

The Sparse Grids Matlab Kit

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February 25, 2022

Outline

- 1 Example
- 2 Basic data structure
- 3 Main features
- 4 Example - reprise
- 5 Conclusions

Contributors, releases

- **main** contributors: Lorenzo Tamellini, Chiara Piazzola

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- **releases:**
 - ▶ 22-2 ("California")
 - ▶ 18-10 ("Esperanza")
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 - ▶ 15-8 ("Woodstock")
 - ▶ 14-12 ("Fenice")
 - ▶ 14-4 ("Ritchie")

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- **BSD2** license

General comments

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- Similar to:
 - ▶ Dakota, PyApprox, MUQ, ChaosPy, UQTK (not Matlab);
 - ▶ SG++, Tasmanian (Matlab wrappers);
 - ▶ UQLab, Spinterp (Matlab).

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Aim of these slides: give rough idea of sparse grids and of the structure of the code, show features by examples

Outline

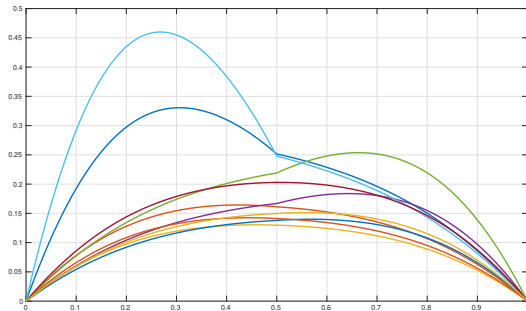
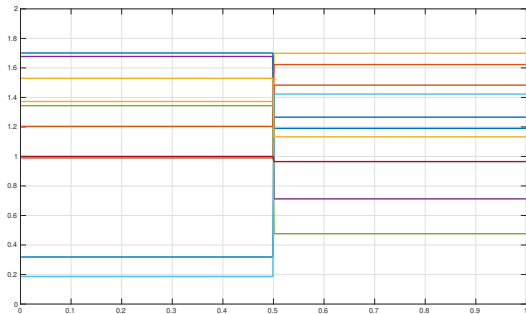
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Forward Uncertainty Quantification

$$\left\{ \begin{array}{l} -\frac{d}{dx} \left[a(x, \mathbf{y}) \frac{d}{dx} u(x, \mathbf{y}) \right] = 1, \quad \text{for } x \in (0, 1) \\ u(0, \cdot) = u(1, \cdot) = 0 \\ a(x, \mathbf{y}) = 1 + \sigma_1 y_1 \mathbb{I}_{[0, 0.5]}(x) + \sigma_2 y_2 \mathbb{I}_{[0.5, 1]}(x) \\ y_1, y_2 \sim \mathcal{U}(-\sqrt{3}, \sqrt{3}) \\ I(\mathbf{y}) = \int_0^1 u(x, \mathbf{y}) dx \end{array} \right.$$

- often, more than $N = 2$ parameters
- ODE and algebraic models are also of interest

Forward Uncertainty Quantification



Forward Uncertainty Quantification

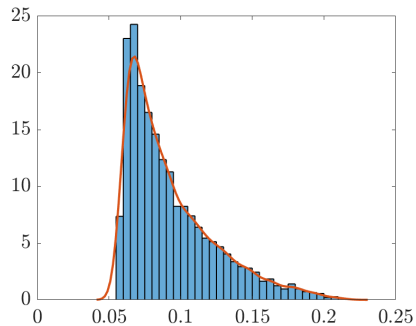
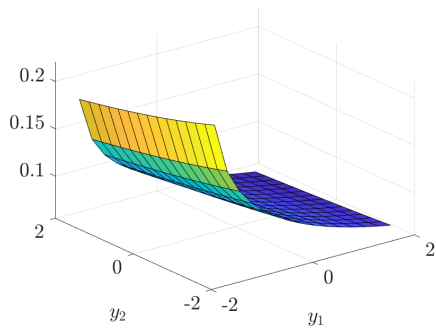
Goals:

- statistics of I (mean, variance, pdf)
- sensitivity analysis for I
- meta-model for $I(y_1, y_2)$ (aka response surface aka surrogate model)

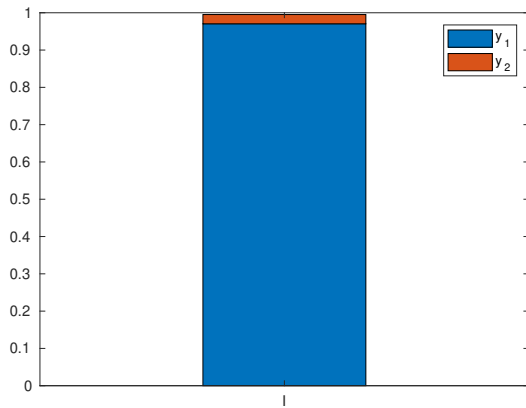
Need:

- High-dimensional quadrature (mean, variance)
- High-dimensional interpolation/approximation (pdf, metamodel)

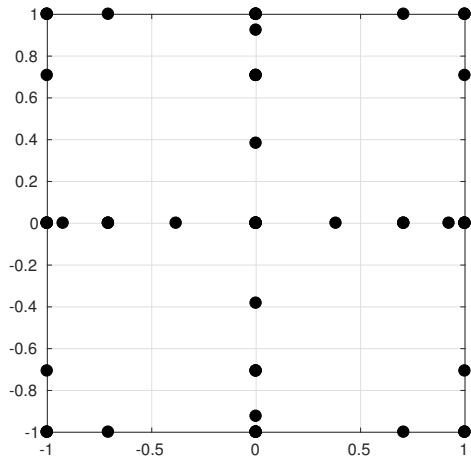
Results



Results



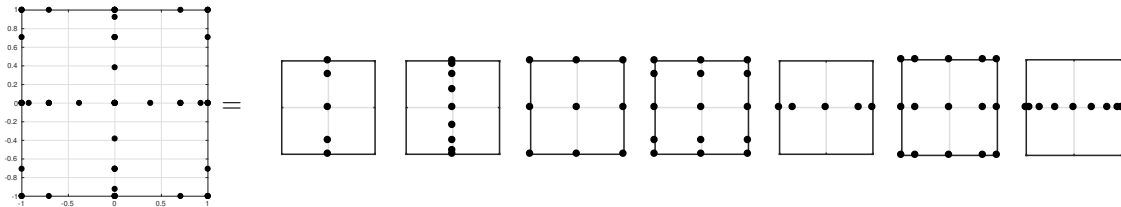
Where do we sample? Sparse grids



Our matlab library handles:

