Uncertainty Quantification in Climate Modeling

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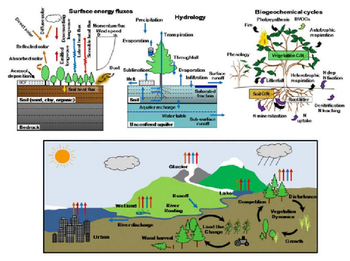
Uncertainty quantification challenges in climate models

- Computationally expensive model simulations
- High-dimensional input parameter space
- Physical constraints and dependencies for some input parameters
- Non-linear dependence of output quantities of interest on inputs



http://www.cesm.ucar.edu/models/clm/

Community Land Model (CLM)

- Nested computational grid hierarchy
- Represents spatial heterogeneity of the land surface
- A single-site, 1000-yr simulation takes $\sim$ 10 hrs on 1 CPU
- Involves $\sim$ 80 input parameters

Problem formulation: surrogate model construction

- Input parameter vector $\boldsymbol{\lambda}$
- Forward function (CLM simulation) $f(\cdot)$
- Given a set of *training* model runs, $(\boldsymbol{\lambda}_i, f(\boldsymbol{\lambda}_i))_{i=1}^N$, build a *surrogate* $f_s(\cdot) \approx f(\cdot)$ that is cheap to evaluate

The surrogate model can be used for

- Global sensitivity analysis
- Optimization
- Forward uncertainty propagation
- Input parameter inference

Polynomial chaos spectral representation serves as a surrogate model

To build a surrogate representation for input-output relationship, Polynomial Chaos (PC) spectral expansions are used; see [1].

- Interprets input parameters as random variables
- Allows propagation of input parameter uncertainties to outputs of interest
- Serves as a computationally inexpensive surrogate for calibration or optimization

Input parameters are represented via their cumulative distribution function (CDF) $F(\cdot)$, such that, with $\eta_i \sim \text{Uniform}[-1,1]$, we have:

$$\lambda_i = F_{\lambda_i}^{-1}\left(\frac{\eta_i+1}{2}\right), \qquad \text{for } i = 1,2,\ldots,d.$$

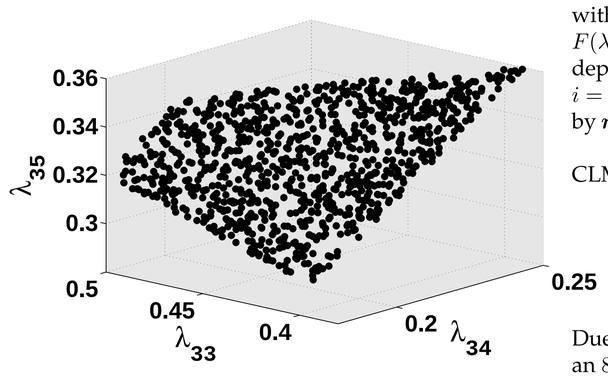
If input parameters are uniform $\lambda_i \sim \text{Uniform}[a_i, b_i]$, then

$$\lambda_i = \frac{a_i+b_i}{2} + \frac{b_i-a_i}{2}\,\eta_i.$$

Output is represented with respect to Legendre polynomials

$$f(\boldsymbol{\lambda}(\boldsymbol{\eta})) \approx y_{\boldsymbol{c}}(\boldsymbol{\eta}) \equiv \sum_{k=0}^{K} c_k \Psi_k(\boldsymbol{\eta}).$$

Rosenblatt transformation maps constrained input parameters to an unconstrained space



Given a vector of random variables $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_{d'})$ with known joint cumulative distribution function (CDF) $F(\lambda_1, \ldots, \lambda_{d'})$, one can obtain a set of η_i's that are independent uniform random variables on $[-1,1]$ for all $i = 1,2,\ldots,d$, using conditional CDFs. This map, denoted by $\boldsymbol{\eta} = R(\boldsymbol{\lambda})$, is called the *Rosenblatt transformation* (RT) [4].

CLM implemented with input parameter constraints

$$\begin{aligned} \lambda_{18} &< \lambda_{22}, \\ \lambda_{30}+\lambda_{31}+\lambda_{32} &= 1, \\ \lambda_{33}+\lambda_{34}+\lambda_{35} &= 1. \end{aligned}$$

Due to the last two mass fraction constraints, the RT maps an 81-dimensional parameter vector $\boldsymbol{\lambda}$ to $\boldsymbol{\eta} \in [-1,1]^{79}$.

Bayesian inference of PC modes allows surrogate construction with uncertainties associated with limited sampling

Bayes formula

$$p(\boldsymbol{c}|D) \propto L_{\mathcal{D}}(\boldsymbol{c}) p(\boldsymbol{c})$$

relates the prior distribution $p(\boldsymbol{c})$ of PC modes to the posterior $p(\boldsymbol{c}|\mathcal{D})$, where the data $\mathcal{D}$ is the set of all training runs $\mathcal{D} = (\boldsymbol{\lambda}_i, f(\boldsymbol{\lambda}_i))_{i=1}^N$.

