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Experiences with Sparse Grids and Smolyak-type Approximations

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(mugshots courtesy of Sandia)

Oxford Numerical Analysis
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Outline

- **Intro/Motivation**
  - Expensive function evaluations with high dimensional input spaces
  - Multivariate polynomial approximation
- **Smolyak's Idea**
  - Picking apart Smolyak's formula
  - Cost and approximation properties
- **Chebyshev transforms**
  - A few examples
- **Discussion**

Motivation

- Need to approximate **expensive** functions in high dimensions – e.g., PDEs that depend on input parameters.
- Assume we can evaluate the function where needed (as opposed to a database of evaluations).

dimension of parameter space (potentially large)

expensive!

$$f : [-1, 1]^d \longrightarrow \mathbb{R}$$

independence assumed.

Motivation

Computing statistics in UQ:

$$\mathbf{E}[f(X)] = \int_{[-1,1]^d} f(x)\,w(x)\,dx$$

- Monte Carlo approximations
- Interpolatory approximation or quadrature
- Gaussian quadrature versus Clenshaw-Curtis

Approximate $f(x)$ by a multivariate polynomial and integrate the approximation!

Multivariate Polynomial Approximation

Total Degree Monomial Basis

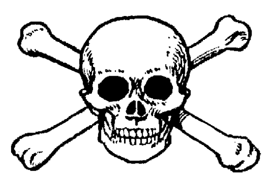
y^2		
y^1	$x^1 y^1$	
1	x^1	x^2

dimension of the polynomial space $\binom{n+d}{d}$

Tensor Product Monomial Basis

y^2	$x^1 y^2$	$x^2 y^2$
y^1	$x^1 y^1$	$x^2 y^1$
1	x^1	x^2

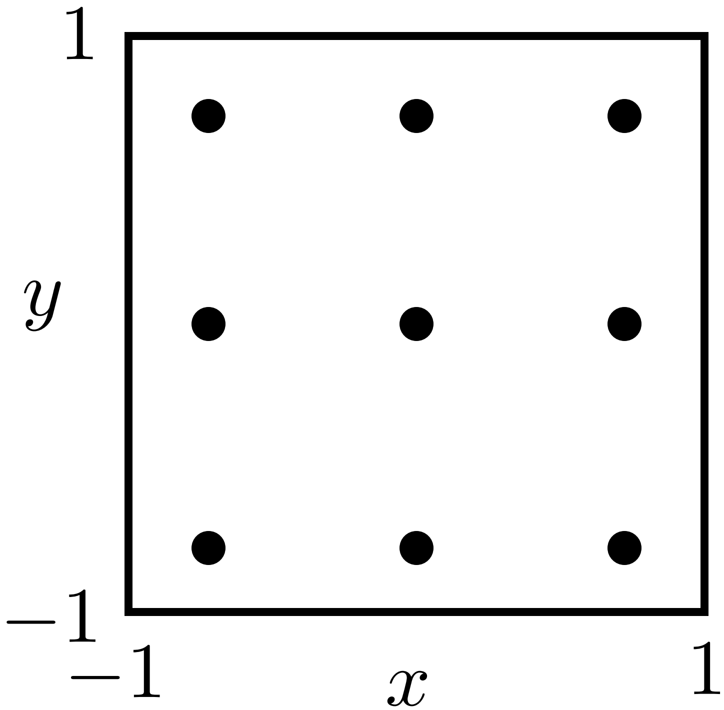
dimension of the polynomial space n^d



the dreaded curse of dimensionality!!!

Multivariate Polynomial Approximation

Tensor Product Point Set



Tensor Product Monomial Basis

y^2	x^1y^2	x^2y^2
y^1	x^1y^1	x^2y^1
1	x^1	x^2

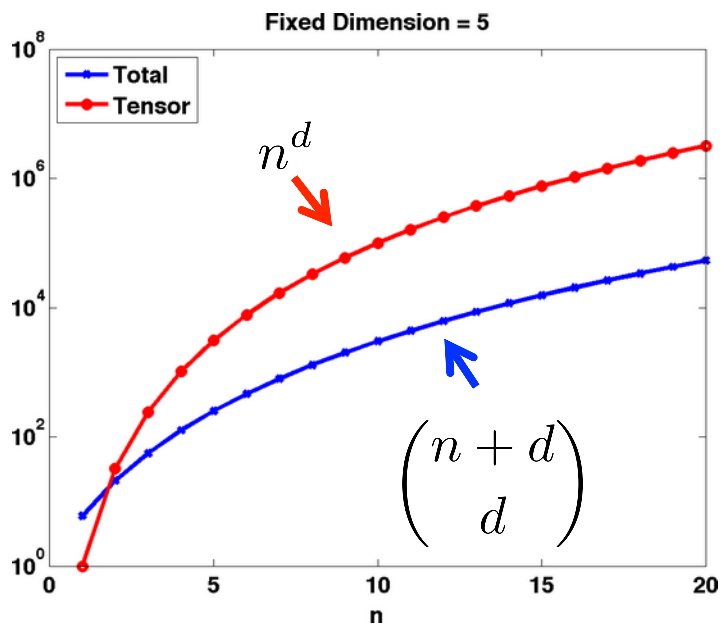
dimension of the polynomial space n^d

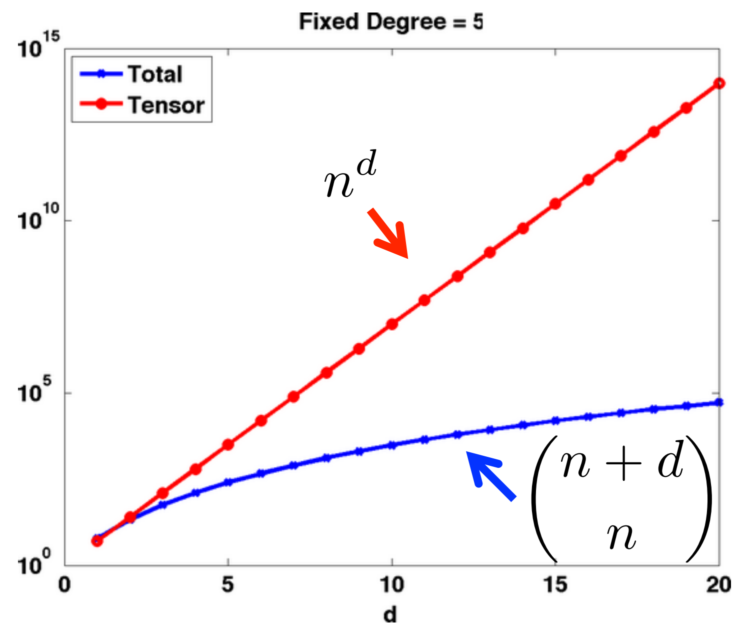
But this construction is not very interesting...

the dreaded curse of dimensionality!!!

