Polynomial optimization on finite sets.

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LECTURE 4: The polynomial kernel method.

Let n be an even integer and $X := \{-1, 1\}^n$. We know that for every quadratic function $f \in \mathbb{R}[X]_{\leq 2}$ and $r \geq \frac{n}{2} + 1$ the equality $f_{\min} = f_{(r)}$ holds where $f_{(r)}$ is the semidefinite programming lower bound of level r,

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Can we bound the gap $f_{\min} - f_{(r)}$ as a function of r?
More precisely we would like to bound the worst-case gap

$$\sup_{f \in \mathbb{R}[X]_{\leq 2}} \frac{f_{\min} - f_{(r)}}{\|f\|_\infty} \leq F(r)$$

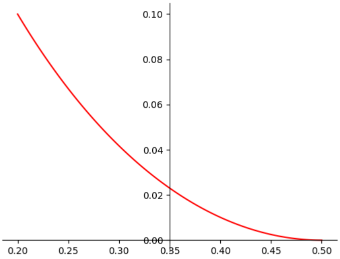
There is a good answer to this question for every d, There is a good answer to this question for every d,

Theorem. (Laurent, Slot (2021))

Suppose $f \in \mathbb{R}[X]_{\leq d}$. There exists a constant $C(d)$ such that

$$\frac{f_{\min} - f_{(r)}}{\|f\|_\infty} \leq C(d)\frac{\zeta_r}{n}$$

where ζ_r is the smallest root of the Krawtchouk polynomial $K_r(t)$. Furthermore $\frac{\zeta_r}{n} \sim \phi(r/n)$.



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- Such perturbations are built by constructing **local averages** of functions, via polynomial kernels.
- There are many possible polynomial kernels and a **good choice**, taking advantage of the symmetries of the problem leads to the proof of the Theorem.

Plan for Lecture 4:

1. The polynomial kernel method.
2. Invariant polynomial kernels on the hypercube.
3. Generalizing the hypercube.

Part 1:
Local averaging via polynomial kernels.

Suppose $X \subseteq \mathbb{R}^n$ is a metric space having distance function $d(x, y)$ and a given probability measure μ.

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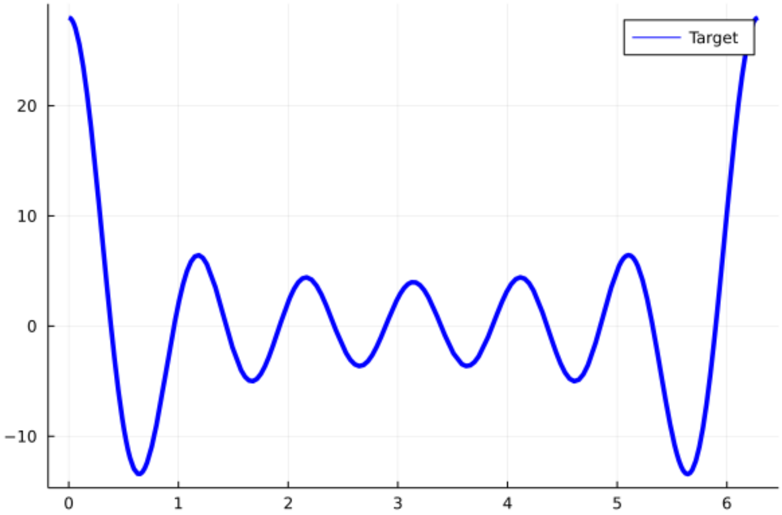
Definition.

