

The Kolmogorov Superposition Theorem:

A framework for multivariate computation

Jonas Actor

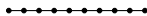
Rice University

7 May 2018

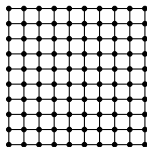
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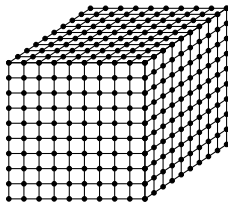
Curse of Dimensionality



10 nodes



10^2 nodes



10^3 nodes

Cost of simulation / computation grows **exponentially**

A Question ¹

Do functions of three variables exist at all?

¹Pólya and Szegő, Problems and Theorems of Analysis, 1925 (German), transl. 1945, reprinted 1978

A Question, Restated

Can functions of three variables be expressed using functions of only two variables?

Example:

Cardano's Formula for roots of a cubic equation

A Better Question

Hilbert's 13th Problem (1900)

Can the solution x to the 7th degree polynomial equation

$$x^7 + ax^3 + bx^2 + cx + 1 = 0$$

be represented by a finite number of compositions of bivariate continuous (algebraic) functions using the three variables a, b, c ?

Answer: Arnol'd 1957 ²

Any **continuous** function of three variables can be expressed using **continuous** functions of only two variables.

² Arnol'd, Dokl. Akad. Nauk SSSR 114:5, 1957

The Next Question

Can continuous functions of three variables be expressed using functions of only **one** variable and addition?

Answer: Kolmogorov 1957³

Any continuous $f : [0, 1]^n \rightarrow \mathbb{R}$ can be written as


$$f(x_1, \dots, x_n) = \sum_{q=0}^{2n} \chi \left(\sum_{p=1}^n \psi_{p,q}(x_p) \right)$$

³ Kolmogorov, Dokl. Akad. Nauk SSSR 114:5, 1957

What's going on here?

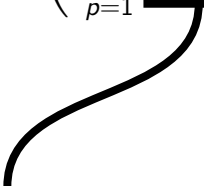
$$f(x_1, \dots, x_n) = \sum_{q=0}^{2n} \chi \left(\sum_{p=1}^n \psi_{p,q}(x_p) \right)$$

What's going on here?

$$\underline{f(x_1, \dots, x_n)} = \sum_{q=0}^{2n} \chi \left(\sum_{p=1}^n \psi_{p,q}(x_p) \right)$$


Original function $f : [0, 1]^n \rightarrow \mathbb{R}$

What's going on here?

$$f(x_1, \dots, x_n) = \sum_{q=0}^{2n} \chi \left(\sum_{p=1}^n \psi_{p,q}(x_p) \right)$$


Inner function $\psi_{p,q} : [0, 1] \rightarrow \mathbb{R}$

What's going on here?

$$f(x_1, \dots, x_n) = \sum_{q=0}^{2n} \chi \left(\sum_{p=1}^n \psi_{p,q}(x_p) \right)$$



Addition

What's going on here?

$$f(x_1, \dots, x_n) = \sum_{q=0}^{2n} \chi \left(\sum_{p=1}^n \psi_{p,q}(x_p) \right)$$

Outer function $\chi : \mathbb{R} \rightarrow \mathbb{R}$

What's going on here?

$$f(x_1, \dots, x_n) = \sum_{q=0}^{2n} \chi \left(\sum_{p=1}^n \psi_{p,q}(x_p) \right)$$



Function composition

Implication

$$\Psi^q(x_1, \dots, x_n) = \sum_{p=1}^n \psi_{p,q}(x_p)$$

(independent of f)

KST: $f \longmapsto \chi$

Traded smoothness for variables:

- No KST⁴ for $\psi_{p,q} \in C^1([0, 1])$
- Current $\psi_{p,q} \in \text{Hölder}([0, 1]) \rightarrow$ bad for computation
- Possible $\psi_{p,q} \in \text{Lip}([0, 1])$

⁴Vituskin, DAN, 95:701–704, 1954.

