Random matrix methods for high-dimensional machine learning models

A statistical limit theory for ML models

Antoine Bodin

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Introduction & motivational example

Why Random Matrix theory needed?

Random matrices are ubuquitous in machine learning theory. **But** using them is not always straightforward. **So** can we develop simple tools to analyze high-dimensional models involving random matrices?

Example: linear-model

- **Data:** $X \in \mathbb{R}^{n \times d}$ with $X_{ij} \sim \mathcal{N}(0, \frac{1}{d})$ (n samples, d features),
- **Output:** $Y = X\beta^* + \xi$ with $\xi \sim \mathcal{N}(0, \sigma^2 I_n)$ and $\frac{1}{d} \|\beta^*\|^2 = r^2$
- **Model:** $\hat{\beta} = (X^T X + \lambda I_d)^{-1} X^T Y$ (ridge regression)

Generalization error

Averaging over new random data points (x and $y = x\beta^* + \epsilon$)

$$\mathcal{E}_{\text{gen}}(\hat{\beta}) = \mathbb{E}_{\epsilon,x}\left[(x^T\beta^* + \epsilon - x^T\hat{\beta})^2\right] = \sigma^2 + \frac{1}{d}\left\|\beta^* - \hat{\beta}\right\|^2$$

The High-dimensional Limit

Average $\mathbb{E}_{X,Y}\mathcal{E}_{\text{gen}}(\hat{\beta})$ can be decomposed with Bias-variance:

$$\frac{1}{d}\mathbb{E}_{X,\xi}\left\|\beta^* - \hat{\beta}\right\|^2 = \mathcal{B}_X(\hat{\beta}) + \mathcal{V}_X(\hat{\beta}) \tag{1}$$

with:

$$\mathcal{B}_X(\hat{\beta}) = \frac{1}{d}\mathbb{E}\left[\left\|\beta^* - \mathbb{E}[\hat{\beta}|X]\right\|^2\right] \qquad \text{and} \qquad \mathcal{V}_X(\hat{\beta}) = \frac{1}{d}\mathbb{E}\left[\left\|\hat{\beta} - \mathbb{E}[\hat{\beta}|X]\right\|^2\right]$$

... After reducing everything with $\frac{1}{d}\left\|\beta^*\right\|^2 = r^2$*:*

$$\mathcal{B}_X(\hat{\beta}) = \lambda^2 r^2 \mathbb{E}_X\left\{\frac{1}{d}\text{Tr}\left[(X^T X + \lambda I)^{-2}\right]\right\} \tag{2}$$

$$\mathcal{V}_X(\hat{\beta}) = \sigma^2 \mathbb{E}_X\left\{\frac{1}{d}\text{Tr}\left[(X^T X + \lambda I)^{-1}\right] - \lambda\frac{1}{d}\text{Tr}\left[(X^T X + \lambda I)^{-2}\right]\right\} \tag{3}$$

Conclusion

- Both terms depend on the trace $\frac{1}{d}\text{Tr}\left[(X^T X + \lambda I)^{-1}\right] = g_d(-\lambda)$
- Simplifies in the high-dimensional limit $d \to \infty$.

Random matrix theory: Marchenko-Pastur law

High-dimensional limit with $\phi = \frac{n}{d}$:

$$g(z) = \lim_{d\to\infty} \frac{1}{d}\mathbb{E}\mathrm{Tr}\left[(X^TX - zI)^{-1}\right]$$

Then [Marchenko and Pastur, 1967]:

$$zg^2 + (1+z-\phi)g + 1 = 0$$

Then also the derivative w.r.t. z:

$$z(2gg' + g^2) + (1+z-\phi)g' + g = 0$$

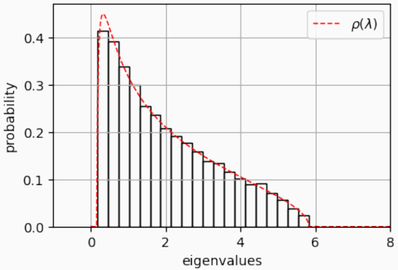


Figure 1: Marchenko-Pastur law with $\phi = 2, n = 2000, d = 1000$ and $\rho(\lambda) = \frac{1}{\pi}\,\mathrm{Im}\,g(\lambda + i0^+)$