Let $g(t)$ be a univariate sum-of-squares. Define $\Gamma_g : \mathbb{R}[X] \to \mathbb{R}[X]$ via $\Gamma_g(f(x)) = h(x)$ where

$$h(x) = \int_X g\left(d(x, y)\right) f(y) d\mu(y).$$

Averaging polynomials



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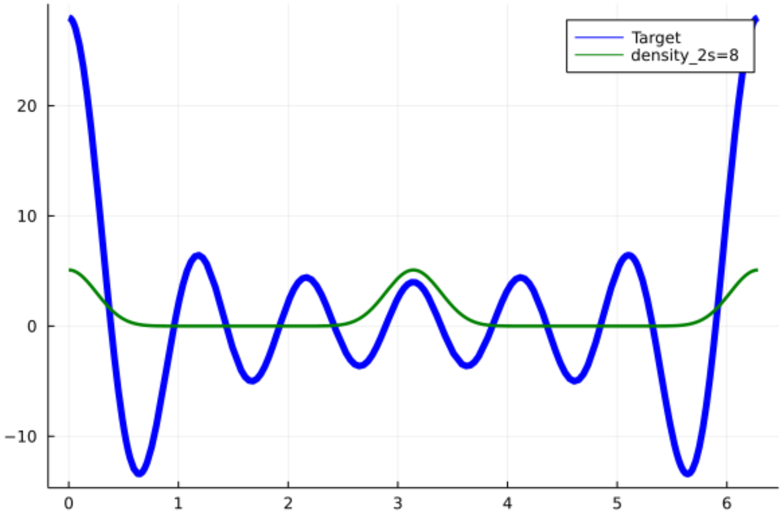

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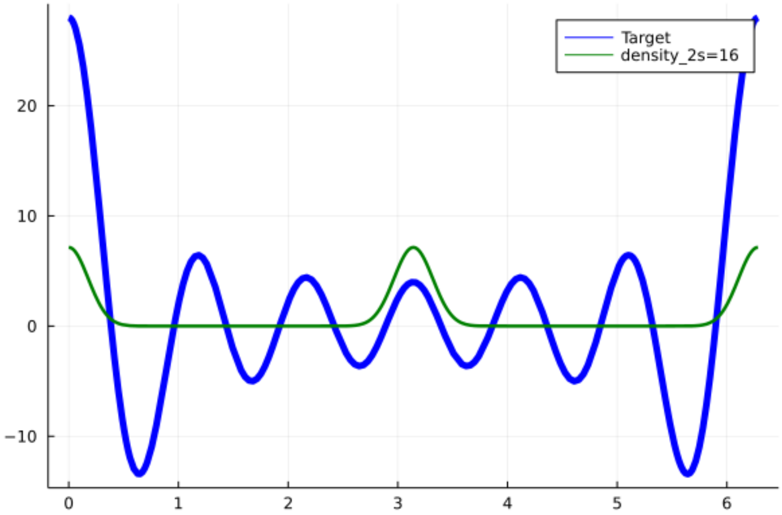

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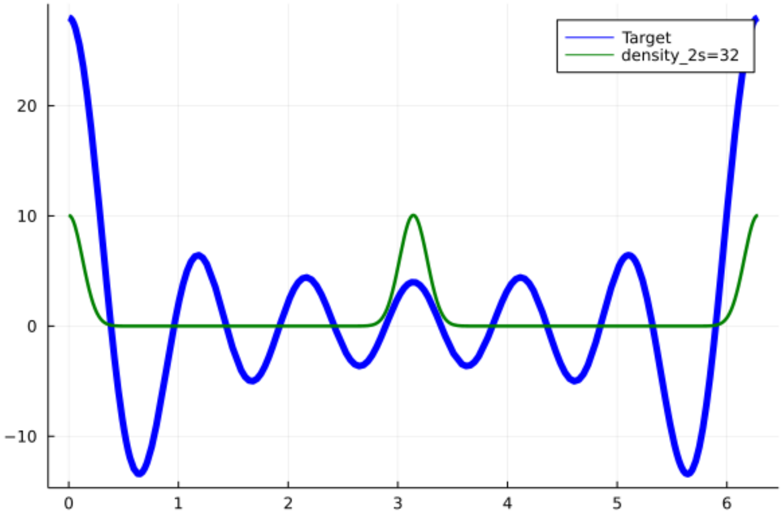

