

Colloquium du CERMICS



Moments, Positive Polynomials, and the Christoffel Function

Jean-Bernard Lasserre

LAAS – CNRS

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Moments, Positive Polynomials, and the Christoffel Function

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... in collaboration with
D. Henrion, M. Korda, V. Magron, S. Marx, E. Pauwels, M.
Putinar, T. Weisser

Vol. 1

Imperial College Press Optimization Series

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Moments, Positive Polynomials and Their Applications

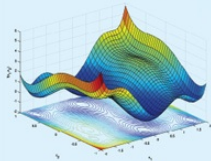
Many important problems in global optimization, algebra, probability and statistics, applied mathematics, control theory, financial mathematics, inverse problems, etc. can be modeled as a particular instance of the *Generalized Moment Problem (GMP)*.

This book introduces, in a unified manual, a new general methodology to solve the GMP when its data are polynomials and basic semi-algebraic sets. This methodology combines semidefinite programming with recent results from real algebraic geometry to provide a hierarchy of semidefinite relaxations converging to the desired optimal values. Applied on appropriate cones, standard duality in convex optimization nicely expresses the duality between moments and positive polynomials.

In the second part of this invaluable volume, the methodology is particularized and described in detail for various applications, including global optimization, probability, optimal control, mathematical finance, multivariate integration, etc., and examples are provided for each particular application.

Moments, Positive Polynomials
and Their Applications

Lasserre



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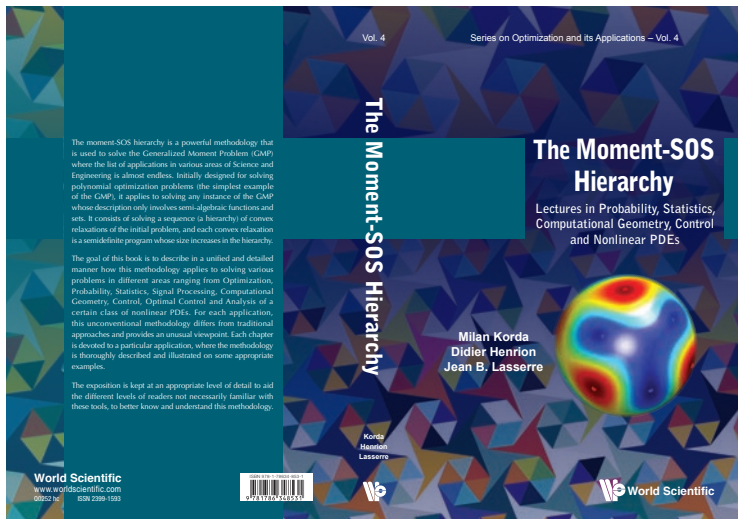
Imperial College Press

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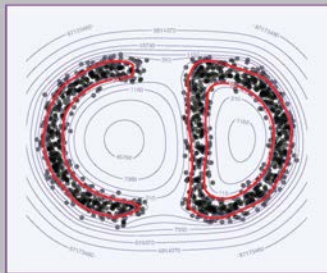
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Cambridge Monographs on Applied and Computational Mathematics

The Christoffel-Darboux Kernel for Data Analysis

Jean Bernard Lasserre, Edouard Pauwels
and Mihai Putinar



- Part I:
 - The **Moment-SOS** hierarchy
 - SOS-based **CERTIFICATES** of **POSITIVITY**
 - Illustration of the Moment-SOS hierarchy for **POLYNOMIAL** optimization
- Part II:
 - The **Christoffel** function
 - Applications and link with Optimization

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A brief overview of the methodology on 3 examples

Let \mathbf{P} be the initial problem to solve, for instance

- Optimization $\min_{\mathbf{x}} \{f(\mathbf{x}) : \mathbf{x} \in \mathbf{K}\}$
- Optimal control

$$\min_u \int_0^1 h(\mathbf{x}(t), u(t)) dt$$

$$\dot{\mathbf{x}}(t) = f(\mathbf{x}(t), u(t)), \quad t \in (0, 1)$$


$$\mathbf{x}(t) \in X; \quad u(t) \in U, \quad t \in [0, 1]$$

- Compute (or approximate)



$$\tau = \int_{\mathbf{K}} \mathbf{x}^\alpha d\lambda(\mathbf{x}), \quad \alpha \in \Gamma,$$

and in particular, $\text{vol}(\mathbf{K})$ ($\Gamma = \{0\}$) where \mathbf{K} is compact basic semi-algebraic set.

basic strategy

-  (i) Search for a measure μ whose **support** is the solution

$$d\mu(\mathbf{x}) = \delta_{x^*}; \quad d\mu(x, u, t) = \delta_{x(t), u(t)}(d(x, u)) dt; \quad d\mu(\mathbf{x}) = \lambda_{\mathbf{K}}(d\mathbf{x})$$

-  (ii) compute its moments, and
-  (iii) recover the solution from moments.

Implementation in Three steps:

I: LIFTING

I: Build up an **infinite-dimensional LP** with μ as unknown:

Constraints of the initial problem become

 **LINEAR constraints**

on the **unknown moments** $(\mu_\alpha)_{\alpha \in \mathbb{N}^n}$ of μ

II: Truncation

Consider only **FINITELY MANY** candidate moments y_α :

- ☞ **Semidefinite constraints** on the scalars y_α 's state **necessary conditions** to qualify them as **moments** of some measure μ
- ☞ Solve the resulting **finite-dimensional convex** (conic) optimization problem to obtain a **guaranteed lower bound**.

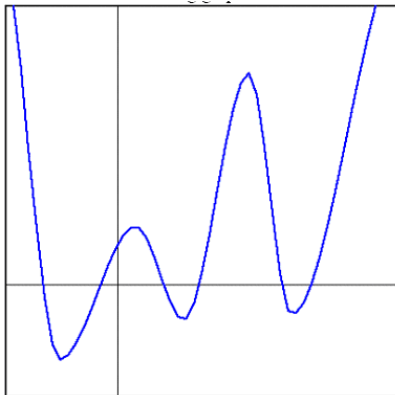
III: Iterate

- ☞ **Increase** the number of moments considered and iterate so as to obtain a **monotone non increasing sequence** of **lower bounds** which **converges to the optimal value**.

Consider the polynomial optimization problem:

$$\mathbf{P} : f^* = \min\{f(\mathbf{x}) : g_j(\mathbf{x}) \geq 0, j = 1, \dots, m\},$$

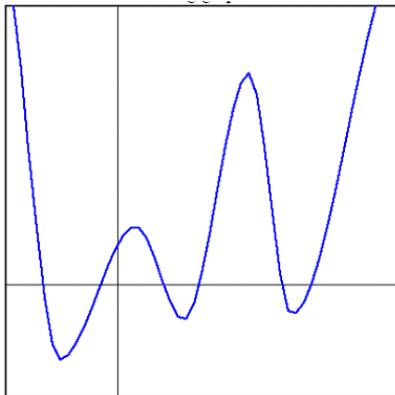
for some polynomials $f, g_j \in \mathbb{R}[\mathbf{x}]$.



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Why Polynomial Optimization?

After all ... **P** is just a particular case of Non Linear Programming (**NLP**)!

True!

... if one is interested with a **LOCAL** optimum only!!

☞ Many minimization algorithms do the job efficiently.

☞ The fact that f, g_j are **POLYNOMIALS** does not help much!

