Introduction to Christoffel-Darboux kernels for polynomial optimization

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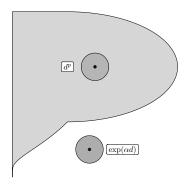






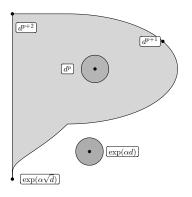
Exponential separation of the support

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Thresholding scheme: C > 0, q > p

$$\{\mathbf{x}, \mathbf{v}_d(\mathbf{x})^T M_{\mu,d}^{-1} \mathbf{v}_d(\mathbf{x}) \leq C d^q\}$$
 " $\underset{d \to \infty}{\longrightarrow}$ " $\operatorname{cl}(\operatorname{int}(S)).$

Extends to positive densities on S. =

Outline

- 1. CD kernel, Christoffel function, orthogonal polynomials, moments
- 2. CD kernel captures measure theoretic properties: univariate case
- 3. Quantitative asymptotics
- 4. The singular case
- 5. Using approximate moments
- 6. An application to polynomial optimal control

The singular case

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

$$(P,Q) \qquad \mapsto \qquad \langle\!\langle P,Q \rangle\!\rangle_{\mu} := \int PQd\mu,$$

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

Specificity of the singular case

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

Moment based computation

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

Then, for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^p$, $K_d^{\mu}(\mathbf{x}, \mathbf{y}) = \mathbf{v}_d(\mathbf{x})^T M_{\mu, d}^{-1} \mathbf{v}_d(\mathbf{y}) \frac{\mathbf{v}_d(\mathbf{x})^T M_{\mu, d}^{-1} \mathbf{v}_d(\mathbf{y})}{\mathbf{v}_d(\mathbf{x})^T M_{\mu, d}^{-1} \mathbf{v}_d(\mathbf{y})}$

Let
$$P(\mathbf{x}) = \sum_{i=1}^{s(d)} \mathbf{p}_i P_i(\mathbf{x}) P \in \mathbb{R}_d[X]$$
. We have

$$\int P^2 d\mu = \mathbf{p}^T M_{\mu,d} \mathbf{p}.$$

If P vanishes on S, if and only if $\mathbf{p} \in \ker(M_{\mu,d})$. Singular moment matrix, morally, CD kernel should be $+\infty$.

Christoffel function to the rescue

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

Variational formulation: for all $z \in \mathbb{R}^p$

$$\frac{1}{\mathcal{K}_d^{\mu}(\mathbf{z},\mathbf{z})} = \Lambda_d^{\mu}(\mathbf{z}) = \min_{P \in \mathbb{R}_d[X]} \ \left\{ \int P^2 d\mu : \quad P(\mathbf{z}) \, = \, 1 \right\}.$$

$$\Lambda_d^\mu(\mathbf{z}) = \min_{P \in \mathbb{R}_d[X]} \left\{ \int P^2 d\mu : \quad P(\mathbf{z}) \, = \, 1
ight\}.$$

Given $\mathbf{z} \in \mathbb{R}^p$, such that there exists $P \in \mathbb{R}_d[X]$ such that

- $P(z) \neq 0$
- P vanishes on S.

Then $\Lambda_d^{\mu}(\mathbf{z}) = 0$.

Getting the CD kernel back (and computation from moments)

 μ : Borel probability measure in \mathbb{R}^p , compact support: S.

 $\mathbb{R}_d[X]$: *p*-variate polynomials of degree at most d (of dimension $s(d) = \binom{p+d}{d}$).

 ${\it V}$ denotes the Zariski closure of ${\it S}$ (smallest algebraic set containing ${\it S}$).

For d large enough, $V = \{ \mathbf{z} \in \mathbb{R}^p, \Lambda_d^{\mu}(\mathbf{z}) > 0 \}.$

Polynomials on $V: L^2_{\mu,d} = \mathbb{R}_d[X] / \{P \in \mathbb{R}_d[X], P \text{ vanishes on } V\}.$

RKHS: $(L^2_{\mu,d}, \langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mu})$ is a Hilbert space of functions on V. K^{μ}_d is its reproducing kernel (defined on V).