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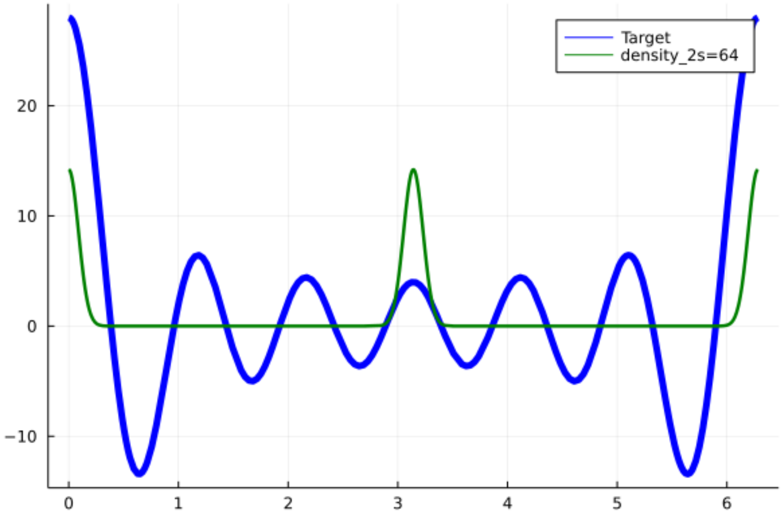

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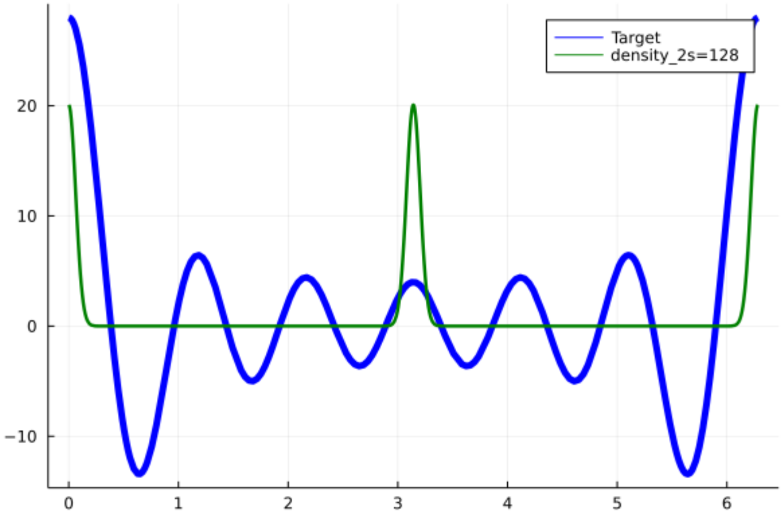

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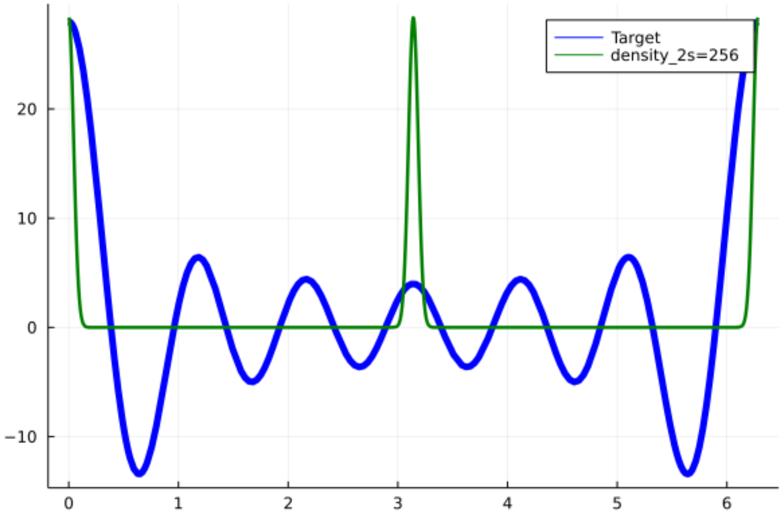