Multivariate Polynomial Approximation

Partly because the asymptotics are trickier.
Partly because it's wasteful.





Can we find a (smaller) set of points that approximates the total degree space?

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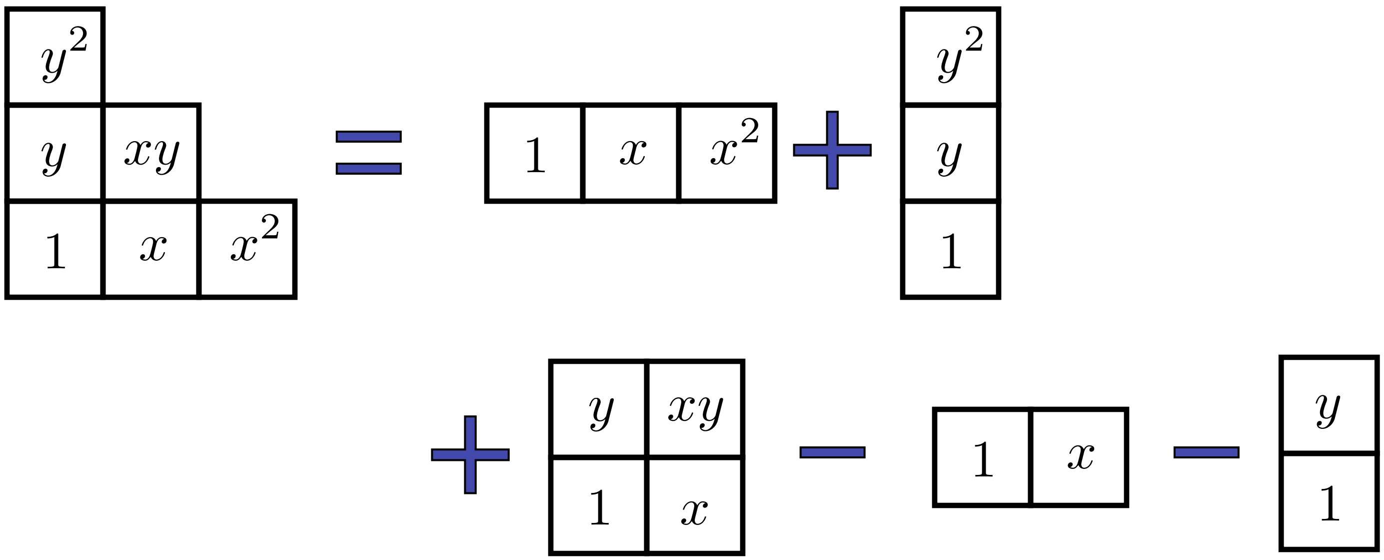
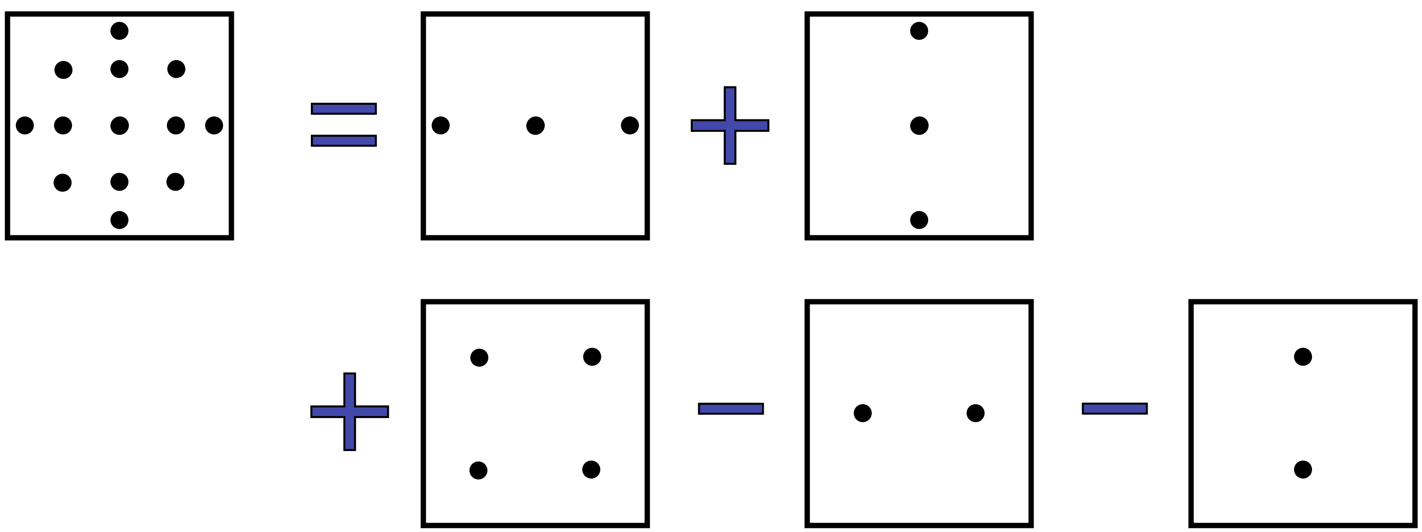
Smolyak's Idea





Smolyak's Formula

$$A(l,d) = \sum_{l+1 \leq |\mathbf{i}| \leq l+d} (-1)^{l+d-|\mathbf{i}|} \binom{d-1}{l+d-|\mathbf{i}|} \left(U^{i_1} \otimes \cdots \otimes U^{i_d}\right)$$

<u>Symbol</u>	<u>Meaning</u>
$f(x)$	The function being approximated
d	The dimension of the inputs
$\mathbf{i}$	A multi-index $\mathbf{i} = (i_1, \ldots, i_d) \in \mathbb{N}^d$
$\lvert\mathbf{i}\rvert$	$= i_1 + \cdots + i_d$
U^{i_j}	A univariate linear operator (projection, interpolation)
$\otimes$	A tensor product operation
l	The so-called **level** parameter

Smolyak's Formula

$$A(l,d) = \sum_{l+1 \leq |\mathbf{i}| \leq l+d} (-1)^{l+d-|\mathbf{i}|} \binom{d-1}{l+d-|\mathbf{i}|} \left(U^{i_1} \otimes \cdots \otimes U^{i_d}\right)$$

Symbol	Meaning
$l+1 \leq \lvert\mathbf{i}\rvert \leq l+d$	A set of admissible multi-indices
$(-1)^{l+d-\lvert\mathbf{i}\rvert} \binom{d-1}{l+d-\lvert\mathbf{i}\rvert}$	A counting coefficient
$\left(U^{i_1} \otimes \cdots \otimes U^{i_d}\right)$	A tensor product linear operator

