Random Matrix Theory: Selected Applications from Statistical Signal Processing and Machine Learning
Ph.D. Thesis Defense

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Introduction
Moore’s law

- The number of transistors that you can fit into a piece of silicon doubles every couple of years.

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1C. M. Bishop, Microsoft research, Cambridge.
We need a tool that embraces these challenges
Random matrix theory (RMT)

Study the behavior of large random matrices

- Allow the prediction of the behavior of random quantities depending on large random matrices
- Key of success: Randomness + High dimensionality
Statistical Signal Processing
  • Large number of antenna arrays vs large number of observations
  $\rightarrow$ Improved signal processing techniques

Wireless Communications
  • Large # of antennas, Large # of users
  $\rightarrow$ Improved transmission and detection strategies
  $\rightarrow$ Low complexity design

Machine learning
  $\rightarrow$ A better fundamental understanding
  $\rightarrow$ Improved classification performance

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$^2$ Z. Liao, R. Couillet, ”A Large Dimensional Analysis of Least Squares Support Vector Machines”, submitted

$^3$ X. Mai, R. Couillet, ”A random matrix analysis and improvement of semi-supervised learning for large dimensional data”, submitted.

RMT: Example

How does this work?

- Self-averaging effect mechanism similar to that met in the law of large numbers

- $h_1, \ldots, h_n \in \mathbb{C}^p$ with i.i.d entries with zero mean and variance $\frac{1}{n}$.

- $HH^H$ is an estimator of the cov. matrix with $H = [h_1, \ldots, h_n]$.

\[ p \text{ fixed, } n \to \infty \]

\[ p, n \to \infty, p/n \to c \]

**Figure 1.1:** Histogram of eigenvalues of $HH^H$

**Figure 1.2:** Histogram of eigenvalues of $HH^H$
Why is this useful?

The same result can be extended in the correlated case\(^5\)

Certain functionals of \( HH^H \) can be evaluated when \( p, n \to \infty, p/n \to c \).

\[
f ( HH^H )
\]

- \( \frac{1}{n} \text{tr} ( HH^H ) \)
- \( \frac{1}{n} \text{tr} ( HH^H )^{-k} \): performance of linear est. techniques
- \( \frac{1}{n} \log \det ( HH^H ) \): MIMO systems, linear estimation (LCE)
- \( \lambda_{\text{min}} ( HH^H ), \lambda_{\text{max}} ( HH^H ), \ldots \): WEV in linear estimation

What happens for the moments in the finite regime?

\[
E_{H \sim D} f ( HH^H )
\]

---

Moments of Correlated Gram matrices
Gram matrices

Linear estimation
Let \( m < n \) and \( H \in \mathbb{C}^{n \times m} \) with i.i.d zero mean unit variance Gaussian entries and \( \Lambda \) is positive definite matrix with \textit{distinct} eigenvalues \( \theta_1, \theta_2, \cdots, \theta_n \).

\[
y_{n \times 1} = H_{n \times m}v_{m \times 1} + \Lambda^{-\frac{1}{2}}z_{n \times 1}.
\]  
(1)

Define the \textit{correlated Gram} matrix

\[
G = H^* \Lambda H.
\] 
(2)

<table>
<thead>
<tr>
<th></th>
<th>LS</th>
<th>LMMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>MSE</td>
<td>( \mathbb{E} \text{ tr } G^{-1} )</td>
<td>( \mathbb{E} \text{ tr } (G + R_v^{-1})^{-1} )</td>
</tr>
</tbody>
</table>

Sample covariance matrix (SCM): \( u(k) = R^{\frac{1}{2}}h(k) \)

\[
\hat{R}(n) = (1 - \lambda) \sum_{k=1}^{n} \lambda^{n-k} u(k) u^*(k) = R^{\frac{1}{2}} \Lambda(n) H^* R^{\frac{1}{2}},
\] 
(3)

\[
\text{Loss}(n) \triangleq \mathbb{E} \left\| R^{\frac{1}{2}} \hat{R}^{-1}(n) R^{\frac{1}{2}} - I_m \right\|_F^2 \\
= m + \mathbb{E} \text{ tr } G_n^{-2} - 2 \mathbb{E} \text{ tr } G_n^{-1}
\]
Define the **negative moments** of $G$ as

$$
\mu_L (-k) \triangleq \mathbb{E} \text{tr} \left( G^{-k} \right), \quad k \in \mathbb{N}.
$$

