# Introduction to Christoffel-Darboux kernels for data analysis

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collaboration with François Bachoc and Jean-Bernard Lasserre and Mihai Putinar and Trang-May Vu.

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# Content of the presentation

Introduction of Christoffel-Darboux kernels and Christoffel function.

Overview of first properties.

Statistical aspects and application to support inference.

# Motivation

**Mathematical context:**

- Christoffel-Darboux (CD) kernels and orthogonal polynomials $\sim$ 19-th century.
- Important in approximation theory (convergence of generalized Fourier series).
- There is still a lot of activity going on.
- Recently used in, data science, polynomial optimization contexts.

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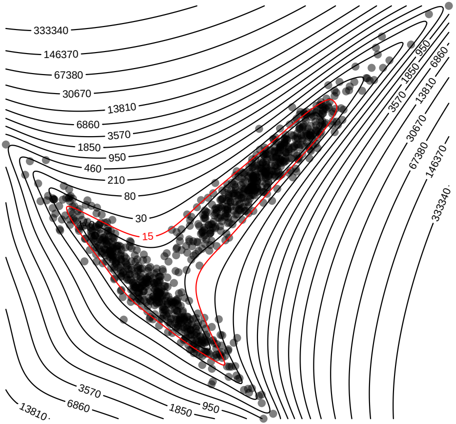
- Moments correspond to empirical averages in a statistical context.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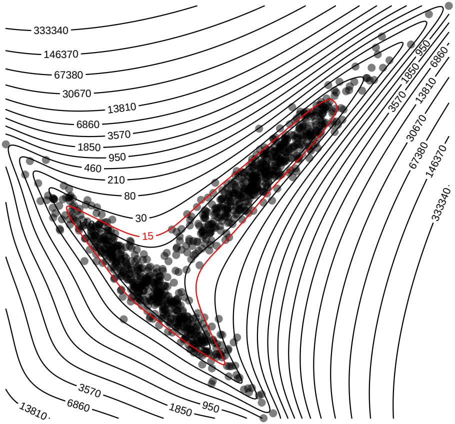
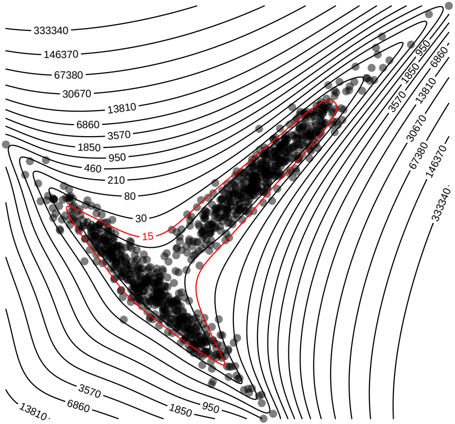
# How does it look like?




- $(\mathbf{x}_i)_{i=1}^N$ is a set of points in $\mathbb{R}^2$ (black dots).
- $\mu$ is the empirical average $\mu = \frac{1}{N}\sum_{i=1}^N \delta_{\mathbf{x}_i}$.
- The CD kernel is a function on $\mathbb{R}^2 \times \mathbb{R}^2$ (level sets of $K_d^\mu(\mathbf{x}, \mathbf{x})$, $d = 4$).

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**Plan for today:** Introduction of these objects and first properties.

# Outline

1. CD kernel, Christoffel function, orthogonal polynomials, moments
2. Quantitative asymptotics
3. Empirical measures statistical aspects
4. Application to support inference from sample

$\mu$: Borel probability measure in $\mathbb{R}^p$ .
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$(\mathbb{R}_d[X], \langle\langle \cdot, \cdot \rangle\rangle_\mu)$ is a *finite dimensional, Hilbert space* of functions from $\mathbb{R}^p$ to $\mathbb{R}$.

# Reproducing Kernel Hilbert Space (RKHS)

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$\mathcal{H}$ is called RKHS and $K$ is *the* reproducing kernel of $\mathcal{H}$.