Conclusion [Belkin et al., 2020, Hastie et al., 2019]

$$\mathcal{E}_{\text{gen}}(r,\sigma,\phi,\lambda) = \sigma^2 + \lambda^2 r^2 g'(-\lambda) + \sigma^2(g(-\lambda) - \lambda g'(-\lambda))$$

Double-descent phenomenon

Take again the algebraic equations:

$$\begin{cases} -\lambda g^2 + (1-\lambda-\phi)g + 1 = 0 \\ -\lambda(2gg' + g^2) + (1-\lambda-\phi)g' + g = 0 \end{cases}$$

Then in the limit $\lambda \to 0$:

$$\mathcal{B}_X(\hat{\beta}) = \begin{cases} r^2(1-\phi) & \text{if } \phi < 1 \\ 0 & \text{if } \phi > 1 \end{cases}$$

$$\mathcal{V}_X(\hat{\beta}) = \begin{cases} \sigma^2 \frac{\phi}{1-\phi} & \text{if } \phi < 1 \\ \sigma^2 \frac{1}{\phi-1} & \text{if } \phi > 1 \end{cases}$$

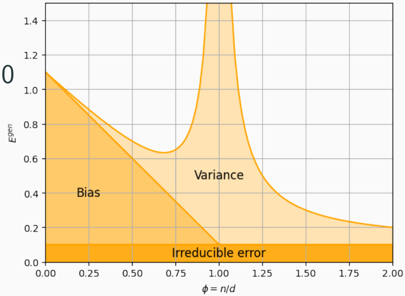


Figure 2: Test error $\sigma^2 = 0.1, r = 1$

Conclusion [Belkin et al., 2020, Hastie et al., 2019]

$$\lim_{\lambda \to 0} \mathcal{E}_{\text{gen}}(r, \sigma, \phi, \lambda) = \begin{cases} \sigma^2 + r^2(1-\phi) + \sigma^2 \frac{\phi}{1-\phi} & \text{if } \phi < 1 \\ \sigma^2 + \sigma^2 \frac{1}{\phi-1} & \text{if } \phi > 1 \end{cases}$$

More general models?

Marchenko-Pastur works well in that case, but what about more complex models?

Non-exhaustive list of interesting models:

1. Teacher-student model $Y = X\beta^*$ and $\hat{Y} = \hat{X}\beta$ with covariation structure $\Sigma = \mathbb{E}[x\hat{x}^T]$
2. Random feature model: $\hat{Y} = \sigma(WX)\beta$ to have a notion of number of parameters
3. Spike Wigner model: $Y = \beta^*{\beta^*}^T + \xi$
4. Matrix denoising: $Y = XX^T + \xi$

Is there a practical tool to analyze them?

Linear-Pencils!

Linear-Pencil Method

Level 1: Linear Pencil, the basics

Let S be a symmetric random matrix ($S_{ij} \sim \mathcal{N}(0, \frac{1}{d})$) and define Stieltjes transform of the spectral density ρ of S:

$$g(z) = \int \frac{\rho(\lambda)\mathrm{d}\lambda}{\lambda - z} = \mathrm{Tr}_d \left[(S - zI)^{-1} \right]$$

Main result [Wigner, 1958]

$$g = (z - g)^{-1} \tag{4}$$

Note 1: above eqn. often represented under the form:

$$g^2 - zg + 1 = 0$$

Note 2: $L = (S - zI)$ *is* a "trivial" linear-pencil of size 1×1! Equation (4) will follow us in the next slides.

Linear-Pencil: 3 examples

Illustration of the method with 3 examples:

1. Marchenko-Pastur:

$$g(z) = \mathrm{Tr}_d\left[(X^T X - zI_d)^{-1}\right]$$

2. Sample Covariance Matrix:

$$g(z) = \mathrm{Tr}_d\left[(C^{\frac{1}{2}} X^T X C^{\frac{1}{2}} - zI_d)^{-1}\right]$$

3. Random Feature Kernel:

$$g(z) = \mathrm{Tr}_d\left[(\sigma(WX)\sigma(WX)^T - zI)^{-1}\right]$$

Each case involves algebraic operations on a matrix level.