Then,

$$
\begin{array}{|c|c|}
\hline
\text{MSE} & \mu_L (-1) & \sum_{k=0}^l \frac{(-1)^k}{\sigma_x^{2k}} \mu_L (-k - 1) + o \left( \sigma_x^{-2l} \right) \\
\hline
\end{array}
$$

$$
\text{Loss} (n) = m + \mu_L(n) (-2) - 2\mu_L(n) (-1).
$$
Theorem (Negative moments)\textsuperscript{a} Let \( p = \min (m, n - m) \), then for \( 1 \leq k \leq p \), we have

\[
\mu_{\Lambda} (-k) = L \sum_{j=1}^{k} \sum_{i=1}^{m} D(i, j) \left( -1 \right)^{k-j} \frac{(k-j)!}{(k-j)!} b_i^t \Psi^{-1} D_i a_{j,k}.
\]

Limitations

\[ \mu_\Lambda (-k) = L \sum_{j=1}^{k} \sum_{i=1}^{m} D(i, j) \frac{(-1)^{k-j}}{(k-j)!} b_i^t \psi^{-1} b_j^t \Psi_{i,j,k} \]

\[ \psi = \begin{bmatrix} 1 & \theta_1 & \cdots & \theta_{n-m-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \theta_{n-m} & \cdots & \theta_{n-m-1} \end{bmatrix} \]

- So complicated formula
- Not useful if the eigenvalues of \( \Lambda \) are close to each other (We treat this issue for positive moments) \(^6\).
- Not numerically stable if the dimensions are large.
- Not insightful!
- Not universal: the result will be different if we change the distribution from Gaussian.

---

Asymptotic moments

Theorem (Silverstein and Bai\textsuperscript{7})

Consider the Gram matrix $G = H^* \Lambda H$ with the following assumptions

- $m, n \to \infty$ with $\frac{m}{n} \to c \in (0, \infty)$
- $\|\Lambda\| = O(1)$ with $\text{rank}(\Lambda) = O(m)$.

\[
\frac{1}{m} \text{tr} G^{-1} - \delta \xrightarrow{a.s.} 0, \quad \delta = \left[ \frac{1}{m} \text{tr} \Lambda (I_n + \delta \Lambda)^{-1} \right]^{-1}.
\]

Higher inverse moments can be computed using an iterative process\textsuperscript{a}


Validation of the inverse moments

\[ m = 3 \]

\[ \mu_\Lambda(r) \text{ in dB} \]

\[ r = -1 \]

\[ r = -2 \]

\[ r = -3 \]

\[ r = -4 \]
Optimal $\lambda$ for SCM estimation

$Loss(\lambda) = m + \mu_\lambda(\neg2) - 2\mu_\lambda(\neg1)$

**Figure 2.1:** The estimation loss as a function of $\lambda$ (Exact formula).
Regularized discriminant analysis with large dimensional data
Supervised learning

- We are provided with labeled data \((\text{features}_i, \text{response}/\text{label}_i)_{1 \leq i \leq n}\).
- Fit a model to the data.
Classification

- Principle: Build a classification rule that allows to assign for an unseen observation its corresponding class.

Let \( x \) be the input data and \( f \) be the classification rule.

\[
\text{Classifier} \triangleq \begin{cases} 
\text{Assign class 1} & \text{if } f(x) > 0 \\
\text{Assign class 2} & \text{if } f(x) \leq 0 
\end{cases}
\]
Model based classification

- Data is assumed to be sampled from a certain distribution.
- The decision rule is constructed based on that.
- The MAP rule is considered in the design.

\[ \hat{k} = \arg \max_{k: \text{classes}} \mathbb{P} [C_k | x] \]

The classifier is designed to satisfy this rule.
Gaussian discriminant analysis

Gaussian mixture model for binary classification (2 classes)

- \( x_1, \ldots, x_n \in \mathbb{R}^p \)
- Class \( k \) is formed by \( x \sim \mathcal{N}(\mu_k, \Sigma_k) \), \( k = 0, 1 \)

Linear discriminant analysis (LDA): \( \Sigma_0 = \Sigma_1 = \Sigma \)

\[
W^{LDA}(x) = \left( x - \frac{\mu_0 + \mu_1}{2} \right)^T \Sigma^{-1}(\mu_0 - \mu_1) - \log \frac{\pi_1}{\pi_0} < 0.
\]

→ Decision rule is linear in \( x \).

Quadratic discriminant analysis: \( \Sigma_0 \neq \Sigma_1 \)

\[
W^{QDA}(x) = -\frac{1}{2} \log \frac{|\Sigma_0|}{|\Sigma_1|} - \frac{1}{2} (x - \mu_0)^T \Sigma_0^{-1}(x - \mu_0) + \frac{1}{2} (x - \mu_1)^T \Sigma_1^{-1}(x - \mu_1) < 0.
\]

→ Decision rule is quadratic in \( x \).

How does this perform?
• Assume $\Sigma$, $\mu_0$ and $\mu_1$ known.

