Sparse grids Matlab kit

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Outline

Contributors, release, general comments

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- Some ad-hoc features and integration with parallel toolbox gives nonetheless reasonable speed
- Geared towards UQ, but flexible enough for other purposes
- Aim of the talk: give rough idea of structure, show by examples features and ease of use

Outline

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

Backbone: combination technique & “reduced” sparse grid

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

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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

Backbone: combination technique & "reduced" sparse grid

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N=2;
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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
- $\mathcal{I} = \left\{ \mathbf{i} \in \mathbb{N}_+^N : \sum_{n=1}^{N} (i_n - 1) \leq w \right\}$

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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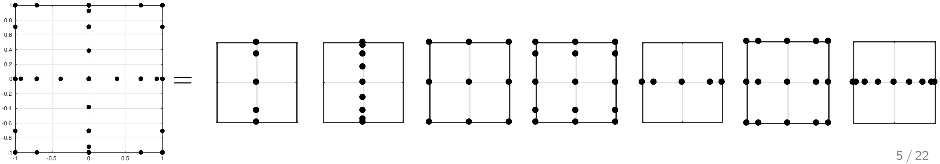

Backbone: combination technique & "reduced" sparse grid

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

```
>> 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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w = 3;
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Ifun = @(i) sum(i-1);
S = smolyak_grid(N,w,knots,m,Ifun);
```

```
>> Sr = reduce_sparse_grid(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, $\mathcal{I}$

```
N=2;
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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`

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

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N=2;
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- `[x,w]=knots_uniform(n,a,b) %Gauss-Legendre`
- `[x,w]=knots_leja(n,a,b,'line')`

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

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

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

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

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

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

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

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

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- `[x,w]=knots_leja(n,a,b,'p_disk')`
- `[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_gaussian(n,mi,sigma) %Gauss-Hermite`
- `[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_kpn(n)%Kronrod Patteron Normal, Genz-Keister`
- `[x,w]=knots_normal_leja(n)%Narayan-Jakeman`

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- **`m = lev2knots_lin(i)`**

  $m(i) = i$

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

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Ifun = @(i) sum(i-1);
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```

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

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```

- `m = lev2knots_lin(i)`
- `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, $\mathcal{I} = \left\{\mathbf{i} \in \mathbb{N}_+^N : \prod_{n=1}^N i_n^{g_n} \leq w\right\}$, $m(i) = i$

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

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- **'TD'** $=$ total deg., $\mathcal{I} = \left\{\mathbf{i} \in \mathbb{N}^N_+ : \sum_{n=1}^N g_n(i_n - 1) \leq w\right\}$, $m(i) = i$
- **'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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N=2;
knots=@(n) knots_CC(n,-1,1,'nonprob');
w = 3;
m = @lev2knots_doubling;
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);
```

Outline

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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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)`**

Main functions

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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)
  ```

Main functions

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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)`**

  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

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f=@(x) x.^2; %vector-valued function
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  same features as **`evaluate`**

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

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       - for nested points: identical to max between sparse grid and true fun.
       - works for non-nested points too
       - over the last added tensor grid

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      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

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  - a buffer of N_b “explored but unused variables” can be set
  - support vector-valued functions, appropriate profits can be set

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  Compare as much as possible indices instead of coordinates, for efficiency

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    - **Idea:** For each tensor grid in the combination technique, compute the equivalent PCE by solving a Vandermonde system

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  - Vandermonde matrix is orthogonal for Gaussian quadrature points
  - several orthogonal polynomials: `'Legendre'`,`'Hermite'`,`'Chebyshev'`

Outline

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**
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2. More on geochemical compaction
   - **convert_to_modal**
   - very easy connection with built-in Matlab routines (**fminsearch**, **polyder**)