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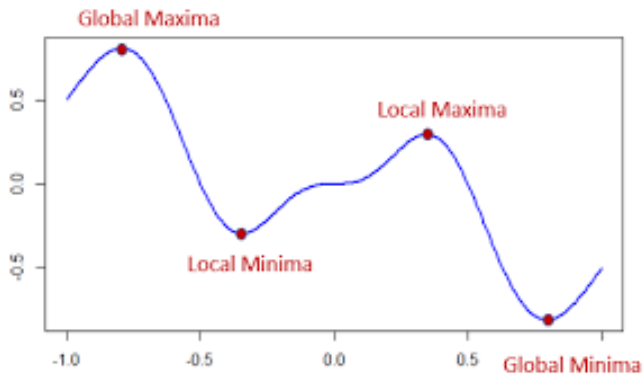
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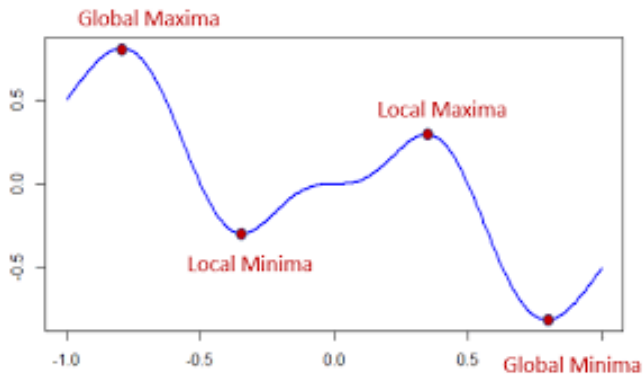
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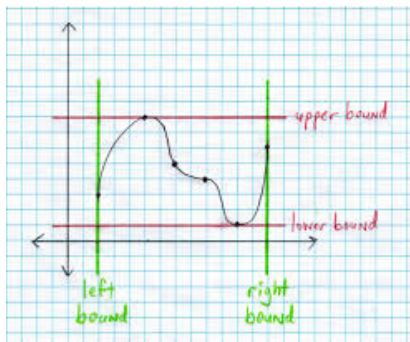
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Remember that for the **GLOBAL** minimum f^* :

$$f^* = \sup_{\lambda} \{ \lambda : f(\mathbf{x}) - \lambda \geq 0 \quad \forall \mathbf{x} \in \mathbf{K} \}.$$

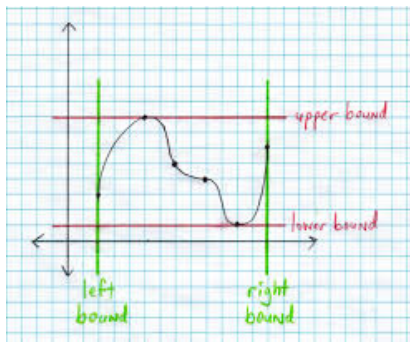
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and so to compute (or approximate) f^* ...

☞ one needs to handle **EFFICIENTLY** the difficult constraint

$$f(\mathbf{x}) - \lambda \geq 0 \quad \forall \mathbf{x} \in \mathbf{K}, \quad (f - \lambda \mathbf{1} \in \mathcal{P}(\mathbf{K})_+)$$

i.e. one needs

☞ **TRACTABLE CERTIFICATES** of **POSITIVITY** on \mathbf{K}
for the polynomial $\mathbf{x} \mapsto f(\mathbf{x}) - \lambda$!

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REAL ALGEBRAIC GEOMETRY helps!!!!

Indeed, **POWERFUL CERTIFICATES OF POSITIVITY** EXIST!

Moreover ... and importantly,

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Such certificates are amenable to **PRACTICAL COMPUTATION!**

SOS-based certificate

A polynomial p is a **sum-of-squares (SOS)** if and only if

$$p(\mathbf{x}) = \sum_{k=1}^s q_k(\mathbf{x})^2, \quad \forall \mathbf{x} \in \mathbb{R}^n,$$

for some polynomials q_k .

☞ Detecting whether a given polynomial p is **SOS** can be done efficiently by solving a **SEMIDEFINITE PROGRAM**

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Illustration for univariate polynomials

Let $v_d(t) = (1, t, t^2, \dots, t^d)$ and let p be of **even** degree $2d$.

$$p(t) = \sum_{k=1}^{2d} p_k t^k \quad (= \langle \mathbf{p}, v_{2d}(t) \rangle)$$

is SOS if and only if there exists $Q \succeq 0$ such that

$$p(t) = \begin{bmatrix} 1 \\ t \\ \dots \\ t^d \end{bmatrix}^T \underbrace{\begin{bmatrix} a & b & c & \dots \\ b & d & e & \dots \\ c & e & f & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix}}_{Q \succeq 0} \begin{bmatrix} 1 \\ t \\ t^2 \\ \dots \\ t^d \end{bmatrix}$$

$$Q \succeq 0 \Rightarrow Q = \sum_{j=1}^s \mathbf{q}_k \mathbf{q}_k^T$$

$$\begin{aligned} \begin{bmatrix} 1 \\ t \\ t^2 \end{bmatrix}^T Q \begin{bmatrix} 1 \\ t \\ \dots \\ t^d \end{bmatrix} &= \sum_{k=1}^s \left(\begin{bmatrix} 1 \\ t \\ \dots \\ t^d \end{bmatrix}^T \mathbf{q}_k \right) \left(\mathbf{q}_k^T \begin{bmatrix} 1 \\ t \\ \dots \\ t^d \end{bmatrix} \right) \\ &= \sum_{k=1}^s \mathbf{q}_k(t)^2 \end{aligned}$$

Conversely if

$$p(t) = \sum_{k=1}^s q_k(t)^2,$$

then write

$$\begin{aligned} p(t) &= \sum_{k=1}^s \left(\begin{bmatrix} 1 \\ t \\ \dots \\ t^d \end{bmatrix}^T \mathbf{q}_k \right) \left(\mathbf{q}_k^T \begin{bmatrix} 1 \\ t \\ \dots \\ t^d \end{bmatrix} \right) \\ &= \sum_{k=1}^s \begin{bmatrix} 1 \\ t \\ \dots \\ t^d \end{bmatrix}^T \underbrace{\left(\sum_{k=1}^s \mathbf{q}_k \mathbf{q}_k^T \right)}_{\mathbf{Q} \succeq 0} \begin{bmatrix} 1 \\ t \\ \dots \\ t^d \end{bmatrix} \end{aligned}$$

Example

Let $t \mapsto f(t) = 6 + 4t + 9t^2 - 4t^3 + 6t^4$. Is f an SOS? Do we have

$$f(t) = \begin{bmatrix} 1 \\ t \\ t^2 \end{bmatrix}^T \underbrace{\begin{bmatrix} a & b & c \\ b & d & e \\ c & e & f \end{bmatrix}}_{Q \succeq 0} \begin{bmatrix} 1 \\ t \\ t^2 \end{bmatrix}$$

We must have:

$$a = 6; 2b = 4; d + 2c = 9; 2e = -4; f = 6.$$

And so we must find a scalar c such that

$$Q = \begin{bmatrix} 6 & 2 & c \\ 2 & 9 - 2c & -2 \\ c & -2 & 6 \end{bmatrix} \succeq 0.$$

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With $c = -4$ we have

$$Q = \begin{bmatrix} 6 & 2 & -4 \\ 2 & 17 & -2 \\ -4 & -2 & 6 \end{bmatrix} \succeq 0.$$

et

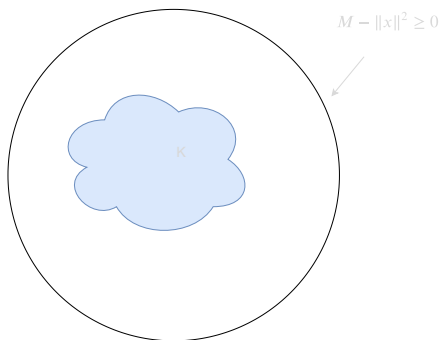
$$Q = 2 \begin{bmatrix} \sqrt{(2/2)} \\ 0 \\ \sqrt{(2)/2} \end{bmatrix} \begin{bmatrix} \sqrt{(2/2)} \\ 0 \\ \sqrt{(2)/2} \end{bmatrix}' + 9 \begin{bmatrix} 2/3 \\ -1/3 \\ -2/3 \end{bmatrix} \begin{bmatrix} 2/3 \\ 1/3 \\ -2/3 \end{bmatrix}'$$

$$+ 18 \begin{bmatrix} 1/\sqrt{(18)} \\ 4/\sqrt{(18)} \\ -1/\sqrt{(18)} \end{bmatrix} \begin{bmatrix} 1/\sqrt{(18)} \\ 4/\sqrt{(18)} \\ -1/\sqrt{(18)} \end{bmatrix}'$$

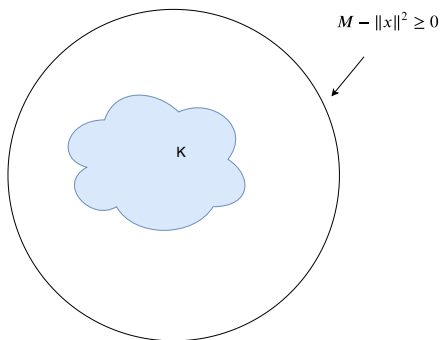
and so

$$f(t) = (1 + t^2)^2 + (2 - t - 2t^2)^2 + (1 + 4t - t^2)^2$$

Let $\mathbf{K} := \{ \mathbf{x} : g_j(\mathbf{x}) \geq 0, \quad j = 1, \dots, m \}$
be compact (with $g_1(\mathbf{x}) = M - \|\mathbf{x}\|^2$, so that $\mathbf{K} \subset \mathbf{B}(0, M)$).



