Understanding Multivariate Computation using the Kolmogorov Superposition Theorem

Matthew Knepley

Computer Science and Engineering
University at Buffalo

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Argonne NATIONAL LABORATORY

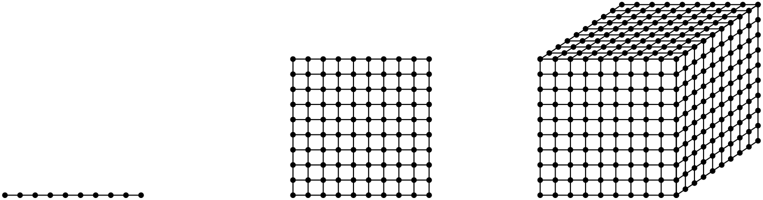
University at Buffalo

Collaborators

KST Representation Collaboration

Jonas Actor

Curse of Dimensionality



10 nodes

10^2 nodes

10^3 nodes

Cost of simulation / computation grows **exponentially**

Main Question

Do functions of three variables exist at all?[1]

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

Q: Can any function of three variables be expressed using functions of only two variables?[2]

[2] Hilbert, Göttinger Nachrichten, 1900

[3] Arnol'd, Dokl. Akad. Nauk SSSR 114:5, 1957

Q: Can any function of three variables be expressed using functions of only two variables?[2]

Ex: Cardano's Formula for roots of a cubic equation

[2] Hilbert, Göttinger Nachrichten, 1900

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Q: Can any function of three variables be expressed using functions of only two variables?[2]

Ex: Cardano's Formula for roots of a cubic equation

A: Any *continuous* function of three variables can be expressed using *continuous* functions of only two variables.[3]

[2] Hilbert, Göttinger Nachrichten, 1900

[3] Arnol'd, Dokl. Akad. Nauk SSSR 114:5, 1957

Q: Can any function of three variables be expressed using only univariate functions and addition?

[4] Kolmogorov, Dokl. Akad. Nauk SSSR 114:5, 1957

Q: Can any function of three variables be expressed using only univariate functions and addition?

A: Yes[4], for any continuous $f : [0,1]^n \to \mathbb{R}$

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

[4] Kolmogorov, Dokl. Akad. Nauk SSSR 114:5, 1957

What's going on here?

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

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

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

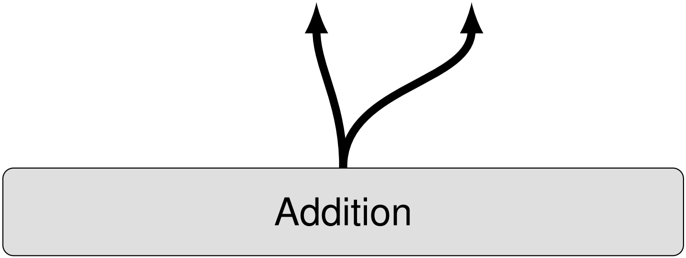
What's going on here?

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

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

What's going on here?

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



What's going on here?

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

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

What's going on here?

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

Function composition

2D: $n = 2$

$$\begin{aligned} f(x, y) = {} & \chi_0\left(\psi_{x,0}(x) + \psi_{y,0}(y)\right) \\ & + \chi_1\left(\psi_{x,1}(x) + \psi_{y,1}(y)\right) \\ & + \chi_2\left(\psi_{x,2}(x) + \psi_{y,2}(y)\right) \\ & + \chi_3\left(\psi_{x,3}(x) + \psi_{y,3}(y)\right) \\ & + \chi_4\left(\psi_{x,4}(x) + \psi_{y,4}(y)\right) \end{aligned}$$

2D: $n = 2$

$$
\begin{aligned}
f(x, y) = \chi_0\big(\lambda_x\psi(x) &+ \lambda_y\psi(y)\big) \\
+ \chi_1\big(\lambda_x\psi(x+\epsilon) &+ \lambda_y\psi(y+\epsilon)\big) \\
+ \chi_2\big(\lambda_x\psi(x+2\epsilon) &+ \lambda_y\psi(y+2\epsilon)\big) \\
+ \chi_3\big(\lambda_x\psi(x+3\epsilon) &+ \lambda_y\psi(y+3\epsilon)\big) \\
+ \chi_4\big(\lambda_x\psi(x+4\epsilon) &+ \lambda_y\psi(y+4\epsilon)\big)
\end{aligned}
$$

Single ψ function (Sprecher)

$$
\begin{aligned}
f(x, y) = &\chi\big(\lambda_x \psi(x) + \lambda_y \psi(y)\big) \\
&+ \chi\big(\lambda_x \psi(x + \epsilon) + \lambda_y \psi(y + \epsilon) + \delta\big) \\
&+ \chi\big(\lambda_x \psi(x + 2\epsilon) + \lambda_y \psi(y + 2\epsilon) + 2\delta\big) \\
&+ \chi\big(\lambda_x \psi(x + 3\epsilon) + \lambda_y \psi(y + 3\epsilon) + 3\delta\big) \\
&+ \chi\big(\lambda_x \psi(x + 4\epsilon) + \lambda_y \psi(y + 4\epsilon) + 4\delta\big)
\end{aligned}
$$

Single χ function (Lorentz) and ψ function (Sprecher)

Universality

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

is independent of f, so that

$$KST : f \to \chi$$

Simple Example

$$xy = \exp^{\ln x + \ln y}$$

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$$xy = \exp^{\ln x + \ln y}$$

Modulus of continuity of *exp* compensates for flatness of *ln*

$$xy = \exp^{\ln x + \ln y}$$

Controlling regularity of ϕ is the key to efficiency

Regularity of Inner Functions

(Vitushkin 1964)
Inner functions ϕ cannot be smooth

$\mathcal{O}(n^2)$ cross-derviatives in f

$\mathcal{O}(n)$ derivatives in ϕ and χ

Regularity of Inner Functions

(Diaconis and Shahshahani 1984)
Exactly characterizes the nullspace for projection pursuit

$$f(x_1, \ldots, x_n) \approx \sum_{q=1}^{Q} \chi_q \left(\sum_{p=1}^{n} \lambda_{pq} x_p \right)$$

(Sprecher 1965)
Explicitly constructs a ϕ
that is Hölder$\left(\frac{\ln 2}{\ln 2n+2}\right)$

(Braün and Griebel 2009)
Demonstrates that such a function
cannot be computed efficiently

(Actor 2018)
Constructs a Lipschitz(2) ϕ

A remapping of Sprecher's ϕ
that is efficiently computable

General Approximations

- Need hierarchy
- Need nonlinearity
- Need to control regularity

Function composition is a powerful nonlinear mechanism missing from FEM

Thank You!

http://cse.buffalo.edu/~knepley