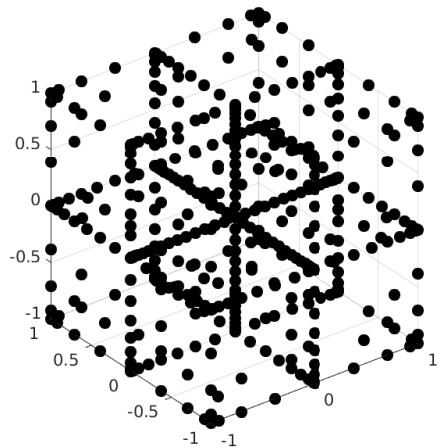
- generation of these schemes
- integration and interpolation on them

Sparse grids in a nutshell



- Linear combination of tensor grids
- Reasonably slows down “curse of dimensionality” up to $N = \text{a few tens}$
- Works well under regularity assumptions on $I(\mathbf{y})$
- Anisotropic and adaptive versions available

Sparse grids in a nutshell



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Backbone: combination technique & “reduced” sparse grid

```
N=2;  
knots=@(n) knots_CC(n,-1,1);  
w = 3;  
m = @lev2knots_doubling;  
Ifun = @(i) sum(i-1);  
S = smolyak_grid(N,w,knots,m,Ifun);
```

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- $S = \sum_{i \in \mathcal{I}} c_i \otimes_{n=1}^N \mathcal{U}^{m(i_n)}$
- $m(i) = "2^{i-1} + 1"$, $\mathcal{U}^{m(i_n)} =$ interpolant on $m(i_n)$ Clenshaw–Cts pts

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- $m(i) = "2^{i-1} + 1"$, $\mathcal{U}^{m(i_n)} =$ interpolant on $m(i_n)$ Clenshaw–Cts pts
- $\mathcal{I} = \left\{ i \in \mathbb{N}_+^N : \sum_{n=1}^N (i_n - 1) \leq w \right\}$

Backbone: combination technique & “reduced” sparse grid

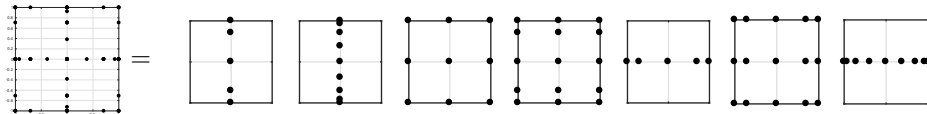
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```

```
>> S  
S =  
1 x 7 struct array with fields:  
knots  
weights  
size  
knots_per_dim  
m  
coeff  
idx
```

Backbone: combination technique & “reduced” sparse grid

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N=2;  
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```

```
>> S(1)  
ans =  
struct with fields:  
  
    knots: [2x5 double] % points are always column vectors  
  weights: [-0.1333 -1.0667 -1.6000 -1.0667 -0.1333]  
    size: 5  
knots_per_dim: {[0] [1 0.7071 6.1232e-17 -0.7071 -1]}  
        m: [1 5]  
   coeff: -1  
    idx: [1 3] %multiidx are always row vectors
```

Backbone: combination technique & “reduced” sparse grid

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```

```
>> Sr = reduce_sparse_grid(S)  
Sr =
```

struct with fields:

```
    knots: [2x29 double]  
        m: [29x1 double]  
weights: [1x29 double]  
        n: [67x1 double]  
    size: 29
```


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Ifun = @(i) sum(i-1);  
S = smolyak_grid(N,w,knots,m,Ifun);
```

```
>> Sr = reduce_sparse_grid(S)    % creates the "uniqued" list of points  
                                % from the set of points of all stensor grids in S.  
                                % Robust to numerical noise (default tol 1e-14)
```

```
Sr =  
  
struct with fields:  
  
    knots: [2x29 double]  
        m: [29x1 double] % map from Sr.knots to [S.knots]  
weights: [1x29 double]  
        n: [67x1 double] % map from [S.knots] to Sr.knots  
    size: 29             % nb of points in the sparse grids
```

Sparse grids “ingredients”: nodes, m , \mathcal{I}

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```

	knots	function	nestedness
uniform	Gauss–Legendre	knots_uniform	No
	Clenshaw–Curtis	knots_CC	Yes
	Leja (standard, symmetric, p-disk)	knots_leja	Yes
	midpoints	knots_midpoint	Yes
	equispaced	knots_trap	Yes
normal	Gauss–Hermite	knots_normal	No
	Genz–Keister	knots_GK	Yes
	weighted Leja (standard, symmetric)	knots_normal_leja	Yes
exponential	Gauss–Laguerre	knots_exponential	No
	weighted Leja	knots_exponential_leja	Yes
gamma	Gauss–generalized Laguerre	knots_gamma	No
	weighted Leja	knots_gamma_leja	Yes
beta	Gauss–Jacobi	knots_beta	No
	weighted Leja (standard, symmetric)	knots_beta_leja	Yes

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- `m = lev2knots_lin(i)`

$$m(i) = i$$

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```

- `m = lev2knots_lin(i)`
- `m = lev2knots_2step(i)`
 $m(i) = 2(i - 1) + 1$

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$$m(1) = 1, m(i) = 2^{i-1} + 1$$

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- `m = lev2knots_doubling(i)`
- `m = lev2knots_trippling(i)`

$$m(i) = 3^{i-1}$$

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- `m = lev2knots_tripling(i)`
- `m = lev2knots_GK(i)`

it is possible to specify different `m` and `knots` in each direction

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presets for m , $Ifun$ are available:

