Sparse grids Matlab kit

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October 15, 2018

Outline

1. Basic data structure
2. Main features
3. Numerical examples
4. Conclusions

Contributors, releases

- main contributors: Lorenzo Tamellini, Fabio Nobile

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  - 17-5 ("Trent")
  - 15-8 ("Woodstock")
  - 14-12 ("Fenice")
  - 14-4 ("Ritchie")

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General comments

- Lightweight, high-level and (hopefully) easy to use, good for quick prototyping and teaching

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Aim of these slides: give rough idea of structure, show by examples features and ease of use

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Backbone: combination technique & “reduced” sparse grid

```
N=2;
knots=@(n) knots_CC(n,-1,1,'nonprob');
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m = @lev2knots_doubling;
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- $S = \sum_{\mathbf{i} \in \mathcal{I}} c_{\mathbf{i}} \bigotimes_{n=1}^{N} \mathcal{U}^{m(i_n)}$

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

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

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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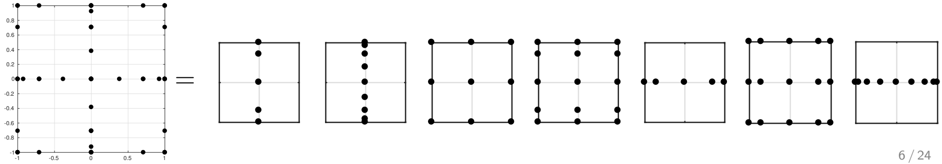

Backbone: combination technique & “reduced” sparse grid

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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
```

Backbone: combination technique & “reduced” sparse grid

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```

```
>> 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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- `[x,w]=knots_CC(n,a,b) %Clenshaw-Curtis`

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- `[x,w]=knots_CC(n,a,b) %Clenshaw-Curtis`
- `[x,w]=knots_uniform(n,a,b) %Gauss-Legendre`

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- `[x,w]=knots_leja(n,a,b,'line')`

  $x_1 = b$

  $x_2 = a$

  $x_3 = (a+b)/2$

  $x_n = \mathrm{argmax}_{[a\ b]} \prod_{k=1}^{n-1} (x - x_k)$

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- `[x,w]=knots_leja(n,a,b,'sym_line')`

$x_1 = b$
$x_2 = a$
$x_3 = (a+b)/2$
$x_{2n} = \text{argmax}_{[a\ b]} \prod_{k=1}^{2n-1} (x - x_k)$
$x_{2n+1} = \text{symmetric of } x_{2n} \text{ wrt } (a+b)/2$

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  compute Leja pts on the complex unit ball, and project on the real line

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- `[x,w]=knots_gaussian(n,mi,sigma) %Gauss-Hermite`

  for gaussian weights with mean μ and st. dev. σ

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- `[x,w]=knots_kpn(n)%Kronrod Patteron Normal, Genz-Keister`

  Tabulated sequence of nested extensions of (n+1) Gauss–Hermite with maximal exactness degree: $m = 1, 3, 9, 19, 35$

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- `[x,w]=knots_gaussian_leja(n)%Narayan-Jakeman, SISC 2014`

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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 = lev2knots_2step(i)`
- `m = lev2knots_doubling(i)`
  $m(1) = 1, m(i) = 2^{i-1} + 1$

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  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., $\mathcal{I} = \left\{\mathbf{i} \in \mathbb{N}_+^N : \max_n g_n(i_n - 1) \leq w\right\}$, $m(i) = i$

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- **'TD'** = total deg., $\mathcal{I} = \left\{\mathbf{i} \in \mathbb{N}_+^N : \sum_{n=1}^N g_n(i_n - 1) \leq w\right\}$, $m(i) = i$

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

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

Sparse grids "ingredients": nodes, m, $\mathcal{I}$

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

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([2 3],1);
T_M = smolyak_grid_multiidx_set(D,knots,m);
```

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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

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- `ev_f = evaluate_on_sparse_grid(f,Sr)`