For any $\mathbf{x} \in V$ and $P \in L^2_{\mu,d}$, $P(\mathbf{x}) = \int P(\mathbf{y}) K_d^{\mu}(\mathbf{x}, \mathbf{y}) d\mu(\mathbf{y})$.

Relation with Christoffel function: $\Lambda_d^{\mu}(z)K_d^{\mu}(z,z)=1$, for $z\in V$.

Pseudo inverse computation: let \mathbf{v}_d be any basis of $\mathbb{R}_d[X]$, $M_{\mu,d}$ moment matrix:

$$\forall \mathbf{x}, \mathbf{y} \in V$$
 $K_d^{\mu}(\mathbf{x}, \mathbf{y}) = \mathbf{v}_d(\mathbf{x}) M_{\mu, d}^{\dagger} \mathbf{v}_d(\mathbf{y}).$

Average value and Hilbert function: $\int K_d^{\mu}(\mathbf{x}, \mathbf{x}) d\mu(\mathbf{x}) = \dim(L_{\mu, d}^2) \leq s(d)$.

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Motivation for approximate moments

"I am a Lasserre hierarchist, I work with pseudo-moments."

"I am a statistician, I work with empirical moments."

"I am a numerician, among others, I care about sensitivity to errors."

A stability result

Choose a basis \mathbf{v}_d of $\mathbb{R}_d[X]$.

Approximation of Christoffel function: Let $Q(\mathbf{x}, \mathbf{y}) = \mathbf{v}_d(\mathbf{x}) M^{-1} \mathbf{v}_d(\mathbf{y})$ where $M \in \mathbb{R}^{s(d) \times s(d)}$ is positive definite, then for all $\mathbf{x} \in \mathbb{R}^p$,

$$|Q(\mathbf{x},\mathbf{x})\Lambda_d^{\mu}(\mathbf{x}) - 1| \leq \|I - M_{\mu,d}^{\frac{1}{2}}M^{-1}M_{\mu,d}^{\frac{1}{2}}\|_{op}$$

If
$$M \simeq M_{\mu,d}$$
, then $\Lambda^\mu_d(\mathbf{x}) \simeq rac{1}{Q(\mathbf{x},\mathbf{x})}$.

Regularization

"Using pseudo inverse is like saying $0=+\infty$ ".

Regularization: Let μ_0 be a simple absolutely continuous measure (moments are easy to compute). Replace μ by $\mu + \beta \mu_0$, $\beta > 0$.

$$egin{aligned} M_{\mu+eta\mu_0,d} &= M_{\mu,d} + eta M_{\mu_0,d} \succ 0 \ & \Lambda^d_{\mu+eta\mu_0} &\geq \Lambda^d_{\mu} + eta \Lambda^d_{\mu_0} \ & \int (\Lambda^d_{\mu+eta\mu_0})^{-1} d\mu \leq \int (\Lambda^d_{\mu+eta\mu_0})^{-1} d(\mu+eta\mu_0) = s(d) = O(d^p) \end{aligned}$$

- The moment matrix is positive definite
- If $\Lambda^d_{\mu+\beta\mu_0}$ is small, then Λ^d_{μ} is also small.
- $\Lambda_{\mu+\beta\mu_0}^d$ stays reasonably big on the support of μ .
- $\Lambda^d_{\mu+\beta\mu_0}$ stays reasonably small outside the support of μ (if β is small).

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Acknowledgement

The content of this section is taken from

Marx, S., Pauwels, E., Weisser, T., Henrion, D., & Lasserre, J. (2019). Tractable semi-algebraic approximation using Christoffel-Darboux kernel. arXiv preprint arXiv:1904.01833.