Ex. 1) Elliptic PDE with lognormal diffusion coefficient

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

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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

$$\|u - U_{\Lambda_N}u\|_{L^2_\mu} \leq CN^{-(q-1.5)} \leq C|\Xi_{\Lambda_N}|^{-\left(\frac{q-1.5}{2}\right)}.$$

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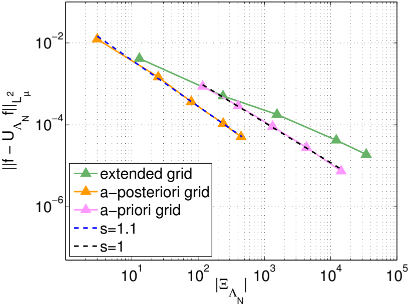
```
% code snippet, a-posteriori heuristic
f = @(y) sol(a_coef(y));
controls.op_vect = @(A,B) H1normALL(A-B); % profit for functions
controls.var_buffer_size = 5;
for nb_pts = [10 100 1000..]
    controls.max_pts = nb_pts;
    adapt = adapt_sparse_grid(f,dim,..,prev_adapt,controls);
    prev_adapt =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

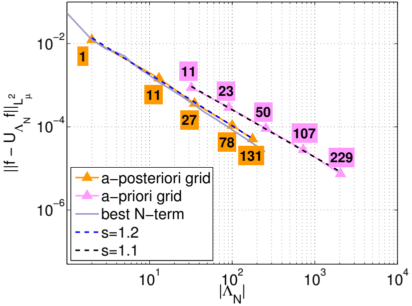
convergence wrt $|\Xi_{\Lambda_N}|$



$q = 2$
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

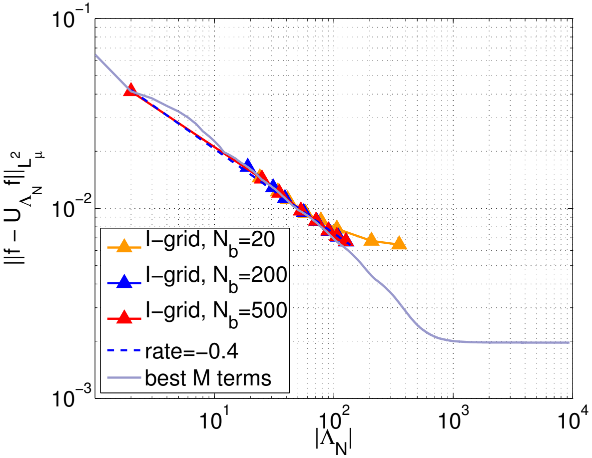
convergence wrt $|\Lambda_N|$



$q = 2$