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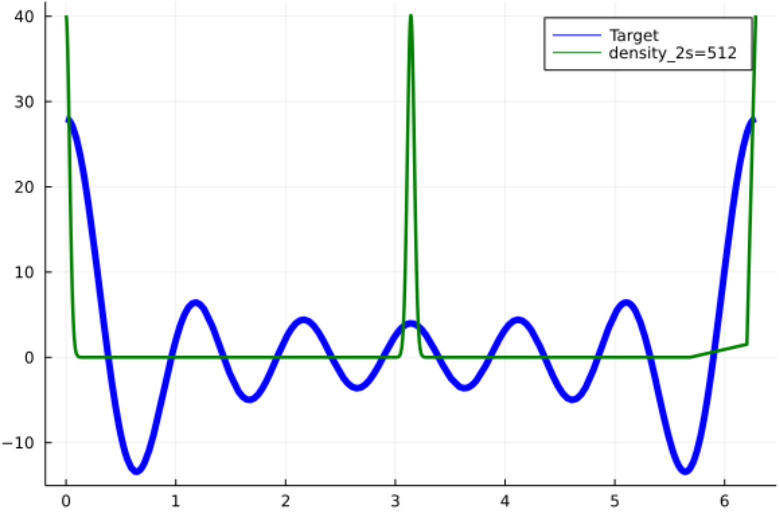

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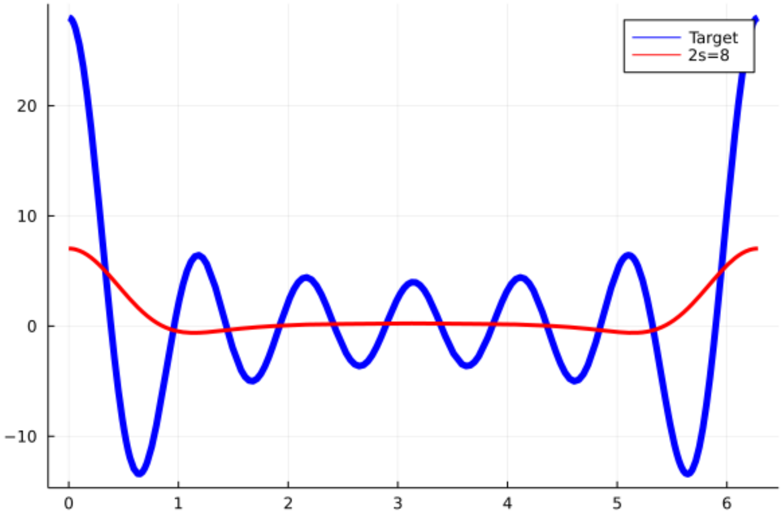

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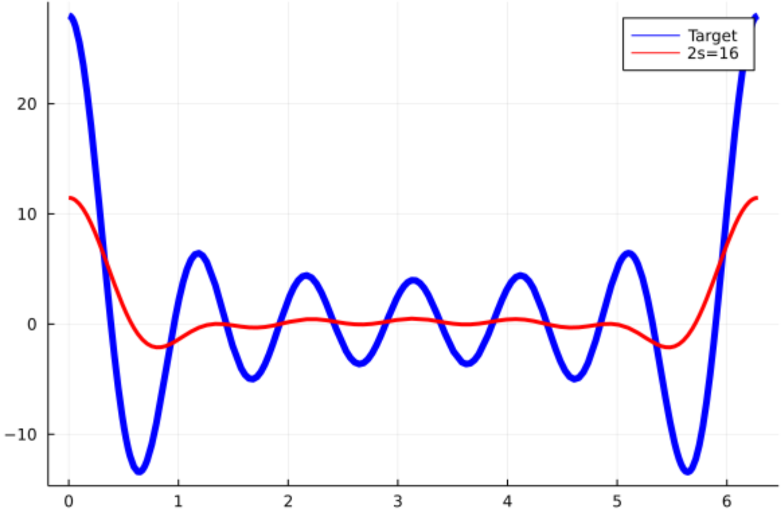