Smolyak's Formula

$$A(l,d) = \sum_{l+1 \le |\mathbf{i}| \le l+d} (-1)^{l+d-|\mathbf{i}|} \binom{d-1}{l+d-|\mathbf{i}|} \left(U^{i_1} \otimes \cdots \otimes U^{i_d}\right)$$

A **linear combination** of **tensor product operators**

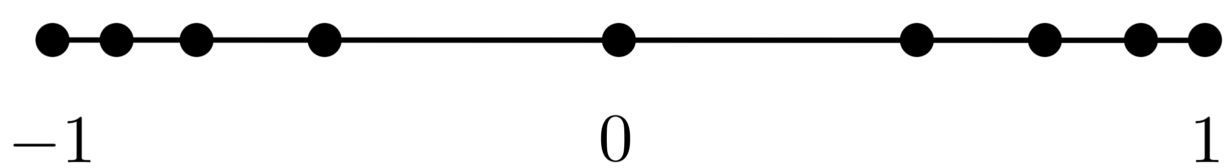
Smolyak's Formula

$$A(l,d) = \sum_{l+1 \le |\mathbf{i}| \le l+d} (-1)^{l+d-|\mathbf{i}|} \binom{d-1}{l+d-|\mathbf{i}|} \left(U^{i_1} \otimes \cdots \otimes U^{i_d}\right)$$

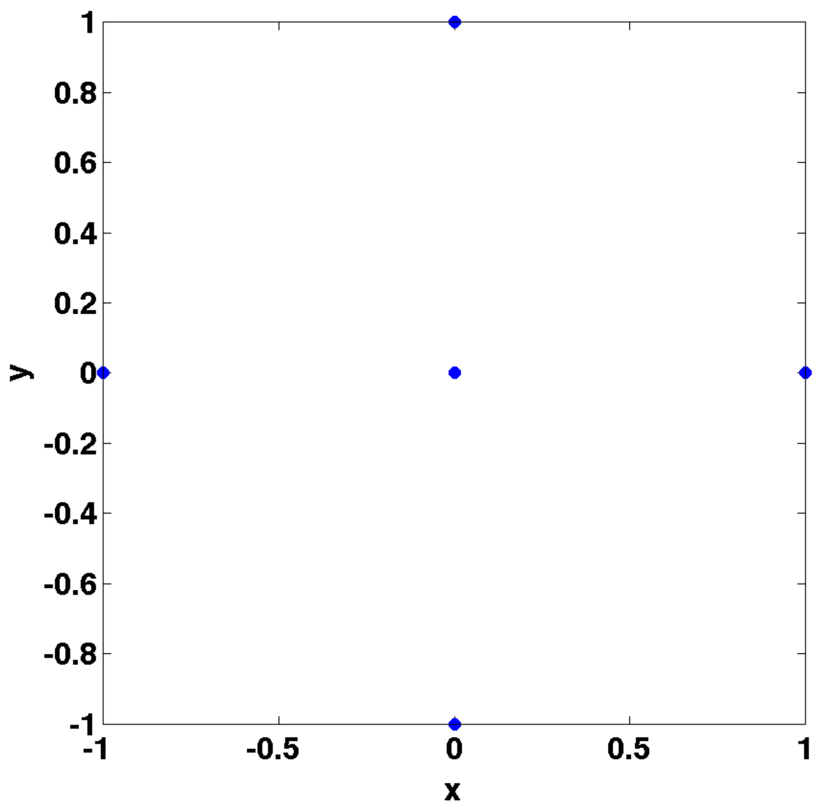
A bit more on the linear operators U^{i_j}:

Univariate integration and interpolation operators can be formed on nested grids -- like Chebyshev points.

$U^1 \; U^2 \; U^3 \; U^4$



Number of Points in the Sparse Grid



d	l	poly. dim.	sparse # points	tensor # points
2	1	3	5	4
	2	6	13	9
	3	10	29	16
	4	15	65	25
10	1	11	21	1024
	2	66	221	59045
	3	286	1581	1048576
20	1	21	41	1048576
	2	231	841	3.5 e+9
50	1	51	101	1.1 e+16
	2	1326	5101	7.2 e+23

For large d and fixed l

$$\dim\left(A(l,d)\right) \approx \frac{2^l}{l!} d^l$$

These are "optimal," since

$$\binom{n+d}{d} \approx \frac{d^l}{l!}$$

Approximation Properties of Sparse Grids (Novak & Ritter)

Polynomial exactness: $A(l,d)$ reproduces polynomials in d variables of order l.

Interpolation error for functions with continuous derivatives of order l in each variable:

$$\|f - A(l,d)(f)\|_\infty \le C_{d,l}\, M^{-l}\, (\log M)^{(l+2)(d-1)+1}$$

number of points

"smoothness"

Integration error for functions with continuous derivatives of order l in each variable:

$$|I(f) - I\big(A(l,d)(f)\big)| = \mathcal{O}\left(M^{-l}\, (\log M)^{(l+1)(d-1)}\right)$$

number of points

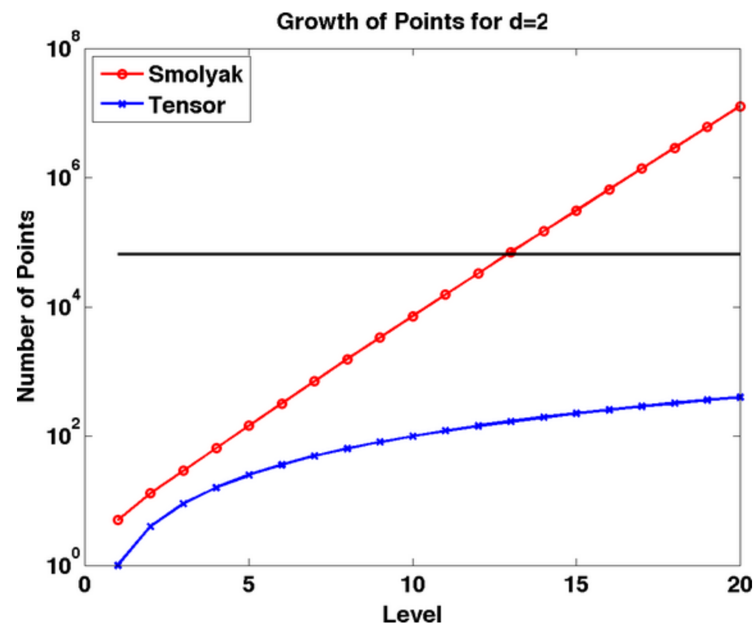
"smoothness"

Sparse Grids – The Bad News

Curse of dimensionality: An ε approximation requires M function evaluations.

$$M \geq c_\varepsilon \, d^{-c \log \varepsilon}$$

The number of points grows quickly for low dimensions.