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Theorem (Putinar's Positivstellensatz)

If $f \in \mathbb{R}[\mathbf{x}]$ is strictly positive ($f > 0$) on \mathbf{K} then:

$$\dagger \quad f(\mathbf{x}) = \sigma_0(\mathbf{x}) + \sum_{j=1}^m \sigma_j(\mathbf{x}) g_j(\mathbf{x}), \quad \forall \mathbf{x} \in \mathbb{R}^n,$$

for some **SOS** polynomials $(\sigma_j) \subset \mathbb{R}[\mathbf{x}]$.

However ... In Putinar's theorem

... nothing is said on the **DEGREE** of the SOS polynomials (σ_j) !

BUT ... GOOD news ..!!

☞ Testing whether \dagger holds
for some SOS $(\sigma_j) \subset \mathbb{R}[\mathbf{x}]$ with a degree bound,
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Immediate application

In ANY application where one need to impose that a polynomial f (to be determined) must be positive on \mathbf{K} , then :



DECLARE

$$\dagger \quad f(\mathbf{x}) = \sigma_0(\mathbf{x}) + \sum_{j=1}^m \sigma_j(\mathbf{x}) g_j(\mathbf{x}), \quad \forall \mathbf{x} \in \mathbb{R}^n,$$

with the additional constraint $\deg(\sigma_j g_j) \leq 2t$ for all $j = 1, \dots, m$.

where the degree-parameter t is **YOUR CHOICE!**

Then identifying both sides of the identity yields :

-  Linear constraints on the coefficients of f and σ_j ,
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- 👉 **Semidefinite constraints** coming from **SOS conditions** on the σ_j 's

- In fact, polynomials **NONNEGATIVE ON A SET** $K \subset \mathbb{R}^n$ are ubiquitous. They also appear in many important applications (outside optimization),

among which

Optimization, Probability, Optimal and Robust Control, non-linear PDEs, Game theory, Signal processing, multivariate integration, etc.

Dual side: The K -moment problem

Given a real sequence $\mathbf{y} = (y_\alpha)$, $\alpha \in \mathbb{N}^n$, does there exist a Borel measure μ on \mathbf{K} such that

$$\dagger \quad y_\alpha = \int_{\mathbf{K}} x_1^{\alpha_1} \cdots x_n^{\alpha_n} d\mu, \quad \forall \alpha \in \mathbb{N}^n \quad ?$$

If yes then \mathbf{y} is said to have a **representing measure** supported on \mathbf{K} .

Let $\mathbf{K} := \{ \mathbf{x} : g_j(\mathbf{x}) \geq 0, \quad j = 1, \dots, m \}$

be compact (with $g_1(\mathbf{x}) = M - \|\mathbf{x}\|^2$, so that $\mathbf{K} \subset \mathbf{B}(0, M)$).

Theorem (Dual side of Putinar's Theorem)

A sequence $\mathbf{y} = (y_\alpha)$, $\alpha \in \mathbb{N}^n$, has a representing measure supported on \mathbf{K} IF AND ONLY IF for every $d = 0, 1, \dots$

$$(*) \quad \mathbf{M}_d(\mathbf{y}) \succeq 0 \quad \text{and} \quad \mathbf{M}_d(g_j \mathbf{y}) \succeq 0, \quad j = 1, \dots, m.$$

☞ The real symmetric matrix $\mathbf{M}_2(\mathbf{y})$ is called the **MOMENT MATRIX** associated with the sequence \mathbf{y}

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the **Necessary & Sufficient conditions** (*) for existence of a representing measure are stated only in terms of **countably many LINEAR MATRIX INEQUALITIES (LMI)** on the sequence y ! (No mention of the unknown representing measure in the conditions.)

☞ Moment matrix $\mathbf{M}_1(\mathbf{y})$ in dimension 2 with $d = 1$:

$$\mathbf{M}_1(\mathbf{y}) = \begin{pmatrix} & 1 & X_1 & X_2 \\ 1 & y_{00} & y_{10} & y_{01} \\ X_1 & y_{10} & y_{20} & y_{11} \\ X_2 & y_{01} & y_{11} & y_{02} \end{pmatrix}$$

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👉 localizing matrix $\mathbf{M}_1(g\mathbf{y})$ in dimension 2 with $d = 1$ and $g(\mathbf{x}) = 1 - x_1^2 - x_2^2$:

$$\begin{pmatrix} & 1 & & X_1 & & X_2 \\ 1 & y_{00} - y_{20} - y_{02} & y_{10} - y_{30} - y_{12} & y_{01} - y_{21} - y_{03} \\ X_1 & y_{10} - y_{30} - y_{12} & y_{20} - y_{40} - y_{22} & y_{11} - y_{31} - y_{13} \\ X_2 & y_{01} - y_{21} - y_{03} & y_{11} - y_{31} - y_{13} & y_{02} - y_{22} - y_{04} \end{pmatrix}$$

ALGEBRAIC SIDE
POSITIVITY ON K

$$f(x) = \sum_{\alpha} f_{\alpha} x^{\alpha}$$

$f > 0$ on K ?

CHARACTERIZE THOSE f

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FUNCTIONAL ANALYSIS
THE K -MOMENT PROBLEM

$$y = (y_{\alpha}), \quad \alpha \in \mathbb{N}^n$$

$$y_{\alpha} \stackrel{?}{=} \int_K x^{\alpha} d\mu \quad \forall \alpha$$

for some μ

CHARACTERIZE THOSE y

$$\text{DUALITY } \langle f, y \rangle = \sum_{\alpha} f_{\alpha} y_{\alpha}$$

- In fact, polynomials **NONNEGATIVE ON A SET** $K \subset \mathbb{R}^n$ are ubiquitous. They also appear in many important applications (outside optimization),

... modeled as

particular instances of the so called
Generalized Moment Problem, among which:
Probability, Optimal and Robust Control, Game theory, Signal processing, multivariate integration, etc.

GMP: The primal view

The **GMP** is the infinite-dimensional LP:

$$\inf_{\mu_i \in M(\mathbf{K}_i)} \left\{ \sum_{i=1}^s \int_{\mathbf{K}_i} f_i d\mu_i : \sum_{i=1}^s \int_{\mathbf{K}_i} h_{ij} d\mu_i \geq b_j, \quad j \in J \right\}$$

with $M(\mathbf{K}_i)$ space of Borel measures on $\mathbf{K}_i \subset \mathbb{R}^{n_i}$, $i = 1, \dots, s$.

GMP: The dual view

The **DUAL GMP*** is the infinite-dimensional LP:

$$\sup_{\lambda_j} \left\{ \sum_{j \in J} \lambda_j b_j : f_i - \sum_{j \in J} \lambda_j h_{ij} \geq 0 \text{ on } \mathbf{K}_i, \quad i = 1, \dots, s \right\}$$

And one can see that ...

the constraints of **GMP*** state that the functions

$$\mathbf{x} \mapsto f_i(\mathbf{x}) - \sum_{j \in J} \lambda_j h_{ij}(\mathbf{x})$$

must be **NONNEGATIVE** on certain sets $\mathbf{K}_i, i = 1, \dots, s$.

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The moment-SOS hierarchy

- is an **iterative numerical scheme** to (help) solve the **GMP**.
- It consists of using a certain type of **positivity certificate** (e.g., **Putinar's** certificate) in potentially any application where such a characterization is needed.
- Global optimization is only one example.

In many situations this amounts to
solving a **HIERARCHY** of **SEMIDEFINITE PROGRAMS**

... of **increasing size!**.