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```

- `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)
  ```

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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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```

- **`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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Main functions

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  - `knots` can be non-nested and on unbounded interval

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N=2; w=3;
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- `res = adapt_sparse_grid(f,N,knots,m,res_old,controls)`
  - **`knots`** can be non-nested and on unbounded interval
  - comes with several definitons of profit/surplus

Main functions

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    1. difference between consecutive quadratures

Main functions

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- `res = adapt_sparse_grid(f,N,knots,m,res_old,controls)`
  - `knots` can be non-nested and on unbounded interval
  - comes with several definitons of profit/surplus
    1. difference between consecutive quadratures
    2. max of difference between two consecutive sparse grid approx

Main functions

```
f=@(x) x.^2; %vector-valued function
N=2; w=3;
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- `ev_f = evaluate_on_sparse_grid(f,Sr)`
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- `int_f = interpolate_on_sparse_grid(S,Sr,ev_f,P)`
- `res = adapt_sparse_grid(f,N,knots,m,res_old,controls)`
  - **knots** can be non-nested and on unbounded interval
  - comes with several definitons of profit/surplus
    1. difference between consecutive quadratures
    2. max of difference between two consecutive sparse grid approx
       - for nested points: identical to max between sparse grid and true fun.
       - works for non-nested points too
       - over the last added tensor grid

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)`
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- `res = adapt_sparse_grid(f,N,knots,m,res_old,controls)`
  - **knots** can be non-nested and on unbounded interval
  - comes with several definitons of profit/surplus
    1. difference between consecutive quadratures
    2. max of difference between two consecutive sparse grid approx
    3. weighting by nb of points and arbitary densities is possible

Main functions

```
f=@(x) x.^2; %vector-valued function
N=2; w=3;
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- `ev_f = evaluate_on_sparse_grid(f,Sr)`
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    3. weighting by nb of points and arbitary densities is possible
  - computation can be stopped, dumped on variables and restarted

Main functions

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    1. difference between consecutive quadratures
    2. max of difference between two consecutive sparse grid approx
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  - computation can be stopped, dumped on variables and restarted
  - a buffer of N_b “explored but unused variables” can be set

Main functions

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    - `knots` can be non-nested and on unbounded interval
    - comes with several definitons of profit/surplus
        1. difference between consecutive quadratures
        2. max of difference between two consecutive sparse grid approx
        3. weighting by nb of points and arbitary densities is possible
    - computation can be stopped, dumped on variables and restarted
    - a buffer of N_b "explored but unused variables" can be set

      the algorithm starts with $N_{curr} = N_b$ dim.; as soon as points are placed in one dim., a new one is taken into account, i.e., $N_{curr} = N_{curr} + 1$.
      In this way, there are always N_b dim. whose "initial profit" is computed but along which no point is placed

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)`
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  - `knots` can be non-nested and on unbounded interval
  - comes with several definitons of profit/surplus
    1. difference between consecutive quadratures
    2. max of difference between two consecutive sparse grid approx
    3. weighting by nb of points and arbitary densities is possible
  - computation can be stopped, dumped on variables and restarted
  - a buffer of N_b “explored but unused variables” can be set
  - support vector-valued functions, appropriate profits can be set

Main functions

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f=@(x) x.^2; %vector-valued function
N=2; w=3;
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- `[coeffs,I] = convert_to_modal(S,Sr,ev_f,'Legendre')`

Main functions

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- `[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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  - 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

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  - 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'`

Main functions

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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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- `res = adapt_sparse_grid(f,N,knots,m,res_old,controls)`
- `[coeffs,I] = convert_to_modal(S,Sr,ev_f,'Legendre')`
- `[Si,Ti]=compute_sobol_indices_from_sparse_grid(S,Sr,ev_f,'Legendre')`

Main functions

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  - `Si` are the principal Sobol indices of x_i (fraction of variability due to x_i only)

Main functions

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- `[coeffs,I] = convert_to_modal(S,Sr,ev_f,'Legendre')`
- `[Si,Ti]=compute_sobol_indices_from_sparse_grid(S,Sr,ev_f,'Legendre')`
    - `Si` are the principal Sobol indices of x_i (fraction of variability due to x_i only)
    - `Ti` are the total Sobol indices of x_i (fraction of variability due to x_i alone and together with any other variable)

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)`
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- `grads = derive_sparse_grid(S,Sr,ev_f,P)`

  uses Finite Differences, increment step can be specified

Main functions