The linearization method

Back to Marchenko-Pastur: $L = (X^T X - zI)$ is not a linear-pencil, because it is not "linear" in X.

But we can linearize it with a block-matrix!

Consider $U_1 = (X^T X - zI)^{-1}$ with:

$$\begin{cases} (X^T X - zI)U_1 & = I \\ U_2 & = XU_1 \end{cases}$$

Then we obtain our linear-pencil L:

$$\underbrace{\begin{pmatrix} -zI & X^T \\ X & -I \end{pmatrix}}_{L} \begin{pmatrix} U_1 \\ U_2 \end{pmatrix} = \begin{pmatrix} I \\ 0 \end{pmatrix}$$

And in particular, $\mathrm{Tr}_d\,[U_1]$ is given by the partial trace of L^{-1} because:

$$U_1 = \begin{pmatrix} I & 0 \end{pmatrix} (L^{-1}) \begin{pmatrix} I \\ 0 \end{pmatrix} = (L^{-1})^{(11)}$$

Linear Pencil: main result

Step 1: Encode matrix into a wider block-matrix (variance $\frac{1}{d}$):

$$L = \begin{pmatrix} -zI_d & X^T \\ X & -I_n \end{pmatrix}$$

Step 2: Extract deterministic blocks from random matrices:

$$L_0 = \begin{pmatrix} -zI_d & 0 \\ 0 & -I_n \end{pmatrix}$$

Step 3: Calculate block-wise covariance structure of L:

$$\sigma_{12}^{21} = \sigma_{21}^{12} = 1 \qquad \sigma_{11}^{11} = \sigma_{22}^{22} = 0$$

Step 4: Define the partial-trace of the inverse, and interesting operator:

$$g_{ij} = \mathrm{Tr}_d \left[(L^{-1})^{(ij)} \right] \qquad [\eta_L(g)]_{il} = \sum_{jk \in \mathbb{S}} \sigma_{ij}^{kl} g_{jk}$$

Here, g_{11} is clearly the quantity of interest, and:

$$\eta_L(g) = \begin{pmatrix} \sigma_{12}^{21} g_{22} & 0 \\ 0 & \sigma_{21}^{12} g_{11} \end{pmatrix}$$

Linear Pencil: Main result

Main result [Rashidi Far et al., 2006, Mingo and Speicher, 2017]

$$g = (J \otimes \mathrm{Tr}_d)\left[(L_0 - (\eta_L \otimes I)(g))^{-1}\right] \tag{5}$$

1. $(\eta_L \otimes I)(\cdot)$ is the matrix operator acting on g:

$$((\eta_L \otimes I)(g))^{(ij)} = \begin{cases} [\eta_L(g)]_{ij} I_{N_i} & \text{if } N_i = N_j \\ 0_{N_i, N_j} & \text{otherwise} \end{cases}$$

So in our example:

$$L_0 - (\eta_L \otimes I)(g) = \begin{pmatrix} -zI_d - [\eta_L(g)]_{11} I_d & 0 \\ 0 & -I_n - [\eta_L(g)]_{22} I_n \end{pmatrix}$$

2. $J \odot \mathrm{Tr}_d\,[\cdot]$ is the partial trace operator:

$$[(J \otimes \mathrm{Tr}_d)\,[G]]_{ij} = \begin{cases} \mathrm{Tr}_d\left[G^{(ij)}\right] & \text{if } N_i = N_j \\ 0 & \text{otherwise} \end{cases}$$

Linear Pencil, example 1: Marchenko-Pastur

- From **step 4** we have defined:

$$g_{11} = \mathrm{Tr}_d\left[(X^T X - zI_d)^{-1}\right] \tag{6}$$

- From application of **Main result** we find:

$$\begin{pmatrix} g_{11} & 0 \\ 0 & g_{22} \end{pmatrix} = (J \otimes \mathrm{Tr}_d)\left[\begin{pmatrix} -zI_d - g_{22} I_d & 0 \\ 0 & -I_n - g_{11} I_n \end{pmatrix}^{-1}\right]$$