• Equal priors : $\pi_0 = \pi_1 = 0.5$

• No asymptotic regime, $p$ is fixed.

The total misclassification rate is given by $^8$

$$\epsilon = \Phi \left(-\frac{\Delta}{2}\right), \quad \Delta = \|\mu_0 - \mu_1\|_{\Sigma^{-1}}$$

What happens when the statistics are not known?

---

LDA: Asymptotic regime (equal covariances)

**Asymptotic growth regime**

Let $n = n_0 + n_1$.

- $n_0, n_1, p \to \infty$ such that $\frac{p}{n} \to c < 1$.
- $\mu_0$ and $\mu_1$ are known.
- $\Sigma$ is replaced by its sample estimate $\hat{\Sigma} = \frac{1}{n-2} \sum_{k=1}^{2} \sum_{i=1}^{n_k} (x_{k,i} - \bar{x}_k)(x_{k,i} - \bar{x}_k)^T$.

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Wang et al. 2018 $^a$

$$\epsilon_{LDA} - \Phi\left[-\frac{\Delta}{2} \sqrt{1 - c}\right] \to_{\text{prob.}} 0$$


$\rightarrow$ When $c \to 1$, the misclassification rate tends to 0.5.

$\rightarrow$ For the LDA to result in acceptable performance, we need $c$ close to 0.

$\rightarrow$ Because its use of the inverse of the pooled covariance matrix, the LDA applies only when $c < 1$.

*What happens if $p > n$?*
LDA: High dimensionality

Regularization

\[ H = \left( I_p + \gamma \hat{\Sigma} \right)^{-1}. \]

Optimal \( \gamma \)?

Dimensionality reduction

\[ \text{data}_{(d)} = W_{d \times p} \times \text{data}_{(p)} \]

Best \( d \)?
LDA with random projections

Random projections

\[ \mathbb{R}^p \rightarrow \mathbb{R}^d \]
\[ x \mapsto W x \]

Projection matrix
We shall assume that the projection matrix \( W \) writes as \( W = \frac{1}{\sqrt{p}} Z \), where the entries \( Z_{i,j} \) (\( 1 \leq i \leq d, 1 \leq j \leq p \)) of \( Z \) are centered with unit variance and independent identically distributed random variables satisfying the following moment assumption. There exists \( \epsilon > 0 \), such that \( \mathbb{E} |Z_{i,j}|^{4+\epsilon} < \infty \).

Johnson-Lindenstrauss Lemma
For a given \( n \) data points \( x_1, \cdots, x_n \) in \( \mathbb{R}^p \), \( \epsilon \in (0,1) \) and \( d > \frac{8 \log n}{\epsilon^2} \), there exists a linear map \( f : \mathbb{R}^p \rightarrow \mathbb{R}^d \) such that
\[
(1 - \epsilon) \|x_i - x_j\|^2 \leq \|W x_i - W x_j\|^2 \leq (1 + \epsilon) \|x_i - x_j\|^2, \tag{4}
\]

Conditional risk after projection
\[
\epsilon^\text{P-LDA}_i = \Phi \left[ -\frac{1}{2} \sqrt{\mu^T W^T (W\Sigma W^T)^{-1} W \mu} + \frac{(-1)^{i+1} \log \frac{\pi_0}{\pi_1}}{\sqrt{\mu^T W^T (W\Sigma W^T)^{-1} W \mu}} \right].
\]
Performance of LDA with random projections

Asymptotic Performance\(^a\)

\[
\epsilon_{i}^{\text{P-LDA}} = \Phi \left[ \frac{-\frac{1}{2} \mu^\top (\Sigma + \delta_d I_p)^{-1} \mu + (-1)^{i+1} \log \frac{\pi_0}{\pi_1}}{\sqrt{\mu^\top (\Sigma + \delta_d I_p)^{-1} \mu}} \right] \rightarrow_{\text{prob.}} 0, \tag{5}
\]

\[
\delta_d \operatorname{tr} (\Sigma + \delta_d I_p)^{-1} = p - d. \tag{6}
\]

\(\delta_d\) can be seen as a penalty on projection.


**LDA**

- **equal priors:** \(\Phi \left[ -\frac{1}{2} \sqrt{\mu^\top \Sigma \mu} \right]\)

- \(\Sigma = I_p\): \(\Phi \left[ -\frac{1}{2} \|\mu\| \right]\)

**P-LDA**

- \(\Phi \left[ -\frac{1}{2} \sqrt{\mu^\top (\Sigma + \delta_d I_p)^{-1} \mu} \right]\)

- \(\Phi \left[ -\frac{1}{2} \sqrt{d/p \|\mu\|} \right]\)
P-LDA: Experiments

- $p = 800$.
- $\mu_0 = 0_p$ and $\mu_1 = \frac{3}{\sqrt{p}} 1_p$.
- $\Sigma = \{0.4|i-j|\}_{i,j}$.

