Polynomial Spectral Decomposition of Conditional Expectation Operators

Anuran Makur and Lizhong Zheng

EECS Department, Massachusetts Institute of Technology

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Outline

1. Introduction
   - Motivation: Regression and Maximal Correlation
   - Preliminaries
   - Spectral Characterization of Maximal Correlation
2. Polynomial Decompositions of Compact Operators
3. Illustrations of Polynomial SVDs

Motivation: Regression and Maximal Correlation

Fix a joint distribution $P_{X,Y}$ on $\mathcal{X} \times \mathcal{Y}$.

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Regression: [Breiman and Friedman, 1985]
Find $f^\star \in \mathcal{F}$ and $g^\star \in \mathcal{G}$ that minimize the mean squared error:

$$\inf_{f \in \mathcal{F},\, g \in \mathcal{G}} \mathbb{E}\left[(f(X) - g(Y))^2\right]$$

where we minimize over:

$$\mathcal{F} \triangleq \left\{f : \mathcal{X} \to \mathbb{R} \,|\, \mathbb{E}[f(X)] = 0,\ \mathbb{E}\left[f^2(X)\right] = 1\right\}$$
$$\mathcal{G} \triangleq \left\{g : \mathcal{Y} \to \mathbb{R} \,|\, \mathbb{E}[g(Y)] = 0,\ \mathbb{E}\left[g^2(Y)\right] = 1\right\}$$

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Maximal Correlation: [Rényi, 1959]
Find $f^\star \in \mathcal{F}$ and $g^\star \in \mathcal{G}$ that maximize the correlation:

$$\rho(X;Y) \triangleq \sup_{f \in \mathcal{F},\, g \in \mathcal{G}} \mathbb{E}[f(X)g(Y)]$$

Equivalence: $\mathbb{E}[(f(X) - g(Y))^2] = 2 - 2\mathbb{E}[f(X)g(Y)]$

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Maximal correlation is a singular value of an operator!

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- Source random variable $X \in \mathcal{X} \subseteq \mathbb{R}$
  with probability density P_X
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- Marginal probability laws: $\mathbb{P}_X$ and $\mathbb{P}_Y$

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- **Hilbert spaces:**

$$\mathcal{L}^2(\mathcal{X}, \mathbb{P}_X) \triangleq \left\{ f : \mathcal{X} \to \mathbb{R} \,\middle|\, \mathbb{E}\left[f^2(X)\right] < +\infty \right\}$$
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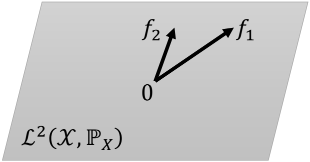

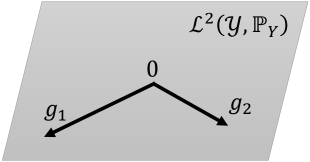

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$$\langle f_1, f_2 \rangle_{\mathbb{P}_X} \triangleq \mathbb{E}\left[f_1(X) f_2(X)\right] \qquad \langle g_1, g_2 \rangle_{\mathbb{P}_Y} \triangleq \mathbb{E}\left[g_1(Y) g_2(Y)\right]$$

Correlation as inner products

Preliminaries

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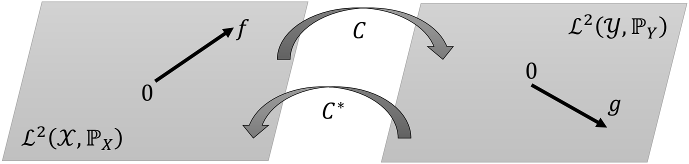

- **Conditional Expectation Operators:**

$C:\mathcal{L}^2(\mathcal{X},\mathbb{P}_X)\to\mathcal{L}^2(\mathcal{Y},\mathbb{P}_Y)$: $(C(f))(y) \triangleq \mathbb{E}[f(X)|Y=y]$

$C^*:\mathcal{L}^2(\mathcal{Y},\mathbb{P}_Y)\to\mathcal{L}^2(\mathcal{X},\mathbb{P}_X)$: $(C^*(g))(x) \triangleq \mathbb{E}[g(Y)|X=x]$

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Proposition (Conditional Expectation Operators)

C and C^* are bounded linear operators with operator norms $\|C\|_{\mathrm{op}} = \|C^*\|_{\mathrm{op}} = 1$. Moreover, C^* is the adjoint operator of C.