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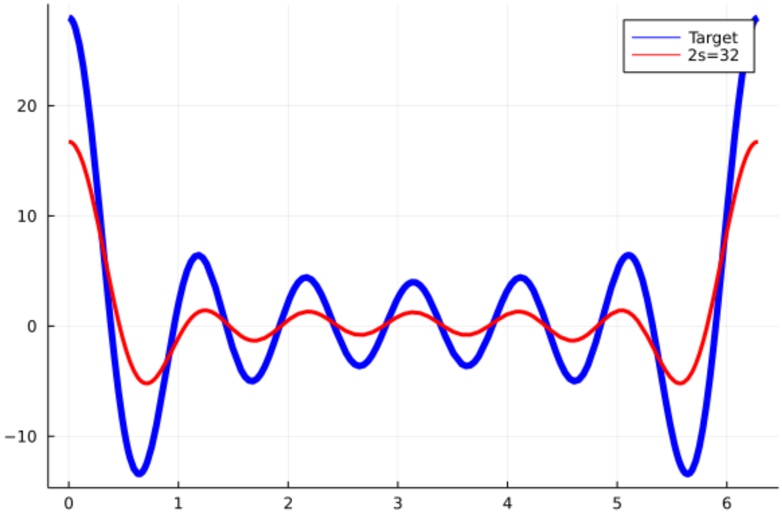

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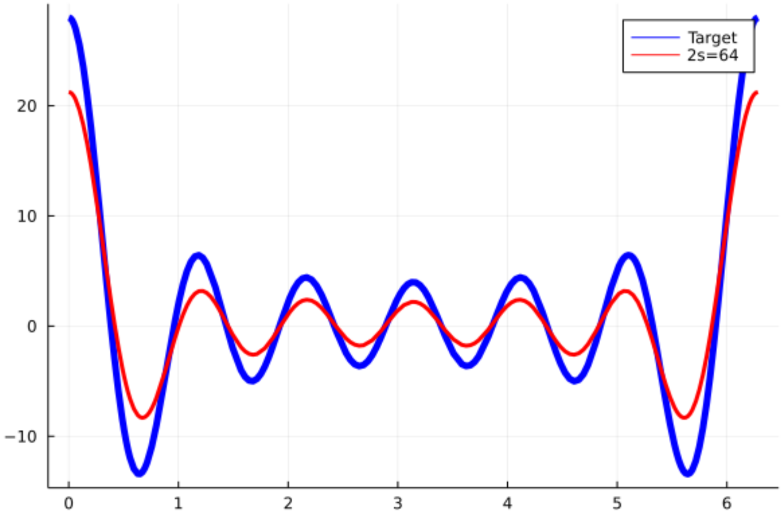

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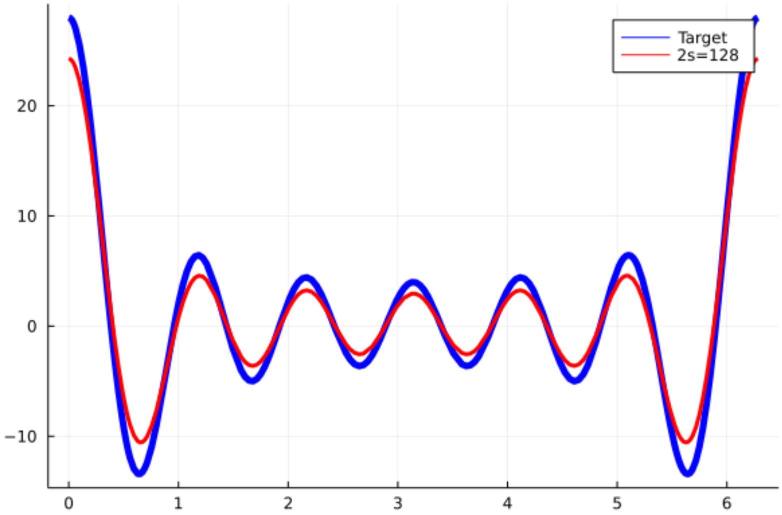