Conclusion

With $g_C(z) = \mathrm{Tr}_d\left[(C - zI_d)^{-1}\right]$:

$$\begin{cases} g_{11} = \mathrm{Tr}_d\left[(-zI_n - g_{22} I_n)^{-1}\right] = -(z + g_{22})^{-1} \\ g_{22} = \mathrm{Tr}_d\left[(-I_n - g_{11} I_n)^{-1}\right] = -\phi\,(1 + g_{11})^{-1} \end{cases}$$

$$g_{11} = -\frac{1}{z - \phi(1 + g_{11})^{-1}} \implies zg_{11}^2 + (1 + z - \phi)g_{11} + 1 = 0$$

Linear-pencil, example 2: Sample covariance Matrix

Linear-pencil works for more general matrices: for instance, the sample covariance matrix.

Quite often, real-world problems come from samples $u \sim \mathcal{N}(0, C)$. An equivalent model is $u = C^{\frac{1}{2}} x$ with $x \sim \mathcal{N}(0, I_d)$.

Problem

Given n samples $U = (u_1, \ldots, u_n)$ an estimation of C is given by:

$$\tilde{C} = \frac{1}{d} U U^T = C^{\frac{1}{2}} X X^T C^{\frac{1}{2}}$$

with X a random matrix. How to characterize the eigenvalue distribution of $\tilde{C}$ compared to C?

Linear-pencils allow the study of the Stieltjes transform of $\tilde{C}$:

$$g(z) = \mathrm{Tr}_d \left[(C^{\frac{1}{2}} X X^T C^{\frac{1}{2}} - z I_d)^{-1} \right]$$

Linear-pencil, example 2: Sample covariance Matrix

Let's consider instead:

$$g(z) = \mathrm{Tr}_d \left[(X^T C X - z I_n)^{-1} \right]$$

In a similar way with $h(z) = \mathrm{Tr}_d \left[U_1 \right]$ and the linearization:

$$\underbrace{\begin{pmatrix} -zI_n & 0 & X \\ 0 & C & I_d \\ X^T & I_d & 0 \end{pmatrix}}_{L} \begin{pmatrix} U_1 \\ U_2 \\ U_3 \end{pmatrix} = \begin{pmatrix} I_n \\ 0 \\ 0 \end{pmatrix}$$

and with $\sigma_{13}^{31} = \sigma_{31}^{13} = 1$:

$$L_0 = \begin{pmatrix} -zI_n & 0 & 0 \\ 0 & C & I \\ 0 & I & 0 \end{pmatrix} \qquad \text{and} \qquad \eta_L(g) = \begin{pmatrix} g_{33} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & g_{11} \end{pmatrix}$$

Linear-pencil, example 2: Sample covariance Matrix

$$M = (L_0 - (\eta_L \otimes I)(g))^{-1} = \begin{pmatrix} (-z - g_{33})I_n & 0 & 0 \\ 0 & C & I_d \\ 0 & I_d & -g_{11} I_d \end{pmatrix}^{-1}$$

Using a block-matrix inversion formula:

$$M = \begin{pmatrix} -(z + g_{33})^{-1} I_n & 0 & 0 \\ 0 & (C + g_{11}^{-1})^{-1} & (g_{11} C + I_d)^{-1} \\ 0 & (g_{11} C + I_d)^{-1} & -g_{11}^{-1}(I_d - (g_{11} C + I_d)^{-1}) \end{pmatrix}$$

Thus, formula $g = (J \otimes \mathrm{Tr}_d)[M]$ from **Main result** yields:

$$\begin{cases} g_{11} & = g(z) = -\phi(z + g_{33})^{-1} \\ g_{33} & = -\frac{1}{g_{11}}(1 - \mathrm{Tr}_d\left[(g_{11} C + I_d)^{-1}\right]) = \frac{1}{g(z)}(\frac{1}{g(z)} g_C(-\frac{1}{g(z)}) - 1) \end{cases}$$

$$\phi + z\phi g(z) + \frac{1}{g(z)} g_C\left(\frac{-1}{g(z)}\right) = 1$$

Linear-pencil, example 3: Gaussian Equivalence Principle

How to calculate $g(z) = \mathrm{Tr}_d\left[(\sigma(WX)\sigma(WX)^T - zI_d)^{-1}\right]$?

