 &= \int \exp \left[\frac{N}{2} \sum_{i,j=1}^N (\sqrt{\omega}M_{ij}x_i x_j - \frac{\omega}{2}x_i^2 x_j^2) \right] d\mathcal{X}(\mathbf{x}) \\
 &= e^{-\omega N/4} \int \exp \left(\frac{\sqrt{\omega}N}{2} \langle \mathbf{x}, M\mathbf{x} \rangle \right) d\mathcal{X}(\mathbf{x})
 \end{aligned}$$

LR with Gaussian noise

From the theory of the Sherrington–Kirkpatrick model of spin glass,

$$\log \mathcal{L}(M; \omega) \Rightarrow \mathcal{N} \left(\pm \frac{1}{4} \log \left(\frac{1}{1 - \omega} \right), \frac{1}{4} \log \left(\frac{1}{1 - \omega} \right) \right).$$

(Aizenman-Lebowitz-Ruelle, Baik-L., El Alaoui-Krzakala-Jordan)

Thus, with the LR test,

$$\text{err}(\omega) \rightarrow \text{erfc} \left(\frac{1}{4} \sqrt{\log \left(\frac{1}{1 - \omega} \right)} \right).$$

$$(\text{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-x^2} dx)$$

LR with non-Gaussian noise

- For the spike \mathbf{x} , we assume that the normalized entries $\sqrt{N}x_i$ are i.i.d. random variables with Rademacher distribution.
- For the noise matrix H , let p and p_d be the densities of the normalized off-diagonal entries $\sqrt{N}H_{ij}$ and the normalized diagonal entries $\sqrt{N}H_{ii}$, respectively. We assume further
 - The density functions p and p_d are smooth, positive everywhere, and symmetric (about 0).
 - The functions p , p_d , and their all derivatives vanish at infinity.
 - The functions $h := -p'/p$, $h_d := -p'_d/p_d$, and their all derivatives are polynomially bounded in the sense that for any s there exist constants $C_s, r_s > 0$, independent of N , such that $|h^{(s)}(w)|, |h_d^{(s)}(w)| \leq C_s |w|^{r_s}$.

$$\mathcal{L}(M; \omega) = \frac{1}{2^N} \sum_{\mathbf{x}} \prod_{i < j} \frac{p(\sqrt{N}M_{ij} - \sqrt{\omega N}x_i x_j)}{p(\sqrt{N}M_{ij})} \prod_k \frac{p_d(\sqrt{N}M_{kk} - \sqrt{\omega N}x_k^2)}{p_d(\sqrt{N}M_{kk})}.$$

LR with non-Gaussian noise

Theorem (Chung-Lee-L.)

Suppose that M is a spiked Wigner matrix with the Rademacher prior. Define

$$F := \int_{-\infty}^{\infty} \frac{(p'(x))^2}{p(x)} dx, \quad F_d := \int_{-\infty}^{\infty} \frac{(p'_d(x))^2}{p_d(x)} dx, \quad G := \int_{-\infty}^{\infty} \frac{(p''(x))^2}{p(x)} dx.$$

If $\omega F < 1$, the log likelihood ratio $\log \mathcal{L}(M; \omega)$ under \mathbf{H}_0 converges in distribution to $\mathcal{N}(-\rho, 2\rho)$ as $N \rightarrow \infty$, where

$$\rho := -\frac{1}{4} \left(\log(1 - \omega F) + \omega(F - 2F_d) + \frac{\omega^2}{4}(2F^2 - G) \right).$$

Remarks

- Applying Le Cam's first lemma, the log likelihood ratio $\log \mathcal{L}(M; \lambda)$ under \mathbf{H}_1 converges in distribution to $\mathcal{N}(\rho, 2\rho)$.
- The result implies the impossibility of the strong detection for $\omega < 1/F$ (first proved by Perry-Wein-Bandeira-Moitra).
- For the GOE noise, $F = 1$, $F_d = \frac{1}{2}$, $G = 2$, and thus the result coincides with the known result.
- The error probability

$$\text{err}(\omega) \rightarrow \text{erfc} \left(\frac{1}{4} \sqrt{\log \left(\frac{1}{1 - \omega F} \right) - \omega(F - 2F_d) - \frac{\omega^2}{4}(2F^2 - G)} \right).$$