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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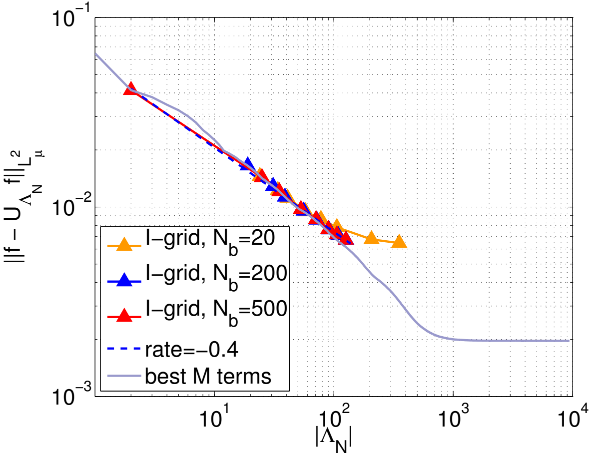

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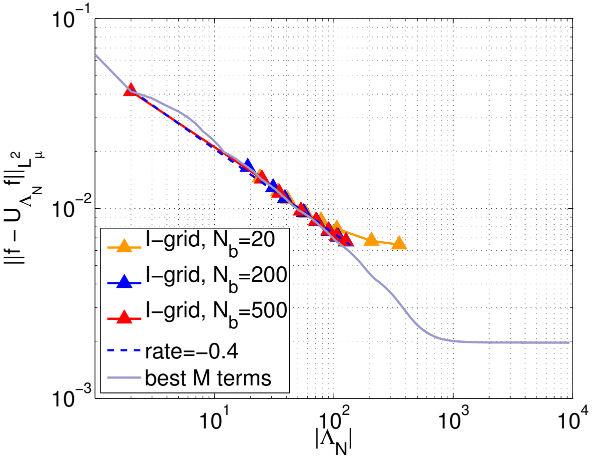

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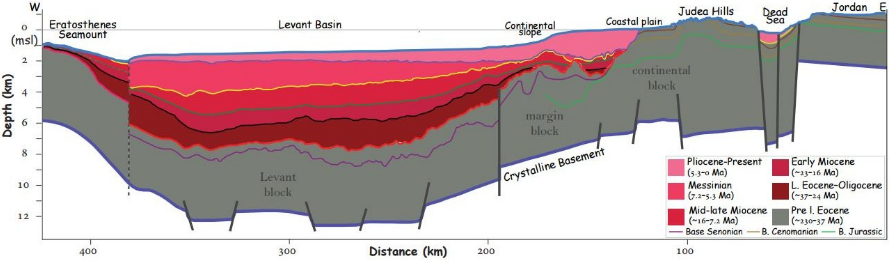
- a-posteriori grid departs from best-M-terms: unsignificant modes have been added to the a-posteriori grid.

Ex. 2) Geochemical compaction problem

How do we get from from sand on the bottom of the sea to sedimentary basins?



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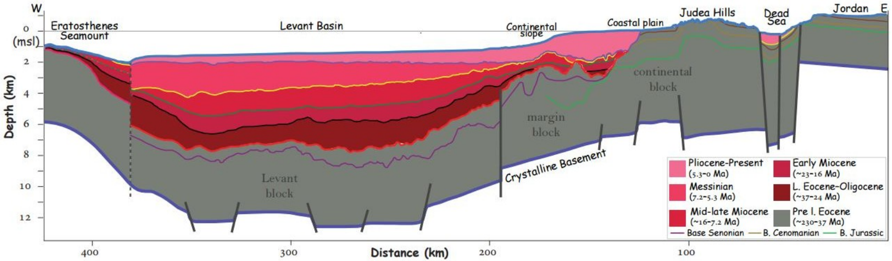

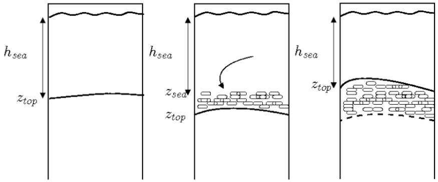

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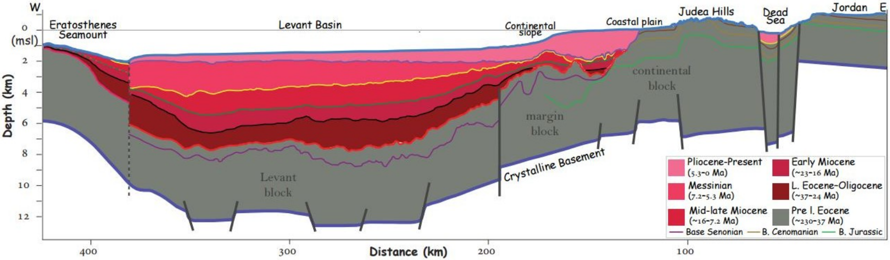

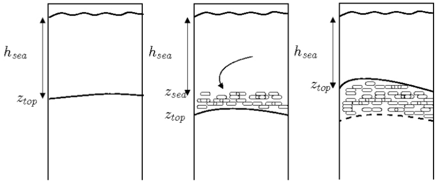

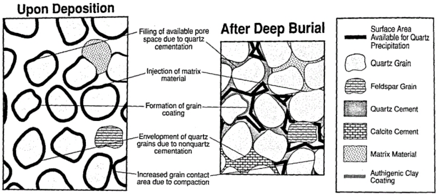

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As temperature, increase chemical reactions which glue grains together are triggered (quartz precipitation)