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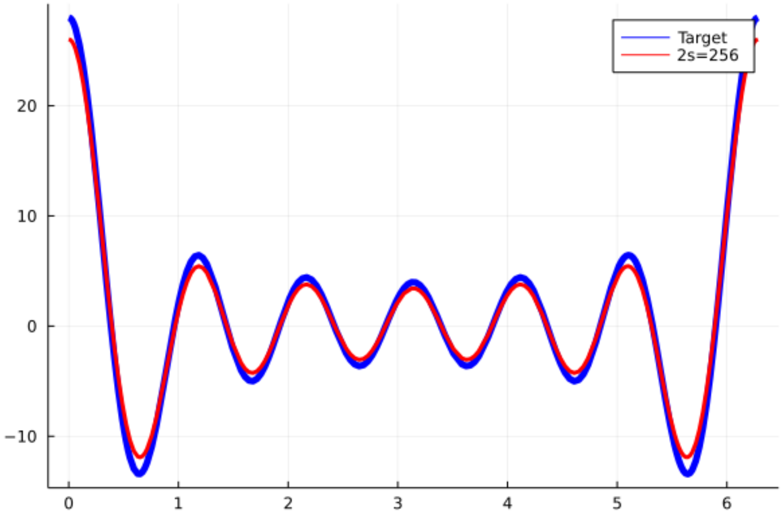

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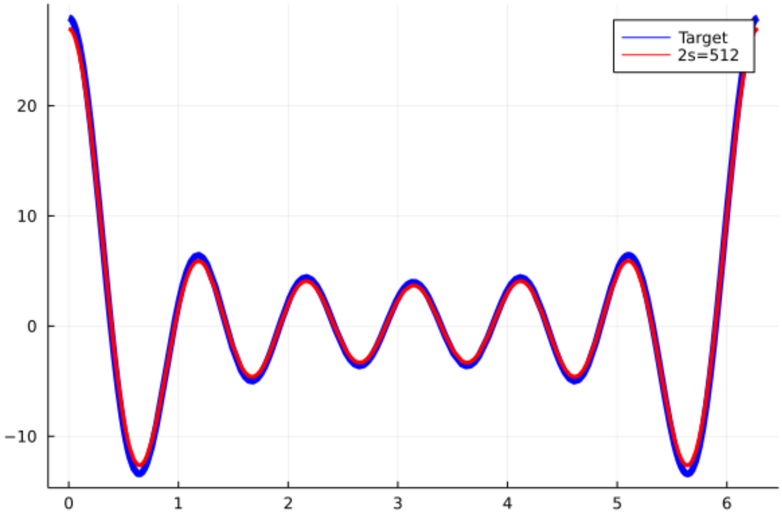

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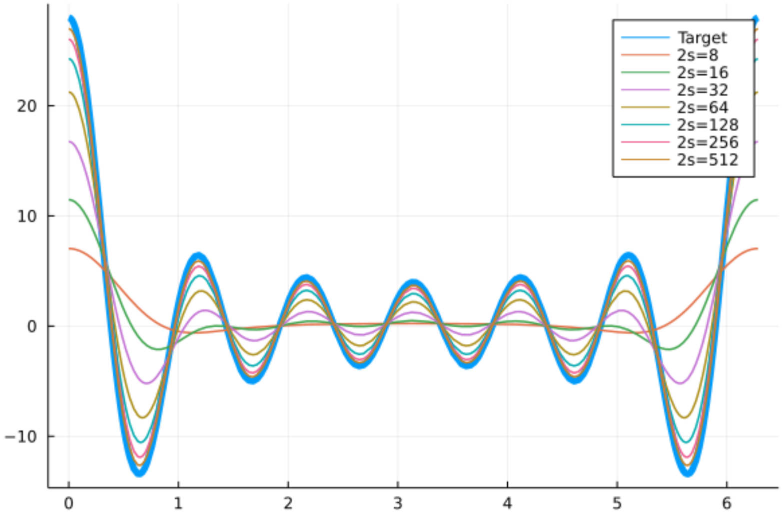

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Assume X is finite, μ is the counting measure and for every y_0 the function $d(x, y_0)$ is affine linear.