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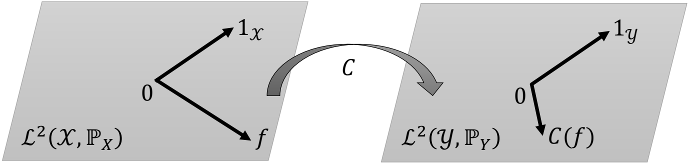
- $\|C\|_{\text{op}} \leq 1$ by Jensen's inequality:

$$\|C(f)\|_{\mathbb{P}_Y}^2 = \mathbb{E}\left[\mathbb{E}\left[f(X)|Y\right]^2\right] \leq \mathbb{E}\left[\mathbb{E}\left[f^2(X)|Y\right]\right] = \|f\|_{\mathbb{P}_X}^2 .$$



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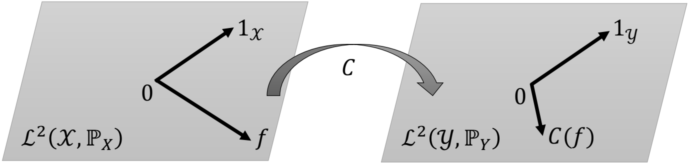
- **Operator Norm:** $\|C\|_{\text{op}} \triangleq \sup_{f \in \mathcal{L}^2(\mathcal{X}, \mathbb{P}_X)} \dfrac{\|C(f)\|_{\mathbb{P}_Y}}{\|f\|_{\mathbb{P}_X}}$
- $\|C\|_{\text{op}} \leq 1$ by Jensen's inequality.
- Let $\mathbf{1}_S : S \to \mathbb{R}$ denote the everywhere unity function: $\mathbf{1}_S(x) = 1$. $C(\mathbf{1}_\mathcal{X}) = \mathbf{1}_\mathcal{Y}$ and $\|\mathbf{1}_\mathcal{X}\|^2_{\mathbb{P}_X} = \|\mathbf{1}_\mathcal{Y}\|^2_{\mathbb{P}_Y} = 1 \Rightarrow \|C\|_{\text{op}} = 1$.



Spectral Characterization of Maximal Correlation

Prop (Spectral Characterization of Maximal Correlation) [Rényi, 1959]

For random variables X and Y as defined earlier:

$$\rho(X;Y) = \sup_{\substack{f \in \mathcal{L}^2(\mathcal{X},\mathbb{P}_X): \\ \mathbb{E}[f(X)]=0}} \frac{\|C(f)\|_{\mathbb{P}_Y}}{\|f\|_{\mathbb{P}_X}}$$

where the supremum is achieved by some $f^\star \in \mathcal{L}^2(\mathcal{X}, \mathbb{P}_X)$ if C is compact.

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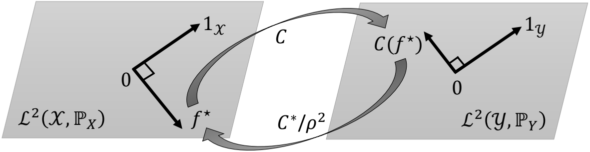

- C has largest singular value $\|C\|_{\text{op}} = 1$: $C(\mathbf{1}_\mathcal{X}) = \mathbf{1}_\mathcal{Y}$, $C^*(\mathbf{1}_\mathcal{Y}) = \mathbf{1}_\mathcal{X}$.

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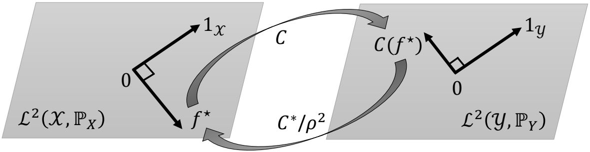

- C has largest singular value $\|C\|_{\text{op}} = 1$: $C(\mathbf{1}_\mathcal{X}) = \mathbf{1}_\mathcal{Y}$, $C^*(\mathbf{1}_\mathcal{Y}) = \mathbf{1}_\mathcal{X}$.
- $\rho(X;Y) =$ second largest singular value of C with singular vectors $f^\star \perp \mathbf{1}_\mathcal{X}$ and $g^\star = C(f^\star)/\rho(X;Y) \perp \mathbf{1}_\mathcal{Y}$ that maximize correlation.