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- For later use $\lambda = \dfrac{\sigma^2}{s^2}$
- Underlying fundamental question: is it better to have porosity or temperature data?

Maximum Likelihood Inversion – details

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

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```
% define @-fun to call interpolate_on_sparse_grid(S,Sr,phi_values,p)
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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
[PCE_coef,I] = convert_to_modal(S,Sr,phi_values(i,:),'legendre')
% PCE => use polyval/polyder, no need for finite diff
Jac_phi(i,:) = derive_PCE(I,PCE_coef,y_MLE);
end
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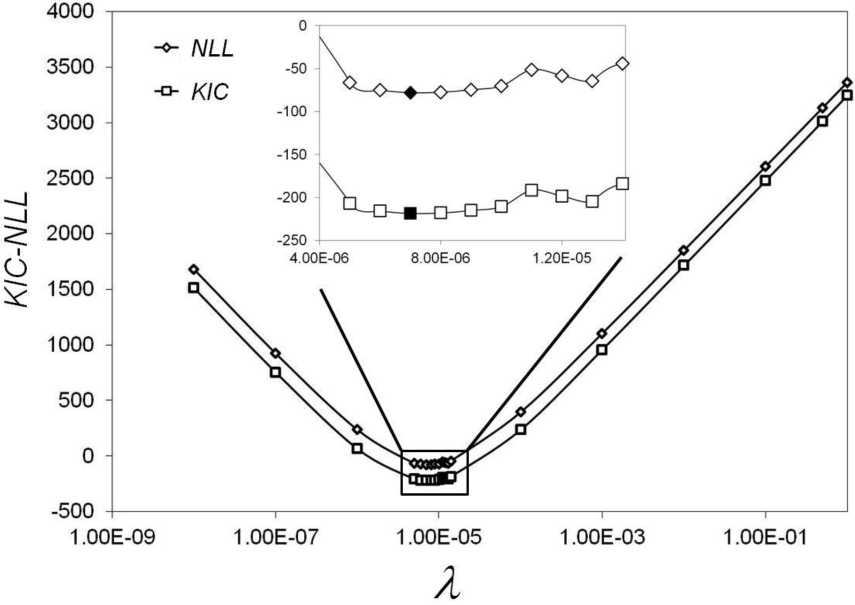
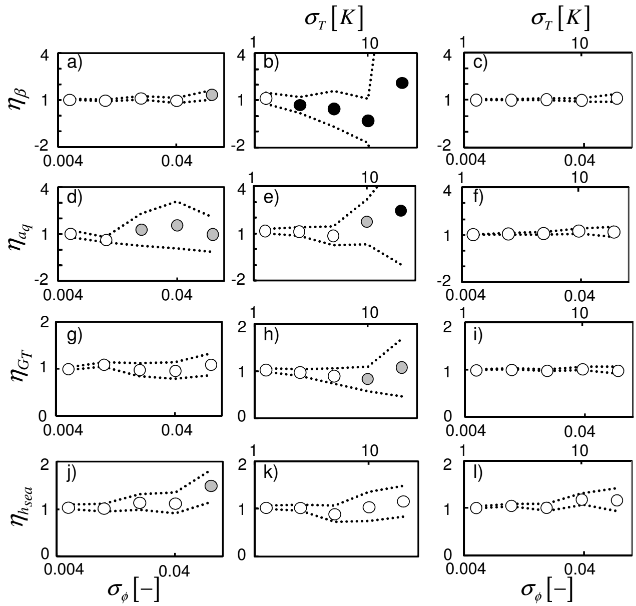
Choose $(\sigma, s, \mathbf{y})$ that yield the minimum KIC



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



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

Outline

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