Idea of proof - Taylor expansion

Set

$$P_{ij}^{(s)} := \frac{p^{(s)}(\sqrt{N}M_{ij})}{p(\sqrt{N}M_{ij})},$$

By the Taylor expansion

$$\begin{aligned} & \frac{p(\sqrt{N}M_{ij} - \sqrt{\omega N}x_i x_j)}{p(\sqrt{N}M_{ij})} \\ &= 1 - \sqrt{\omega N}P_{ij}^{(1)}x_i x_j + \frac{\omega P_{ij}^{(2)}}{2N} - \frac{\omega\sqrt{\omega}}{6\sqrt{N}}P_{ij}^{(3)}x_i x_j + \frac{\omega^2 P_{ij}^{(4)}}{24N^2} + \mathcal{O}(N^{-\frac{5}{2}}), \end{aligned}$$

Idea of proof - Taylor expansion

$$P_{ij}^{(s)} := \frac{p^{(s)}(\sqrt{NM}x_{ij})}{p(\sqrt{NM}x_{ij})},$$

Taking the logarithm and Taylor expanding it again,

$$\begin{aligned} & \log \left(\frac{p(\sqrt{NM}x_{ij} - \sqrt{\omega N}x_i x_j)}{p(\sqrt{NM}x_{ij})} \right) \\ &= -\sqrt{\omega N}x_i x_j \left(P_{ij}^{(1)} + \frac{\omega}{6N} \left(P_{ij}^{(3)} - 3P_{ij}^{(1)}P_{ij}^{(2)} + 2(P_{ij}^{(1)})^3 \right) \right) \\ & \quad + \frac{\omega}{2N} \left(P_{ij}^{(2)} - (P_{ij}^{(1)})^2 \right) \\ & \quad + \frac{\omega^2}{24N^2} \left(P_{ij}^{(4)} - 3(P_{ij}^{(2)})^2 - 4P_{ij}^{(1)}P_{ij}^{(3)} + 12(P_{ij}^{(1)})^2P_{ij}^{(2)} - 6(P_{ij}^{(1)})^4 \right) \\ & \quad + \mathcal{O}(N^{-\frac{5}{2}}). \end{aligned}$$

Idea of proof - Taylor expansion

$$\begin{aligned}
 & \log \frac{1}{2^N} \sum_{\mathbf{x}} \prod_{i < j} \frac{p(\sqrt{N}M_{ij} - \sqrt{\omega N}x_i x_j)}{p(\sqrt{N}M_{ij})} \\
 &= \log \frac{1}{2^N} \sum_{\mathbf{x}} \exp \left(\sum_{i < j} \log \left(\frac{p(\sqrt{N}M_{ij} - \sqrt{\omega N}x_i x_j)}{p(\sqrt{N}M_{ij})} \right) \right) \\
 &= \log \frac{1}{2^N} \sum_{\mathbf{x}} \exp \left(\sum_{i < j} A_{ij} x_i x_j + \sum_{i < j} (B_{ij} + C_{ij}) + \mathcal{O}(N^{-\frac{1}{2}}) \right). \\
 & A_{ij} := -\sqrt{\omega N} \left(P_{ij}^{(1)} + \frac{\omega}{6N} \left(P_{ij}^{(3)} - 3P_{ij}^{(1)} P_{ij}^{(2)} + 2(P_{ij}^{(1)})^3 \right) \right). \\
 & (A_{ij} = \mathcal{O}(\sqrt{N}), \quad B_{ij} = \mathcal{O}(N^{-1}), \quad C_{ij} = \mathcal{O}(N^{-2}))
 \end{aligned}$$

Idea of proof - Spin glass part

Proposition

Set

$$Z := \frac{1}{2^N} \sum_{\mathbf{x}} \exp \left(\sum_{i < j} A_{ij} x_i x_j \right).$$

Then, there exist random variables ζ and ζ' such that

$$\log Z = \zeta + \zeta' + \mathcal{O}(N^{-1}),$$

where ζ and ζ' are asymptotically orthogonal to each other under L_B^2 , the conditional distribution of ζ given B converges in distribution to $\mathcal{N}(-\nu, 2\nu)$, where

$$\nu := \sum_{k=3}^{\infty} \frac{(\omega F)^k}{4k} = -\frac{1}{4} \left(\log(1 - \omega F) + \omega F + \frac{\omega^2 F^2}{2} \right),$$

Idea of proof - Spin glass part

Proposition

and conditional on B ,

$$\zeta' = \frac{1}{2N^2} \sum_{i < j} \mathbb{E}_B[A_{ij}^2] - \frac{\omega^2}{24} \mathbb{E}[(P_{12}^{(1)})^4] + U,$$

where U is a random variable whose asymptotic law is a centered Gaussian with variance

$$\theta := \frac{\omega^2}{8} \mathbb{E} \left[\text{Var}_B((P_{12}^{(1)})^2) \right].$$