Outline

The Hermite SVD

Gaussian Channel: $P_{Y|X=x} = \mathcal{N}(x, \nu)$ with expectation parameter $x \in \mathbb{R}$ and fixed variance $\nu \in (0, \infty)$

$$\forall x, y \in \mathbb{R}, \quad P_{Y|X}(y|x) = \frac{1}{\sqrt{2\pi\nu}} \exp\left(-\frac{(y-x)^2}{2\nu}\right)$$

Gaussian Source: $P_X = \mathcal{N}(0, p)$ with fixed variance $p \in (0, \infty)$

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Remark: (AWGN channel) $Y = X + W$ with $X \perp\!\!\!\perp W \sim \mathcal{N}(0, \nu)$

Gaussian Output Marginal: $P_Y = \mathcal{N}(0, p + \nu)$

$$\forall y \in \mathbb{R}, \quad P_Y(y) = \frac{1}{\sqrt{2\pi(p+\nu)}} \exp\left(-\frac{y^2}{2(p+\nu)}\right)$$

The Hermite SVD

Prop (Hermite SVD) [Abbe & Zheng, 2012], [Makur & Zheng, 2016]

For the Gaussian channel $P_{Y|X}$ and Gaussian source P_X, the conditional expectation operator $C : \mathcal{L}^2(\mathbb{R}, \mathbb{P}_X) \to \mathcal{L}^2(\mathbb{R}, \mathbb{P}_Y)$ has SVD:

$$\forall k \in \mathbb{N}, \;\; C\left(H_k^{(p)}\right) = \sigma_k H_k^{(p+\nu)}$$

with singular values: $\{\sigma_k \in (0,1] : k \in \mathbb{N}\}$ where $\sigma_0 = 1$ and $\lim_{k\to\infty} \sigma_k = 0$, and singular vectors:

- $\{H_k^{(p)}$ with degree $k : k \in \mathbb{N}\}$ - Hermite polynomials that are orthonormal with respect to $\mathbb{P}_X$,
- $\{H_k^{(p+\nu)}$ with degree $k : k \in \mathbb{N}\}$ - Hermite polynomials that are orthonormal with respect to $\mathbb{P}_Y$.

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For which joint distributions $P_{X,Y}$ are the singular vectors of C orthonormal polynomials?

Assumptions and Definitions

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Assumptions and Definitions

Definition (Closure over Polynomials and Degree Preservation)

An operator $T : \mathcal{L}^2(\mathcal{X}, \mathbb{P}_X) \rightarrow \mathcal{L}^2(\mathcal{Y}, \mathbb{P}_Y)$ is closed over polynomials if for any polynomial $p \in \mathcal{L}^2(\mathcal{X}, \mathbb{P}_X)$, $T(p)$ is also a polynomial. Furthermore, T is degree preserving if:

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Convolution preserves polynomials!

Polynomial EVD of Compact Self-Adjoint Operators

Theorem (Condition for Orthonormal Polynomial Eigenbasis) [Makur and Zheng, 2016]

Let $T : \mathcal{L}^2(\mathcal{X}, \mathbb{P}_X) \rightarrow \mathcal{L}^2(\mathcal{X}, \mathbb{P}_X)$ be a compact self-adjoint operator. T is closed over polynomials and degree preserving if and only if:

$$\forall k \in \mathbb{N}, \quad T(p_k) = \alpha_k p_k$$

where $\{\alpha_k \in \mathbb{R} : k \in \mathbb{N}\}$ are eigenvalues satisfying $\lim_{k \rightarrow \infty} \alpha_k = 0$.

Polynomial SVD of Conditional Expectation Operators

Theorem (Condition for Orthonormal Polynomial Singular Vectors) [Makur and Zheng, 2016]

Suppose $C : \mathcal{L}^2(\mathcal{X}, \mathbb{P}_X) \rightarrow \mathcal{L}^2(\mathcal{Y}, \mathbb{P}_Y)$ is compact and $C^* : \mathcal{L}^2(\mathcal{Y}, \mathbb{P}_Y) \rightarrow \mathcal{L}^2(\mathcal{X}, \mathbb{P}_X)$ is its adjoint operator.
C and C^* are closed over polynomials and *strictly* degree preserving if and only if:

$$\forall k \in \mathbb{N}, \quad C(p_k) = \beta_k q_k$$

where $\{\beta_k \in (0, \infty) : k \in \mathbb{N}\}$ are the singular values such that $\lim_{k \to \infty} \beta_k = 0$.