![Gaussian projection matrix](image)
![Bernoulli projection matrix](image)

![Gaussian projection matrix](image)
![Bernoulli projection matrix](image)

![MNIST (2, 3)](image)
![MNIST (2, 3)](image)
R-LDA: Asymptotic regime (equal covariances)

Asymptotic growth regime

- \( n_0, n_1, p \to \infty \) such that \( p/n \to c \in (0, \infty) \).
- \( \mu_k \) are replaced by \( \bar{x}_k = \frac{1}{n_k} \sum_{x_i \in C_k} x_i \).
- \( \Sigma^{-1} \) is replaced by its ridge estimate \( H = \left( I_p + \gamma \hat{\Sigma} \right)^{-1} \).

Hachem et al 2008.

\[
H \sim T = (I_p + \rho \Sigma)^{-1},
\]
in the sense that \( a^T (H - T) b \to_{\text{prob.}} 0 \) and \( \frac{1}{n} \text{tr} A (H - T) \to_{\text{prob.}} 0 \).


Zollanvari and Dougherty 2015

\[
\epsilon_{R-LDA}^{\text{equal}} = \Phi \left[ -\mu^T (I_p + \rho \Sigma)^{-1} \mu \right] \sqrt{D} \to_{\text{prob.}} 0
\]


What if the covariances are different?
R-LDA: Asymptotic regime (dist. covariances)

Asymptotic growth regime

- \( n_0, n_1, p \to \infty \) such that \( \frac{p}{n} \to c \in (0, \infty) \).
- \( \mu_k \) are replaced by \( \bar{x}_k = \frac{1}{n_k} \sum_{x_i \in C_k} x_i \).
- \( \Sigma^{-1} \) is replaced by its ridge estimate \( H = \left( I_p + \gamma \hat{\Sigma} \right)^{-1} \).

---

**Benaych and Couillet 2016**

\[
H \sim T_{0,1} \propto (I_p + \rho_0 \Sigma_0 + \rho_1 \Sigma_1)^{-1}
\]

---

**Elkhalil et al. 2018**

\[
\varepsilon_{\text{dist.}R-LDA} \sim \left\{ \frac{1}{2} \Phi \left[ \frac{-\mu^T T_{0,1} \mu + \beta}{\sqrt{D_0}} \right] + \frac{1}{2} \Phi \left[ \frac{-\mu^T T_{0,1} \mu - \beta}{\sqrt{D_1}} \right] \right\} \to_{\text{prob.}} 0
\]

---

*How is this different from the case of equal covariances?*
R-LDA: Asymptotic regime (dist. covariances)

\[
\epsilon_{\text{R-LDA}}^{\text{dist.}} = \left\{ \frac{1}{2} \Phi \left[ -\frac{\mu^T T_{0,1} \mu + \beta}{\sqrt{D_0}} \right] + \frac{1}{2} \Phi \left[ -\frac{\mu^T T_{0,1} \mu - \beta}{\sqrt{D_1}} \right] \right\} \rightarrow_{\text{prob.}} 0
\]

Some insights

• If \( \|\Sigma_0 - \Sigma_1\| = o(1) \)

\[
\epsilon_{\text{R-LDA}}^{\text{dist.}} = \epsilon_{\text{R-LDA}}^{\text{equal}} + o(1).
\]

→ R-LDA is robust against small perturbations.

• Different misclassification rates across classes.

• The enhancement in the misclassification rate in one class is likely to be lost by the other class.

• R-LDA does not leverage well the information about the covariance differences.

What about R-QDA?
### R-QDA: Asymptotic regime

<table>
<thead>
<tr>
<th>R-LDA</th>
<th>R-QDA</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_0, n_1$ samples</td>
<td>$n_0, n_1$ samples</td>
</tr>
</tbody>
</table>

$$\hat{\Sigma} = \frac{1}{n-2} \sum_{k=1}^{2} \sum_{i=1}^{n_k} (x_{k,i} - \bar{x}_k)(x_{k,i} - \bar{x}_k)^T$$

$$\hat{\Sigma}_0 = \frac{1}{n_0-1} \sum_{i=1}^{n_0} (x_{0,i} - \bar{x}_0)(x_{0,i} - \bar{x}_0)^T$$

$$\hat{\Sigma}_1 = \frac{1}{n_1-1} \sum_{i=1}^{n_1} (x_{1,i} - \bar{x}_1)(x_{1,i} - \bar{x}_1)^T$$

$$\epsilon_i = P \left[ \omega^T B_i \omega + 2 \omega^T y_i < \xi_i \right]$$, where $\omega \sim \mathcal{N}(0_p, I_p)$.