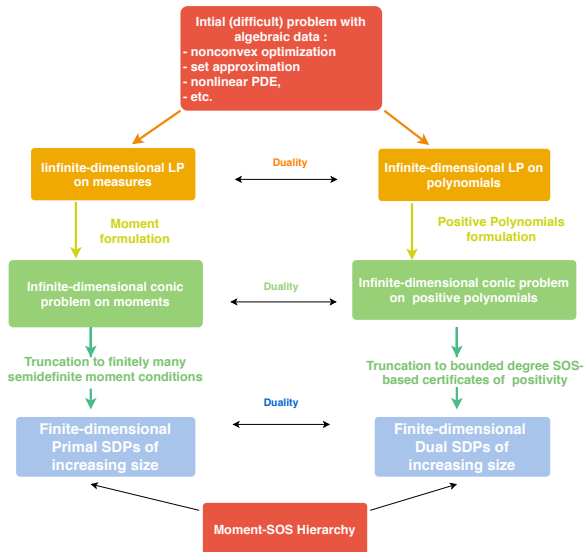
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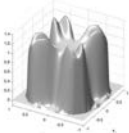


- Has already been proved successful in applications with **modest problem size**, notably in **optimization**, **control**, **robust control**, **optimal control**, **estimation**, **computer vision**, etc.
- ☞ If **sparsity** then problems of larger size can be addressed

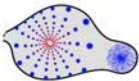
Global optimization



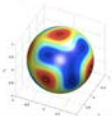
Volume of semialgebraic set



Reachable set



Super resolution



Optimal control



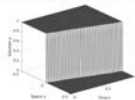
Region of attraction



Maximum invariant sets



PDE analysis & control



Example: Global optimization

Global OPTIM $\rightarrow f^* = \inf_{\mathbf{x}} \{ f(\mathbf{x}) : \mathbf{x} \in \mathbf{K} \}$

is the SIMPLEST example of the GMP

because ...

$$f^* = \inf_{\mu \in \mathcal{M}(\mathbf{K})_+} \left\{ \int_{\mathbf{K}} f d\mu : \int_{\mathbf{K}} 1 d\mu = 1 \right\}$$

☞ A GMP with only one unknown measure μ and only one moment-constraint $\int_{\mathbf{K}} 1 d\mu = 1$

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Remember also that for the **GLOBAL** minimum f^* :

$$f^* = \sup_{\lambda} \{ \lambda : f(\mathbf{x}) - \lambda \geq 0 \quad \forall \mathbf{x} \in \mathbf{K} \}.$$

Then for each t solve:

$$\rho_t = \sup_{\lambda, \sigma_j} \{ \lambda : f(\mathbf{x}) - \lambda = \sigma_0(\mathbf{x}) + \sum_{j=1}^m \sigma_j(\mathbf{x}) g_j(\mathbf{x}), \forall \mathbf{x} \in \mathbb{R}^n \\ \deg(\sigma_j g_j) \leq t, \quad j = 0, \dots, m \}$$

👉 $\rho_t \leq \rho_{t+1} \leq f^*$ for all t and $\rho_t \uparrow f^*$ as $t \rightarrow \infty$.

Alternatively, for each t solve:

$$\rho_t^* = \inf_y \left\{ L_y(f) : \begin{array}{l} \text{(think of } \int f d\mu) \\ y_0 = 1 \\ \mathbf{M}_t(y) \succeq 0 \\ \mathbf{M}_{t-t_j}(g_j y) \succeq 0 \quad \forall j = 1, \dots, m \end{array} \right\} \leftarrow y_\alpha = \int_{\mathbf{K}} x^\alpha d\mu$$

Theorem (Lasserre 2000)

$\rho_t \leq \rho_t^* \leq f^*$ for all t and $\rho_t^* \uparrow f^*$ as $t \rightarrow \infty$.

Moreover, generically $\rho_t^* = f^*$ and one may extract global minimizers from the optimal (truncated moment) solution y^* .

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Theorem (Lasserre 2000)

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Moreover, generically $\rho_t^* = f^*$ and one may extract global minimizers from the optimal (truncated moment) solution \mathbf{y}^* .

Ex: Consider the optimization problem: $\min\{f(x) : x \in [0, 1]\}$:

$$x \mapsto f(x) := \sum_{j=1}^4 a_j x^j; \quad [0, 1] = \{x : x(1-x) \geq 0\}, .$$

SDP relaxation

$$\text{SDP } f^* = \min_y \left\{ \sum_{j=1}^4 a_j y_j : \begin{bmatrix} y_0 & y_1 & y_2 \\ y_1 & y_2 & y_3 \\ y_2 & y_3 & y_4 \end{bmatrix} \succeq 0 \right.$$

$$\left. \text{SDP } \begin{bmatrix} y_1 - y_2 & y_2 - y_3 \\ y_2 - y_3 & y_3 - y_4 \end{bmatrix} \succeq 0; y_0 = 1. \right\}$$

👉 $y^* = (1, x^*, (x^*)^2, (x^*)^3, (x^*)^4)$, and

$$f(x) - f^* = \underbrace{\sigma_0(x)}_{\text{SOS of degree 4}} + \underbrace{\sigma_1(x)}_{\text{SOS of degree 2}} x(1-x).$$

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- **Finite convergence** is “generic”
 - **Extraction of minimizers** from an **optimal solution of the dual** (linear algebra)
 - If the problem is **SOS-convex** then convergence takes place at the first step of the hierarchy
 - The “**same algorithm**” for many **combinatorial optimization problems** (just use $x_i^2 = x_i$ to model boolean variables) which still provides better lower bounds than ad-hoc tailored algorithms.
- ☞ Has become **key tool** to **prove/disprove Khot's Unique Games Conjecture** in computational complexity.
- ☞ The **NPA-hierarchy** is a **non-commutative** version of the Moment-SOS hierarchy to address some quantitative problems in **Quantum Information**.

A recovery issue

In static optimization, an optimal solution is a **point** $\mathbf{x}^* \in \mathbb{R}^n$.

Generically, some semidefinite relaxation at step t of the Moment-SOS hierarchy is **exact** and:

☞ To recover \mathbf{x}^* from its optimal solution $\mathbf{y}^* = (y_\alpha^*)_{\alpha \in \mathbb{N}_{2t}^n}$ can be done via a linear algebra subroutine.

☞ If \mathbf{x}^* is unique then it is even trivial as \mathbf{x}^* is just the subvector of degree-1 moments of \mathbf{y}^*

However,

in many other problems like optimal control, PDE's, computational geometry, an optimal solution is a **function** $f : \Omega \rightarrow \mathbb{R}$ (e.g. a trajectory $\{\mathbf{x}(t) : t \in [0, 1]\}$)

... and the Moment-SOS hierarchy provides a sequence of scalars $(\mu_{\alpha,j})_{\alpha,j}$ which approximates moments

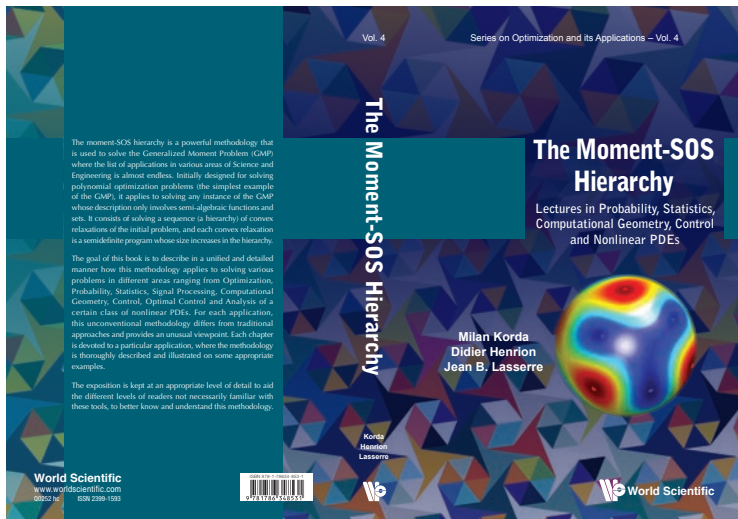
$$\mu_{\alpha,j}^* = \int_{\Omega} \mathbf{x}^{\alpha} y^j d\mu^*(\mathbf{x}, y), \quad \alpha \in \mathbb{N}^n, j \in \mathbb{N},$$

of the measure $d\mu^*(\mathbf{x}, y) = \delta_{\{f(\mathbf{x})\}}(dy) \phi(d\mathbf{x})$
whose support IS the **graph**
 $\{(\mathbf{x}, f(\mathbf{x})) : \mathbf{x} \in \Omega\}$ of the optimal solution f .