```
f=@(x) x.^2; %vector-valued function
N=2; w=3;
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- `[Si,Ti]=compute_sobol_indices_from_sparse_grid(S,Sr,ev_f,'Legendre')`
- `grads = derive_sparse_grid(S,Sr,ev_f,P)`
- `export_sparse_grid_to_file(Sr,'filename')`

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)`
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- `grads = derive_sparse_grid(S,Sr,ev_f,P)`
- `export_sparse_grid_to_file(Sr,'filename')`

  save points (and optionally quad weights) on an ascii file, one point per row

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)`
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- `[Si,Ti]=compute_sobol_indices_from_sparse_grid(S,Sr,ev_f,'Legendre')`
- `grads = derive_sparse_grid(S,Sr,ev_f,P)`
- `export_sparse_grid_to_file(Sr,'filename')`
- `plot_sparse_grids_interpolant(S,Sr,f_ev)`

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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- `[Si,Ti]=compute_sobol_indices_from_sparse_grid(S,Sr,ev_f,'Legendre')`
- `grads = derive_sparse_grid(S,Sr,ev_f,P)`
- `export_sparse_grid_to_file(Sr,'filename')`
- `plot_sparse_grids_interpolant(S,Sr,f_ev)`

  plots the sparse grids interpolant of `f`. Different plots are produced for the cases $N = 2, N = 3, N > 3$ (see next slide)

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)`
- `res = adapt_sparse_grid(f,N,knots,m,res_old,controls)`
- `[coeffs,I] = convert_to_modal(S,Sr,ev_f,'Legendre')`
- `[Si,Ti]=compute_sobol_indices_from_sparse_grid(S,Sr,ev_f,'Legendre')`
- `grads = derive_sparse_grid(S,Sr,ev_f,P)`
- `export_sparse_grid_to_file(Sr,'filename')`
- `plot_sparse_grids_interpolant(S,Sr,f_ev)`
- `plot_sparse_grids(S)` or `plots_sparse_grids(Sr)`

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)`
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- `[coeffs,I] = convert_to_modal(S,Sr,ev_f,'Legendre')`
- `[Si,Ti]=compute_sobol_indices_from_sparse_grid(S,Sr,ev_f,'Legendre')`
- `grads = derive_sparse_grid(S,Sr,ev_f,P)`
- `export_sparse_grid_to_file(Sr,'filename')`
- `plot_sparse_grids_interpolant(S,Sr,f_ev)`
- `plot_sparse_grids(S)` or `plots_sparse_grids(Sr)`

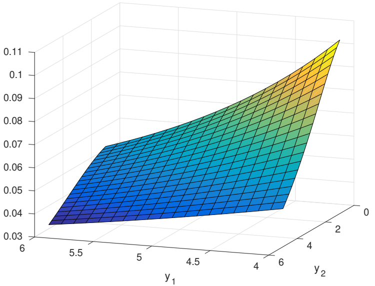
  plots (selected coordinates of) the sparse grid points in a 2d plane