#### Asymptotic growth regime

1. Data scaling: $\frac{n_i}{p} \to c \in (0, \infty)$, with $|n_0 - n_1| = o(p)$.
2. Mean scaling: $\|\mu_0 - \mu_1\|^2 = O(\sqrt{p})$.
3. Covariance scaling: $\|\Sigma_i\| = O(1)$.
4. $\Sigma_0 - \Sigma_1$ has exactly $O(\sqrt{p})$ eigenvalues of $O(1)$.

#### CLT (Lyapunov)

$$\epsilon_i^{R-QDA} - \Phi \left[ (-1)^i \frac{1/ \sqrt{p} \xi_i - 1/ \sqrt{p} \text{tr} B_i}{\sqrt{1/p2 \text{tr} B_i^2 + 1/p4 y_i^T y_i}} \right] \to_{\text{prob.}} 0.$$
Elkhalil et al. 2017/2018 $^a$ $^b$

\[
\epsilon_{i}^{R-QDA} = \left\{ \frac{1}{2} \Phi \left[ \frac{\xi_0 - b_0}{\sqrt{2B_0}} \right] + \frac{1}{2} \Phi \left[ \frac{-\xi_1 + b_1}{\sqrt{2B_1}} \right] \right\} \rightarrow \text{prob. 0.}
\]

$\bar{\xi}_i$, $\bar{b}_i$ and $\bar{B}_i$ depend on the classes’ statistics.


Recall that R-QDA needs $\|\mu_0 - \mu_1\|^2 = O(\sqrt{p})$

$\|\mu_0 - \mu_1\| = O(1)$

The information on the distance between the means is asymptotically useless!
Discussion

\[ \Sigma_0 - \Sigma_1 \text{ has more than } O\left(\sqrt{p}\right) \text{ eigenvalues of } O(1) \]

\[ \parallel \mu_0 - \mu_1 \parallel^2 = O(\sqrt{p}) \]

R-QDA achieves asymptotic perfect classification.
Discussion

\[ \| \Sigma_0 - \Sigma_1 \| = o(1) \]

\[ \| \mu_0 - \mu_1 \| = O(1) \]

Classification is asymptotically impossible.
Discussion

- Unbalanced training: \( n_0 - n_1 = O(p) \).

R-QDA is equivalent to the naive classifier.

\[ \epsilon \rightarrow \pi_0 \Phi(\infty) + \pi_1 \Phi(-\infty) \]
Parameter tuning

- Prone to estimation errors due to insufficiency in the number of observations.
- The tuning of the regularization parameter is very important.

Model selection

Given a set of candidate regularization factors:

- Evaluate the performance using the test data for each regularization value\(^9\)
- Select the value that presents the lowest mis-classification rate

Consistent estimator of the classification error

Exploiting the asymptotic equivalent

- If \( p = O(1) \) and \( n \to \infty \), then \( \| \hat{\Sigma}_i - \Sigma_i \| = o_p(1) \).
- When \( p, n \to \infty \), then \( \| \hat{\Sigma}_i - \Sigma_i \| \neq o_p(1) \).

\[
\hat{\epsilon}_{R-LDA} - \Phi \left[ \frac{(1)^i G (\hat{\mu}_i, \hat{\mu}_0, \hat{\mu}_1, H)}{\sqrt{D (\hat{\mu}_0, \hat{\mu}_1, H, \hat{\Sigma}_i)}} \right] \to_p 0
\]

\[
\hat{\epsilon}_{R-QDA} - \Phi \left[ \frac{(1)^i (\hat{\xi}_i - \hat{b}_i)}{\sqrt{2B_i}} \right] \to_p 0
\]

Optimal regularizer

\[ \hat{\gamma}^* = \arg \min_{\gamma > 0} \hat{\epsilon}(\gamma). \]

- These results provides a glimpse on the region where the optimal \( \gamma \) is likely to belong.
- Perform a cross validation or testing in that region.

How well does this perform?
Performance

Benchmark estimation techniques:

- 5-fold cross-validation with 5 repetitions (5-CV).
- 0.632 bootstrap (B632).
- 0.632+ bootstrap (B632+)
- Plugin estimator consisting of replacing the stats. in the DEs by their sample estimates.