Idea of proof - CLT part

The terms involving B in the decomposition of $\log \mathcal{L}(M; \omega)$ are

$$\sum_{i < j} B_{ij} + \frac{1}{2N^2} \sum_{i < j} \mathbb{E}[A_{ij}^2 | B_{ij}],$$

which is the sum of i.i.d. random variables that depend only on B_{ij} . By the central limit theorem, it converges to a Gaussian random variable with the mean

$$\frac{\omega^2}{12} \mathbb{E} \left[P_{12}^{(1)} P_{12}^{(3)} \right]$$

and the variance

$$\frac{\omega^2}{8} \mathbb{E} \left[(P_{12}^{(2)})^2 - \text{Var}((P_{12}^{(1)})^2 | B_{12}) \right]$$

LR with Gaussian noise

Assume that the noise H is GOE and the prior is spherical.

$$\begin{aligned}
 \mathcal{L}(M; \omega) &= e^{-\omega N/4} \int_{S^N} \exp\left(\frac{\sqrt{\omega}N}{2} \langle \mathbf{x}, M\mathbf{x} \rangle\right) d\mathcal{X}(\mathbf{x}) \\
 &= e^{-\omega N/4} \int_{S^N} \exp\left(\frac{\sqrt{\omega}N}{2} \sum_i \mu_i x_i^2\right) d\mathcal{X}(\mathbf{x}) \\
 &\approx e^{-\omega N/4} \int_{\mathbb{R}^N} \prod_i \exp\left(\frac{\sqrt{\omega}N}{2} \mu_i x_i^2\right) \sqrt{\frac{N}{2\pi}} e^{-Nx_i^2/2} dx_i \\
 &= \prod_i \frac{1}{N(1 - \sqrt{\omega}\mu_i + \omega)}.
 \end{aligned}$$

Thus,

$$\log \mathcal{L}(M; \omega) \approx \frac{1}{N} \sum_i \log \left(\frac{1}{1 - \sqrt{\omega}\mu_i + \omega} \right).$$

Linear spectral statistics (LSS)

- Denoting by μ_1, \dots, μ_N the eigenvalues of M , LSS is defined as

$$L_N(f) = \sum_{i=1}^N f(\mu_i)$$

for any sufficiently smooth f on an open interval containing $[-2, 2]$.

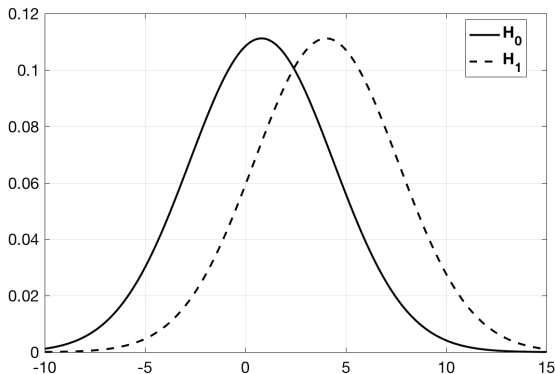
CLT for LSS

Theorem (Chung-L.)

$$\left(\sum_{i=1}^N f(\mu_i) - N \int_{-2}^2 \frac{\sqrt{4-x^2}}{2\pi} f(x) dx \right) \Rightarrow \mathcal{N}(m_M(f), V_M(f)).$$

- CLT holds if $\lambda = 0$. (Bai-Yao, Chatterjee, Lytova-Pastur)
- CLT holds if $\lambda > 0$ and $\mathbf{x} = 1 = \frac{1}{\sqrt{N}}(1, 1, \dots, 1)^T$. (Baik-L.)
- CLT holds if M is the adjacency matrix of a (sparse) Erdős-Rényi graph and f is a polynomial. (Banerjee-Ma)
- The mean depends on λ , but the variance does not.