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);
```

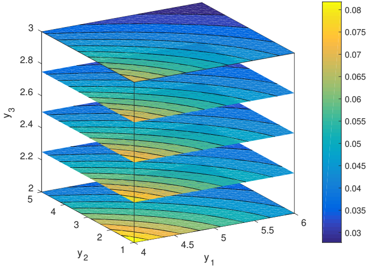
- `ev_f = evaluate_on_sparse_grid(f,Sr)`
- `q_f = quadrature_on_sparse_grid(f,Sr)`
- `int_f = interpolate_on_sparse_grid(S,Sr,ev_f,P)`
- `res = adapt_sparse_grid(f,N,knots,m,res_old,controls)`
- `[coeffs,I] = convert_to_modal(S,Sr,ev_f,'Legendre')`
- `[Si,Ti]=compute_sobol_indices_from_sparse_grid(S,Sr,ev_f,'Legendre')`
- `grads = derive_sparse_grid(S,Sr,ev_f,P)`
- `export_sparse_grid_to_file(Sr,'filename')`
- `plot_sparse_grids_interpolant(S,Sr,f_ev)`
- `plot_sparse_grids(S)` or `plots_sparse_grids(Sr)`

plot_sparse_grids_interpolant - examples



case N=2: surf of sparse grid interpolant.

Above, $f(x) = 1/(1 + 0.5x_1^2 + 0.5x_2^2)$



case N=3: several contourf plots of the sparse grid interpolant obtained fixing x_3 at different values will be plotted in the same axes.

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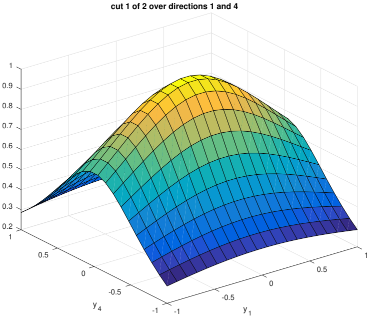

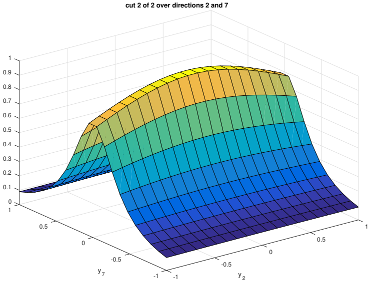

case N>3: several two-dimensional surf plots will be produced. In each of them, all variables are frozen to their average value but 2, and the value of the interpolant with respect of those will be plotted.

Above, $f(x) = 1./(1 + 0.5x_1^2 + 0.25x_2^2 + 5x_3^2 + 2x_4^2 + 0.001x_5^2 + 10x_6^2 + 10x_7^2)$. We plot the two-dimesional cuts (x_1, x_4) and (x_2, x_7)

Outline

1. Basic data structure
2. Main features
3. Numerical examples
4. Conclusions

Examples of applications

1. Convergence of sparse grids approximation of lognormal problem:
    - **adapt_sparse_grid** with non-nested knots on unbounded domains
    - **smolyak_grid_multiidx_set**
    - **convert_to_modal**

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2. Geochemical compaction
   - very easy connection with built-in Matlab routines (in this case, **`fminsearch`**)
   - **`derive_sparse_grid`**

Ex. 1) Elliptic PDE with lognormal diffusion coefficient

$$\begin{cases} -\dfrac{\mathrm{d}}{\mathrm{d}x}\left(a(x,\boldsymbol{\xi})\,\dfrac{\mathrm{d}}{\mathrm{d}x}u(x,\boldsymbol{\xi})\right) = 0.03\sin(2\pi x), \qquad u(0,\boldsymbol{\xi}) = u(1,\boldsymbol{\xi}) = 0 \\ \log a(x,\boldsymbol{\xi}) = 0.1\displaystyle\sum_{m=1}^{\infty} \underbrace{\frac{\sqrt{2}}{(\pi m)^{q}}\sin(m\pi x)}_{=:\phi_m(x)}\,\xi_m, \qquad q \geq 1,\ \text{smoothed Brownian bridge} \end{cases}$$

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Convergence Theorem

- Under assumptions on $a(x,\boldsymbol{\xi})$ and knots, $\exists$ a multiidx set Λ_N with $|\Lambda_N| = N$ st

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\|u - U_{\Lambda_N}u\|_{L^2_\mu} \;\leq\; CN^{-(q-1.5)} \;\leq\; C|\Xi_{\Lambda_N}|^{-\left(\frac{q-1.5}{2}\right)}.
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$$\Lambda_N = \{\boldsymbol{\nu} \in \mathbb{N}^{\mathbb{N}} \text{ with N largest } \hat{c}_{\boldsymbol{\nu}}\}, \qquad \hat{c}_{\boldsymbol{\nu}} = \hat{c}_{\boldsymbol{\nu}}(q)$$

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- technical assumptions on knots proved for Gauss–Hermite knots (so far).

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```
% code snippet, a-priori heuristic
Lambda = buildLambda_prior(..);
for iter = 1:P
    C = Lambda(1:P,:);
    C = sortrows(C);
    S = smolyak_grid_multiidx_set(C,..);
    Sr = reduce_sparse_grid(S);
    f_grid=evaluate_on_sparse_grid(f,S,Sr,evals_old,..);
    evals_old = f_grid;
    err = ... % calls interpolate_on_sparse_grid over an MC sample
 end
```