Synthetic data

- $[\Sigma_0]_{i,j} = 0.6|i-j|$
- $\Sigma_1 = \Sigma_0 + 3 \begin{bmatrix} I_{\lceil \sqrt{p} \rceil} & 0_{k \times (p-k)} \\ 0_{(p-k) \times k} & 0_{(p-k) \times (p-k)} \end{bmatrix}$
- $\mu_0 = [1, 0_{1 \times (p-1)}]^T$
- $\mu_1 = \mu_0 + \frac{0.8}{\sqrt{p}} 1_{p \times 1}$

Real data

- USPS dataset.
- $p = 256$ features ($16 \times 16$) grayscale images.
- $n = 7291$ training examples.
- $n_{test} = 2007$ testing examples.
Performance: Synthetic data

Figure 3.1: \( n_0 = n_1 \) and \( \gamma = 1 \).
Figure 3.2: $p = 100$ features with equal training size ($n_0 = n_1 = p$).
Figure 3.3: \( n_0 = n_1 \) and \( \gamma = 1 \). The first row gives the performance for the USPS data with digits (5, 2) whereas the second row considers the digits (5, 6).
Performance: USPS dataset

$n_0 = 100$

$n_0 = 400$

$n_0 = 100$

$n_0 = 400$

Figure 3.4: Equal training size ($n_0 = n_1$).
Centered Kernel Ridge Regression (CKRR)
KRR: Kernel trick

\[ y = w^T x \]

\[ y = w^T \phi(x) \]
KRR: Kernel trick

- \( \{ \mathbf{x}_i, y_i \}_{i=1}^n \) in \( \mathcal{X} \times \mathcal{Y} \) s.t. \( y_i = f(\mathbf{x}_i) + \sigma \epsilon_i \) with \( \epsilon_i \sim \text{i.i.d. } \mathcal{N}(0, 1) \).
- Feature map: \( \phi : \mathcal{X} \rightarrow \mathcal{H} \), with \( \mathcal{H} \) is a RKHS.
- Learning problem

\[
\begin{align*}
\min_{\alpha} & \quad \frac{1}{2} \| \mathbf{y} - \Phi \alpha \|^2 + \frac{\lambda}{2} \| \alpha \|^2 \\
\Phi & = [\phi(\mathbf{x}_1), \ldots, \phi(\mathbf{x}_n)]^T \in \mathbb{R}^{\mathcal{H} \times n}
\end{align*}
\]

\[
\alpha^* = \left( \Phi^T \Phi + \lambda I |\mathcal{H}| \right)^{-1} \Phi^T \mathbf{y} \in \mathbb{R}^{|\mathcal{H}|}
\]

Woodbury
\[
\begin{align*}
f^*(\mathbf{x}) &= \phi(\mathbf{x})^T \left( \Phi^T \Phi + \lambda I |\mathcal{H}| \right)^{-1} \Phi^T \mathbf{y} \\
f^*(\mathbf{x}) &= \phi(\mathbf{x})^T \Phi^T \left( \Phi \Phi^T + \lambda I_n \right)^{-1} \mathbf{y}
\end{align*}
\]

\[
\{ \Phi \Phi^T \}_{i,j} = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)
\]

\[
f^*(\mathbf{x}) = \kappa(\mathbf{x})^T (\mathbf{K} + \lambda I_n)^{-1} \mathbf{y}
\]

with \( \kappa(\mathbf{x})_i = \phi(\mathbf{x})^T \phi(\mathbf{x}_i) \) and \( \mathbf{K}_{i,j} = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j) \).
Inner-product kernels

\[ k(x, x') = \phi(x)^T \phi(x') = g\left(x^T x / p\right), \text{ } x \text{ and } x' \in \mathcal{X}. \]

Asymptotic growth regime

Assumption 1.

- \( p/n \to c(0, \infty) \).
- \( \mathbb{E}x_i = 0 \) and \( \text{cov}x_i = \Sigma \) unif. bounded in \( p \) (e.g. \( x_i \sim \mathcal{N}(0, \Sigma) \)).

El Karoui 2010\(^a\)

\[ \| K - K^\infty \| \to a.s. 0 \]

with \( K^\infty = g(0) 11^T + g'(0) \frac{XX^T}{p} + \text{constant}(g, \Sigma). \)

Centered KRR: Motivation

Inner-product kernels

\[ k(x, x') = \phi(x)^T \phi(x') = g\left(\frac{x^T x}{p}\right), \text{ } x \text{ and } x' \in \mathcal{X}. \]

Asymptotic growth regime

Assumption 1.

- \( p/n \rightarrow c(0, \infty). \)
- \( \mathbb{E}x_i = 0 \) and \( \text{cov}x_i = \Sigma \) unif. bounded in \( p \) (e.g. \( x_i \sim \mathcal{N}(0, \Sigma) \)).