From the tutorial of Didier

Controled ODE,

$$\dot{x}(t) = f(x(t), u(t)),$$

 $x(t) \in X,$
 $u(t) \in U,$
 $t \in [0, 1],$
 $x(0) = 0$

Occupation measure, given a classical trajectory

$$d\mu(x, u, t) = d\delta_{x(t)}(x)d\delta_{u(t)}(u)dt$$

Relaxation: Replace classical trajectories satisfying an ODE by measures satisfying a linear transport PDE.

A heuristic argument

Hierarchy: f polynomial, X, U basic semi-algebraic: level d provides pseudo-moments up to degree 2d in variables t, u, x.

 PM_d

Heuristic: As d grows PM_d should get close to $M_{\mu,d}$ where μ is an occupation measure supported on optimal trajectories.

Use the Christoffel Darboux kernel:

"
$$(x, u, t)^T PM_d^{-1}(x, u, t)$$
"

- The measure is singular, we only have pseudo moments . . .
- ullet Morally, it is small on the support of μ and large outside the support.
- Morally, it is small on the optimal trajectory and large outside.

A semi-algebraic estimator

Hierarchy: f polynomial, X, U basic semi-algebraic: level d provides pseudo-moments up to degree 2d in variables t, u, x.

 PM_d

Christoffel Darboux kernel:

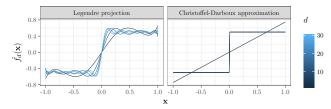
$$((x, u, t)^{T} PM_{d}^{-1}(x, u, t)) = Q_{d}(x, u, t)$$

Morally, it is small on the optimal trajectory and large outside.

A semi-algebraic estimator: For all $t \in [0,1]$

$$(\hat{u}(t),\hat{x}(t))\in \operatorname{argmin}_{(x,u)}Q(x,u,t).$$

An example with $x(t) = \operatorname{sign}(t)/2$ and exact moments



Convergence guaranties

A semi-algebraic estimator: $Q_d(x, u, t) = "(x, u, t)^T PM_d^{-1}(x, u, t)"$

$$(\hat{u},\hat{x})$$
: $t\mapsto (\hat{u}(t),\hat{x}(t))\in \operatorname{argmin}_{(x,u)}Q(x,u,t)$.

Assumption: x, u in L^1 , bounded, continuous almost everywhere, exact moments. Strong convergence in L^1 .

Assumption: x, u Lipschitz, exact moments. Rate of order $O(1/\sqrt{d})$.

Nate of order $O(1/\sqrt{a})$.

Assumption: x, u have bounded total variation, exact moments.

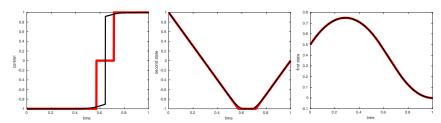
Conjecture: Rate of order $O(1/d^{\frac{1}{4}})$.

Illustration on the double integrator with constraints

Minimal time to reach the origin. $u \in [-1, 1]$, $x_1 \ge -1$.

$$\dot{x}_2(t)=x_1(t)$$

$$\dot{x}_1(t)=u(t)$$



With True moments:

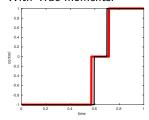
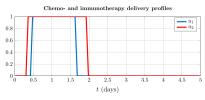
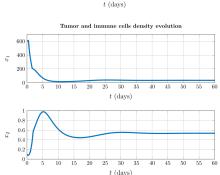


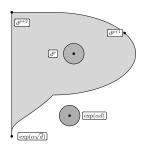
Illustration in Chemo-Immuno therapy modeling

Moussa, K., Fiacchini, M., & Alamir, M. (2019). Robust Optimal Control-based Design of Combined Chemo-and Immunotherapy Delivery Profiles. IFAC-PapersOnLine, 52(26), 76-81.





Conclusion



- ullet CD kernel is computed from moments of a measure $\mu.$
- ullet It captures the support of $\mu.$
- Century old mathematical history and still active.
- Proper set up, proof guaranties, require some subtleties.
- Can be combined with Lassere's Hierarchy: example in polynomial optimal control.