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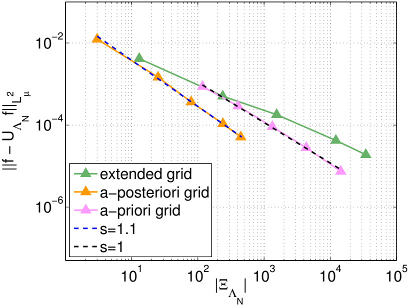
```
% code snippet, a-posteriori heuristic
f = @(y) sol(a_coef(y));
controls.op_vect = @(A,B) H1normALL(A-B); % profit for functions
controls.var_buffer_size = 5;
for nb_pts = [10 100 1000..]
    controls.max_pts = nb_pts;
    adapt = adapt_sparse_grid(f,dim,..,prev_adapt,controls);
    prev_adapt = adapt;
    err = .. % calls interpolate_on_sparse_grid over an MC sample
end
```

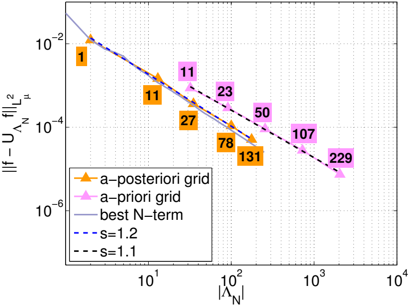
convergence wrt $|\Xi_{\Lambda_N}|$



$q = 2$
expect $s = 0.25$;
a-priori $s = 1.0$;
a-posteriori $s = 1.1$

- Extended grid = a-posteriori with evaluations in the neighbourhood
- Expected rate smaller than observed:
  - summability argument could be improved
  - bound between number of elements and points not sharp

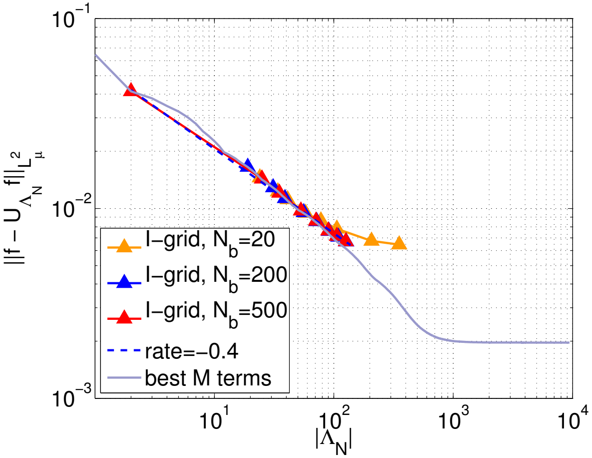
convergence wrt $|\Lambda_N|$



$q = 2$
expect $s = 0.5$;
a-priori $s = 1.1$;
a-posteriori $s = 1.2$

- Labels show the number of activated random variables
- Similar rate to before $\Rightarrow$ growth of points linear in $|\Lambda_N|$
- best-N-terms obtained by converting sparse grid into Hermite polynomials with **`convert_to_modal`** and sorting the coefficients

The importance of the buffer size N_b



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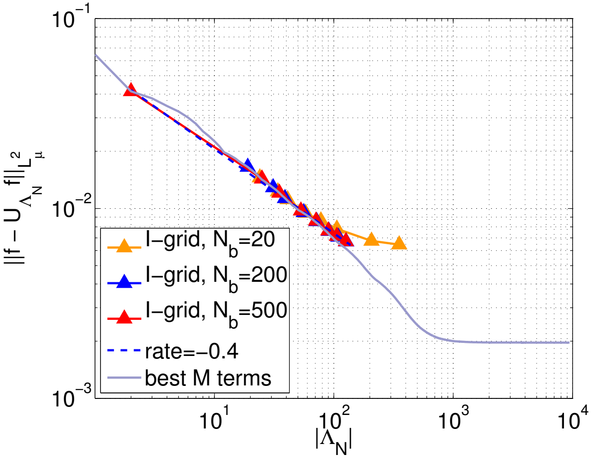