Goal: Construct Lipschitz functions $\psi_{p,q}$

Rest of the Talk

- 1 Constructive KST
- 2 The Fridman Strategy
- 3 Reparameterization Approach
- 4 Conclusions and Outstanding Tasks

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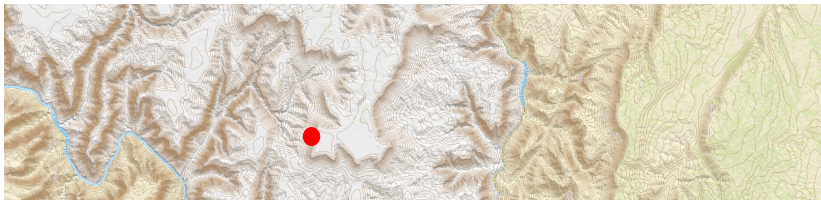
An Analogy

$f(x, y) =$ elevation of Grand Canyon at (x, y)

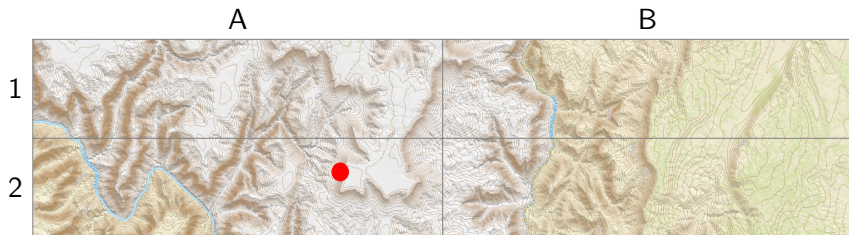


An Analogy

$$f(\text{Thor's Temple}) = ?$$



An Analogy



Bright Angel Point A1

Desert View B2

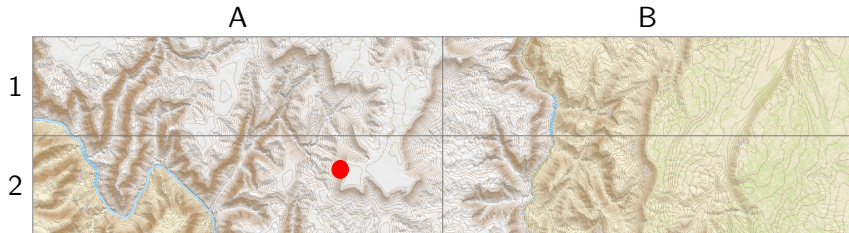
Grand Canyon Lodge A1

Kaibab Nat'l Forest B1

Thor's Temple A2

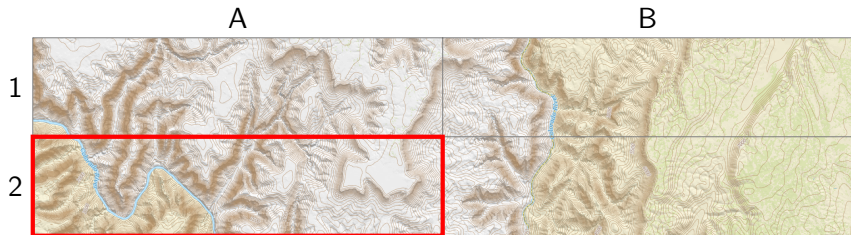
Walhalla's Overlook A2

An Analogy

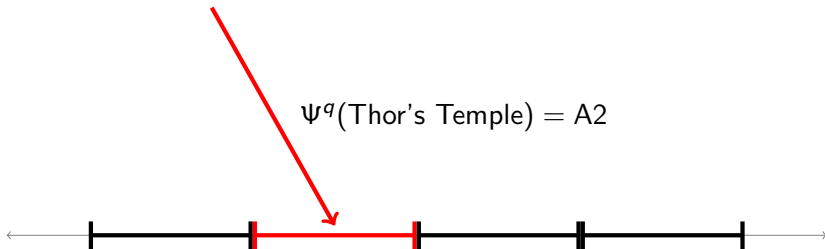


Elevation (ft)	A1	8200	B1	8000
	A2	9000	B2	7600

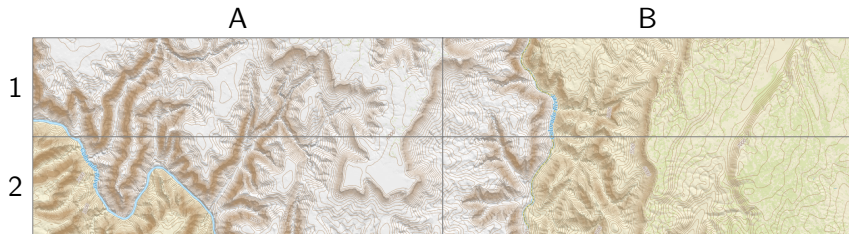
An Analogy



$$\Psi^q(\text{Thor's Temple}) = A2$$



An Analogy



$$f(\text{Thor's Temple}) = \chi(A2)$$



An Analogy

A

B

1



2



An Analogy

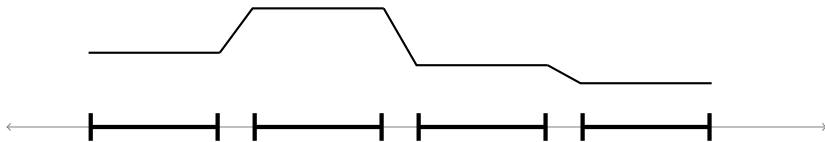
A

B

1



2



An Analogy

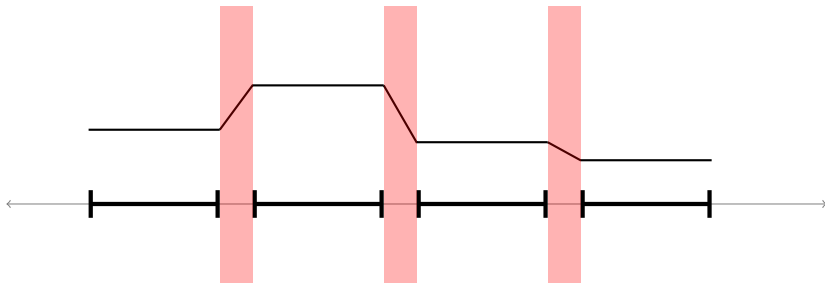
A

B

1



2



Decomposition Process

Strategy

