Efficient UQ and Global Time-Varying SA Using the Spatially Adaptive Combination Technique

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Motivation

- Final Goal:
  Doing UQ and SA of complex dynamical models (e.g., HBV-SASK Hydrological model[1])
- Impediments:
  - High-dimensionality
  - Model as a black box
  - Possible discontinuities in the parameter space; anisotropic or decoupled parameters
  - Output of the model - time signal
- Scientific Approach:
  Use (Adaptive) SG to investigate the stochastic parameter space efficiently

Non-intrusive UQ

General Polynomial Chaos Expansion (gPCE)[2]

$$f(x,\boldsymbol{\theta}) \approx \mathcal{P}_{\boldsymbol{p}}^{\boldsymbol{N}} = f_N(x,\boldsymbol{\theta}) = \sum_{\boldsymbol{p}=0}^{N-1} c_p(x)\boldsymbol{\Phi_p}(\boldsymbol{\theta}) = \sum_{p=0}^{N-1} < f(x,\boldsymbol{\theta}), \boldsymbol{\Phi_p}(\boldsymbol{\theta}) >_{\boldsymbol{\rho}} \boldsymbol{\Phi_p}(\boldsymbol{\theta})$$

Where $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_d)^T$; $\quad \boldsymbol{\theta} : \Omega \to \Gamma$ and $\boldsymbol{\rho}(\boldsymbol{\theta}) := \prod_{i=1}^{d} \rho_i(\theta_i)$

And $\boldsymbol{\Phi}_{p_i}(\boldsymbol{\theta})$ are orthonormal multivariate polynomials constructed via a tensor product basis of the univariate polynomials $\boldsymbol{\Phi_p}(\boldsymbol{\theta}) := \Phi_{p_1}(\theta_1) \cdot \ldots \cdot \Phi_{p_d}(\theta_d)$
Coefficients:

$$c_{\boldsymbol{p}}(x) = \mathbb{E}[f(x,\boldsymbol{\theta})\boldsymbol{\Phi}_p(\boldsymbol{\theta})] = \int_{\boldsymbol{\Gamma}} f(x,\boldsymbol{\theta})\boldsymbol{\Phi}_p(\boldsymbol{\theta})\boldsymbol{\rho}(\boldsymbol{\theta})d\boldsymbol{\theta}$$

(Isotropic Full Tensor) Pseudo-spectral projection (PSP)

$$\boldsymbol{\mathcal{S}_p^N} = \sum_{q=0}^{N-1} \mathcal{Q}(f\boldsymbol{\Phi_p})\boldsymbol{\Phi_p}(\boldsymbol{\theta}) = \sum_{q=0}^{N-1} \hat{c}_{\boldsymbol{p}}(x)\boldsymbol{\Phi_p}(\boldsymbol{\theta})$$

Post-processing

Quantify uncertainty of Output of Interest (OoI)

$$E[\mathcal{O}] = \int_{\boldsymbol{\Gamma}} \mathcal{O}(f(x,\boldsymbol{\theta}))\boldsymbol{\rho}(\boldsymbol{\theta})d\boldsymbol{\theta}; \quad Var[\mathcal{O}] = E[\mathcal{O}^2] - (E[\mathcal{O}])^2$$

Variance based sensitivity analysis

$$S_i^T = \frac{Var(f) - Var(E(f|\boldsymbol{\theta}_{-i}))}{Var(f)} = \frac{E(Var(f|\boldsymbol{\theta}_{-i}))}{Var(f)}$$

Use gPCE coeff. to compute expectation and variance:

$$\mathbb{E}[f_N(x,\boldsymbol{\theta})] = c_0(x) \qquad Var[f_N(x,\boldsymbol{\theta})] = \sum_{p=1}^{N-1} c_{\boldsymbol{p}}^2(x)$$

Use gPCE coeff. to compute Sobol' indices:[3]

$$S_i^T = \frac{\sum_{p \in A_i} c_p^2(x)}{Var[f_N(x,\boldsymbol{\theta})]}, \qquad i = 1, \ldots, d$$