# Reproducing Kernel Hilbert Space (RKHS)

$\mathcal{H} = (\mathbb{R}_d[X], \langle\!\langle \cdot, \cdot \rangle\!\rangle_\mu)$ is a Reproducing Kernel Hilbert Space (RKHS):

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**Reproducing property:** For all $d \in \mathbb{N}$, there exists $K_d^\mu : \mathbb{R}^p \times \mathbb{R}^p \mapsto \mathbb{R}$, symmetric such that for all $\mathbf{z} \in \mathbb{R}^p$,

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**Christoffel-Darboux kernel**: $K_\mu^d$ is *the* reproducing kernel of $\mathcal{H}$.

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$$\left\langle\!\left\langle P(\cdot), K_d^\mu(\mathbf{z}, \cdot) \right\rangle\!\right\rangle_\mu = \int P(\mathbf{x}) K_d^\mu(\mathbf{z}, \mathbf{x}) d\mu(\mathbf{x}) = \int c_P^T \mathbf{v}_d(\mathbf{x}) \mathbf{v}_d(\mathbf{x})^T M_{\mu,d}^{-1} \mathbf{v}_d(\mathbf{z}) d\mu(\mathbf{x})$$

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# Computation from moments

$\mu$: Borel probability measure in $\mathbb{R}^p$ (compact support, density).
$\mathbb{R}_d[X]$: $p$-variate polynomials of degree at most $d$ (of dimension $s(d) = \binom{p+d}{d}$).

- Let $\{P_i\}_{i=1}^{s(d)}$ be any basis of $\mathbb{R}_d[X]$,
- $\mathbf{v}_d : \mathbf{x} \mapsto (P_1(\mathbf{x}), \dots, P_{s(d)}(\mathbf{x}))^T$.
- $M_{\mu,d} = \int \mathbf{v}_d \mathbf{v}_d^T d\mu \in \mathbb{R}^{s(d)\times s(d)}$ (integral coordinate-wise).
- Let $P : \mathbf{x} \mapsto c_P^T \mathbf{v}_d(\mathbf{x})$, and $Q : \mathbf{x} \mapsto c_Q^T \mathbf{v}_d(\mathbf{x})$, then

$$c_Q^T M_{\mu,d} c_P = \int (c_Q^T \mathbf{v}_d(\mathbf{x}))(\mathbf{v}_d(\mathbf{x})^T c_P) d\mu(\mathbf{x}) = \int P(\mathbf{x}) Q(\mathbf{x}) d\mu(\mathbf{x}).$$

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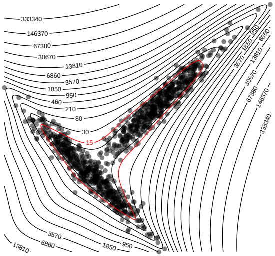
**Remark:**

- It does not depend on the choice of the basis.
- If $\mathbf{v}_d$ is the monomial basis, then we recover the usual moment matrix.

# (Practical computation: empirical measures)




**Empirical measure:** $\mu_N = \frac{1}{N} \sum_{i=1}^{N} \delta_{x_i}$.

**Polynomial basis:** Choose $\mathbf{v}_d : \mathbf{x} \mapsto (P_1(\mathbf{x}), \ldots, P_{s(d)}(\mathbf{x}))^T$.

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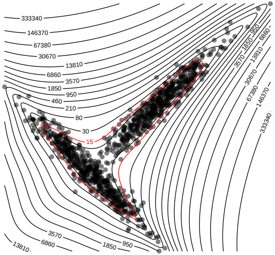


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**Empirical moments:** $D \in \mathbb{R}^{N \times s(d)}$ rows given by $\mathbf{v}_d(X_i)$, $i = 1 \ldots N$ (design matrix)

$$M_{\mu_N,d} = \frac{1}{N} D^T D.$$

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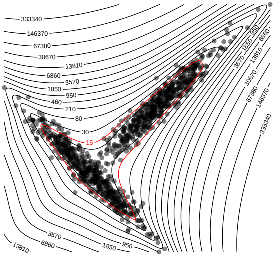