- Leave gaps between squares \rightarrow gives room to vary continuously
- Duplicate and slightly shift the squares to cover the gaps
- Define functions $\psi_{p,q}$ as we refine squares

Decisions

- How big to make the gaps
- How to assign values to functions

Sprecher's Reduction⁵

Define 1 function instead of $2n^2 + n$ functions:

$$\psi_{p,q}(x_p) = \lambda_p \psi(x_p + q\varepsilon)$$

$\lambda_1, \dots, \lambda_n$ integrally independent

⁵Sprecher, Trans. AMS, 115:340–355, 1965

Requirements (1/2)

Refinement:

Squares \mathcal{S}^k get smaller as $k \rightarrow \infty$

More Than Half:

Each point in at least $\frac{n+1}{2n+1}$ sets of shifted squares

Requirements (2/2)

Disjoint Image:

Image of squares under Ψ^q disjoint

Monotonicity:

Function ψ strictly monotonic increasing

Bounded Slope:

Function ψ Lipschitz

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First proof of Lipschitz inner KST functions⁶

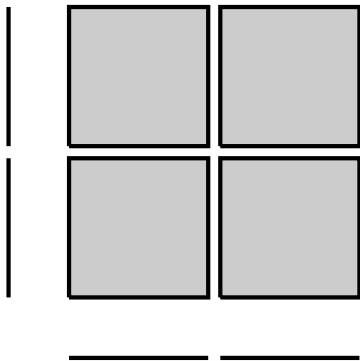
Predominant approach for Lipschitz KST functions

Never successfully implemented

⁶Dokl. Akad. Nauk SSR, 177:5:1019–1022, 1967.