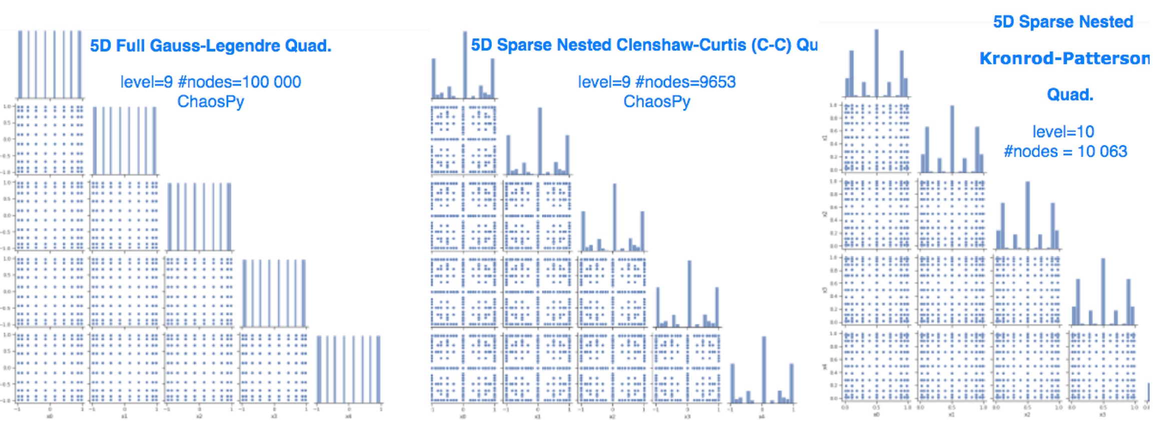
Sparse Grid (SG) and Combination Technique (CT)

- **Main problem:** Curse of dimension with full grids
- **Idea:** Reduce point numbers by removing point sets that contribute least

⇒ Reduction of point numbers from $\mathcal{O}(N^d)$ to $\mathcal{O}(Nlog(N)^{d-1})$

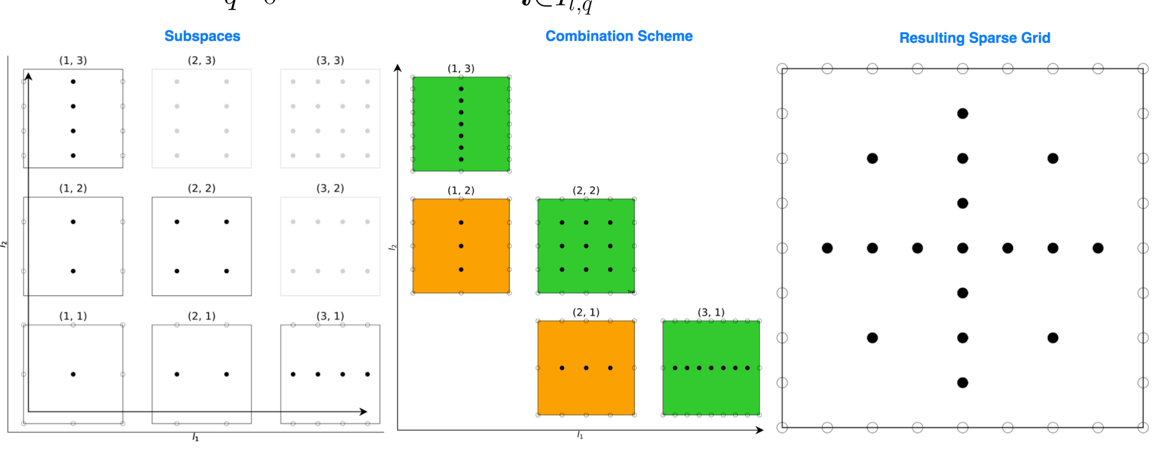
Sparse Grids can be constructed in various ways:

- different basis functions (e.g., linear hat, Lagrange poly, etc.)
- or the point positions (e.g., Clenshaw-Curtis, Leja)