Negative quadrature weights!

In practice, we need **a lot** of smoothness.

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Sparse Grids and Chebyshev Coefficients

How can one compute Chebyshev coefficients with a sparse grid?

$$a_{\mathbf{i}} = \int_{[-1,1]^d} f(x)\, T_{\mathbf{i}}(x)\, w_d(x)\, dx$$

multi-index

product-type Chebyshev polynomial

product-type Chebyshev weight

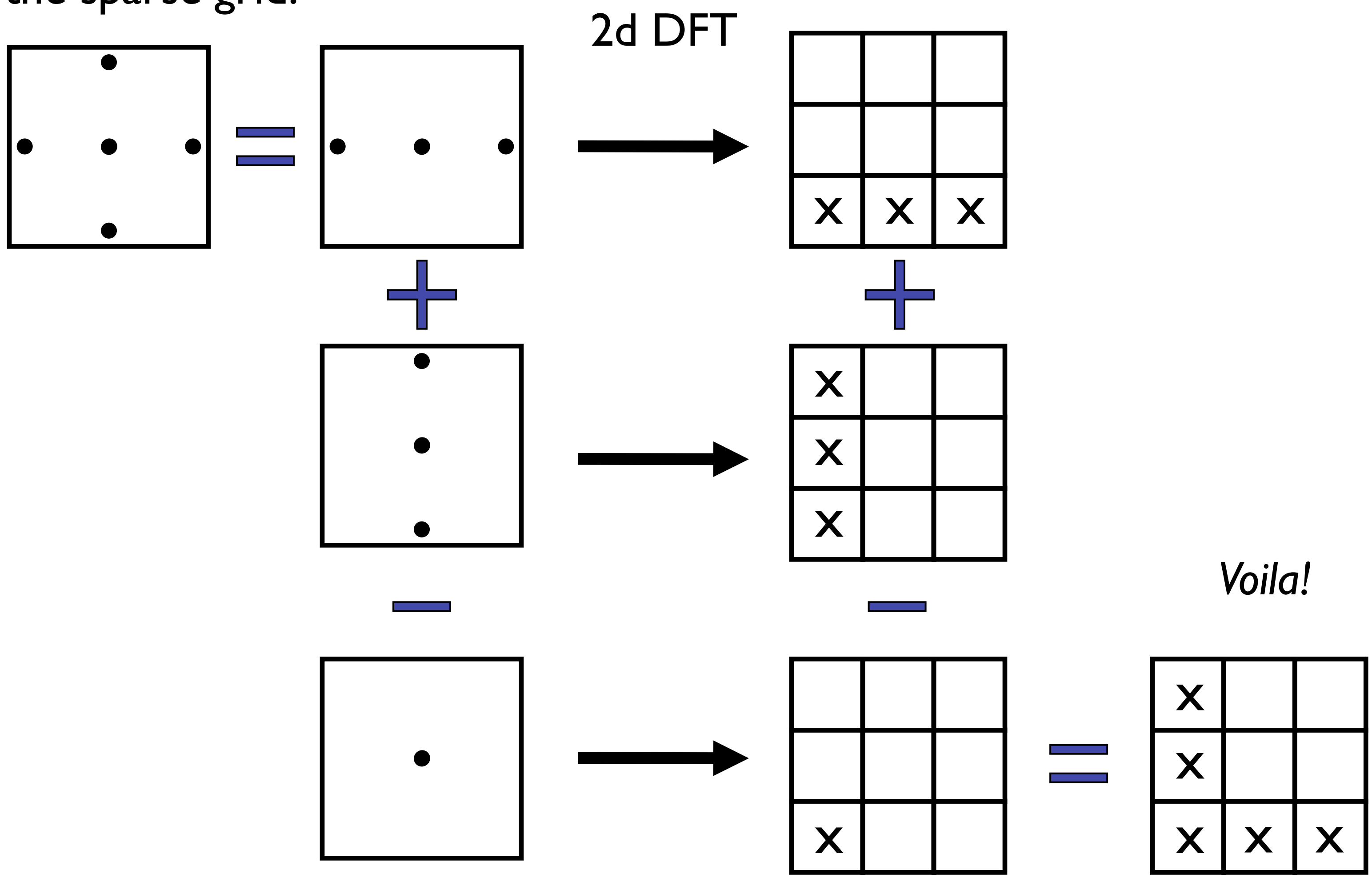
Can we use a sparse grid integration rule to approximate the multivariate Chebyshev coefficients?

(Please don't.)

Sparse Grids and Chebyshev Coefficients

"Physical space" **"Coefficient space"**

Building the sparse grid:



But this isn't terribly surprising. Remember…

$$A(l,d) = \sum_{l+1\leq|\mathbf{i}|\leq l+d} (-1)^{l+d-|\mathbf{i}|} \binom{d-1}{l+d-|\mathbf{i}|} \left(U^{i_1} \otimes \cdots \otimes U^{i_d}\right)$$