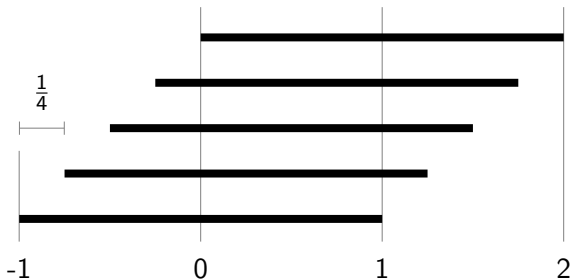
Defining our Squares

Squares: Cartesian product of 1D family of intervals



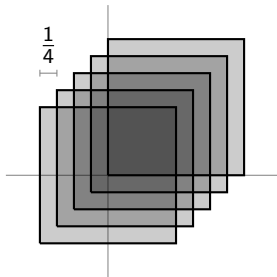
Space Decomposition

5 copies of the same family of intervals, shifted by $\frac{1}{4}$



Space Decomposition

Cartesian product for each shifted family of intervals



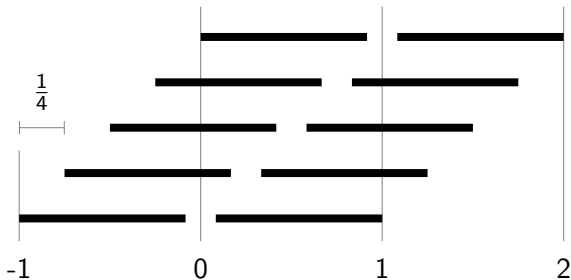
Space Decomposition

Each *refinement level* $k \in \mathbb{N}$,
break largest intervals roughly in half



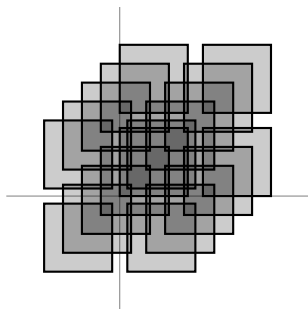
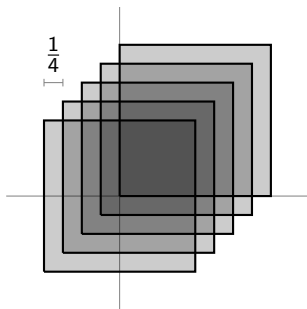
Space Decomposition

Breaks are copied in **each** shifted family of intervals ...



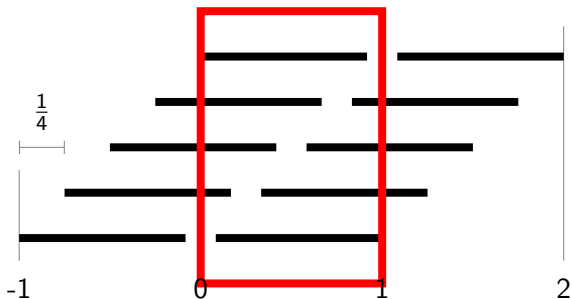
Space Decomposition

... and each shifted family of squares.



Requirements on Breaks

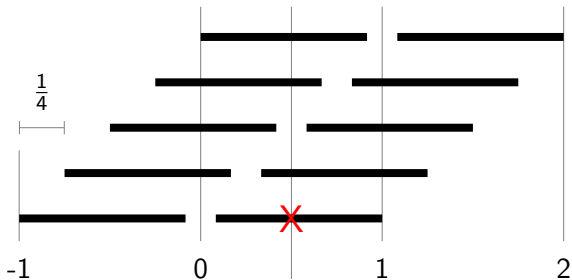
Every $x \in [0, 1]$ in at least **All But One** of shifted families



All But One on intervals \iff More Than Half on squares

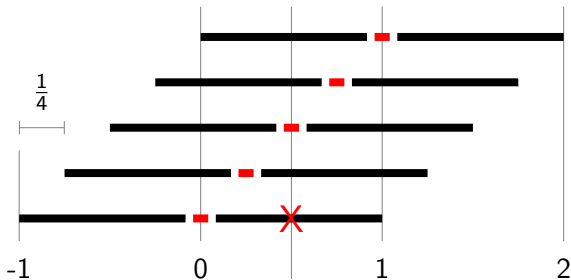
Choosing Breaks

Keep inserting breaks \longrightarrow lose All But One Condition



Choosing Breaks

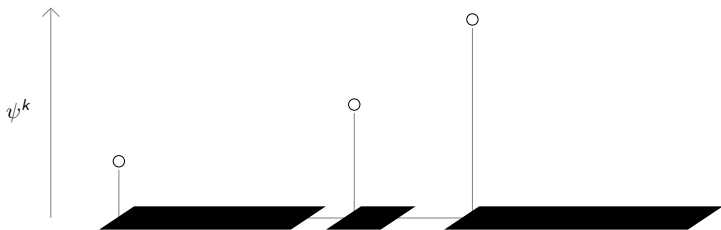
Solution: plug the gaps that cause problems



Inner Function ψ

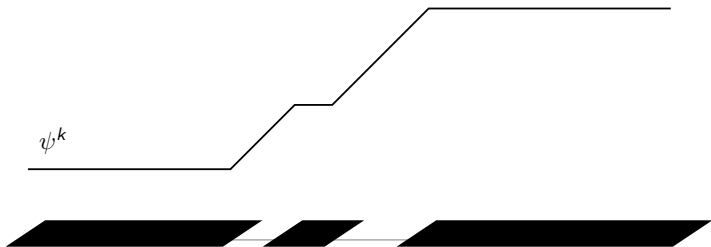
At each refinement level k :