```
[m,Ifun]=define_functions_for_rule(<'TP','TD','HC','SM'>,<N,g>)
```

where for $g \in \mathbb{R}_+^N$, $w \in \mathbb{N}$

- **'TP'** = tensor prod., $\mathcal{I} = \{i \in \mathbb{N}_+^N : \max_n g_n(i_n - 1) \leq w\}$, $m(i) = i$

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- **'HC'** = hyperbolic cross, $\mathcal{I} = \{i \in \mathbb{N}_+^N : \prod_{n=1}^N i_n^{g_n} \leq w\}$, $m(i) = i$
- **'SM'** = Smolyak, $\mathcal{I} = \{i \in \mathbb{N}_+^N : \sum_{n=1}^N g_n(i_n - 1) \leq w\}$, $m(i) = 2^{i-1} + 1$

Sparse grids “ingredients”: nodes, m , \mathcal{I}

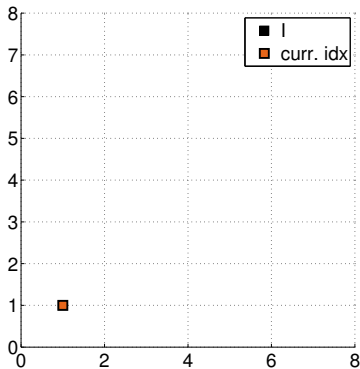
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It is also possible to define sparse grids directly by a multi-idx set

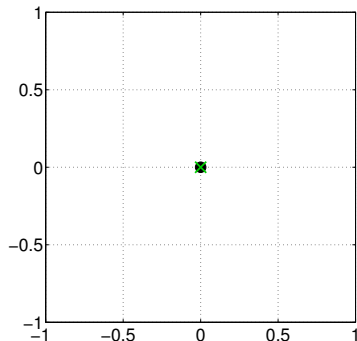
```
% ex. 1) 'hand-typed' set  
C=[1 1; 1 3; 4 1]; % non downward-closed set  
[adm,C_compl] = check_set_admissibility(C); % fix C  
S_M = smolyak_grid_multiidx_set(C_compl,knots,m);  
  