A **linear combination** of **tensor product operators**

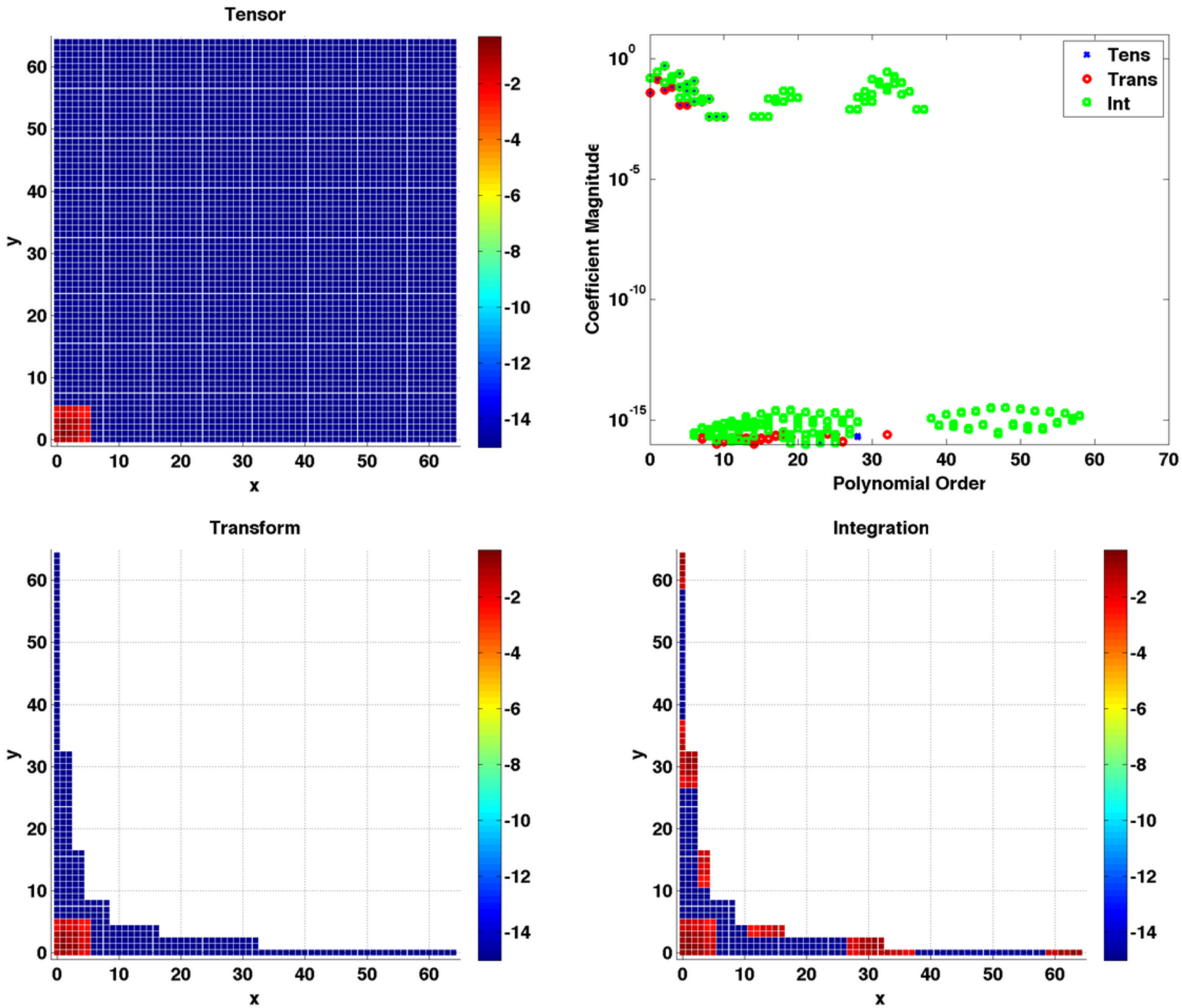
Numerical Examples

<u>Test Functions</u>

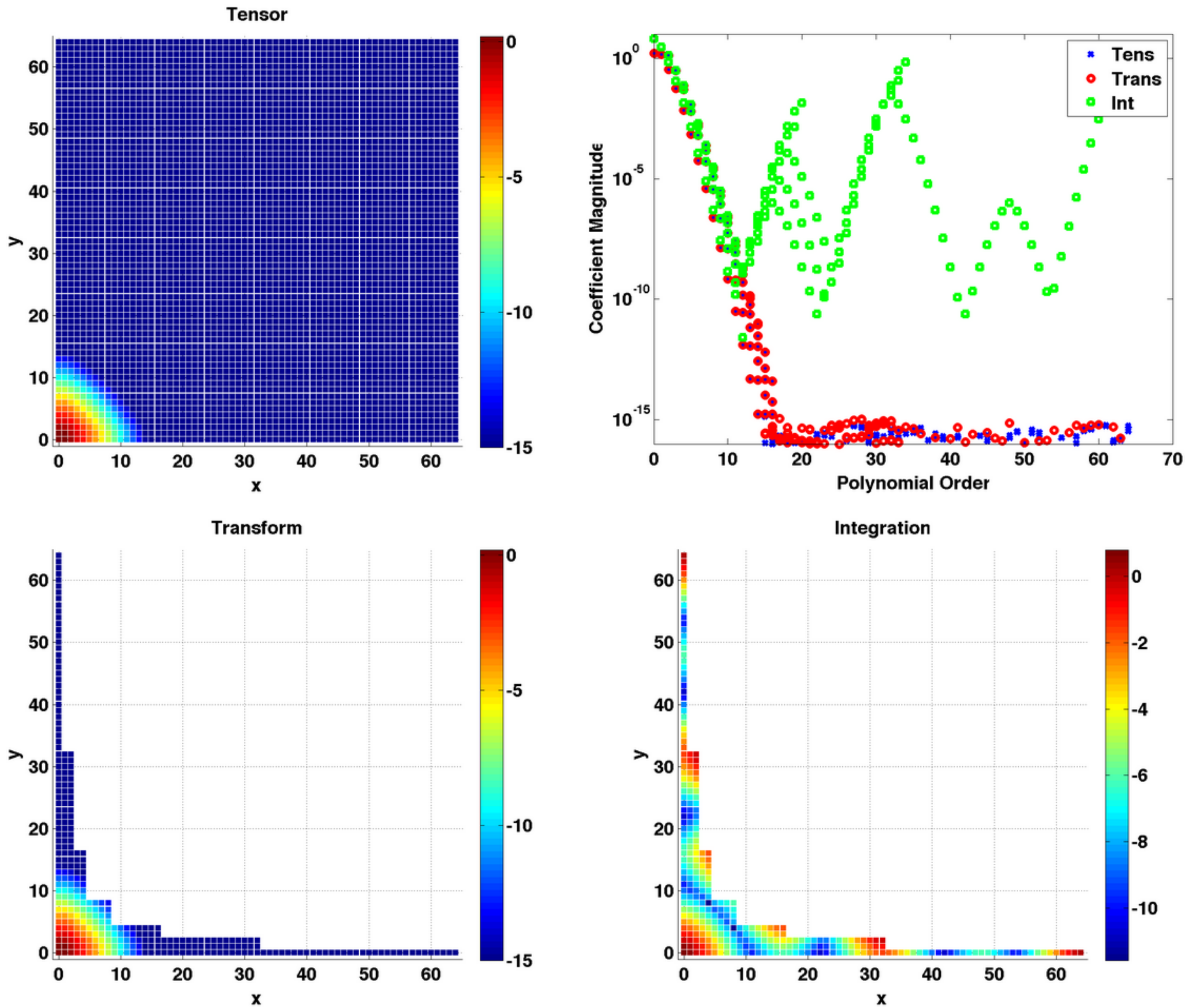
1. [(x+0.1)(y+0.1)]^5
2. exp(x+y)
3. sin(5(x-0.1)) + cos(3(y-0.1))
4. 1 / (6 + 16(x-0.1) + 25(y-0.1))
5. (|x-0.1| + |y-0.1|)^3

For each function we compute (i) the 2d Chebyshev coefficients with a tensor product DFT, (ii) the integral form of the coefficients approximated with the sparse grid quadrature rule, and (iii) the proper transform coefficients from the points of the sparse grid.