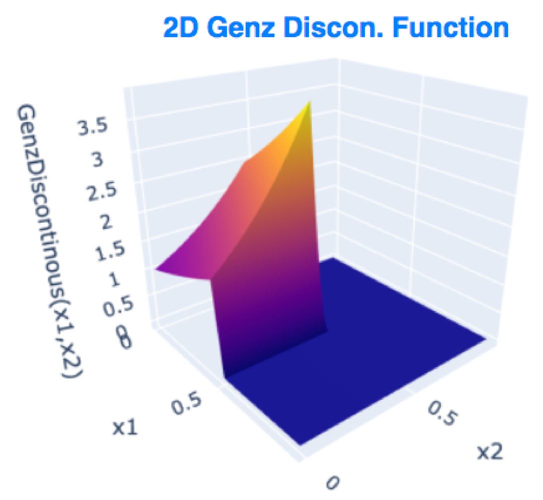


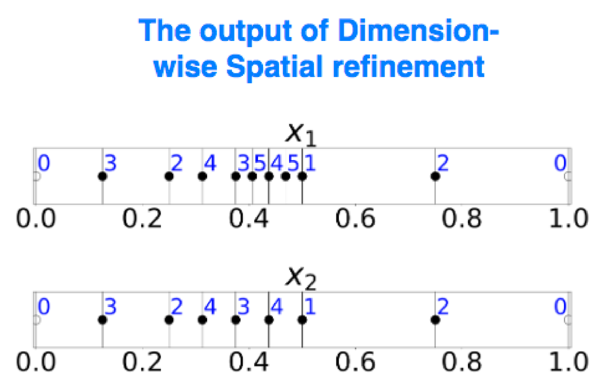
- **Combination Technique:** Efficient SG computation by linearly combining computations on cheap anisotropic full grids (e.g., component grids)

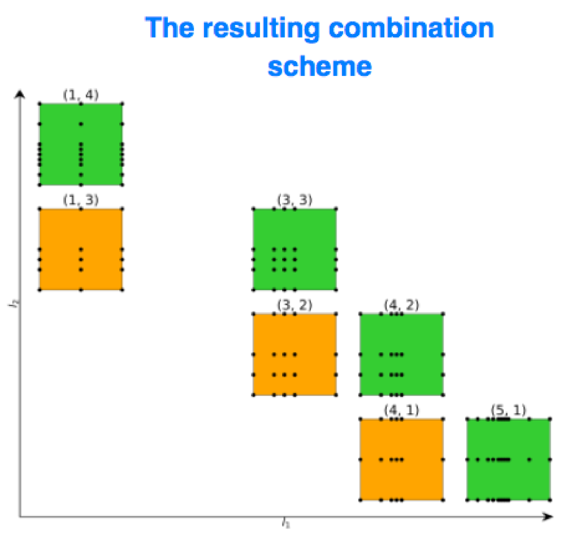
$$u_l^c = \sum_{q=0}^{d-1} (-1)^q \binom{d-1}{q} \sum_{\boldsymbol{l} \in I_{l,q}} u_{\boldsymbol{l}}, \qquad I_{l,q} = \{\boldsymbol{l} \in \mathbb{N}_0^d \| \boldsymbol{l} \|_1 = l + d - 1 - q\}$$

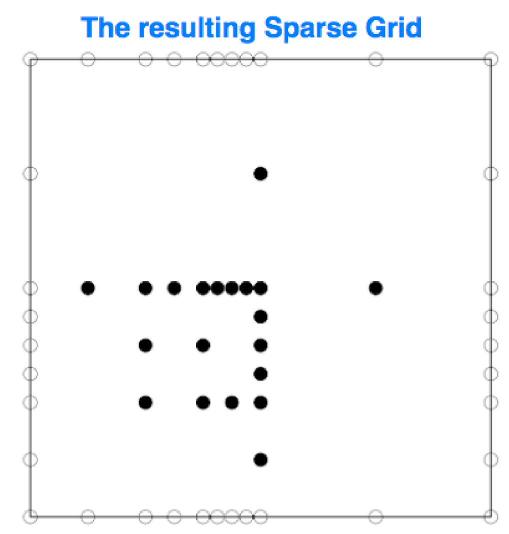


Dimension-Wise Spatially Adaptive SG CT[4]









Drawback: Standard CT offers no spatial adaptivity

CT with Spatial Adaptivity - use rectilinear grids constructed via a tensor product of refined 1-D grids[4]

Key components:

- 1D refinements define the adaptive process
- Creating a global scheme from these 1D point sets
- Special error estimators guide the refinement

UQ with Sparse Grids

Multiple ways how to combine the gPCE and SG!