- Assign a value of ψ^k on left endpoint of each interval
- Value is fixed for all future k



Inner Function ψ

ψ^k constant on intervals, linear on gaps



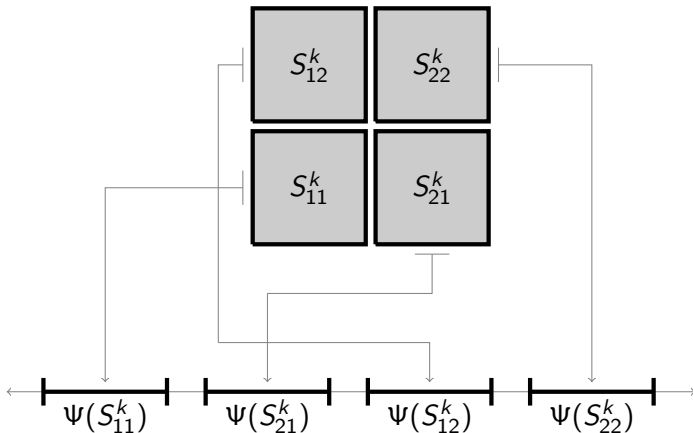
large plugs \rightarrow small gaps \rightarrow steep ψ^k

Fixing Values: Disjoint Image Condition

For any two squares $S, S' \in \mathcal{S}^k$,

$$\Psi(S) \cap \Psi(S') = \emptyset.$$

Disjoint Image Condition



Disjoint Image Condition

Don't know ψ at level k

Can't enforce Disjoint Image Condition without ψ

Two remedies:

- Fridman's Disjoint Image Condition
- Conservative Disjoint Image Condition

Fridman's Disjoint Image Condition

For any two squares $S, S' \in \mathcal{S}^k$,

$$\Psi^k(S) \cap \Psi^k(S') = \emptyset.$$

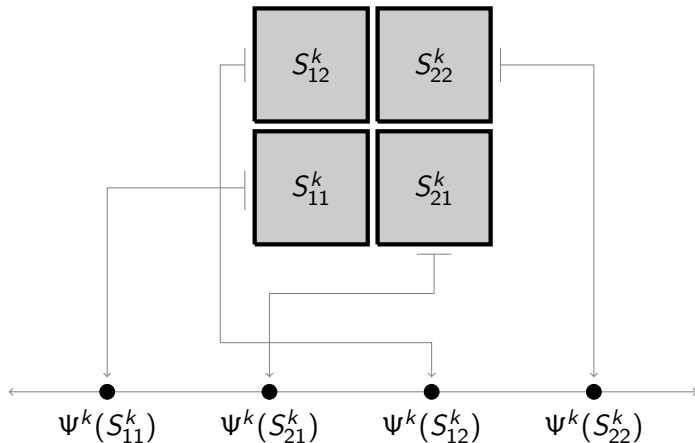
Fridman's Disjoint Image Condition

For any two squares $S, S' \in \mathcal{S}^k$,

$$\Psi^k(S) \cap \Psi^k(S') = \emptyset.$$

Not $\Psi(S), \Psi(S')$

Fridman's Disjoint Image Condition



Fridman's Disjoint Image Condition

$$\Psi(x) = \sum_{p=1}^n \lambda_p \psi(x_p + q\varepsilon)$$

$\lambda_1, \dots, \lambda_n$ integrally independent

ψ^k rational values at left endpoints

Fridman's Condition is always met!
Does not enforce disjointness in limit

Conservative Disjoint Image Condition

Use Lipschitz bound to define intervals Δ_i^k that are guaranteed to contain $\Psi(S_i^k)$