%ex. 2) create a box in  $N^2$  with top-right corner at [2 3]  
jj=[2 3];  
D=multiidx_box_set(jj,1);  
T_M = smolyak_grid_multiidx_set(D,knots,m);
```

Sparse grids “ingredients”: adaptive algorithm

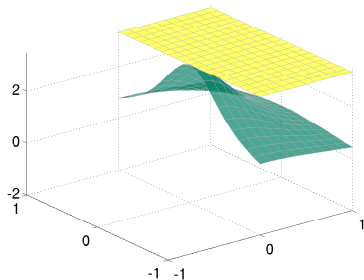
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



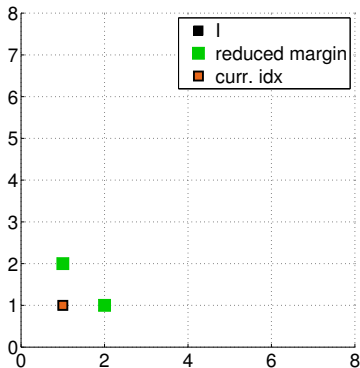
Sparse grid set



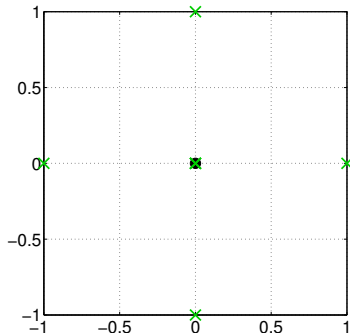
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

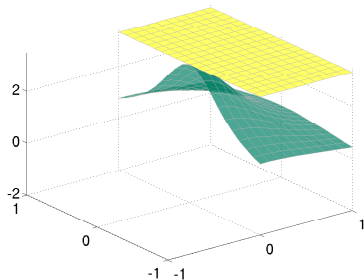
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```



Multi-index set



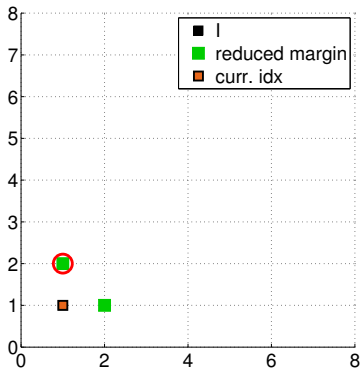
Sparse grid set



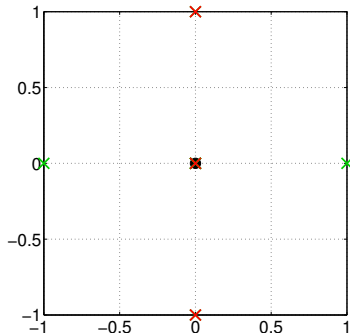
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

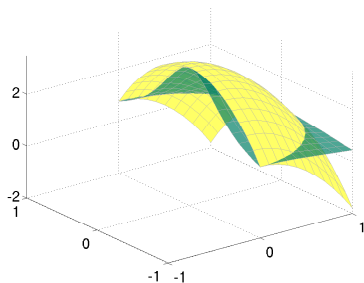
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



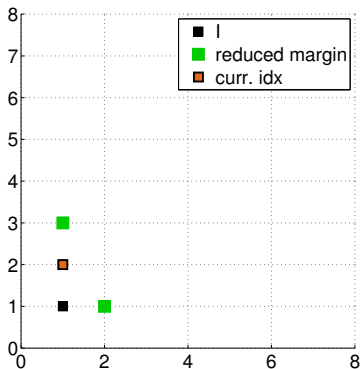
Sparse grid set



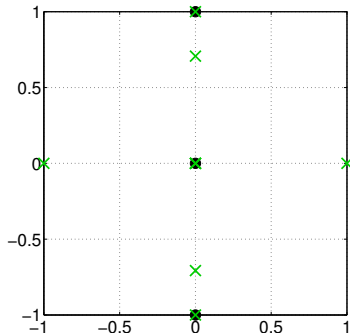
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

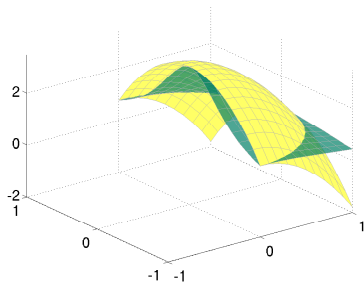
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



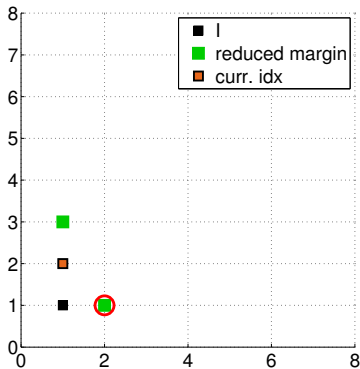
Sparse grid set



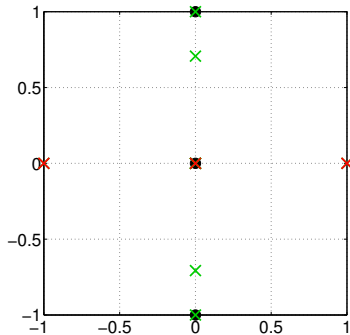
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

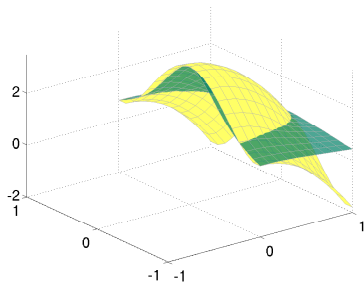
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



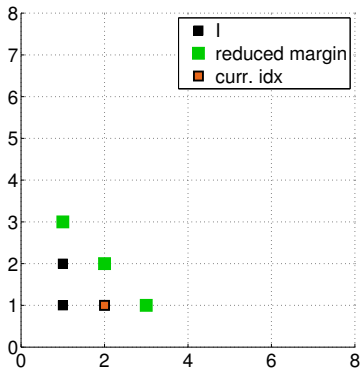
Sparse grid set



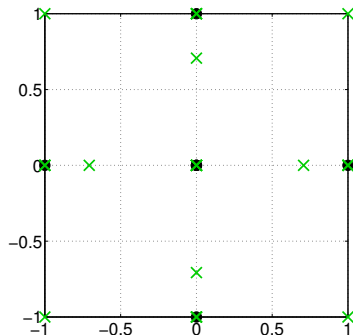
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

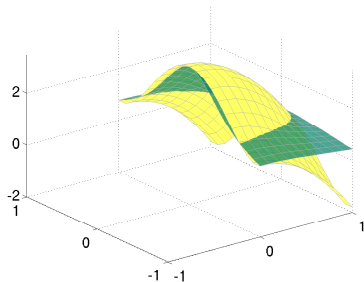
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



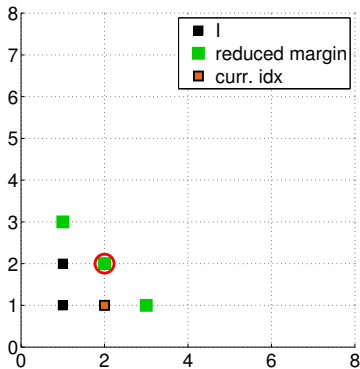
Sparse grid set



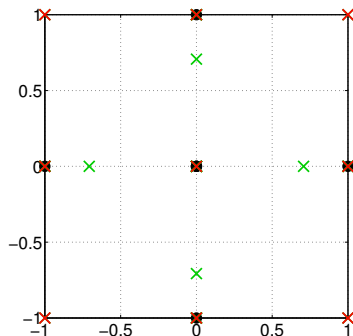
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

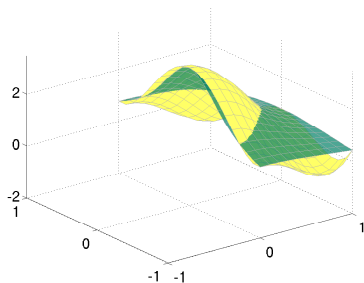