Var 1: Sparse PSP[5,6]

- Approximate all the weighted integrals of f via some sparse interpolatory quadrature scheme (i.e., sparse quadrature scheme generated with CT)

$\hat{c}_{\boldsymbol{p}}(x) = \sum_m \cdots \sum_m f(x, \Theta_m^1, \ldots, \Theta_m^d)\boldsymbol{\Phi_p}(\Theta_m^1, \ldots, \Theta_m^d)\omega_m^1 \ldots \omega_m^d$

Var2: SG Interpolation Surrogate + gPCE

- SG Interpolation of $f(x,\boldsymbol{\theta})$

$$f(x,\boldsymbol{\theta}) \approx \boldsymbol{\mathcal{U}_{SGI}} = f_{SGI}(x,\boldsymbol{\theta}) = \sum_{\boldsymbol{l} \in j, \boldsymbol{i} \in \boldsymbol{l}} \alpha_{\boldsymbol{l},\boldsymbol{i}}(x)\boldsymbol{\varphi}_{l,i}(\boldsymbol{\theta})$$

Where $\alpha_{\boldsymbol{l},\boldsymbol{i}}(x,t)$ are hierarchical surpluses, and $\boldsymbol{\varphi}_{l_j,i_j}(\boldsymbol{\theta}) = \boldsymbol{\varphi}_{l,i}(\boldsymbol{\theta}) = \prod_j^d \varphi_{l_j,i_j}(\theta_j)$ are d-variate hierarchical basis functions

- Use SG model surrogate to compute gPCE coefficients[7]

$$\hat{c}_{\boldsymbol{p}}(x) = \int_{\boldsymbol{\Gamma}} f_{\mathcal{SGI}}(x,\boldsymbol{\theta})\boldsymbol{\Phi_p}(\boldsymbol{\theta})\boldsymbol{\rho}(\boldsymbol{\theta})d\boldsymbol{\theta}$$
$$= \sum_{\boldsymbol{l},\boldsymbol{i}} \alpha_{\boldsymbol{l},\boldsymbol{i}}(x) \prod_{j=1}^{d} \int_{\Gamma_j} \boldsymbol{\Phi}_j(\theta_j)\varphi_{l_j,i_j}(\theta_j)d\theta_j$$

- Variants:
  - Use some quadrature rule to approximate inner integrals
  - Analytical computation of 1D integrals where the integrand is a product of polynomials

Var 3: Spatially Adaptive Sparse Interpolatory Quadrature

- Approximate all weighted integrals of f,
  e.g., $c_{\boldsymbol{p}}(x)$ (Spatially Adaptive PSP), $E[\mathcal{O}(f)], Var[\mathcal{O}(f)]$
  with spatially adaptive SG quadrature scheme

UQ Designed Strategies

Variant	Method	Interpolation method (SGI)	quadrature method	gPCE
Var 1	m1	no	Full Gauss-Legendre	yes
	m2	no	(Sparse) Clenshaw-Curtis	yes
	m3	no	(Sparse) delayed Kronrod-Patterson[8]	yes
Var 2	m4	piecewise linear, standard CT	Gauss-Legendre (high order)	yes
	m5	piecewise linear, spatially adaptive CT	Gauss-Legendre (high order)	yes
	m6	piecewise linear, standard CT	analytical computation	yes
	m7	piecewise linear, spatially adaptive CT	analytical computation	yes
Var 3	m8	spatially adaptive sparse interpolatory quad. for $c_{\boldsymbol{p}}(x)$		yes
	m9	spatially adaptive sparse interpolatory quad. for $E[\mathcal{O}(f)], \quad Var[\mathcal{O}(f)]$		no

Some implementation aspects:

- Libraries used - **SparseSpACE** & **ChaosPy**
- Parallel aspect - parallel model runs inside one component grid
- Avoiding aliasing errors in PSP
  (i.e., taking care of polynomial exactness of quad. rules)[6]
- Linear and non-linear transformations of nodes

Open question - Building Adaptive SG Surrogate

- of the model itself?
- some likelihood function (suitable for inversion)?

First Results

Benchmark Convergence of different methods

- (gPCE or SG) Surrogate construction of Genz function set, including discontinuous fun. (5D)
- SA of Ishigami Function (3D)
- Convergence results as expected - adaptive approaches comparable to or better than non-adaptive
- For simple cases, 2 stages approach (Var2) is not much beneficial

Time-wise UQ SA of Hydrological Model with Var 2 m5

- Single Adaptive SG Surrogate for all the time-steps

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