Polynomial SVD of Conditional Expectation Operators

Theorem (Condition for Orthonormal Polynomial Singular Vectors) [Makur and Zheng, 2016]

Suppose $C \triangleq \mathbb{E}[\cdot|Y] : \mathcal{L}^2(\mathcal{X}, \mathbb{P}_X) \rightarrow \mathcal{L}^2(\mathcal{Y}, \mathbb{P}_Y)$ is compact and $C^* = \mathbb{E}[\cdot|X] : \mathcal{L}^2(\mathcal{Y}, \mathbb{P}_Y) \rightarrow \mathcal{L}^2(\mathcal{X}, \mathbb{P}_X)$ is its adjoint operator. For every $n \in \mathbb{N}$, $\mathbb{E}[X^n|Y]$ is a polynomial in Y with degree n and $\mathbb{E}[Y^n|X]$ is polynomial in X with degree n if and only if:

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Gaussian Example Proof Sketch:

- $Y = X + W$ with $X \sim \mathcal{N}(0, p) \perp\!\!\!\perp W \sim \mathcal{N}(0, \nu)$.

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- C, C^* are defined by *convolution kernels* which preserve polynomials.

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Theorem (Condition for Orthonormal Polynomial Singular Vectors) [Makur and Zheng, 2016]

Suppose $C \triangleq \mathbb{E}[\cdot|Y] : \mathcal{L}^2(\mathcal{X}, \mathbb{P}_X) \to \mathcal{L}^2(\mathcal{Y}, \mathbb{P}_Y)$ is compact and $C^* = \mathbb{E}[\cdot|X] : \mathcal{L}^2(\mathcal{Y}, \mathbb{P}_Y) \to \mathcal{L}^2(\mathcal{X}, \mathbb{P}_X)$ is its adjoint operator. For every $n \in \mathbb{N}$, $\mathbb{E}[X^n|Y]$ is a polynomial in Y with degree n and $\mathbb{E}[Y^n|X]$ is polynomial in X with degree n if and only if:

$$\forall k \in \mathbb{N}, \ \ C(p_k) = \beta_k q_k$$

where $\{\beta_k \in (0,1] : k \in \mathbb{N}\}$ are the singular values such that $\beta_0 = 1$ and $\lim_{k \to \infty} \beta_k = 0$.

Gaussian Example Proof Sketch:

- $Y = X + W$ with $X \sim \mathcal{N}(0,p) \perp\!\!\!\perp W \sim \mathcal{N}(0,\nu)$.
- C, C^* are defined by *convolution kernels* which preserve polynomials.
- By above theorem, C has Hermite polynomial singular vectors.

Outline

1. Introduction
2. Polynomial Decompositions of Compact Operators
3. Illustrations of Polynomial SVDs
   - The Laguerre SVD
   - The Jacobi SVD
   - Natural Exponential Families and Conjugate Priors

The Laguerre SVD

Poisson Channel: $P_{Y|X=x} = \text{Poisson}(x)$ with rate parameter $x \in (0, \infty)$

$$\forall x \in (0,\infty), \forall y \in \mathbb{N}, \;\; P_{Y|X}(y|x) = \frac{x^y e^{-x}}{y!}$$

Gamma Source: $P_X = \text{gamma}(\alpha, \beta)$ with shape parameter $\alpha \in (0, \infty)$ and rate parameter $\beta \in (0, \infty)$

$$\forall x \in (0,\infty), \;\; P_X(x) = \frac{\beta^\alpha x^{\alpha-1} e^{-\beta x}}{\Gamma(\alpha)}$$

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Negative Binomial Output Marginal:
$P_Y = \text{negative-binomial}\left(p = \frac{1}{\beta+1}, \alpha\right)$ with success probability parameter $p \in (0,1)$ and number of failures parameter $\alpha \in (0, \infty)$

$$\forall y \in \mathbb{N}, \;\; P_Y(y) = \frac{\Gamma(\alpha+y)}{\Gamma(\alpha) y!} \left(\frac{1}{\beta+1}\right)^y \left(\frac{\beta}{\beta+1}\right)^\alpha$$

The Laguerre SVD

Proposition (Laguerre SVD) [Makur and Zheng, 2016]

For the Poisson channel $P_{Y|X}$ and gamma source P_X, the conditional expectation operator $C : \mathcal{L}^2\left((0,\infty), \mathbb{P}_X\right) \rightarrow \mathcal{L}^2\left(\mathbb{N}, \mathbb{P}_Y\right)$ has SVD:

$$\forall k \in \mathbb{N}, \;\; C\left(L_k^{(\alpha,\beta)}\right) = \sigma_k M_k^{\left(\alpha, \frac{1}{\beta+1}\right)}$$

with singular values: $\{\sigma_k \in (0,1] : k \in \mathbb{N}\}$ where $\sigma_0 = 1$ and $\lim_{k\rightarrow\infty} \sigma_k = 0$, and singular vectors:

- $\{L_k^{(\alpha,\beta)}$ with degree $k : k \in \mathbb{N}\}$ - generalized Laguerre polynomials that are orthonormal with respect to $\mathbb{P}_X$,
- $\{M_k^{\left(\alpha, \frac{1}{\beta+1}\right)}$ with degree $k : k \in \mathbb{N}\}$ - Meixner polynomials that are orthonormal with respect to $\mathbb{P}_Y$.