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



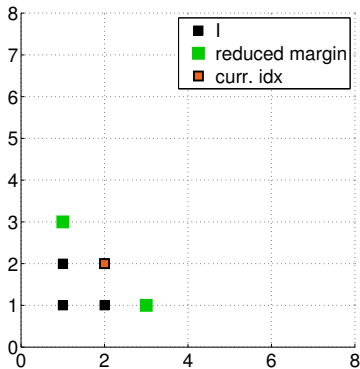
Sparse grid set



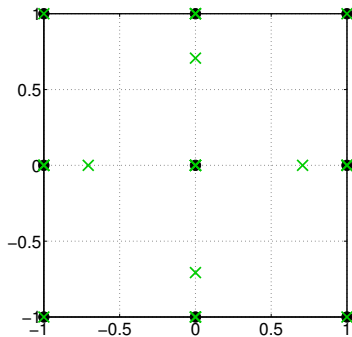
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

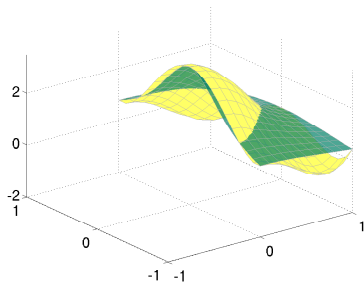
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



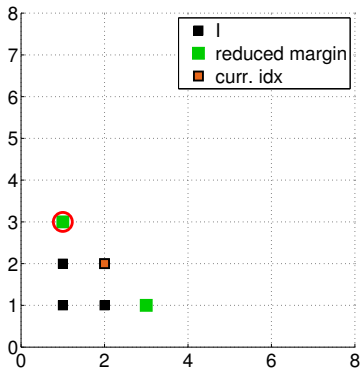
Sparse grid set



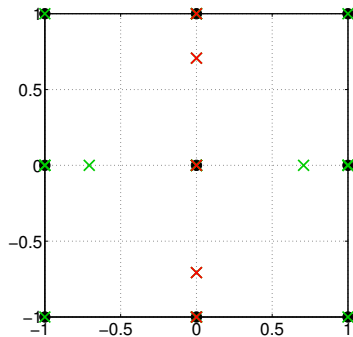
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

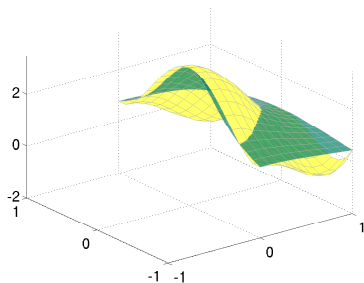
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



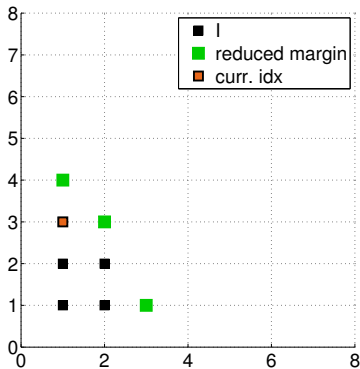
Sparse grid set



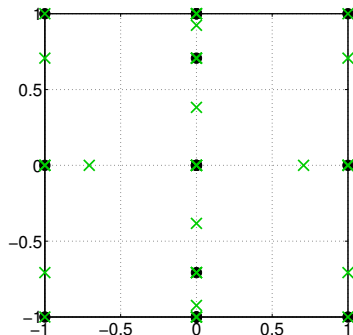
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

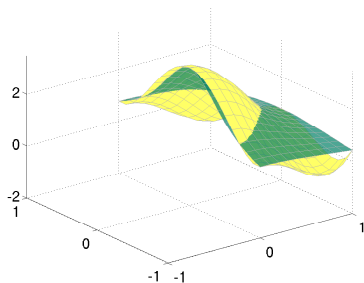
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



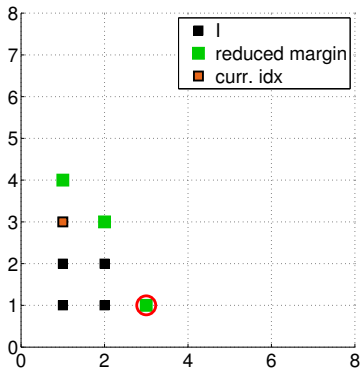
Sparse grid set



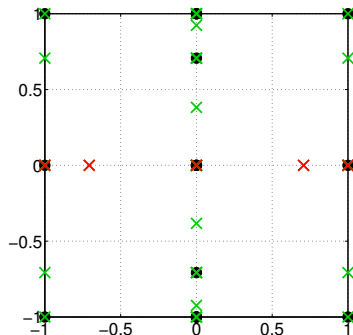
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

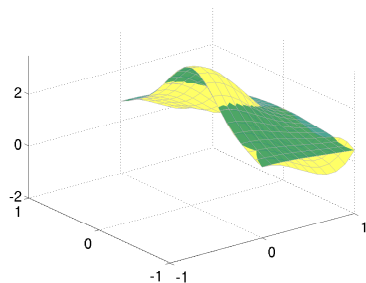
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



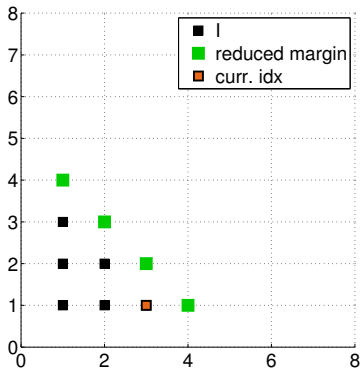
Sparse grid set



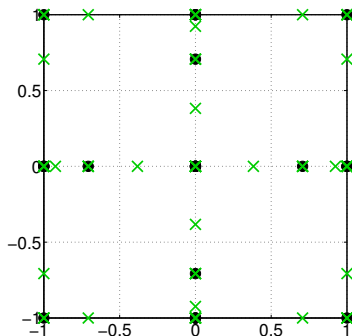
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

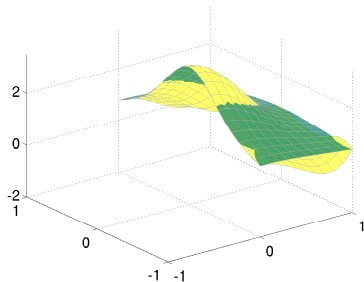
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



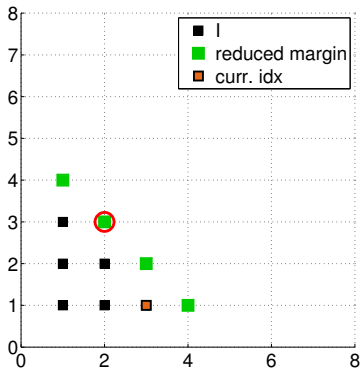
Sparse grid set



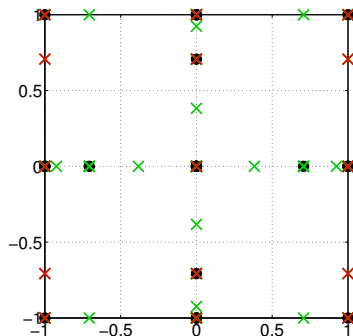
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

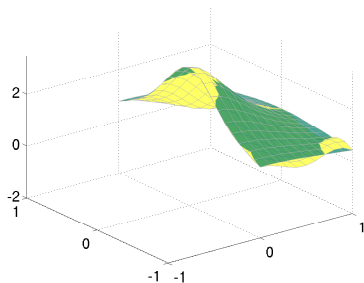
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



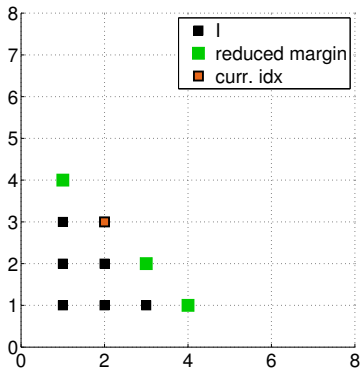
Sparse grid set



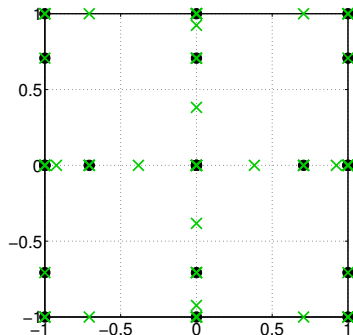
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

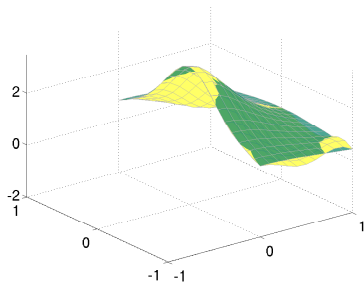
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