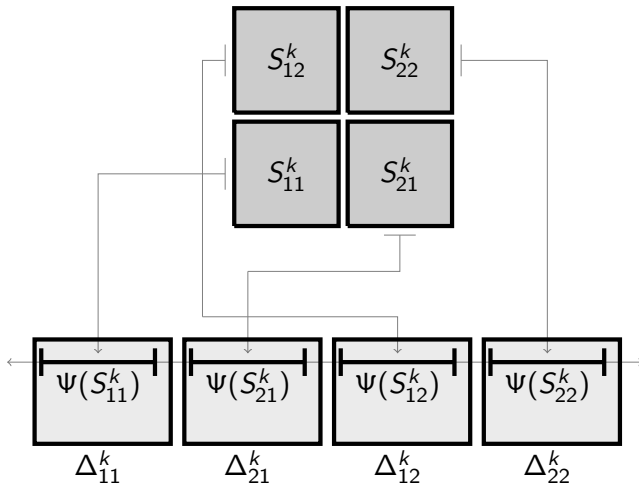
$$\psi^k(S_i^k) \subseteq \Psi(S_i^k) \subseteq \Delta_i^k.$$

Conservative Disjoint Image Condition

For any two squares $S_{\mathbf{i}}^k, S_{\mathbf{i}'}^k \in \mathcal{S}^k$
and corresponding intervals $\Delta_{\mathbf{i}}^k, \Delta_{\mathbf{i}'}^k$,

$$\Delta_{\mathbf{i}}^k \cap \Delta_{\mathbf{i}'}^k = \emptyset.$$

Conservative Disjoint Image Condition



Conservative Disjoint Image Condition

Requires removing **at least half** of each interval

Points not contained in enough shifted copies of \mathcal{S}^k to
reconstruct χ

Implications

Choose 2 of 3:

- (Conservative) Disjoint Image Condition
- All But One Condition
- Bounded Slope Condition

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KST inner functions are strictly monotonic increasing

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... which are of Bounded Variation

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... so they define rectifiable curves

KST inner functions are strictly monotonic increasing

... which are of Bounded Variation

... so they define rectifiable curves

... which have Lipschitz reparameterizations.

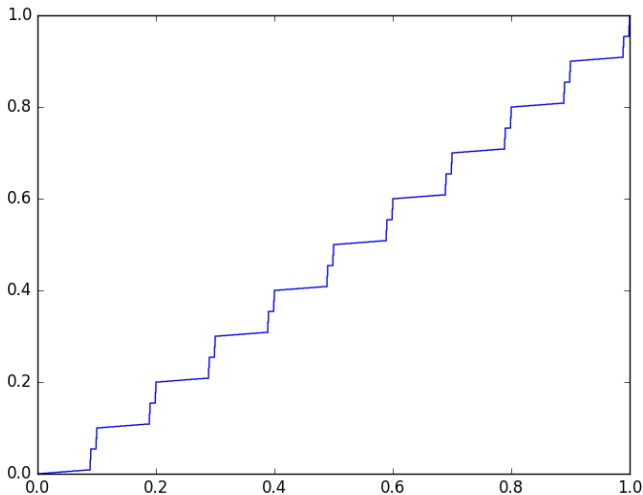
Approach

- ① Find (non-Lipschitz) function $\hat{\psi}$
- ② Define reparameterization σ
- ③ Create Lipschitz ψ from $\hat{\psi}$ using σ
- ④ Construct squares \mathcal{S}^k that meet conditions

Hölder Continuous $\hat{\psi}$

- Define iteratively: $\hat{\psi} = \lim_{k \rightarrow \infty} \hat{\psi}^k$
- Fix values at points with k digits in base γ expansion
 - Small increase for most points
 - Large increase for expansions ending in $\gamma - 1$
- Linearly interpolate between fixed values

Köppen's KST Inner Function $\hat{\psi}^7$



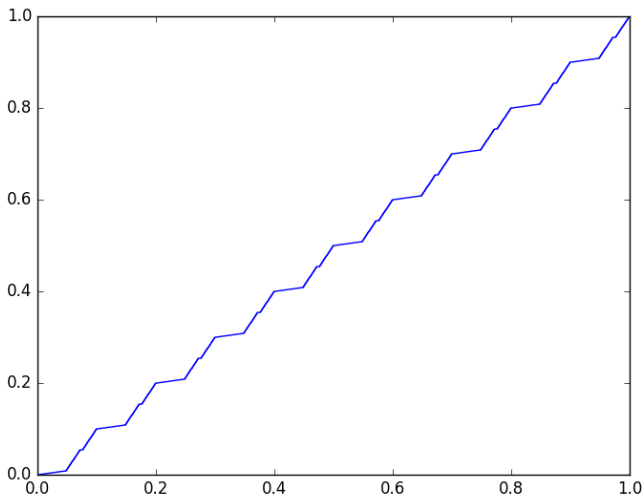
Lipschitz Reparameterization

Reparameterization $\sigma : [0, 1] \rightarrow [0, 1]$

$$\sigma(x) = \frac{\text{arclength of } \hat{\psi} \text{ from } 0 \text{ to } x}{\text{total arclength of } \hat{\psi} \text{ from } 0 \text{ to } 1}$$