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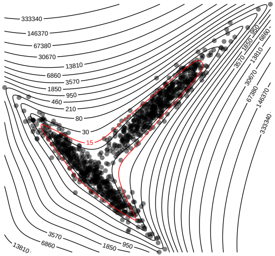
**What's wrong?**

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**Remark:** monomial basis, Gram-Schmitt provides a canonical way to construct such a basis. This is at the heart of the (rich) theory of orthogonal polynomials.

# Christoffel function

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reproducing property, Cauchy-Schwartz

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reproducing property, Cauchy-Schwartz , reproducing property.

Equality for $P(\cdot) = K_d^\mu(\mathbf{z},\cdot)/K_d^\mu(\mathbf{z},\mathbf{z})$.

# Historical remarks

Univariate case (complex and real) since beginning of 20-th century:

- quadrature, interpolation, approximation
- orthogonal polynomials
- potential theory
- random matrices/polynomials
- ...

A few contributors

- Szegö, Erdös, Turan, Freud, Totik, Máté, Nevai, ...

Still an object of very active research (asymptotics, multivariate case).

# Outline

1. CD kernel, Christoffel function, orthogonal polynomials, moments

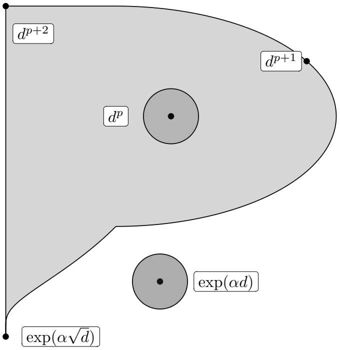
2. Quantitative asymptotics

3. Empirical measures statistical aspects

4. Application to support inference from sample

# Main idea

$\mu$: Lebesgue restricted to $S \subset \mathbb{R}^p$, compact, non-empty interior.
Order of growth of the CD kernel.



# The unit euclidean ball (Bos, Xu)

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**Lebesgue measure on the ball:** Let $\lambda_B$ be the restriction of Lebesgue measure to the unit Euclidean ball $B \subset \mathbb{R}^p$. We have

$$K_d^{\lambda_B}(0,0) \leq \frac{s(d)}{\omega_p} \frac{(d+p+1)(d+p+2)(2d+p+6)}{(d+1)(d+2)(d+3)} = O(d^p)$$

$$K_d^{\lambda_B}(\mathbf{x},\mathbf{x}) = 2\binom{p+d+1}{d} - \binom{p+d}{d} = O(d^{p+1}), \qquad \|\mathbf{x}\| = 1.$$

**Exercise:** Show that if $\mu(A) \geq \nu(A)$ for all measurable set $A$, then for all $d$, $K_d^\mu \leq K_d^\nu$.

# Smooth boundary

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**Tubular neighborhood theorem:** There exists $r > 0$ such that for all $\mathbf{x} \in S$, there is a ball of radius $r$, $B_r \subset S$ such that $x \in B_r$. Consider $\lambda_{B_r} \leq \lambda_S$.

# Explicit construction: the cube $[-1,1]^p$

**Legendre Polynomials:** $P_0(t) = 0$, $P_1(t) = t$

$$(n+1)P_{n+1}(t) = (2n+1)tP_n(t) - nP_{n-1}(t)$$

$\max_{t\in[-1,1]} P_n(t) = 1$.