Centering with \( P = I_n - \frac{11^T}{n} \)

\[ K_c = PKP \]

El Karoui 2010

\[ \|K - K^\infty\| \to_{a.s.} 0 \]

with \( K^\infty = g(0)11^T + g'(0)\frac{XX^T}{p} + \text{constant}(g, \Sigma). \)

\[ \|\cdot\| = O(p), \|\cdot\| = O(1) \]

Centered KRR

\[ P = I_n - \frac{11^T}{n}. \]

Learning problem

\[
\begin{align*}
\min_{\alpha_0, \alpha} & \quad \frac{1}{2} \| y - \Phi \alpha - \alpha_0 1_n \|^2 + \frac{\lambda}{2} \| \alpha \|^2 \\
\iff \quad & \min_{\alpha} \frac{1}{2} \| P (y - \Phi \alpha) \|^2 + \frac{\lambda}{2} \| \alpha \|^2
\end{align*}
\]

\[ \alpha^* = \Phi^T P \left( PKP + \lambda I_n \right)^{-1} (y - \bar{y} 1_n) \]

\[ f_c^* (x) = \kappa_c (x)^T (K_c + \lambda I_n)^{-1} P y + \bar{y}. \]

\[ \kappa_c (x) = P \kappa (x) - \frac{1}{n} PK 1_n, \quad \phi_c (x) = \phi (x) - \frac{1}{n} \sum_{i=1}^{n} \phi (x_i). \]

Centered KRR \sim KRR with centered kernels

What about the performance?
### Performance metrics

\[
\mathcal{R}_{\text{train}} = \frac{1}{n} \mathbb{E} \left\| \hat{f}_c (X) - f (X) \right\|_2^2
\]

\[
\mathcal{R}_{\text{test}} = \mathbb{E}_{s \sim \mathcal{D}, \epsilon} \left\| \hat{f}_c (s) - f (s) \right\|_2^2
\]

### Assumption 1. (Growth rate)
As \( p, n \to \infty \) we assume the following

- **Data scaling**: \( p/n \to c \in (0, \infty) \).
- **Covariance scaling**: \( \lim \sup_p \| \Sigma \| < \infty \).

### Assumptions 2. (Kernel function)

\[
\mathbb{E} \left| g^{(3)} \left( \frac{1}{p} x_i^T x_j \right) \right|^k < \infty.
\]

### Assumption 3. (Data generating function)

- \( \mathbb{E}_{x \sim \mathcal{N}(0, \Sigma)} |f(x)|^k < \infty \),

- \( \mathbb{E}_{x \sim \mathcal{N}(0, \Sigma)} \| \nabla f (x) \|_2^k < \infty \), where \( \nabla f (x) = \left\{ \frac{\partial f (x)}{\partial x_l} \right\}_{l=1}^p \).
CKRR: Limiting risk

Let \( z = -\frac{\lambda + g(\tau) - g(0) - \tau g'(0)}{g'(0)} \) with \( \tau = \frac{1}{p} \text{tr} \Sigma \).

\begin{align*}
R_{\text{train}} - R_{\text{train}}^\infty & \rightarrow_{\text{prob.}} 0, \\
R_{\text{test}} - R_{\text{test}}^\infty & \rightarrow_{\text{prob.}} 0, \\
R_{\text{train}}^\infty &= \left( \frac{c\lambda m_z}{g'(0)} \right)^2 \frac{n (1 + m_z)^2 (\sigma^2 + \text{var}_f) - nm_z (2 + m_z) \|\mathbb{E} [\nabla f]\|^2}{n (1 + m_z)^2 - pm_z^2} + \sigma^2 - 2\sigma^2 \frac{c\lambda m_z}{g'(0)} \\
R_{\text{test}}^\infty &= \frac{n (1 + m_z)^2 (\sigma^2 + \text{var}_f) - nm_z (2 + m_z) \|\mathbb{E} [\nabla f]\|^2}{n (1 + m_z)^2 - pm_z^2} - \sigma^2. 
\end{align*}


Bad news ☹ Minimim prediction risk is achieved by all kernels!! ~ Linear kernel

Good news ☺ kernel/regularizer can be jointly optimized!
Interesting relation between $\mathcal{R}_\infty^{\text{train}}$ and $\mathcal{R}_\infty^{\text{test}}$

$$
\mathcal{R}_\infty^{\text{test}} = \left( \frac{c\lambda m_z}{g'(0)} \right)^{-2} \mathcal{R}_\infty^{\text{train}} - \sigma^2 \left( \frac{g'(0)}{c\lambda m_z} - 1 \right)^2.
$$

Consistent estimator of $\hat{\mathcal{R}}^{\text{test}}$

$$
\hat{\mathcal{R}}^{\text{test}} = \left( \frac{c\lambda \hat{m}_z}{g'(0)} \right)^{-2} \hat{\mathcal{R}}^{\text{train}} - \sigma^2 \left( \frac{g'(0)}{c\lambda \hat{m}_z} - 1 \right)^2,
$$

$$
\hat{m}_z = \frac{1}{p} \text{tr} \left( \frac{XX^T}{p} - zI_n \right)^{-1}.
$$