[(x+0.1)(y+0.1)]^5


Tensor
Transform
Integration
x
y
Coefficient Magnitude
Polynomial Order
Tens
Trans
Int

exp(x+y)


Tensor
Transform
Integration
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x
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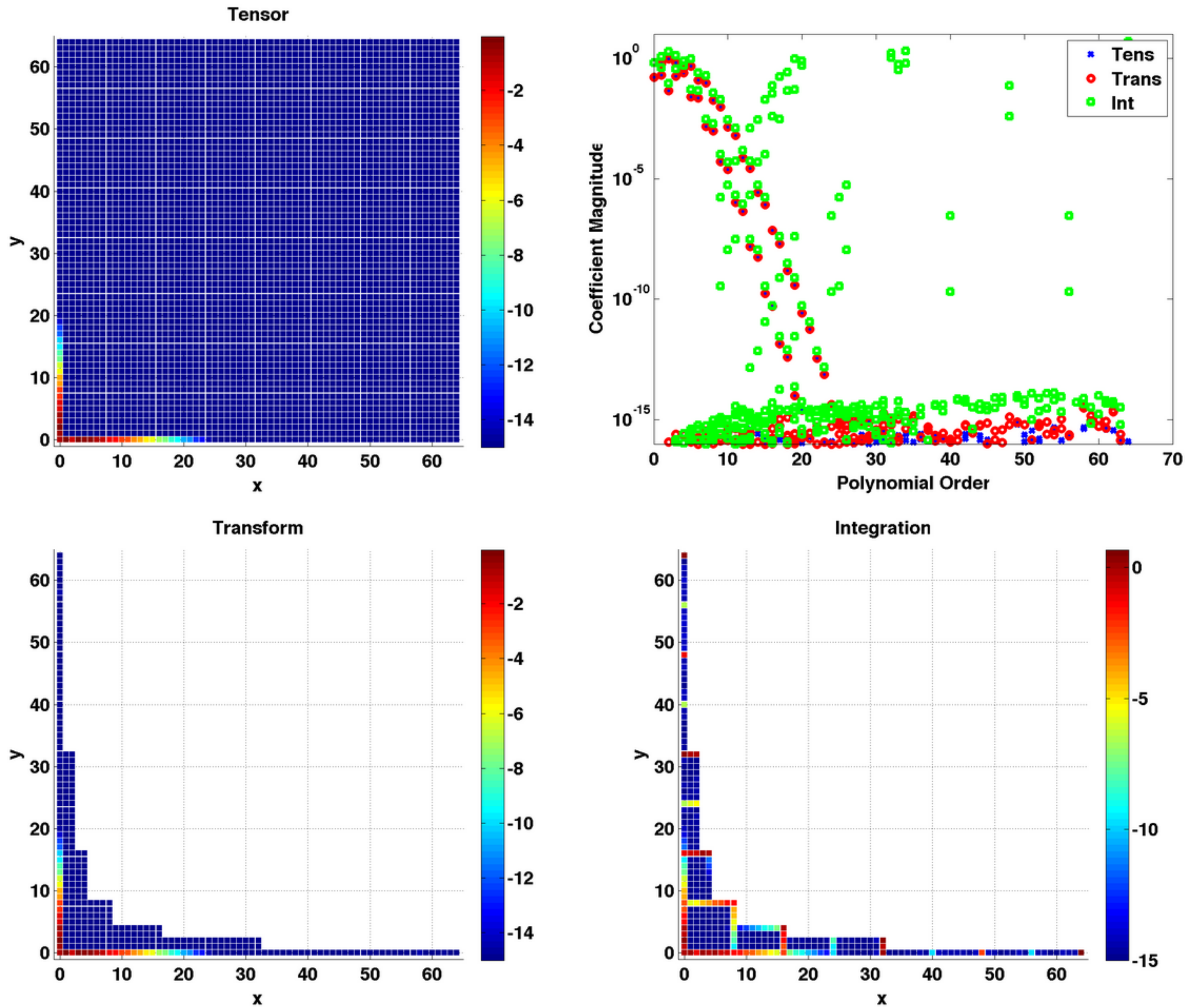
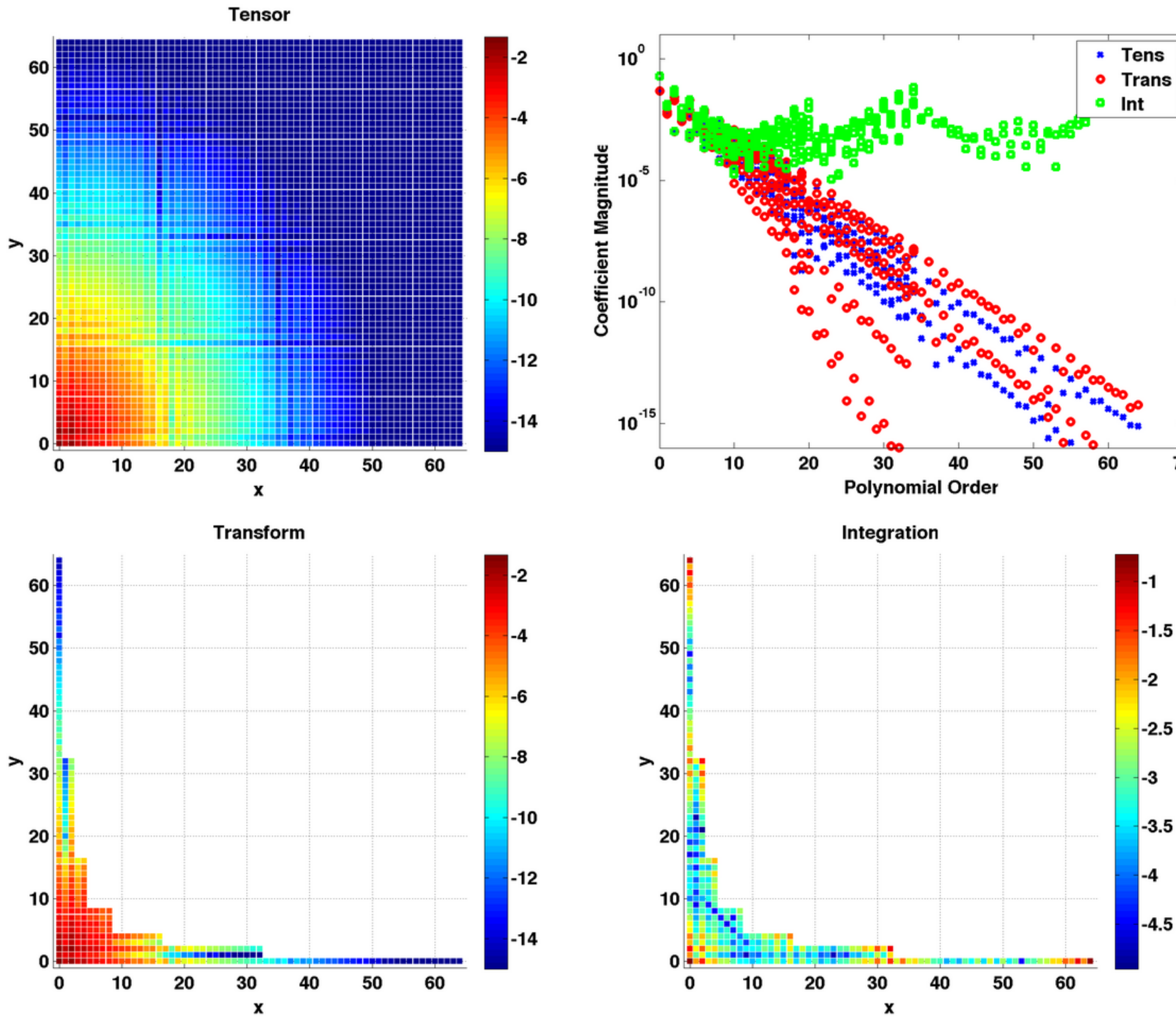
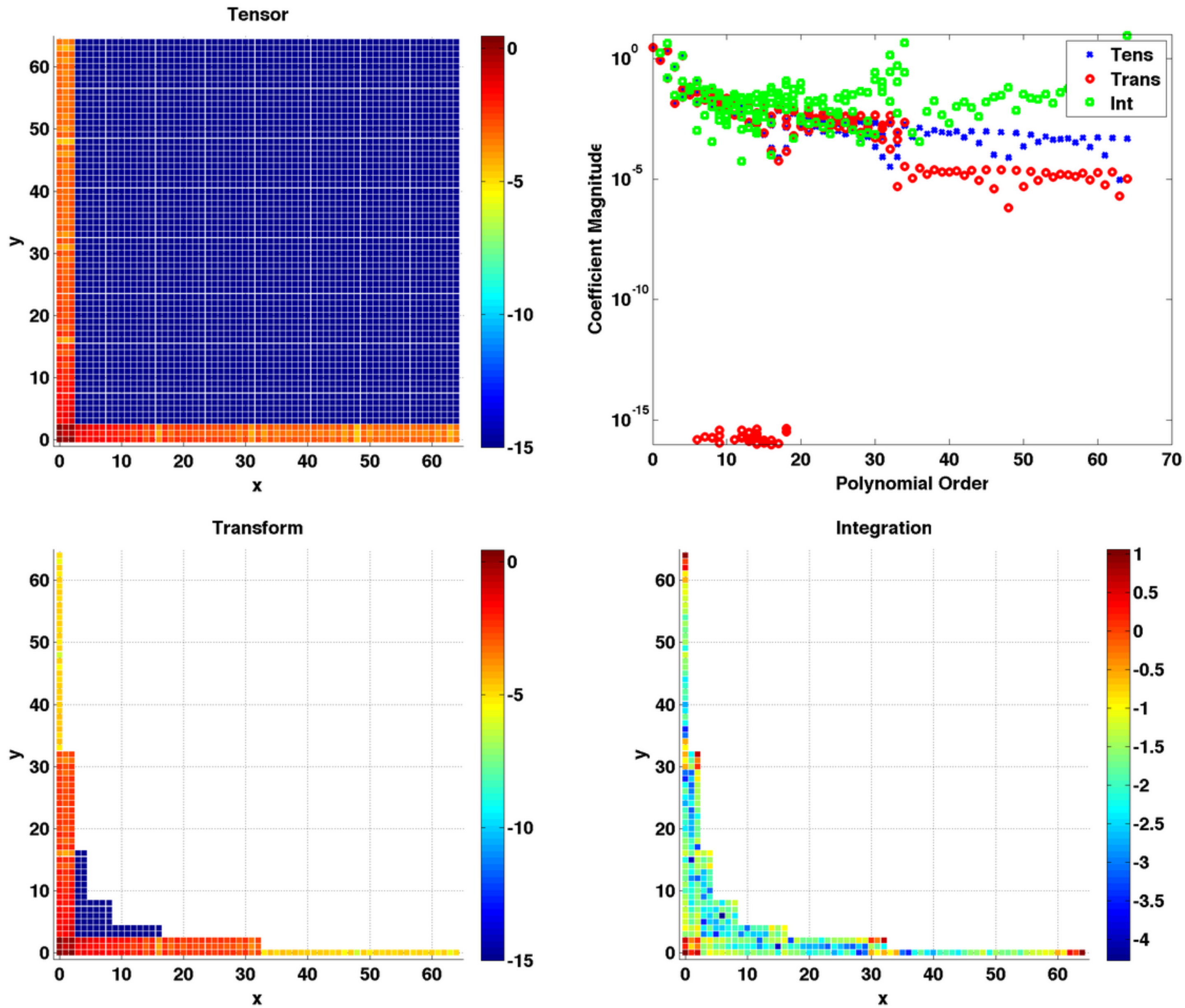
sin(5(x-0.1)) + cos(3(x-0.1))