Lemma.

Assume $g(t) = s(t)^2$ is a square of a polynomial of degree $\leq r$. If $f(x)$ is nonnegative on X then $h(x)$ is a sum-of-squares of functions of degree $\leq r$.

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Lemma.

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Proof.

$$h(x) = \int_X s_i(d(x, y))^2 f(y) d\mu(y) = \frac{1}{|X|} \sum_{y_0 \in X} s_i(d(x, y_0))^2 f(y_0)$$

$\square$

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To measure distances between operators $L : \mathbb{R}[X] \to \mathbb{R}[X]$ we will use the operator norm

$$\|L\| := \sup_{\|p\|_\infty \leq 1} \|L(p)\|_\infty$$

where $\|p\|_\infty := \sup_{x \in X} |p(x)|$.

Theorem. (Reznick / Fang-Fawzi)

Assume $g(t) = s(t)^2$ is the square of a polynomial of degree $\leq r$. If $\Gamma_g(1) = 1$ and $\|\Gamma_g^{-1} - I\| \leq \delta$ then $\sup_f \frac{f_{\min} - f_{(r)}}{\|f\|_\infty} \leq \delta$.

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$$= \Gamma_g^{-1}(f) - f_{\min} + \delta \geq f - \delta - f_{\min} + \delta = f - f_{\min} \geq 0$$

The result follows since the nonnegativity of $\Gamma_g^{-1}(h)$ implies that $h = \Gamma_g(\Gamma_g^{-1}(h)) \in \Sigma_{\leq r}$. □

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This suggests the following two questions:

1. Given $g(t)$, how to compute $\|\Gamma_g^{-1} - I\|$?
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For the hypercube $X = \{-1, 1\}^n \subseteq \mathbb{R}^n$ both questions have good answers...

Part 2:
Invariant kernels on the hypercube $X := \{-1, 1\}^n$.

Theorem. (Laurent, Slot, 2021)

There exists a collection of univariate orthogonal polynomials $\hat{K}_j(t)$ for $j = 0, \ldots, n$ and a decomposition

$$\mathbb{R}[X] = W_0 \oplus \cdots \oplus W_n$$

into orthogonal subspaces having the following property: If $g(t) = \sum \lambda_i \hat{K}_i(t)$ is the unique expression of a polynomial $g(t)$ then, in any basis for $\mathbb{R}[X]$ compatible with the above decomposition we have

$$[\Gamma_g] = \begin{pmatrix} \lambda_1 I_{d_1} & 0 & 0 & \ldots & 0 \\ 0 & \lambda_2 I_{d_2} & 0 & \ldots & 0 \\ 0 & 0 & \lambda_3 I_{d_3} & \ldots & 0 \\ \vdots & \vdots & \vdots & \ldots & 0 \\ 0 & 0 & \ldots & \ldots & \lambda_n I_{d_n} \end{pmatrix}$$

Why is this useful?

- The block-diagonal structure of Γ_g allows us to get a simple estimate of the norm [Fang-Fawzi],

$$\|\Gamma_g^{-1} - I\| \leq \gamma \sum_{i=1}^{n} (1 - \lambda_i)$$

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$$\min_{g(t)} \left\{ \sum_{j=1}^{n} \left(1 - \langle \hat{K}_j(t), g(t) \rangle\right) : g(t) \in \Sigma_{\leq r}^{\mathbb{R}[t]} \ , \ \langle 1, g(t) \rangle = 1 \right\}$$

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With the inner product that makes the $\hat{K}_j$ orthonormal.

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Remark.

The analysis of Laurent-Slot is a discrete analogue to the work of [Fang-Fawzi, 2020] on the sphere.