Issues with $\lambda$ small 😊
Consistent estimator of $\hat{R}_{\text{test}}$

$$\hat{R}_{\text{test}} = \frac{1}{(cz\hat{m}_z)^2} \left[ \frac{1}{np} y^T P X \left( z\hat{Q}_z^2 - \hat{Q}_z \right) X^T P y + \text{var}(y) \right] - \sigma^2.$$ 

$$\hat{Q}_z = \left( \frac{X^T P X}{p} - z I_p \right)^{-1}.$$ 

More stable with respect to $\lambda \circledast$

$$\hat{R}_{\text{test}}^* = \min_{z \notin \text{Supp}\{XX^T/p\}} \hat{R}_{\text{test}}(z), \ z^* = -\frac{\lambda^* + g^*(\tau) - g^*(0) - \tau g'^*(0)}{g'^*(0)}.$$
Kernels

- Linear kernels: \( k(x, x') = \alpha x^T x' / p + \beta \).
- Polynomial kernels: \( k(x, x') = \left( \alpha x^T x'/p + \beta \right)^d \).
- Sigmoid kernels: \( k(x, x') = \tanh \left( \alpha x^T x'/p + \beta \right) \).
- Exponential kernels: \( k(x, x') = \exp \left( \alpha x^T x'/p + \beta \right) \).

Synthetic data

- \( x \sim \Sigma^{1/2} z \) with \( z \{z_i\}_{i=1}^P, \mathbb{E} z_i = 0, \text{var} z_i = 1 \) and \( \mathbb{E} z_i^k = O(1) \).
- Generating function: \( f(x) = \sin \left( \frac{1}{\sqrt{\beta}} x \right) \).

Real data

- Communities and Crime dataset.
- \( p = 122, n_{\text{train}} = 73 \) and \( n_{\text{test}} = 50 \).
- Prediction risk is computed by averaging over 500 data shuffling.
CKRR: Synthetic data

- **Linear kernel, $\alpha = 1, \beta = 1$**
  - $p = 100, n = 200$
  - $p = 200, n = 100$
  - Bernoulli data
  - Gaussian data

- **Polynomial kernel, $\alpha = 1, \beta = 1, d = 2$**
  - $p = 100, n = 200$
  - $p = 200, n = 100$
  - Bernoulli data
  - Gaussian data

- **Sigmoid kernel, $\alpha = 1, \beta = -1$**
  - $p = 100, n = 200$
  - $p = 200, n = 100$
  - Bernoulli data
  - Gaussian data

- **Exponential kernel, $\alpha = 1, \beta = 0$**
  - $p = 100, n = 200$
  - $p = 200, n = 100$
  - Bernoulli data
  - Gaussian data
Figure 4.1: CKRR risk with respect to the regularization parameter $\lambda$ on Gaussian data $(x \sim \mathcal{N}(\mathbf{0}_p, \{0.4^{|i-j|}\}_{i,j}), n = 200$ training samples and $p = 100$ predictors.
Figure 4.2: CKRR risk with respect to $\lambda$ where independent zero mean Gaussian noise samples with variance $\sigma^2 = 0.05$ are added to the true response.
Conclusion
Random matrix theory is a powerful tool that has been applied with success to the fields wireless communications and signal processing, providing solutions to very challenging problems.

High dimensionality along with stochasticity are the sole prerequisite of this tool.

Successful application of this tool has been demonstrated in the context of RDA.

Fundamental limits of Centered kernel ridge regression.
Future research directions
Future research directions

- We can also consider the performance analysis of kernel LDA/QDA.
- Extend the analysis to *Homogenous* kernels.
Important results on Homogenus Kernel matrices

- $\phi(x)$ is a fixed non linear feature space mapping. The kernel function is given by
  $$k(x, x') = \phi(x)^T \phi(x').$$

- Homogeneous kernels
  $$k(x, x') = f\left(\frac{\|x - x'\|^2}{p}\right).$$

- $\{K\}_{i,j} = k(x_i, x_j)$.

**Theorem (Spectrum of kernel random matrices, El-Karoui 2010)**

**[Informal statement]**

$$\hat{K} = f(\tau) 11^T + f'(\tau) W + f''(\tau) Q, \quad \frac{\|x - x'\|^2}{p} \to_{a.s.} \tau.$$  

$$\|K - \hat{K}\| \xrightarrow{p} 0.$$  

(7)

This might help to analyze the performance of some kernel methods in regression or classification.

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That’s it

Thank you for your time and attention!