1 / (6 +16(x-0.1)^2 + 25(y-0.1)^2)



(|x-0.1| + |y-0.1|)^3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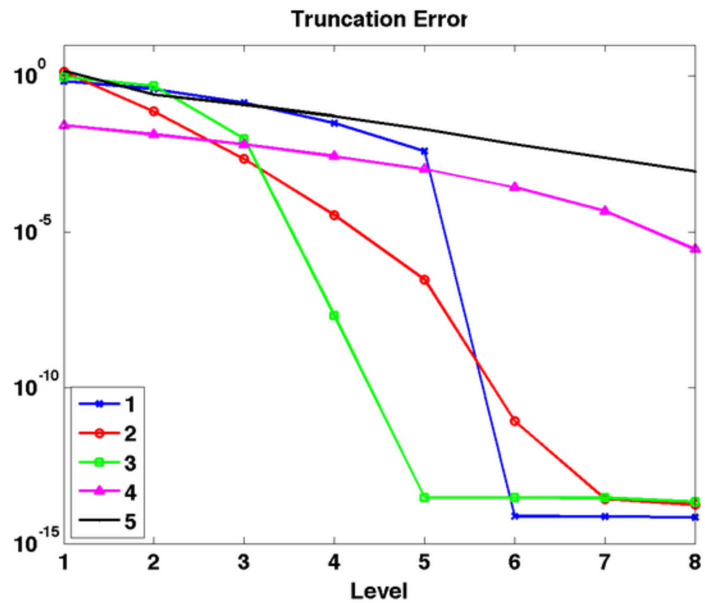
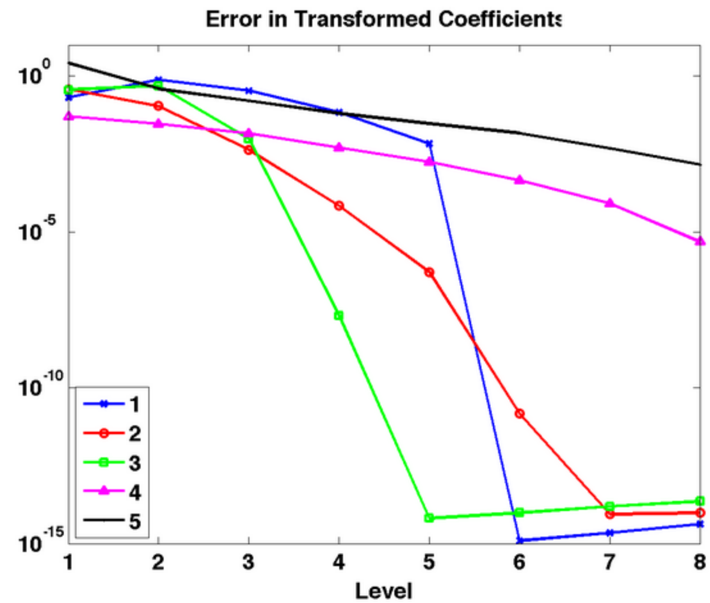
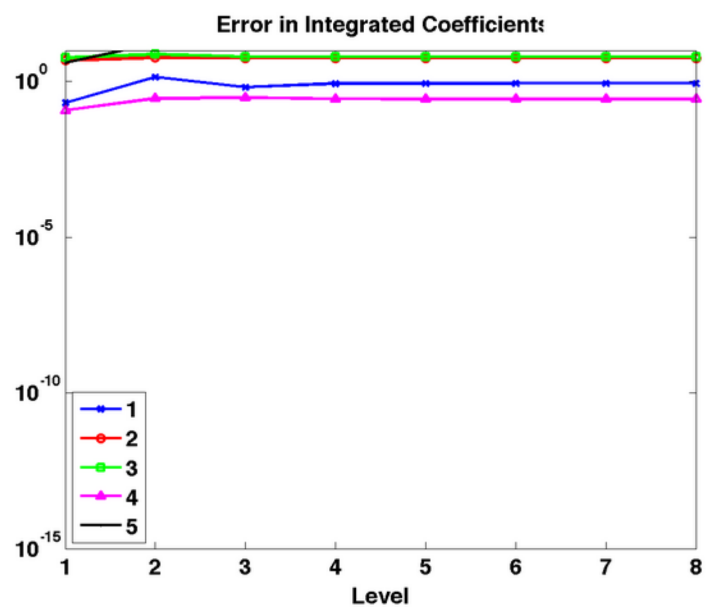
x
y

Errors



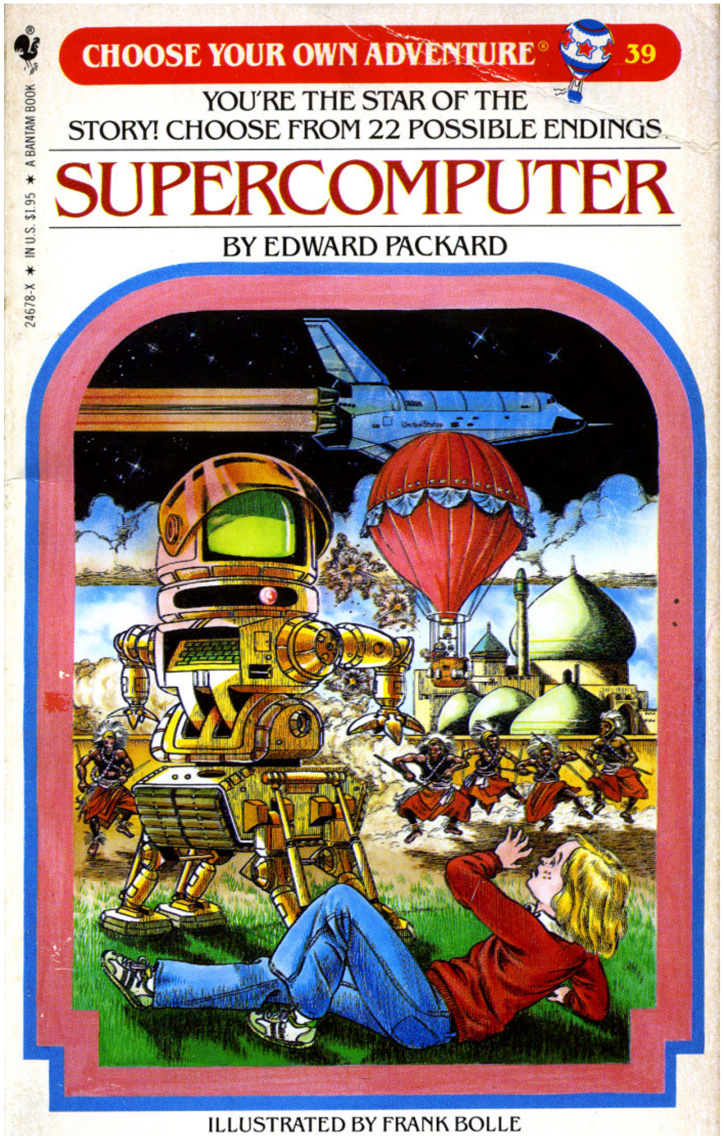




<u>Function legend</u>

1. [(x+0.1)(y+0.1)]^5
2. exp(x+y)
3. sin(5(x-0.1)) + cos(3(y-0.1))
4. 1 / (6 + 16(x-0.1) + 25(y-0.1))
5. (|x-0.1| + |y-0.1|)^3

Discussion



- *Is Smolyak right for Chebfun?*
- *What other options are there in 2d?*
- *How about irregular domains?*
- *What if the function depends primarily on a smaller set of variables?*
- *What if those variables are not the original coordinates?*
- *Can we see a demo?*

For Further Reading

Smolyak-like sparse grids

• Barthelmann, Novak, & Ritter. *High dimensional polynomial interpolation on sparse grids*. (2000).
• Novak & Ritter. *Simple cubature formulas with high polynomial exactness*. (1999).
• Novak & Ritter. *High dimensional integration of smooth functions over cubes*. (1996).
• Griebel. *Sparse grids and related approximation schemes for higher dimensional problems*. (FOCM, 2005).

In high dimensional PDEs

• Shen & Yu. *Efficient spectral sparse grid methods and applications to high-dimensional elliptic problems*. (SISC, 2010).

In UQ

• Xiu & Hesthaven. *High order collocation methods for differential equations with random inputs*. (SISC, 2005).