$$\psi(x) = \hat{\psi}(\sigma^{-1}(x))$$

Lipschitz Reparameterization ψ^7



Correct Squares

$$\psi = \hat{\psi} \circ \sigma^{-1}$$

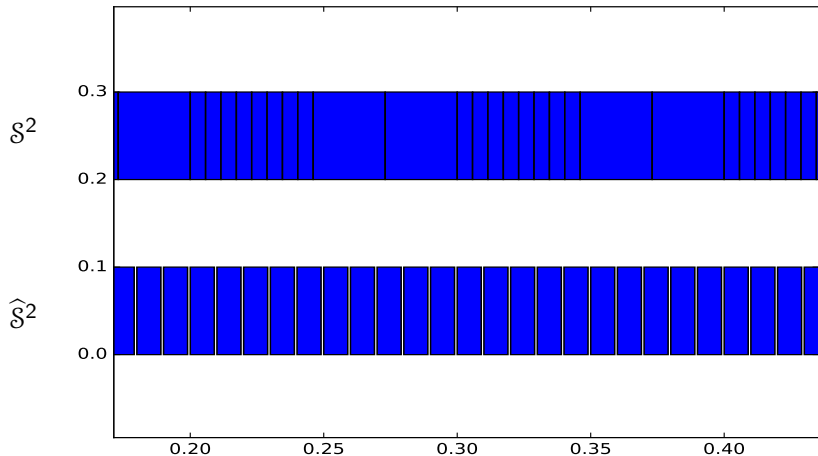
Intervals for $\hat{\psi}$ are $\hat{\mathcal{S}}^k$

Intervals for ψ are $\mathcal{S}^k = \sigma(\hat{\mathcal{S}}^k)$

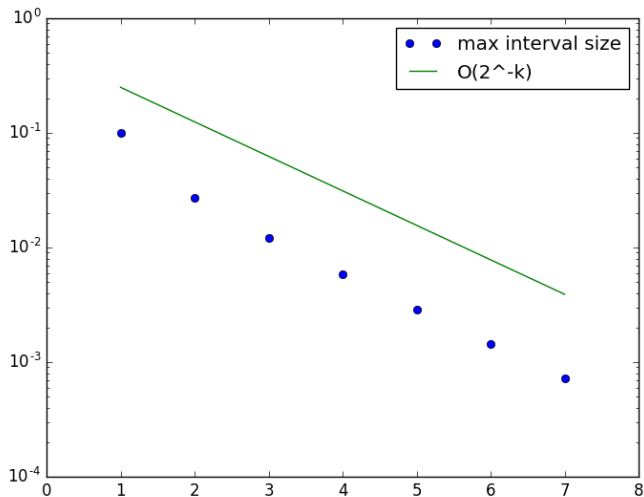
$\hat{\psi}$ satisfies Disjoint Image Condition on $\hat{\mathcal{S}}^k$

ψ satisfies Disjoint Image Condition on \mathcal{S}^k

Comparing $\widehat{\mathcal{S}}^k$ and \mathcal{S}^k



Largest Interval Size for \mathcal{S}^k



Reparameterized Intervals

Refinement Condition:

Intervals shrink at $O(2^{-k})$ not $O(\gamma^{-k})$

All But One Condition:

Gaps between intervals get smaller under σ

Takeaway

Function $\psi = \hat{\psi} \circ \sigma^{-1}$ is a Lipschitz KST inner function

Squares $\mathcal{S}^k = \sigma(\hat{\mathcal{S}}^k)$ are KST squares

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Review

- Motivated why KST is interesting, hard
- Illustrated how KST works
- Outlined Fridman Strategy
- Showed where Fridman Strategy fails
- Posed new reparameterization approach
- Justified reparameterization meets requirements

Outstanding Tasks

Complete proofs for reparameterization argument for ψ

Framework for computing outer function χ

- Requires squares at each level k
- Requires final Ψ

First Application: Image compression