Test based on linear spectral statistics (LSS)



Goal: find $f = f_{\omega}^*$ that maximizes

$$\left| \frac{m_M(f) - m_H(f)}{\sqrt{V_M(f)}} \right|$$

Hypothesis Testing - Algorithm 1

$$f_{\omega}^*(x) = \log \left(\frac{1}{1 - \sqrt{\omega}x + \omega} \right) + \sqrt{\omega} \left(\frac{2}{w_2} - 1 \right) x + \omega \left(\frac{1}{w_4 - 1} - \frac{1}{2} \right) x^2.$$

- Compute the test statistic

$$\begin{aligned} L_{\omega} &= \sum_{i=1}^N f_{\omega}^*(\mu_i) - N \int_{-2}^2 \frac{\sqrt{4 - z^2}}{2\pi} f_{\omega}^*(z) dz \\ &= -\log \det \left((1 + \omega)I - \sqrt{\omega}M \right) + \frac{\omega N}{2} \\ &\quad + \sqrt{\omega} \left(\frac{2}{w_2} - 1 \right) \text{Tr } M + \frac{\omega}{2} \left(\frac{1}{w_4 - 1} - \frac{1}{2} \right) (\text{Tr } M^2 - N). \end{aligned}$$

- Set $m_{\omega} = \frac{1}{2}(m_M(f_{\omega}^*) + m_H(f_{\omega}^*))$
- Accept \mathbf{H}_0 if $L_{\omega} \leq m_{\omega}$; Accept \mathbf{H}_1 if $L_{\omega} > m_{\omega}$

Hypothesis Testing - Algorithm 1

- Universality:

- For any \mathbf{x} with $\|\mathbf{x}\|_2 = 1$, the proposed test and its error do not change, and thus the test **does not need any prior information on \mathbf{x}** .
- The proposed test **does not depend on the distribution of the noise H** except on $\mathbb{E}[H_{ii}^2]$ and $\mathbb{E}[H_{ij}^4]$.

- Optimality:

- The proposed test is with the lowest error among all tests based on LSS.
- For Gaussian noise, the proposed test achieves the optimal error (under a fairly weak assumption on the prior).
- For Gaussian noise, if the prior is sparse enough, the (optimal) error from the LR test is lower than that of the proposed test. Nevertheless, in this case, it is conjectured that no polynomial time tests can perform better than the proposed test. (Moitra-Wein)

Hypothesis Testing - Algorithm 2

$$h(x) := -\frac{p'(w)}{p(w)}, \quad \tilde{M}_{ij} = \frac{1}{FHN} h(\sqrt{N} M_{ij})$$

Theorem (Chung-L.)

Denoting by $\tilde{\mu}_1, \dots, \tilde{\mu}_N$ the eigenvalues of \tilde{M}

$$\left(\sum_{i=1}^N f(\tilde{\mu}_i) - N \int_{-2}^2 \frac{\sqrt{4-z^2}}{2\pi} f(z) dz \right) \Rightarrow \mathcal{N}(m_{\tilde{M}}(f), V_{\tilde{M}}(f))$$

- Find $f = \tilde{f}_\omega^*$ that maximizes $\left| \frac{m_{\tilde{M}}(f) - m_{\tilde{M}_0}(f)}{\sqrt{V_{\tilde{M}}(f)}} \right|$
- Proposed test (Algorithm 2):
 - Compute the test statistic $\tilde{L}_\omega := \sum_{i=1}^N \tilde{f}_\omega^*(\tilde{\mu}_i) - N \int_{-2}^2 \frac{\sqrt{4-z^2}}{2\pi} \tilde{f}_\omega^*(z) dz$
 - Set $\tilde{m}_\omega = \frac{1}{2}(m_{\tilde{M}}(\tilde{f}_\omega^*) + m_{\tilde{M}_0}(\tilde{f}_\omega^*))$
 - Accept \mathbf{H}_0 if $\tilde{L}_\omega \leq \tilde{m}_\omega$; Accept \mathbf{H}_1 if $\tilde{L}_\omega > \tilde{m}_\omega$

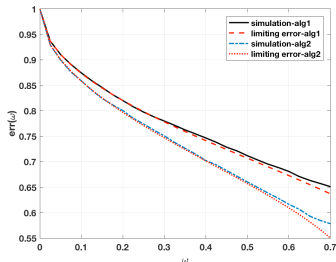
Example: Limiting errors of the two tests

- Suppose that the density function of the noise matrix is given by

$$p(x) = \frac{1}{2 \cosh(\pi x/2)} = \frac{1}{e^{\pi x/2} + e^{-\pi x/2}}$$

- Apply the entrywise transformation

$$h(x) = -\frac{p'(x)}{p(x)} = \frac{\pi}{2} \tanh \frac{\pi x}{2}, \quad \tilde{M}_{ij} = \sqrt{\frac{2}{N}} \tanh \left(\frac{\pi \sqrt{N}}{2} M_{ij} \right)$$



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