GEP [Pennington and Worah, 2017]

$$\sigma(WX) \equiv \mu WX + \nu\Omega \tag{7}$$

With: $0 = \langle \sigma, H_{e_0} \rangle$ $\quad \mu = \langle \sigma, H_{e_1} \rangle$ $\quad \mu^2 + \nu^2 = \langle \sigma, \sigma \rangle$

Ex.: $U = (\mu W, \nu\Omega)$, $V = (X^T, I)$ so $g(z) = \mathrm{Tr}_d\left[(UV^TVU^T - zI_d)^{-1}\right]$

$$L = \begin{pmatrix} -zI & 0 & 0 & U \\ 0 & 0 & V^T & I \\ 0 & V & I & 0 \\ U^T & I & 0 & 0 \end{pmatrix} = \begin{pmatrix} -zI & 0 & 0 & 0 & \mu W & \nu\Omega \\ 0 & 0 & 0 & X & I & 0 \\ 0 & 0 & 0 & I & 0 & I \\ 0 & X^T & I & I & 0 & 0 \\ \mu W^T & I & 0 & 0 & 0 & 0 \\ \nu\Omega^T & 0 & I & 0 & 0 & 0 \end{pmatrix}$$

Note: no unique encoding! In fact, possible with a 4×4 linear-pencil

GEP: Construction of 4×4 linear pencil

Consider $\mathrm{Tr}_d\left[(\sigma(XW)\sigma(XW)^T - zI)^{-1}\right] = \mathrm{Tr}_d\left[U_0\right]$:

$$\begin{aligned}((\mu WX + \nu\Omega)(\mu X^T W^T + \nu\Omega^T) - zI)U_0 &= I \\ U_1 &= \mu W^T U_0 \\ U_2 &= X^T U_1 + \nu\Omega^T U_0 \\ U_3 &= XU_2\end{aligned}$$

So first equation is: $\mu WU_3 + \nu\Omega U_2 - zU_0 = I$, so:

$$\begin{pmatrix} -zI & 0 & \nu\Omega & \mu W \\ 0 & 0 & X & -I \\ \nu\Omega^T & X^T & -I & 0 \\ \mu W^T & -I & 0 & 0 \end{pmatrix} \begin{pmatrix} U_0 \\ U_1 \\ U_2 \\ U_3 \end{pmatrix} = \begin{pmatrix} I \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

The dynamics of general linear models

Random Feature Model is just a structured linear model

Gaussian covariate model [Loureiro et al., 2021]

A mutual source of randomness Z, and two structures A and B:

$$Y = X\beta^* = (ZB)\beta^* \qquad \hat{Y} = \tilde{X}\beta = (ZA)\beta$$

With the generalization error:

$$\mathcal{E}_{\text{gen}}(\beta) = \mathbb{E}\left[(x^T\beta^* - \tilde{x}^T\beta)^2\right]$$

Ex. Random feature model with $Z = \begin{pmatrix} X_0 & \Omega & \xi \end{pmatrix}$ and:

$$\beta^* = \begin{pmatrix} \beta_0^* \\ 1 \end{pmatrix} \qquad B = \begin{pmatrix} I_d & O \\ O & O \\ 0 & \sigma \end{pmatrix} \qquad A = \begin{pmatrix} \mu W \\ \nu I_N \\ 0 \end{pmatrix}$$

Then:

$$Y = X_0\beta_0^* + \xi \qquad \hat{Y} = (\mu W X_0 + \nu\Omega)\,\beta \equiv \sigma(WX_0)\beta$$

The dynamics of the Gaussian covariate model

Main result [Bodin and Macris, 2022]