The Jacobi SVD

Binomial Channel: $P_{Y|X=x} = \text{binomial}(n, x)$ with number of trials parameter $n \in \mathbb{N}\backslash\{0\}$ and success probability parameter $x \in (0, 1)$

$$\forall x \in (0,1), \forall y \in [n] \triangleq \{0, \ldots, n\}\,, \;\; P_{Y|X}(y|x) = \binom{n}{y} x^y (1-x)^{n-y}$$

Beta Source: $P_X = \text{beta}(\alpha, \beta)$ with shape parameters $\alpha \in (0, \infty)$ and $\beta \in (0, \infty)$

$$\forall x \in (0,1), \;\; P_X(x) = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{\mathrm{B}(\alpha, \beta)}$$

The Jacobi SVD

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Beta-Binomial Output Marginal: $P_Y = \text{beta-binomial}(n, \alpha, \beta)$

$$\forall y \in [n], \;\; P_Y(y) = \binom{n}{y} \frac{\mathrm{B}(\alpha + y, \beta + n - y)}{\mathrm{B}(\alpha,\beta)}$$

The Jacobi SVD

Proposition (Jacobi SVD) [Makur and Zheng, 2016]

For the binomial channel $P_{Y|X}$ and beta source P_X, the conditional expectation operator $C : \mathcal{L}^2\left((0,1), \mathbb{P}_X\right) \rightarrow \mathcal{L}^2\left([n], \mathbb{P}_Y\right)$ has SVD:

$$\forall k \in [n], \;\; C\left(J_k^{(\alpha,\beta)}\right) = \sigma_k Q_k^{(\alpha,\beta)}$$

$$\forall k \in \mathbb{N} \backslash [n], \;\; C\left(J_k^{(\alpha,\beta)}\right) = 0$$

with singular values: $\{\sigma_k \in (0,1] : k \in [n]\}$ where $\sigma_0 = 1$, and singular vectors:

- $\{J_k^{(\alpha,\beta)}$ with degree $k : k \in \mathbb{N}\}$ - Jacobi polynomials that are orthonormal with respect to $\mathbb{P}_X$,
- $\{Q_k^{(\alpha,\beta)}$ with degree $k : k \in [n]\}$ - Hahn polynomials that are orthonormal with respect to $\mathbb{P}_Y$.

Why are these joint distributions special?

- $P_{Y|X}$ is a natural exponential family with quadratic variance function (introduced in [Morris, 1982]):

$$\forall x \in \mathcal{X}, \forall y \in \mathcal{Y}, \;\; P_{Y|X}(y|x) = \exp\left(xy - \alpha(x) + \beta(y)\right)$$

  where $P_{Y|X}(y|0) = \exp\left(\beta(y)\right)$ is the *base distribution*, $\alpha(x)$ is the *log-partition function* with $\alpha(0) = 0$, and $\mathbb{VAR}(Y|X = x)$ is a *quadratic* function of $\mathbb{E}\left[Y|X = x\right]$.

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- P_X belongs to the corresponding conjugate prior family:

$$\forall x \in \mathcal{X}, \;\; P_X(x; y', n) = \exp\left(y'x - n\alpha(x) - \tau(y', n)\right)$$

where $\tau(y', n)$ is the *log-partition function*.

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- All moments exist and are finite:
  - Gaussian likelihood with Gaussian prior,
  - Poisson likelihood with gamma prior,
  - binomial likelihood with beta prior.

Conclusion

Summary:

1. Regression and maximal correlation
   $\Rightarrow$ conditional expectation operators
2. Closure over polynomials and degree preservation
   $\Leftrightarrow$ orthogonal polynomial eigenvectors or singular vectors
3. Check conditional moments are polynomials
   $\Rightarrow$ Gaussian-Gaussian, Gamma-Poisson, Beta-Binomial examples
4. Examples have natural exponential family/conjugate prior structure


That's all Folks!