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$$Q_\alpha(\mathbf{x}) = \prod_{i=1}^{p} \sqrt{\alpha_i + \frac{1}{2}} P_{\alpha_i}(x_i), \qquad \alpha \in \mathbb{N}_+^p, \quad |\alpha| < d$$

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Let $\lambda_C$ be the restriction of Lebesgue measure to the unit cube $C = [-1,1]^p$, then

$$\sup_{\mathbf{x}\in C} K_d^{\lambda_C}(\mathbf{x},\mathbf{x}) \leq \sum_{|\alpha|\leq d} \prod_{i=1}^{p} \left(\alpha_i + \frac{1}{2}\right) = O(d^{2p})$$

# Exponential lower bounds

Let $S \subset \mathbb{R}^p$ be compact and $\mu$ be a probability measure supported on $S$. Then for all $\mathbf{x}$ with $\mathrm{dist}(\mathbf{x}, S) \geq \delta > 0$, and $d \in \mathbb{N}$

$$K_d^{\mu}(\mathbf{x}, \mathbf{x}) \geq 2^{\frac{\delta d}{\delta + \mathrm{diam}(S)} - 3}.$$

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$$K_\mu^d(\mathbf{x}, \mathbf{x}) \geq \left( \int P^2 d\mu \right)^{-1}.$$

Choose $P$ such that $P(\mathbf{x}) = 1$ and the integral is small.

*Kroó's needle polynomial*, for any $\delta > 0$, $d \in \mathbb{N}^*$, $\exists Q \in \mathbb{R}_{2d}[X]$

$$Q(0) = 1, \qquad |Q(\mathbf{x})| \leq 1 \text{ if } \|\mathbf{x}\| \leq 1, \qquad |Q(\mathbf{x})| \leq 2^{1-\delta d} \text{ if } \delta \leq \|\mathbf{x}\| \leq 1.$$

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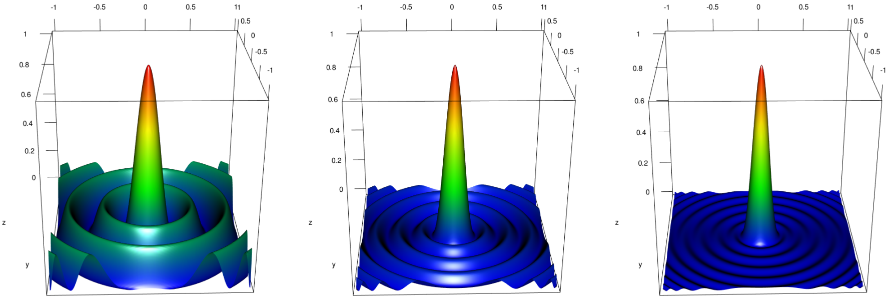
Example for $\delta = 0.2$ and $d = 20, 30, 40$.



# Exponential separation of the support

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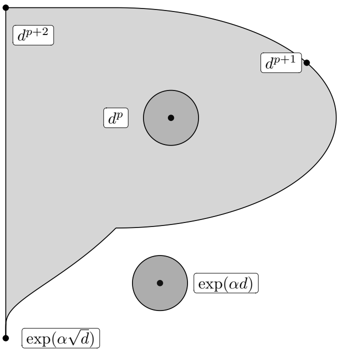


**Exponential growth dichotomy:** Growth of the CD kernel is

- At most polynomial in the degree $d$ in the interior of the support.
- Exponential in the degree $d$ outside the support.
- In between on the boundary of the support of $\mu$: depending on local geometry.

# Outline

# Empirical christoffel-Darboux kernel

$\mu$: Borel probability measure in $\mathbb{R}^p$ (compact support, density).
$\mathbb{R}_d[X]$: $p$-variate polynomials of degree at most $d$ (of dimension $s(d) = \binom{p+d}{d}$).
(dimension $p$ and degree $d$ are fixed).

$$(P, Q) \quad \mapsto \quad \langle\langle P, Q \rangle\rangle_\mu := \int PQ d\mu,$$

defines a valid scalar product on $\mathbb{R}_d[X]$.

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**Example:** $P \colon \mathbf{x} \mapsto \prod_{i=1}^n \|\mathbf{x} - \mathbf{x}_i\|^2$, $\qquad \langle\!\langle P, P \rangle\!\rangle_{\mu_N} = 0$ but $P \neq 0$.