With gradient flow on: $\mathcal{E}_{\text{train}}^{\lambda}(\beta) = \frac{1}{n}\|Y - \hat{Y}(\beta)\|^2 + \frac{\lambda}{n}\|\beta\|^2$

$$\bar{\mathcal{E}}_{\text{gen}}(t) = c_0 + r_0^2 \mathcal{B}_0(t) + \mathcal{B}_1(t)$$

With random initialization $\beta(t=0) \sim \mathcal{N}(0, r_0^2 \frac{1}{d} I_d)$:

$$\mathcal{B}_1(t) = \frac{-1}{4\pi^2} \oint_\Gamma \oint_\Gamma \frac{(1-e^{-t(x+\lambda)})(1-e^{-t(y+\lambda)})}{(x+\lambda)(y+\lambda)} f_1(x,y)\mathrm{d}x\mathrm{d}y + \frac{1}{i\pi}\oint_\Gamma \frac{1-e^{-t(z+\lambda)}}{z+\lambda} f_2(z)\mathrm{d}z$$

$$\mathcal{B}_0(t) = \frac{-1}{2i\pi}\oint_\Gamma e^{-2t(z+\lambda)} f_0(z)\mathrm{d}z$$

And with $V = B\beta^*\beta^{*T}B^T$, $U = AA^T$, $c_0 = \mathrm{Tr}_d[V]$ and the self-consistent equations:

$$\begin{aligned}
f_1(x,y) &= f_2(x) + f_2(y) + \tilde{f}_1(x,y) - c_0 \\
\tilde{f}_1(x,y) &= \mathrm{Tr}_d\left[(\phi U + \zeta_x I)^{-1}(\zeta_x\zeta_y V^* + \tilde{f}_1(x,y)\phi U^2)(\phi U + \zeta_y I)^{-1}\right] \\
f_2(z) &= c_0 - \mathrm{Tr}_d\left[\zeta_z V^*(\phi U + \zeta_z I)^{-1}\right] \\
f_0(z) &= -\left(1 + \frac{\zeta_z}{z}\right) \\
\zeta_z &= -z + \mathrm{Tr}_d\left[\zeta_z U(\phi U + \zeta_z I)^{-1}\right]
\end{aligned}$$

The limit $t \to +\infty$ of the Gaussian covariate model

Secondary result [Bodin and Macris, 2022]

$$\bar{\mathcal{E}}_{\text{gen}}(+\infty) = c_0 + f_1(-\lambda, -\lambda) + 2f_2(-\lambda) = \tilde{f}_1$$
$$\bar{\mathcal{E}}^0_{\text{train}}(+\infty) = \lambda^2 \zeta^{-2} \bar{\mathcal{E}}_{\text{gen}}(+\infty)$$

With $U_\star = \phi A^T A$ and $\Xi = \phi A^T B$ and:

$$f_1 = 2f_2 + \tilde{f}_1 - c_0$$
$$f_1 = \mathrm{Tr}_n \left[((\Xi \beta^* \beta^{*T} \Xi^T) + \tilde{f}_1 U_\star) U_\star (U_\star + \zeta I)^{-2} \right]$$
$$f_2 = \mathrm{Tr}_n \left[(\Xi \beta^* \beta^{*T} \Xi^T)(U_\star + \zeta I)^{-1} \right]$$
$$\zeta = \lambda + \mathrm{Tr}_n \left[\zeta U_\star (U_\star + \zeta I)^{-1} \right]$$

See also [Loureiro et al., 2021]

Example 1: Random feature - model/sample double-descents

Ex.: Triple descent [d'Ascoli et al., 2020, Bodin and Macris, 2021]

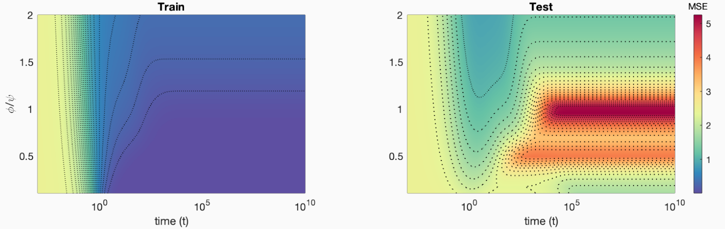


Figure 3: Parameters: $(\mu, \nu, \psi, r, s, \lambda) = (0.9, 0.1, 2, 1, 0.8, 0.0001)$