For instance in optimal control (OC), one uses the **weak formulation** of OC

☞ **infinite-dimensional LP** on **occupation (Young) measure μ**

- Controlled dynamics of OC
 - ☞ **linear constraints** on **moments** of μ via integration of **polynomial test functions**
- integral cost functional
 - ☞ **linear criterion** $\langle h, \mu \rangle$ on μ .
- state/control constraints = **support constraints** on μ
 - ☞ **semidefinite conditions** on moments of μ (by Putinar theorem)

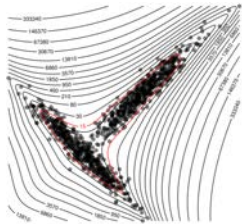


Then it remains to extract f from knowledge of the $(\mu_{\alpha,j}) \dots$

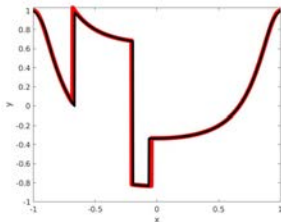
☞ This can be done by several techniques (including L^2 -polynomial approximation via a standard application of the Christoffel-Darboux kernel) not detailed here.

👉 We claim that a **non-standard** application of the CD kernel provides a **simple** and **easy to use** tool (with no optimization involved) which can help solve problems not only in **data analysis**, but also in **approximation** and **interpolation** of (possibly discontinuous) functions. In particular one is able to recover a discontinuous function with no **Gibbs phenomenon**.

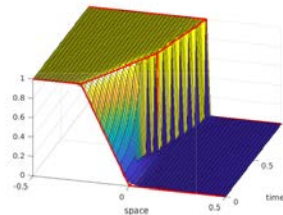
Outlier detection



Interpolation



Recovery



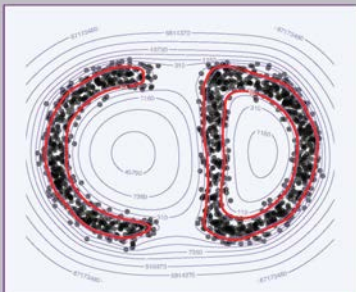
Part two:

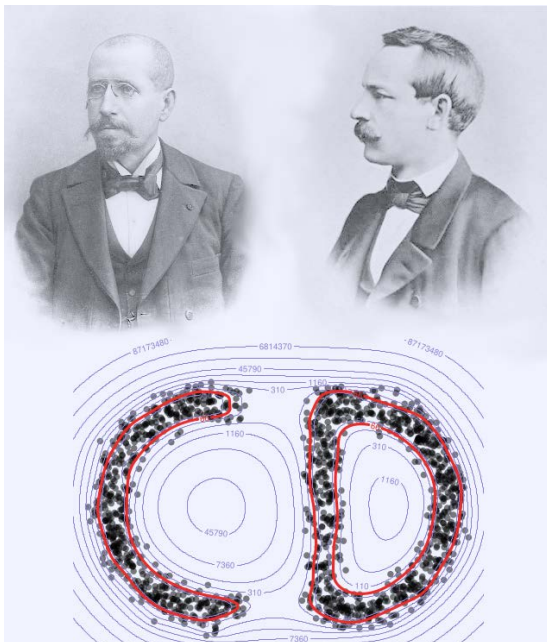
The Christoffel function

Cambridge Monographs on Applied and Computational Mathematics

The Christoffel-Darboux Kernel for Data Analysis

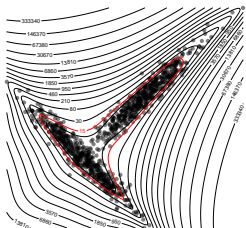
Jean Bernard Lasserre, Edouard Pauwels
and Mihai Putinar





Motivation

Consider the following cloud of 2D-points (data set) below



The **red curve** is the level set

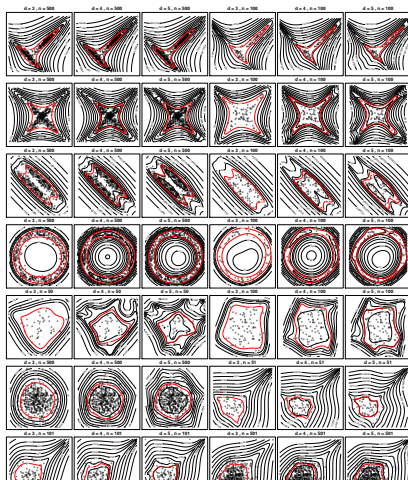
$$S_\gamma := \{ \mathbf{x} : Q_d(\mathbf{x}) \leq \gamma \}, \quad \gamma \in \mathbb{R}_+$$

of a certain polynomial $Q_d \in \mathbb{R}[x_1, x_2]$ of degree $2d$.

👉 Notice that S_γ captures quite well the shape of the cloud.

Not a coincidence!

👉 Surprisingly, low degree d for Q_d is often enough to get a pretty good idea of the shape of Ω (at least in dimension $p = 2, 3$)



Cook up your own convincing example

Perform the following simple operations on a preferred cloud of $2D$ -points: So let $d = 2$, $p = 2$ and $s(d) = \binom{p+d}{p}$.

- Let $\mathbf{v}_d(\mathbf{x})^T = (1, x_1, x_2, x_1^2, x_1x_2, \dots, x_1x_2^{d-1}, x_2^d)$. be the vector of all monomials $x_1^i x_2^j$ of total degree $i + j \leq d$
- Form the real symmetric matrix of size $s(d)$

$$\mathbf{M}_d := \frac{1}{N} \sum_{i=1}^N \mathbf{v}_d(\mathbf{x}(i)) \mathbf{v}_d(\mathbf{x}(i))^T,$$

where the sum is over all points $(\mathbf{x}(i))_{i=1, \dots, N} \subset \mathbb{R}^2$ of the data set.

☞ Note that \mathbf{M}_d is the **MOMENT-matrix** $\mathbf{M}_d(\mu^N)$ of the **empirical measure**

$$\mu^N := \frac{1}{N} \sum_{i=1}^N \delta_{\mathbf{x}(i)}$$

associated with a sample of size N , drawn according to an unknown measure μ .

☞ The (usual) notation $\delta_{\mathbf{x}(i)}$ stands for the **DIRAC** measure supported at the point $\mathbf{x}(i)$ of \mathbb{R}^2 .

Recall that the moment matrix $\mathbf{M}_d(\mu)$ is real symmetric with rows and columns indexed by $(\mathbf{x}^\alpha)_{\alpha \in \mathbb{N}_d^p}$, and with entries

$$\mathbf{M}_d(\mu)(\alpha, \beta) := \int_{\Omega} \mathbf{x}^{\alpha+\beta} d\mu = \mu_{\alpha+\beta}, \quad \forall \alpha, \beta \in \mathbb{N}_d^p.$$

☞ Illustrative example in dimension 2 with $d = 1$:

$$\mathbf{M}_1(\mu) := \begin{pmatrix} & 1 & X_1 & X_2 \\ 1 & \mu_{00} & \mu_{10} & \mu_{01} \\ X_1 & \mu_{10} & \mu_{20} & \mu_{11} \\ X_2 & \mu_{01} & \mu_{11} & \mu_{02} \end{pmatrix}$$

is the *moment matrix of μ of "degree $d=1$ "*.

- Next, form the SOS polynomial:

$$\mathbf{x} \mapsto Q_d(\mathbf{x}) := \mathbf{v}_d(\mathbf{x})^T \mathbf{M}_d^{-1}(\mu^N) \mathbf{v}_d(\mathbf{x}).$$

$$= (1, x_1, x_2, x_1^2, \dots, x_2^d) \mathbf{M}_d^{-1}(\mu^N) \begin{pmatrix} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ \dots \\ x_2^d \end{pmatrix}$$

- Plot some level sets

$$\mathcal{S}_\gamma := \{ \mathbf{x} \in \mathbb{R}^2 : Q_d(\mathbf{x}) = \gamma \}$$

for some values of γ , the thick one representing the particular value $\gamma = \binom{2+d}{2}$.