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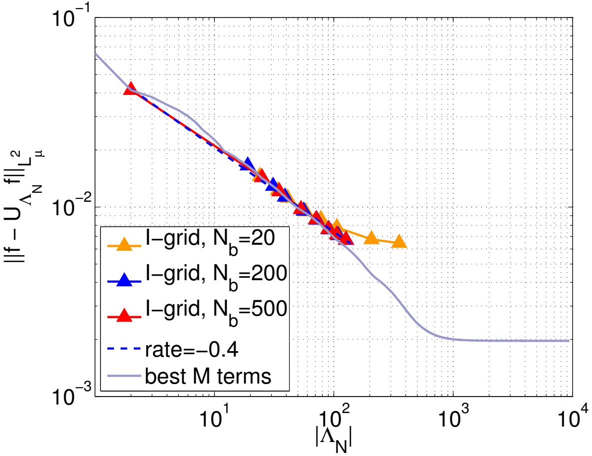

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- use large N_b, or convengence will stagnate
- a-posteriori grid departs from best-M-terms: unsignificant modes have been added to the a-posteriori grid.

Ex. 2) Geochemical compaction problem

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3. This process is described by a set of coupled, time-dependent, non-linear, monodimensional (depth-only) PDEs.

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- Underlying fundamental question: is it better to have porosity or temperature data?

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Eval: `[phi_values,T_values] = evaluate_on_sparse_grids(@model,S,Sr,..)`

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```
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2. $\sigma = \dfrac{J_\Phi(\mathbf{y}^*) + \lambda J_\mathrm{T}(\mathbf{y}^*)}{K+L}, s^2 = \dfrac{\sigma^2}{\lambda}$

Maximum Likelihood Inversion – details

Then, a MLE procedure to estimate $\mathbf{y}, \sigma, s$ is

Eval:
```
[phi_values,T_values] = evaluate_on_sparse_grids(@model,S,Sr,..)
```

For $\lambda = \lambda_1, \ldots, \lambda_N$

1. $\mathbf{y}^* = \mathrm{argmin}_{\mathbf{y}\in\Gamma} J_\Phi + \lambda J_\mathrm{T}$ (i.e., $\mathrm{argmin}_{\mathbf{y}\in\Gamma} NLL$ for fixed σ, s)

```
% define @-fun to call interpolate_on_sparse_grid(S,Sr,phi_values,p)
f = @(y) eval_J_phi(S,Sr,phi_values,phi_data,y) + eval_J_T ..
y_MLE = fminsearch(f,p0);
```

2. $\sigma = \dfrac{J_\Phi(\mathbf{y}^*) + \lambda J_\mathrm{T}(\mathbf{y}^*)}{K+L}, s^2 = \dfrac{\sigma^2}{\lambda}$
3. $KIC = NLL - N \log 2\pi - \ln det(C)$
   - $C = \sigma^2 (D_\mathbf{y}\phi^\top D_\mathbf{y}\phi + \lambda D_\mathbf{y} T^\top D_\mathbf{y} T)^{-1}$
   - $D_\mathbf{y}\phi, D_\mathbf{y} T$ Jacobian matrices of ϕ and T wrt to $\mathbf{y}$, evaluated at $\mathbf{y}^*$ (sensitivity)

```
for i=1:nb_z_nodes
  Jac_phi(i,:) = derive_sparse_grid(S,Sr,phi_values(i,:),y_MLE);
end
```