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How to ensure that $\Lambda_d^{\mu_N}$ retains the favorable properties of $\Lambda_d^{\mu}$?

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**Strong law of large numbers:** for any continuous $f$, almost surely

$$\lim_{N\to\infty} \int f(\mathbf{z}) d\mu_N(\mathbf{z}) = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} f(X_i) = \int f(\mathbf{z}) d\mu(\mathbf{z}),$$

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**Statistical tools:** Concentration for random matrices (non commutative Bernstein).

# Outline

## Leveraging the exponential growth dichotomy

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**Hausdorff Distance:** $d_H(X, Y)$ between two compact sets $X, Y$:

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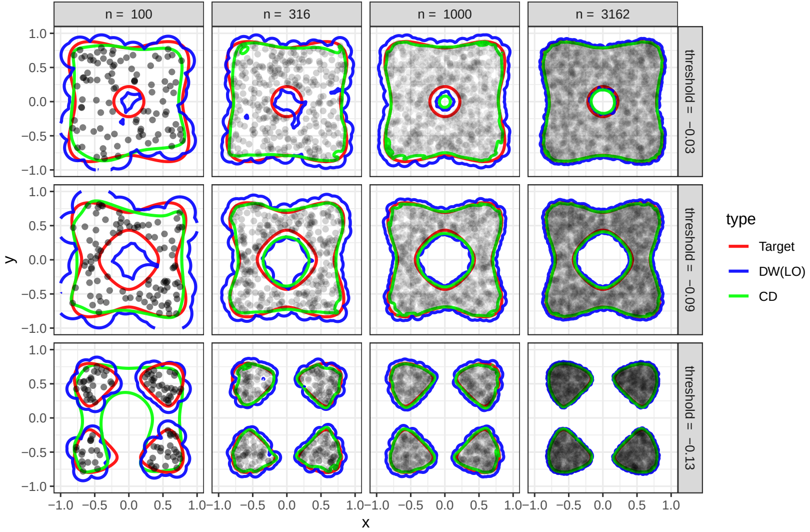
# Numerical illustration



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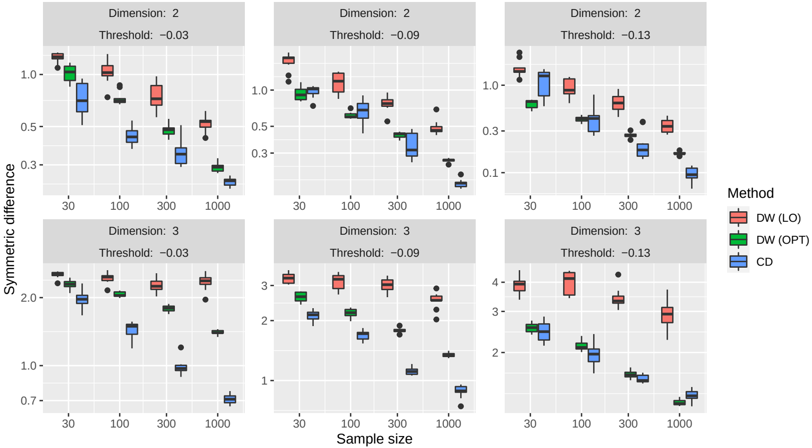

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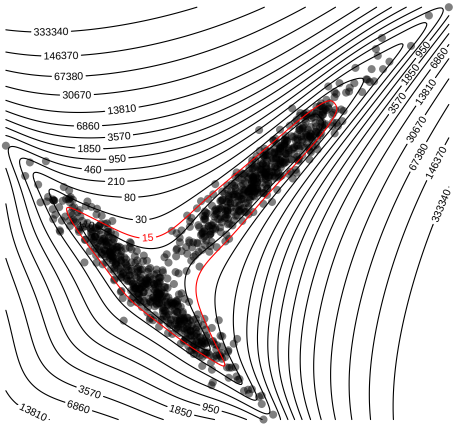
# Thanks



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