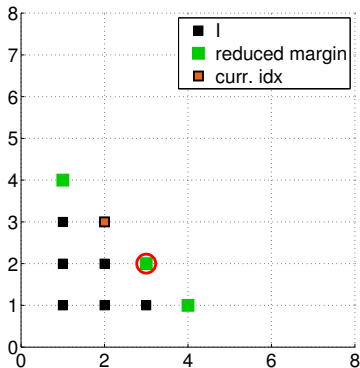
Sparse grid set



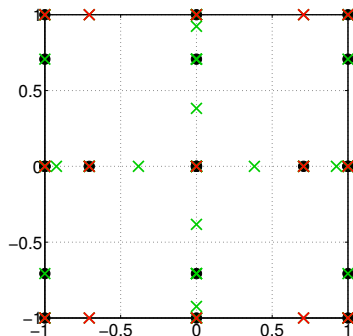
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

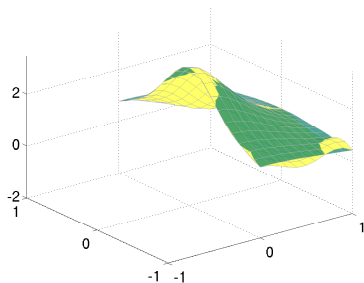
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



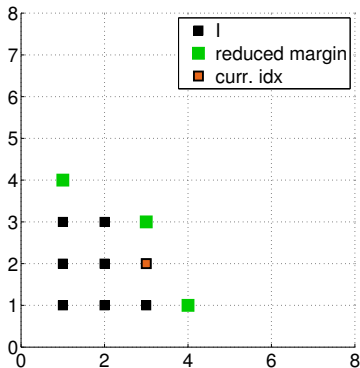
Sparse grid set



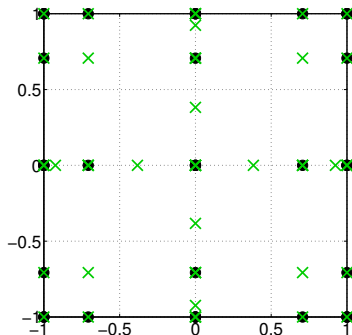
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

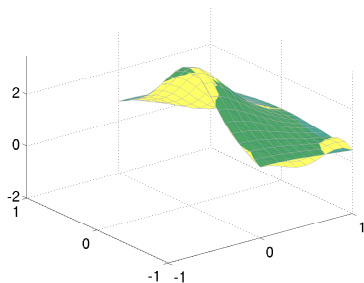
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



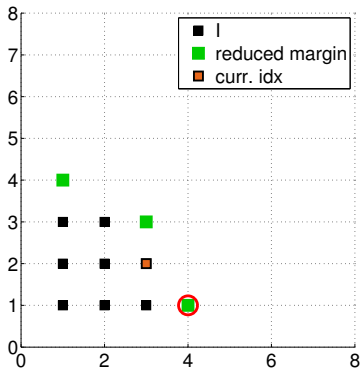
Sparse grid set



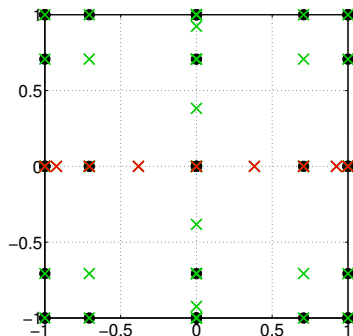
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

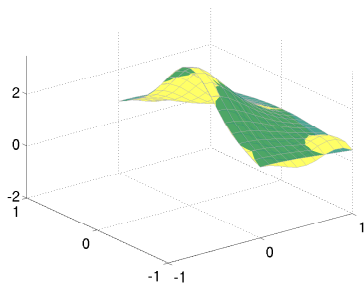
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



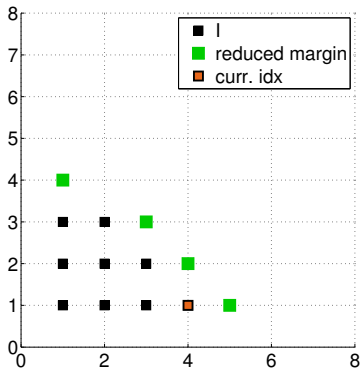
Sparse grid set



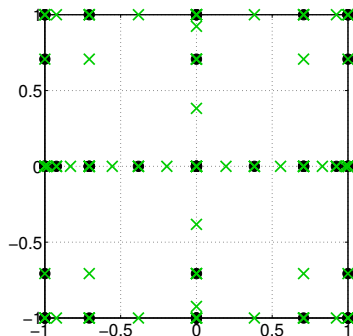
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

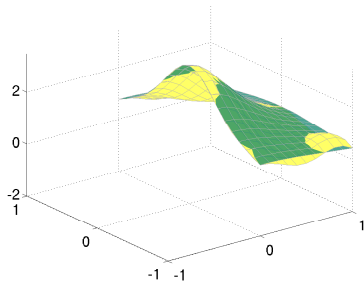
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



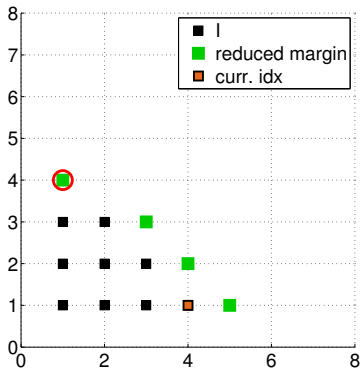
Sparse grid set



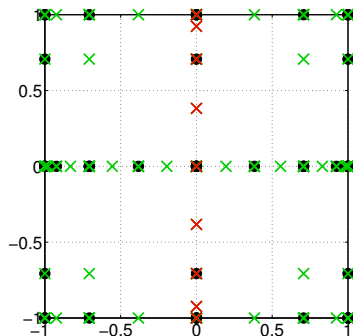
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

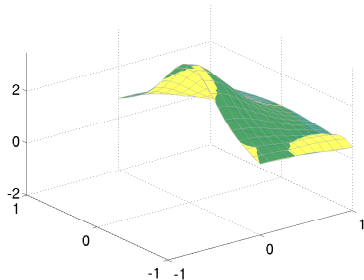
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



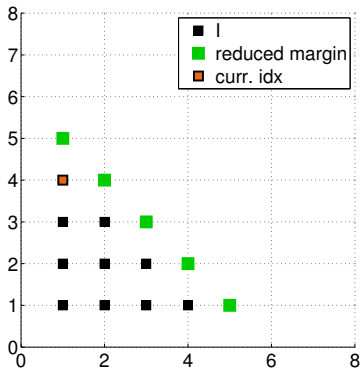
Sparse grid set



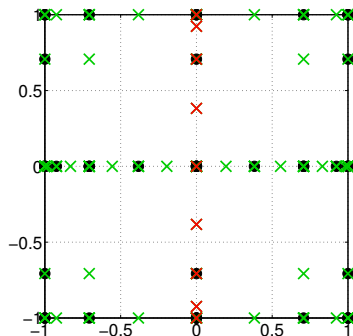
interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Sparse grids “ingredients”: adaptive algorithm

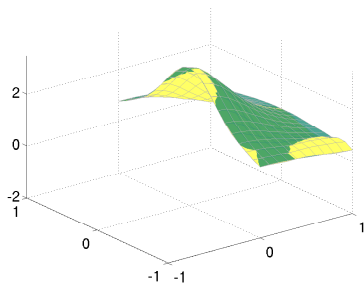
```
res = adapt_sparse_grid(f,N,knots,m,res_old,controls)
```



Multi-index set



Sparse grid set



interpolation of $f(\mathbf{y}) = \frac{1}{y_1^2 + y_2^2 + 0.3}$

Outline

- 1 Example
- 2 Basic data structure
- 3 Main features**
- 4 Example - reprise
- 5 Conclusions

Main functions