The **Christoffel function** $\Lambda_d : \mathbb{R}^p \rightarrow \mathbb{R}_+$ is the **reciprocal**

$$\mathbf{x} \mapsto Q_d(\mathbf{x})^{-1}, \quad \forall \mathbf{x} \in \mathbb{R}^p$$

of the SOS polynomial Q_d .

☞ It has a rich history in **Approximation theory**
and **Orthogonal Polynomials**.

☞ Among main contributors: **Nevai, Totik, Króó, Lubinsky, Simon, ...**

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Simon, ...

Let $\Omega \subset \mathbb{R}^p$ be the compact support of μ with nonempty interior, and $(P_\alpha)_{\alpha \in \mathbb{N}^p}$ be a family of orthonormal polynomials w.r.t. μ .

The vector space $\mathbb{R}[\mathbf{x}]_d$ viewed as a subspace of $L^2(\mu)$ is a **Reproducing Kernel Hilbert Space (RKHS)**.

Its *reproducing kernel*

$$(\mathbf{x}, \mathbf{y}) \mapsto K_d^\mu(\mathbf{x}, \mathbf{y}) := \sum_{|\alpha| \leq d} P_\alpha(\mathbf{x}) P_\alpha(\mathbf{y}), \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^p,$$

is called the *Christoffel-Darboux kernel*.

The reproducing property

$$\mathbf{x} \mapsto q(\mathbf{x}) = \int_{\Omega} K_d^{\mu}(\mathbf{x}, \mathbf{y}) q(\mathbf{y}) d\mu(\mathbf{y}), \quad \forall q \in \mathbb{R}[\mathbf{x}]_d.$$

☞ useful to determinate the **best degree- d** polynomial approximation

$$\inf_{q \in \mathbb{R}[\mathbf{x}]_d} \|f - q\|_{L^2(\mu)}$$

of f in $L^2(\mu)$. Indeed:

$$\begin{aligned} \mathbf{x} \mapsto \widehat{f}_d(\mathbf{x}) &:= \sum_{\alpha \in \mathbb{N}_d^p} \overbrace{\left(\int_{\Omega} f(\mathbf{y}) P_{\alpha}(\mathbf{y}) d\mu \right)}^{\widehat{f}_{d,\alpha}} P_{\alpha}(\mathbf{x}) \in \mathbb{R}[\mathbf{x}]_d \\ &= \arg \min_{q \in \mathbb{R}[\mathbf{x}]_d} \|f - q\|_{L^2(\mu)} \end{aligned}$$

Theorem

The Christoffel function $\Lambda_d^\mu : \mathbb{R}^p \rightarrow \mathbb{R}_+$ is defined by:

$$\xi \mapsto \Lambda_d^\mu(\xi)^{-1} = \sum_{|\alpha| \leq d} P_\alpha(\xi)^2 = K_d^\mu(\xi, \xi), \quad \forall \xi \in \mathbb{R}^p,$$

and it also satisfies the variational property:

$$\Lambda_d^\mu(\xi) = \min_{P \in \mathbb{R}[\mathbf{x}]_d} \left\{ \int_{\Omega} P^2 d\mu : P(\xi) = 1 \right\}, \quad \forall \xi \in \mathbb{R}^p.$$

☞ Alternatively

$$\Lambda_d^\mu(\xi)^{-1} = \mathbf{v}_d(\xi)^T \mathbf{M}_d(\mu)^{-1} \mathbf{v}_d(\xi), \quad \forall \xi \in \mathbb{R}^p.$$

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☞ Importantly, and crucial for applications, the **Christoffel function** identifies the **support** Ω of the underlying measure μ .

Theorem

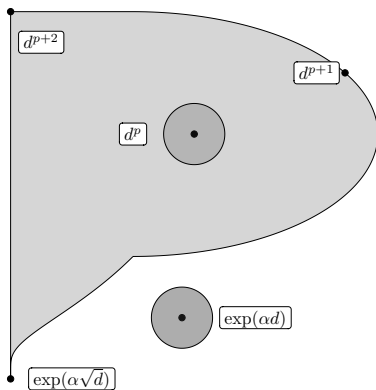
Let the support Ω of μ be compact with nonempty interior.
Then:

- For all $\mathbf{x} \in \text{int}(\Omega)$: $K_d^\mu(\mathbf{x}, \mathbf{x}) = O(d^p)$.
- For all $\mathbf{x} \in \text{int}(\mathbb{R}^p \setminus \Omega)$: $K_d^\mu(\mathbf{x}, \mathbf{x}) = O(\exp(-\alpha d))$ for some $\alpha > 0$.

☞ In particular, as $d \rightarrow \infty$,

$$d^p K_d^\mu(\mathbf{x}) \rightarrow 0 \text{ very fast whenever } \mathbf{x} \notin \Omega.$$

Growth rates for $K_d^\mu(\mathbf{x}, \mathbf{x}) = \Lambda_d^\mu(\mathbf{x})^{-1}$.



Some other properties

- Under some (restrictive) assumption on Ω and μ

$$\lim_{d \rightarrow \infty} s(d) \Lambda_d^\mu(\xi) = f_\mu(\xi) \omega(\xi)^{-1}$$

where ω is the density of an **equilibrium measure** intrinsically associated with Ω .

For instance with $p = 1$ and $\Omega = [-1, 1]$, $\omega(\xi) = \sqrt{1 - \xi^2}$.

- If μ and ν have same support Ω and respective densities f_μ and f_ν w.r.t. Lebesgue measure on Ω , positive on Ω , then:

$$\lim_{d \rightarrow \infty} \frac{\Lambda_d^\mu(\xi)}{\Lambda_d^\nu(\xi)} = \frac{f_\mu(\xi)}{f_\nu(\xi)}, \quad \forall \xi \in \Omega.$$

 useful for **density approximation**

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$$\lim_{d \rightarrow \infty} s(d) \Lambda_d^\mu(\xi) = f_\mu(\xi) \omega(\xi)^{-1}$$

where ω is the density of an **equilibrium measure** intrinsically associated with Ω .

For instance with $p = 1$ and $\Omega = [-1, 1]$, $\omega(\xi) = \sqrt{1 - \xi^2}$.

- If μ and ν have same support Ω and respective densities f_μ and f_ν w.r.t. Lebesgue measure on Ω , positive on Ω , then:

$$\lim_{d \rightarrow \infty} \frac{\Lambda_d^\mu(\xi)}{\Lambda_d^\nu(\xi)} = \frac{f_\mu(\xi)}{f_\nu(\xi)}, \quad \forall \xi \in \Omega.$$

 useful for **density approximation**

☞ For instance one may decide to classify as **outliers** all points ξ such that $\Lambda_d^{\mu^N}(\xi) < \binom{p+d}{p}^{-1}$.

☞ Such a strategy (even with relatively low degree d) is as efficient as more elaborated techniques, **with only one parameter** (the degree d), and **with no optimization involved**.

☞ [Lass. & Pauwels \(2016\)](#) Sorting out typicality via the inverse moment matrix SOS polynomial, [NIPS 2016](#).
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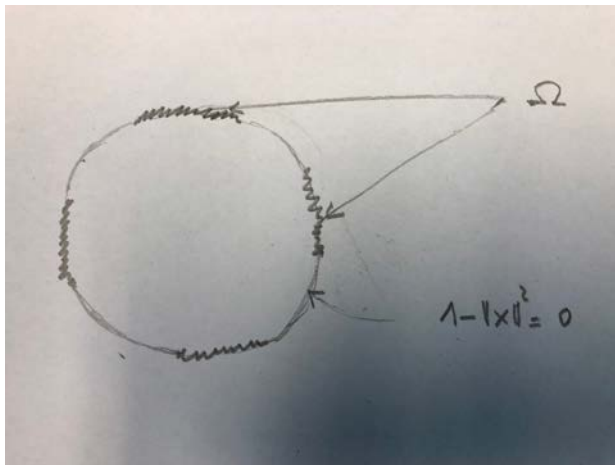
Manifold learning

A measure μ on compact set Ω is completely determined by its moments and therefore it should not be a surprise that its moment matrix $\mathbf{M}_d(\mu)$ contains a lot of information.

☞ We have already seen that its inverse $\mathbf{M}_d(\mu)^{-1}$ defines the Christoffel function.