Remark.

Explicit polynomial kernels combined with quadrature rules can be used to create novel optimization algorithms on spaces admitting both (see [Cristancho, -, 2022] on the sphere).

Why do Krawtchouk polynomials exist?

- We think of the hypercube $X = \{-1, 1\}^n$ as a metric space with the Hamming distance:

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- If $x_0 = (1, \ldots, 1)$ the subgroup $H \subseteq \mathbb{B}$ of elements fixing x_0 is precisely the permutations.

We thus have a pair group, subgroup $(\mathbb{B}, H)$.

This pair has several miraculous properties:

1. The isotypical decomposition of $\mathbb{R}[X]$ as a $\mathbb{B}$-representation is **of multiplicity one**.

$$\mathbb{R}[X] = W_0 \oplus W_1 \oplus \cdots \oplus W_n$$

2. For any $g(t)$ the map $\Gamma_g : \mathbb{R}[X] \to \mathbb{R}[X]$ is a morphism of representations so behaves **like a multiple λ_i of the identity** in each W_i.
3. Each W_i contains a unique copy of the trivial representation, when seeing as an H-representation (this follows from the Frobenius character formula).

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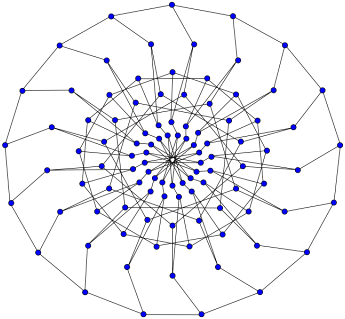
Remark.

The last two properties follow from the first. A pair $(\mathbb{B}, H)$ with the first property is called a **Gelfand pair**.

Hypercubes in the multiverse

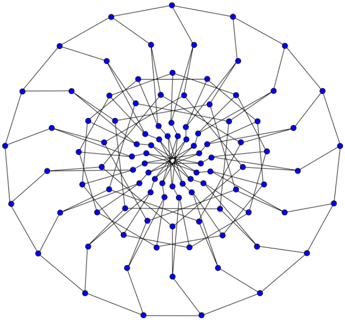
Let X be a finite metric space and let $\mathbb{B}$ be the group of distance-preserving bijections. Fix $x_0 \in X$ and let $H := \mathrm{Stab}(x_0)$.



Definition.

A finite metric space X is **doubly-transitive** *if for any $x_1, x_2, y_1, y_2 \in X$ with $d(x_1, x_2) = d(y_1, y_2)$ there exists an element $g \in \mathbb{B}$ with $y_1 = gx_1$ and $y_2 = gx_2$.*

Hypercubes in the multiverse



There are at least 19 infinite families of doubly transitive graphs, including **hypercubes**, *Cocktail party graphs, Johnson graphs, Grassmann graphs, Paley graphs, etc.*

Hypercubes in the multiverse

For a finite metric space X let $\mathbb{B} := \mathrm{Aut}(X)$ and $n := \mathrm{diam}(\mathrm{X})$.

Theorem. (-)

If X is doubly transitive then the following statements hold:

1. $\mathbb{R}[X]^H = \mathbb{R}[d(x_0, x)] = \mathbb{R}[\ell]/\prod_{j \in \mathrm{range}(d)}(\ell - j)$.
2. $\mathbb{R}[X]$ *decomposes into* $\mathbb{B}$*-irreducibles* W_j *in a multiplicity free manner and every* $\mathbb{B}$*-irreducible contains a unique copy of the* H*-trivial representation.*
3. *There are unique univariate polynomials* $\hat{K}_j(t)$ *such that* $\hat{K}_j(d(x,y))$ *is the Christoffel-Darboux kernel in* W_j.
4. *There is an embedding* $X \subseteq \mathbb{R}^e$ *uniquely specified up to orthogonal transformations. The speed of convergence of the SOS hierarchy on this embedding is bounded by a univariate SDP using the* $\hat{K}_j(t)$.