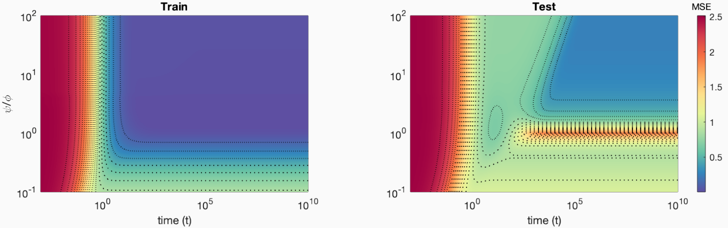
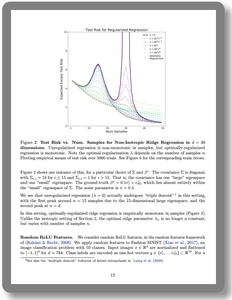


Figure 4: Parameters $(\mu, \nu, \phi, r, s, \lambda) = (0.5, 0.3, 3, 2., 0.4, 0.001)$.

Example 2: Non-Isotropic regression - Descent structures

$$B = I \quad \text{and} \quad A = \mathrm{diag}(\underbrace{\alpha^{-\frac{0}{2}}, \dots, \alpha^{-\frac{0}{2}}}_{\frac{d}{p}\text{times}}, \underbrace{\alpha^{-\frac{1}{2}}, \dots, \alpha^{-\frac{1}{2}}}_{\frac{d}{p}\text{times}}, \alpha^{-\frac{2}{2}}, \dots, \alpha^{-\frac{p-1}{2}})$$



Test Risk for Regularized Regression

Expected Excess Test Risk

Num Samples

Figure 2: **Test Risk vs. Num. Samples for Non-Isotropic Ridge Regression in $d = 30$ dimensions.** Unregularized regression is non-monotonic in samples, but optimally-regularized regression is monotonic. Note the optimal regularization λ depends on the number of samples n. Plotting empirical means of test risk over 5000 trials. See Figure 6 for the corresponding train errors.

Figure 2 shows one instance of this, for a particular choice of Σ and β^*. The covariance Σ is diagonal, with $\Sigma_{i,i} = 10$ for $i \leq 15$ and $\Sigma_{i,i} = 1$ for $i > 15$. That is, the covariance has one "large" eigenspace and one "small" eigenspace. The ground-truth $\beta^* = 0.1\vec{e_1} + \vec{e_{30}}$, which lies almost entirely within the "small" eigenspace of Σ. The noise parameter is $\sigma = 0.5$.

We see that unregularized regression ($\lambda = 0$) actually undergoes "triple descent"[2] in this setting, with the first peak around $n = 15$ samples due to the 15-dimensional large eigenspace, and the second peak at $n = d$.

In this setting, optimally-regularized ridge regression is empirically monotonic in samples (Figure 2). Unlike the isotropic setting of Section 2, the optimal ridge parameter λ_n is no longer a constant, but varies with number of samples n.

Random ReLU Features. We consider random ReLU features, in the random features framework of (Rahimi & Recht, 2008). We apply random features to Fashion-MNIST (Xiao et al., 2017), an image classification problem with 10 classes. Input images $x \in \mathbb{R}^d$ are normalized and flattened to $[-1, 1]^d$ for $d = 784$. Class labels are encoded as one-hot vectors $y \in \{\vec{e_1}, \dots \vec{e_{10}}\} \subset \mathbb{R}^{10}$. For a

[2] See also the "multiple descent" behavior of kernel interpolants in Liang et al. (2020).