☞ When μ is degenerate and its support Ω is contained in a zero-dimensional real algebraic variety V then the kernel of $\mathbf{M}_d(\mu)$ identifies the generators of a corresponding ideal of $\mathbb{R}[\mathbf{x}]$ (the vanishing ideal of V).

For instance let $\Omega \subset \mathbb{S}^{p-1}$ (the Euclidean unit sphere of \mathbb{R}^p)



Then the **kernel** of $\mathbf{M}_d(\mu)$ contains vectors of coefficients of polynomials in the ideal generated by the quadratic polynomial $\mathbf{x} \mapsto g(\mathbf{x}) := 1 - \|\mathbf{x}\|^2$.

In fact and remarkably,

$$\text{rank } \mathbf{M}_d(\mu) = p(d)$$

for some **univariate polynomial** p (the **Hilbert polynomial** associated with the algebraic variety) which is of degree t if t is the dimension of the variety.

For instance $t = p - 1$ if the support is contained in the sphere \mathbb{S}^{p-1} of \mathbb{R}^p .

👉 **Pauwels E., Putinar M., Lass. J.B. (2021). [Data analysis from empirical moments and the Christoffel function](#), Found. Comput. Math. 21, pp. 243–273.**

- 👉 Again this illustrates how quite sophisticated concepts of algebraic geometry are hidden and **encapsulated** in the **moment matrix** $\mathbf{M}_d(\mu)$.
- 👉 They can be exploited to extract **various useful information** on the data set.
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👉 However

for non modest dimension of data, matrix inversion of \mathbf{M}_d^{-1} does not scale well ...

👉 On the other hand

for evaluation $\Lambda_d^\mu(\xi)$ at a point $\xi \in \mathbb{R}^p$, the variational formulation

$$\Lambda_d^\mu(\xi) = \min_{P \in \mathbb{R}[\mathbf{x}]_d} \left\{ \int_{\Omega} P^2 d\mu : P(\xi) = 1 \right\}, \quad \forall \xi \in \mathbb{R}^p.$$

is the simple quadratic programming problem.

$$\min_{p \in \mathbb{R}^{s(d)}} \left\{ p^T \mathbf{M}_d p : \mathbf{v}_d(\xi)^T p = 1 \right\},$$

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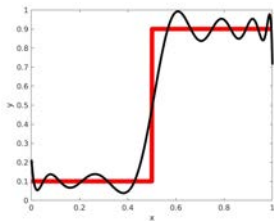
which can be solved quite efficiently.

The Christoffel function for approximation

A typical approach is to approximate $f : [0, 1] \rightarrow \mathbb{R}$ in some function space, e.g. its projection on $\mathbb{R}[\mathbf{x}]_n \subset L^2([0, 1])$:

$$x \mapsto \hat{f}_n(x) := \sum_{j=0}^n \left(\int_0^1 f(y) L_j(y) dy \right) L_j(x),$$

with an orthonormal basis $(L_j)_{j \in \mathbb{N}}$ of $L^2([0, 1])$.



BUT ...

Ex: Chebyshev interpolant

☞ Typical **Gibbs** phenomenon occurs.

Alternative **Positive Kernels** with better convergence properties have been proposed, still in the same framework:

Féjer, Jackson kernels, etc.

- **Reproducing property** of the **CD kernel** is **LOST**
- **Preserve positivity** (e.g when approximating a density)
- **Better convergence properties** than the **CD kernel**, in particular uniform convergence (for continuous functions) on arbitrary compact subsets

An alternative approach, still via the CD-kernel

A counter-intuitive detour: Instead of considering $f : [0, 1] \rightarrow \mathbb{R}$, and the associated measure

$$d\mu(x) := f(x) dx$$

on the **real line**, whose support is $[0, 1] \in \mathbb{R}$,

☞ Rather consider the **graph** $\Omega \subset \mathbb{R}^2$ of f , i.e., the set

$$\Omega := \{(x, f(x)) : x \in [0, 1]\}.$$

and the measure

$$d\phi(x, y) := \delta_{f(x)}(dy) 1_{[0,1]}(x) dx$$

on \mathbb{R}^2 with **degenerate support** $\Omega \subset \mathbb{R}^2$.

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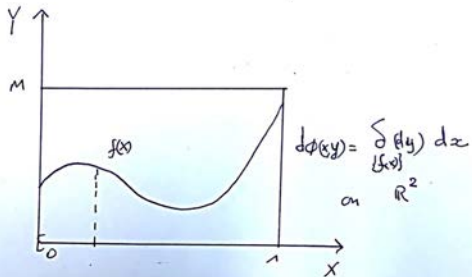
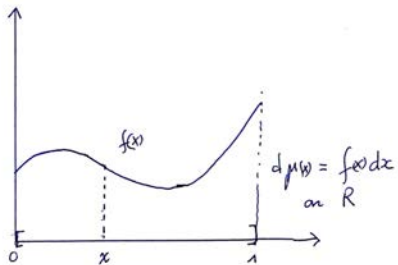
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on \mathbb{R}^2 with **degenerate support** $\Omega \subset \mathbb{R}^2$.



Why should we do that as it implies going to \mathbb{R}^2 instead of staying in \mathbb{R} ?

 ... because

- The support of ϕ is **exactly** the graph of f , and
- The CF $(x, y) \mapsto \Lambda_n^\phi(x, y)$ **identifies the support** of ϕ !

So suppose that we know the moments

$$\phi_{i,j} = \int x^i y^j d\phi(x, y) = \int_{[0,1]} x^i f(x)^j dx, \quad i + j \leq 2d,$$

and let $\varepsilon > 0$ and λ be the Lebesgue measure on $[0, 1]$.

- ☞ Compute the degree- d **moment matrix** of ϕ :

$$\mathbf{M}_d(\phi) := \int \mathbf{v}_d(x, y) \mathbf{v}_d(x, y)^T d\phi(x, y),$$

- ☞ Compute the **Christoffel function**

$$x \mapsto \Lambda_d^{\phi, \varepsilon}(x, y)^{-1} := \mathbf{v}_d(x, y)^T \mathbf{M}_d(\phi + \varepsilon\lambda)^{-1} \mathbf{v}_d(x, y).$$

- Approximate $f(x)$ by $\hat{f}_{d,\varepsilon}(x) := \arg \min_y \Lambda_d^{\phi, \varepsilon}(x, y)^{-1}$.

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Interpolation: same story

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$$\mathbf{v}_d(x, y) := (1, x, y, x^2, x y, y^2, \dots, x y^{d-1}, y^d).$$

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Choosing

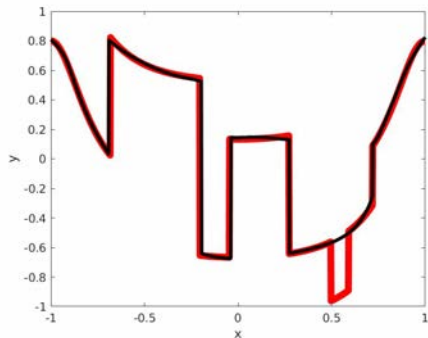
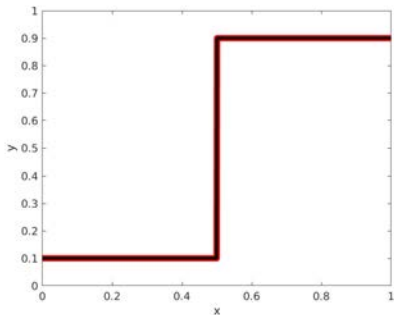
$$\varepsilon := 2^{3-\sqrt{d}}$$

ensures convergence properties for bounded measurable functions, e.g. **pointwise** on open sets with no point of discontinuity.

Convergence properties as $d \uparrow$

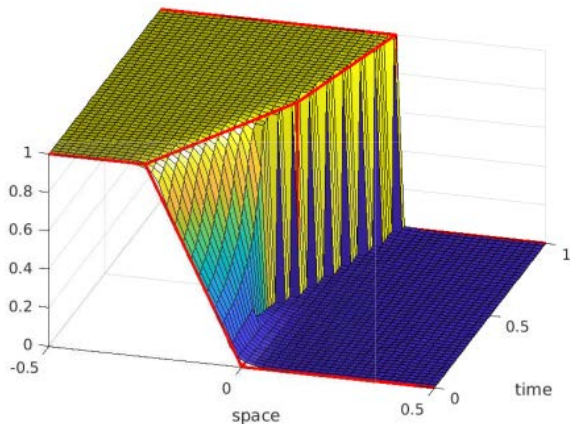
-  **L^1 -convergence**
-  **pointwise convergence** on open sets with no point of discontinuity, and so **almost uniform convergence**.
-  **L^1 -convergence** at a rate $O(d^{-1/2})$ for Lipschitz continuous f .