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end
```
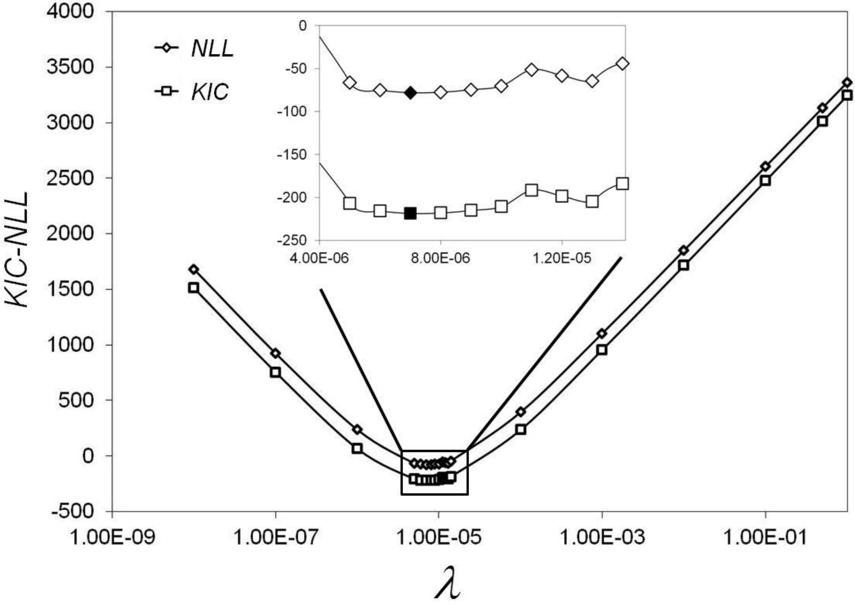
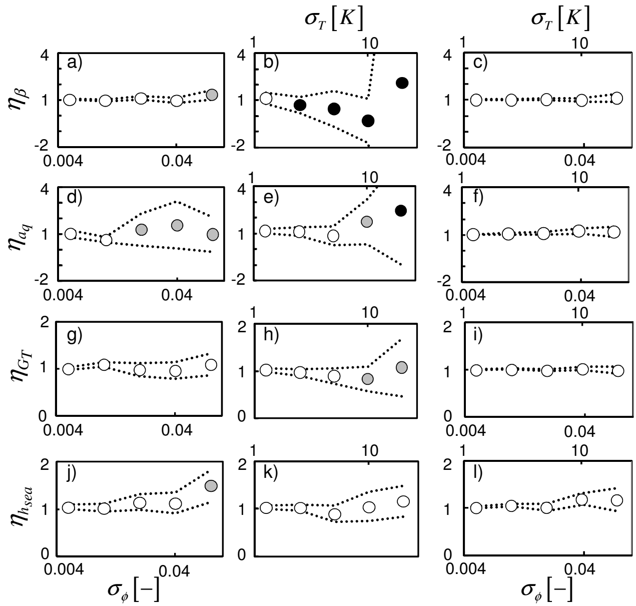

Choose $(\sigma, s, \mathbf{y})$ that yield the minimum KIC



NLL
KIC
KIC-NLL
λ
4000
3500
3000
2500
2000
1500
1000
500
0
-500
1.00E-09
1.00E-07
1.00E-05
1.00E-03
1.00E-01
0
-50
-100
-150
-200
-250
4.00E-06
8.00E-06
1.20E-05

Results



$\sigma_T\,[K]$
$\sigma_T\,[K]$
a)
b)
c)
d)
e)
f)
g)
h)
i)
j)
k)
l)
η_β
η_{aq}
η_{GT}
η_{hsea}
4
1
-2
2
0
0.004
0.04
10
$\sigma_\phi\,[-]$
$\sigma_\phi\,[-]$

Outline

1. Basic data structure
2. Main features
3. Numerical examples
4. Conclusions

Concluding remarks

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Bibliography

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- G. Porta, L. Tamellini, V. Lever, M. Riva. *Inverse modeling of geochemical and mechanical compaction in sedimentary basins through polynomial chaos expansion.* Water Resources Research, 2014.
- J. Martnez-Frutos, F. Periago Esparza, *Optimal Control of PDEs under Uncertainty,* Springer 2018. Uses Matlab Sparse Grids Kit