```
f=@(x) x.^2; %vector-valued function
N=2; w=3;
S=smolyak_grid(N,w,@(n) knots_uniform(n,-1,1),@lev2knots_lin);
Sr= reduce_sparse_grid(S);
```

Main functions

```
f=@(x) x.^2; %vector-valued function
N=2; w=3;
S=smolyak_grid(N,w,@(n) knots_uniform(n,-1,1),@lev2knots_lin);
Sr= reduce_sparse_grid(S);
```

- `ev_f = evaluate_on_sparse_grid(f, Sr)`

Main functions

```
f=@(x) x.^2; %vector-valued function
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S=smolyak_grid(N,w,@(n) knots_uniform(n,-1,1),@lev2knots_lin);
Sr= reduce_sparse_grid(S);
```

- `ev_f = evaluate_on_sparse_grid(f, Sr)`

can **recycle evaluations** from previous results if available (regardless of nestedness)

```
ev_f = evaluate_on_sparse_grid(f, S, Sr, ev_f_old, S_old, Sr_old)
```

Main functions

```
f=@(x) x.^2; %vector-valued function
N=2; w=3;
S=smolyak_grid(N,w,@(n) knots_uniform(n,-1,1),@lev2knots_lin);
Sr= reduce_sparse_grid(S);
```

- `ev_f = evaluate_on_sparse_grid(f, Sr)`

evaluate `f` in **parallel** if more than `X` evals are required, uses **Matlab parallel toolbox**

```
ev_f = evaluate_on_sparse_grid(f, S, Sr, [], [], [], X)
```

Main functions

```
f=@(x) x.^2; %vector-valued function
N=2; w=3;
S=smolyak_grid(N,w,@(n) knots_uniform(n,-1,1),@lev2knots_lin);
Sr= reduce_sparse_grid(S);
```

- `ev_f = evaluate_on_sparse_grid(f, Sr)`
- `q_f = quadrature_on_sparse_grid(f, Sr)`

Main functions

```
f=@(x) x.^2; %vector-valued function
N=2; w=3;
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Sr= reduce_sparse_grid(S);
```

- `ev_f = evaluate_on_sparse_grid(f, Sr)`
- `q_f = quadrature_on_sparse_grid(f, Sr)`
same features as `evaluate`

Main functions

```
f=@(x) x.^2; %vector-valued function
N=2; w=3;
S=smolyak_grid(N,w,@(n) knots_uniform(n,-1,1),@lev2knots_lin);
Sr= reduce_sparse_grid(S);
```

- `ev_f = evaluate_on_sparse_grid(f, Sr)`
- `q_f = quadrature_on_sparse_grid(f, Sr)`
- `int_f = interpolate_on_sparse_grid(S, Sr, ev_f, P)`

`P` is a matrix of eval. points (stored as columns)

Main functions

```
f=@(x) x.^2; %vector-valued function
N=2; w=3;
S=smolyak_grid(N,w,@(n) knots_uniform(n,-1,1),@lev2knots_lin);
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```

- `ev_f = evaluate_on_sparse_grid(f, Sr)`
- `q_f = quadrature_on_sparse_grid(f, Sr)`
- `int_f = interpolate_on_sparse_grid(S, Sr, ev_f, P)`
- `[coeffs, I] = convert_to_modal(S, Sr, ev_f, 'Legendre')`
 - ▶ Converts a sparse grid into its **equivalent Polynomial Chaos Exp.**