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[Nakkiran et al., 2020]

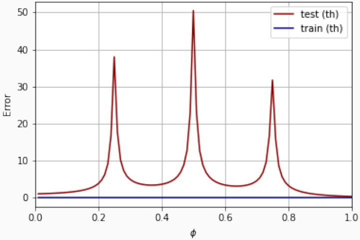

Figure 5: $p = 4, \lambda = 10^{-13}$, $\alpha = 10^4$

Result with $\alpha \to +\infty$ [Bodin and Macris, 2022]

$$\bar{\mathcal{E}}_{\text{gen}}(+\infty) = \frac{1}{p} \sum_{k=0}^{p-1} \frac{\phi(1-\phi)}{\left(\phi - \frac{k}{p}\right)\left(\frac{k+1}{p} - \phi\right)} \mathbb{1}_{]\frac{k}{p}; \frac{k+1}{p}[}(\phi) - \phi + o_\alpha(1)$$

Example 3: Realistic datasets

- **Data:** MNIST dataset $X_0 \in \mathbb{R}^{n_{tot} \times d}$ with normalized entries and $n_{tot} = 60'000$ and $d = 28 \times 28 = 784$
- **Aim:** Learning the parity ($y = \pm 1$ for even/odd numbers)
- **Structure:** cov. matrix $U_\star \simeq \frac{1}{n_{tot}} X^T X$ and $\Xi \beta^* \simeq X^T Y$ (since $X^T X = A^T (Z^T Z) A$ and $X^T Y = A(Z^T Z) B \beta^*$ and $n_{tot} \gg d$)

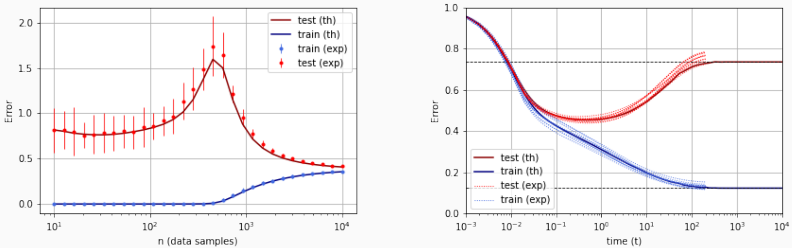

Figure 6: Comparison between the analytical and experimental learning profiles for the minimum least-squares estimator at $\lambda = 10^{-3}$ on the left (20 runs) and the time evolution at $\lambda = 10^{-2}$, $n = 700$ on the right (10 runs).

Questions?

Appendix: Gaussian Equivalence Principle

From [Lu and Yau, 2022, Mei and Montanari, 2019] with $y, x \in \mathbb{S}^{d-1}$, decomposition with Gegenbauer polynomials:

$$\sigma(\sqrt{d}x^T y) = \sum_{k=1}^{p} \alpha_k q_k(\sqrt{d}x^T y)$$

(In high-dimenion, α_k are related to the coefficients of the Hermite polynomials decomposition).
Decoupling with spherical harmonics $Y_{k,a}$:

$$q_k(\sqrt{d}x^T y) = \frac{1}{\sqrt{N_k}} \sum_{a=0}^{N_k} Y_{k,a}(x) Y_{k,a}(y)$$

Appendix: Bias-variance decomposition

Classical bias-variance decomposition over new data point x:

$$\mathbb{E}[(y-\hat{y})^2] = \mathbb{E}[y-\hat{y}]^2 + \mathrm{Var}(\hat{y}) + \mathrm{Var}(y) \tag{8}$$

Is true when:

$$\mathrm{Var}(y-\hat{y}) = \mathrm{Var}(\hat{y}) + \mathrm{Var}(y) \implies \mathrm{Cov}(y,\hat{y}) = 0 \tag{9}$$

This is true for the R.V. $\beta_0, \xi, X, \epsilon$ (because each of them only affect either y and $\hat{y}$) but not for x (and β^* if considered random). So in fact we implicitly always require the conditional expectation on x:

$$\mathbb{E}[(y-\hat{y})^2] = \mathbb{E}_x\left[\mathbb{E}[y-\hat{y}|x]\right]^2 + \mathbb{E}_x\mathrm{Var}(\hat{y}|x) + \mathbb{E}_x\mathrm{Var}(y|x) \tag{10}$$

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