In non trivial exemples, the approximation is quite good with small values of d , and with no Gibbs phenomenon .



Ex: Recovery

Below : **Recovery** of a (discontinuous) solution of the **Burgers Equation** from knowledge of approximate moments of the occupation measure supported on the solution.



Again note the central role played by the **Moment Matrix!**

S. Marx, E. Pauwels, T. Weisser, D. Henrion, J.B. Lasserre.
Semi-algebraic approximation using Christoffel-Darboux kernel,
[Constructive Approximation](#), 2021

Christoffel function and Positive polynomials

Let $\Omega \subset \mathbb{R}^n$ be the basic semi-algebraic set (with nonempty interior)

$$\Omega := \{\mathbf{x} \in \mathbb{R}^n : g_j(\mathbf{x}) \geq 0, \quad j = 1, \dots, m\}$$

with $g_j \in \mathbb{R}[\mathbf{x}]_{d_j}$ and let $s_j = \lceil \deg(g_j)/2 \rceil$. Let $g_0 = 1$ with $s_0 = 0$.

With t fixed, its associated quadratic module

$$Q_t(\Omega) := \left\{ \sum_{j=0}^m \sigma_j g_j : \sigma_j \in \Sigma[\mathbf{x}]_{t-s_j} \right\} \subset \mathbb{R}[\mathbf{x}]$$

is a convex cone with nonempty interior,

and with dual convex cone of pseudo-moments

$$Q_t(\Omega)^* := \{ \mathbf{y} \in \mathbb{R}^{s(t)} : \mathbf{M}_{t-s_j}(\mathbf{g}_j \mathbf{y}) \succeq 0, \quad j = 0, \dots, m \},$$

where $s(t) = \binom{n+t}{n}$.

Notice that if $\mathbf{M}_t(\mathbf{y})^{-1} \succ 0$ for all t ,

then one may define a family of polynomials $(P_\alpha)_{\alpha \in \mathbb{N}^n} \subset \mathbb{R}[\mathbf{x}]$ orthonormal w.r.t. \mathbf{y} , meaning that

$$L_{\mathbf{y}}(P_\alpha \cdot P_\beta) = \delta_{\alpha=\beta}, \quad \alpha, \beta \in \mathbb{N}^n,$$

and exactly as for measures, the Christoffel function $\Lambda_t^{\mathbf{y}}$

$$\mathbf{x} \mapsto \Lambda_t^{\mathbf{y}}(\mathbf{x})^{-1} := \sum_{|\alpha| \leq t} P_\alpha(\mathbf{x})^2.$$

Theorem

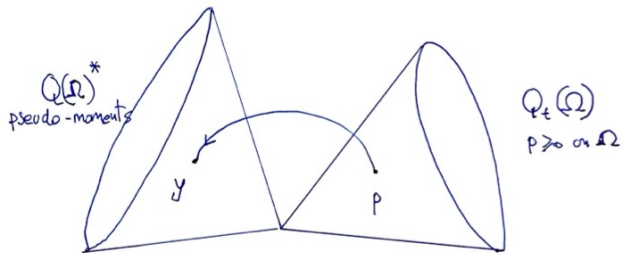
For every $p \in \text{int}(Q_t(\Omega))$ there exists a sequence of pseudo-moments $y \in \text{int}(Q_t(\Omega)^*)$ such that

$$\begin{aligned} p(\mathbf{x}) &= \sum_{j=0}^m \left(\mathbf{v}_{t-s_j}(\mathbf{x})^T \mathbf{M}_t(\mathbf{g}_j y)^{-1} \mathbf{v}_{t-s_j}(\mathbf{x}) \right) g_j(\mathbf{x}) \\ &= \sum_{j=0}^m \Lambda_{t-s_j}^{\mathbf{g}_j \cdot y}(\mathbf{x})^{-1} g_j(\mathbf{x}) \end{aligned}$$



where $(\mathbf{g} \cdot y)$ is the sequence of pseudo-moments

$$(\mathbf{g} \cdot y)_\alpha := \sum_{\gamma} g_\gamma y_{\alpha+\gamma}, \quad \alpha \in \mathbb{N}^n \quad (\text{if } g(\mathbf{x}) = \sum_{\gamma} g_\gamma \mathbf{x}^\gamma).$$

In addition $L_y(p) = \sum_{j=0}^m \binom{n+t-s_j}{n}$.





The proof combines

-  a result by Nesterov on a one-to-one correspondence between $\text{int}(Q_t(\Omega))$ and $\text{int}(Q_t(\Omega)^*)$, and
-  the fact that

$$\mathbf{v}_{t-s_j}(\mathbf{x})^T \mathbf{M}_t(\mathbf{g}_j \mathbf{y})^{-1} \mathbf{v}_{t-s_j}(\mathbf{x}) = \Lambda_{t-s_j}^{\mathbf{g}_j \cdot \mathbf{y}}(\mathbf{x})^{-1}.$$

-  Lass (2022) [A Disintegration of the Christoffel function](#), *Comptes Rendus Math.* (2022)

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In other words:

If $p \in \text{int}(Q_t(\Omega))$ then in **Putinar's certificate**

$$p = \sum_{j=0}^m \sigma_j g_j, \quad \sigma_j \in \mathbb{R}[\mathbf{x}]_{t-s_j},$$

of **positivity** of p on Ω ,

☞ one may always choose the SOS weights σ_j in the form

$$\sigma_j(\mathbf{x}) := \Lambda_{t-s_j}^{g_j \cdot \mathbf{y}}(\mathbf{x})^{-1}, \quad j = 0, \dots, m,$$

for some sequence of pseudo-moments $\mathbf{y} \in \text{int}(Q_t(\Omega)^*)$.

 In particular,

every SOS polynomial p of degree $2d$, in the **interior of the SOS-cone**, is the reciprocal of the **CF** of some linear functional

$y \in \mathbb{R}[\mathbf{x}]_{2d}^*$. That is:

$$p(\mathbf{x}) = \mathbf{v}_d(\mathbf{x})^T \mathbf{M}_d(\mathbf{y})^{-1} \mathbf{v}_d(\mathbf{x}) = \Lambda_d^y(\mathbf{x})^{-1}, \quad \forall \mathbf{x} \in \mathbb{R}^n.$$

CF – Pell's equation – equilibrium measure

☞ What is the link between $p \in \text{int}(Q_t(\Omega))$ and the mysterious linear functional y ?

Theorem

For some sets Ω , $1 \in \text{int}(Q_t(\Omega))$ and

$$1 = \frac{1}{\sum_{j=0}^m s(t-t_j)} \sum_{j=0}^m \Lambda_{t-s_j}^{g_j \cdot \phi}(\mathbf{x})^{-1} g_j(\mathbf{x}) \quad (1)$$

where ϕ is the *equilibrium measure* of Ω .

(1) can be called a *generalized polynomial Pell's equation* satisfied by the CFs $\Lambda_{t-s_j}^{g_j \cdot \phi}(\mathbf{x})^{-1}$.

Disintegration

Recall that if μ is a measure on a Borel set $\Omega := X \times Y$, then it disintegrates as

$$d\mu(x, y) = \underbrace{\hat{\mu}(dy | x)}_{\text{conditional}} \underbrace{\phi(dx)}_{\text{marginal}}$$

with marginal ϕ on X and conditional $\hat{\mu}(dy|x)$ on Y given $x \in X$.

Theorem (Lasserre (2022))

The Christoffel function $\Lambda_d^\mu(x, y)$ disintegrates into

$$\Lambda_d^\mu(x, y) = \Lambda_d^\phi(x) \cdot \Lambda_d^{\nu_{x,d}}(y)$$

for some measure $\nu_{x,d}$ on \mathbb{R} .

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Crucial in the proof is the use of the previous duality result of Nesterov.

THANK YOU !