Main functions

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f=@(x) x.^2; %vector-valued function
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S=smolyak_grid(N,w,@(n) knots_uniform(n,-1,1),@lev2knots_lin);
Sr= reduce_sparse_grid(S);
```

- `ev_f = evaluate_on_sparse_grid(f, Sr)`
- `q_f = quadrature_on_sparse_grid(f, Sr)`
- `int_f = interpolate_on_sparse_grid(S, Sr, ev_f, P)`
- `[coeffs, I] = convert_to_modal(S, Sr, ev_f, 'Legendre')`
 - ▶ Converts a sparse grid into its **equivalent Polynomial Chaos Exp.**
 - ▶ **Idea:** For each tensor grid in the combination technique, compute the equivalent PCE by solving a Vandermonde system

Main functions

```
f=@(x) x.^2; %vector-valued function
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```

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- `[coeffs, I] = convert_to_modal(S, Sr, ev_f, 'Legendre')`
 - ▶ Converts a sparse grid into its **equivalent Polynomial Chaos Exp.**
 - ▶ **Idea:** For each tensor grid in the combination technique, compute the equivalent PCE by solving a **Vandermonde system**
 - ▶ Vandermonde matrix is orthogonal for Gaussian quadrature points

Main functions

```
f=@(x) x.^2; %vector-valued function
N=2; w=3;
S=smolyak_grid(N,w,@(n) knots_uniform(n,-1,1),@lev2knots_lin);
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```

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- `int_f = interpolate_on_sparse_grid(S, Sr, ev_f, P)`
- `[coeffs, I] = convert_to_modal(S, Sr, ev_f, 'Legendre')`
 - ▶ Converts a sparse grid into its **equivalent Polynomial Chaos Exp.**
 - ▶ **Idea:** For each tensor grid in the combination technique, compute the equivalent PCE by solving a **Vandermonde system**
 - ▶ Vandermonde matrix is orthogonal for Gaussian quadrature points
 - ▶ several orthogonal polynomials:
`'Legendre', 'Hermite', 'Chebyshev', 'Laguerre', 'Jacobi', 'Generalized Laguerre'`

Main functions

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f=@(x) x.^2; %vector-valued function
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- plus of course, plotting and exporting on file...

Outline

- 1 Example
- 2 Basic data structure
- 3 Main features
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- 5 Conclusions

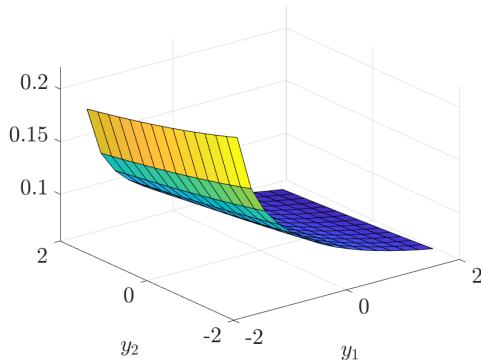
Results with code

```
N = 2;
knots = @(n) knots_CC(n,-sqrt(3),sqrt(3));
lev2knots = @lev2knots_doubling;
rule = @(ii) sum((ii-1));
w=4;
S = smolyak_grid(N,w,knots,lev2knots,rule);
Sr = reduce_sparse_grid(S);

% solve PDEs on sparse grid (expensive part)
I_on_Sr = evaluate_on_sparse_grid(I,Sr);

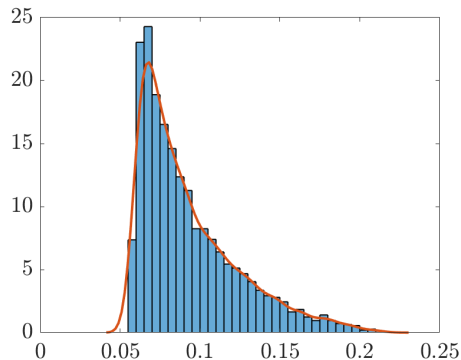
% task 1: expected value
exp_I = quadrature_on_sparse_grid(I_on_Sr,Sr);

% task 2: evaluate metamodel
yy = linspace(-sqrt(3),sqrt(3),15);
[Y1,Y2] = meshgrid(yy,yy);
eval_points = [Y1(:)';Y2(:)'];
I_vals = interpolate_on_sparse_grid(S,Sr,...
                                   I_on_Sr,eval_points);
```



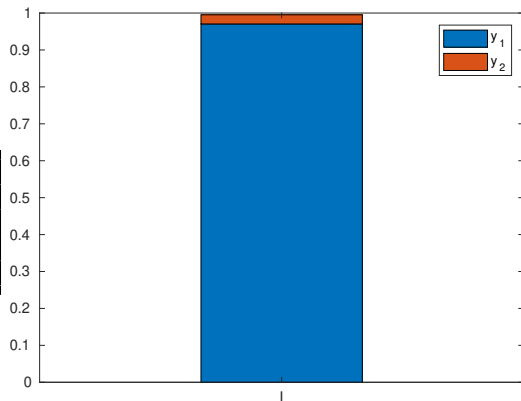
Results with code

```
% task 3: pdf
M = 5000;
y_samples = -sqrt(3)+2*sqrt(3)*rand(N,M);
I_vals_rand = interpolate_on_sparse_grid(S,Sr,...
                                         I_on_Sr,y_samples);
H = histogram(I_vals_rand,'Normalization','pdf');
[pdf_vals,pdf_pts] = ksdensity(I_vals_rand);
```



Results with code

```
% task 4: sensitivity analysis (Sobol indices)
domain = [-sqrt(3) -sqrt(3);sqrt(3) sqrt(3)];
Sob = compute_sobol_indices_from_sparse_grid(...
    S,Sr,I on Sr ,domain,'legendre');
bar(1,Sob','stacked')
```



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- J. Martínez-Frutos, F. Periago Esparza, *Optimal Control of PDEs under Uncertainty*, Springer 2018. Uses Matlab Sparse Grids Kit