The likelihood accounts for the discrepancy between the simulation data and the surrogate model [5],

$$L_{\mathcal{D}}(\boldsymbol{c}) \propto \exp\left(-\sum_{i=1}^{N} \frac{(f(\boldsymbol{\lambda}_i) - y_{\boldsymbol{c}}(\boldsymbol{\eta}_i))^2}{2\sigma^2}\right)$$

Iterative Bayesian compressive sensing (BCS): dimensionality reduction by using sparsity priors

The number of polynomial basis terms grows fast; a p-th order, d-dimensional basis has a total of $(p+d)!/(p!d!)$ terms. With large d, one can not afford to build a PC basis of order greater than two.
In order to use as few basis terms as possible, Gaussian *sparsity* priors are taken

$$p(\boldsymbol{c}) \propto \prod_{k=0}^{K} \exp\left(-\frac{c_k^2}{2s_k^2}\right).$$

Then, the posterior is an analytically tractable multivariate normal distribution. The parameters $(\sigma^2, s_0^2, \ldots, s_K^2)$ are fixed by evidence maximization. The optimization leads to very small s_i^2 for some indices i - the corresponding bases are discarded. For details, see [2].

Iterative BCS: We propose and implement an iterative procedure that allows increasing the order for the relevant basis terms while maintaining the dimensionality reduction. Only basis elements best explained by the data are retained [3].

Number of training runs needed for reliable detection of important dimensions

Assume $\boldsymbol{\lambda} \sim \text{Uniform}[-1,1]^d$ and consider test function

$$y = \exp\left(\sum_{i=1}^{d} a_i \lambda_i\right),$$

Dimensionality 'importances' dialed-in

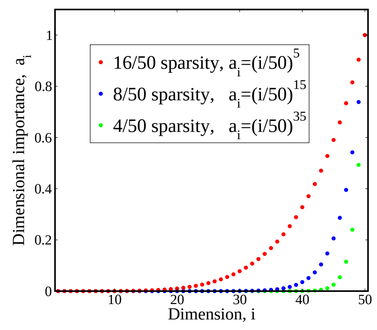
$$a_i = \begin{cases} 1 & \text{if } 1 \le i \le d_{\text{imp}}, \\ 0.1 & \text{if } d_{\text{imp}} < i \le d, \end{cases}$$

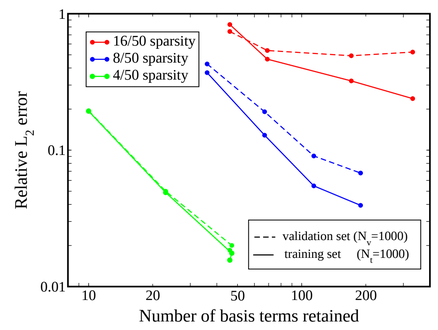
d_{imp}	d	N
1	any	20
2	any	50
5	any	130
10	any	980

Error for different model sparsity levels

Dimensionality 'importances' are chosen so that 90% of energy is in a small subset of dimensions, i.e. model is 'sparse'.

Validation error increase indicates overfitting. $N_t = 1000$ training runs are sufficient if ~ 10 dimensions matter.

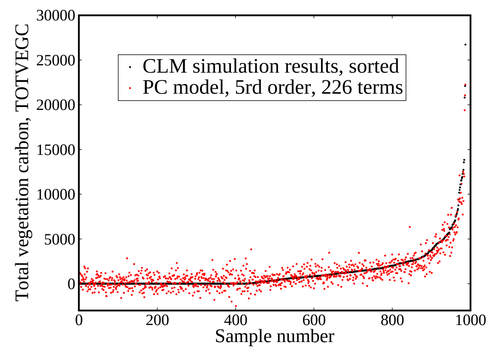




Results based on $N = 987$ training runs of CLM

- Single-site mode, $N = 987$ training runs
- Outputs: steady-state, 10-year averages of 7 quantities

Name	Units	Description
TOTVEGC	gC/m^2	Total vegetation carbon
TOTSOMC	gC/m^2	Total soil carbon
GPP	$gC/m^2/s$	Gross primary production
ERR	W/m^2	Energy conservation error
TLAI	none	Total leaf area index
EFLX_LH_TOT	W/m^2	Total latent heat flux
FSH	W/m^2	Sensible heat flux

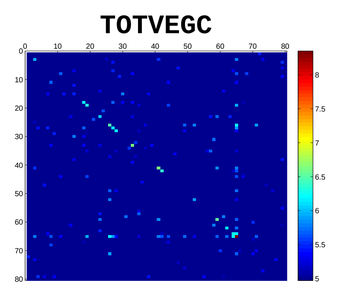


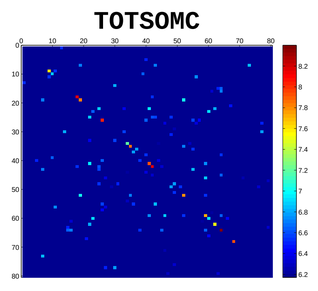
First order BCS: ranking of the most important input parameters for each output

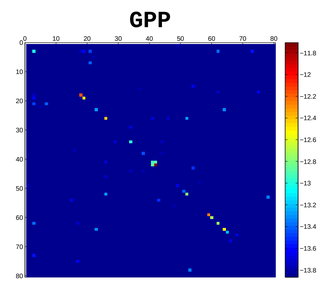
rank	TOTVEGC	TOTSOMC	GPP	ERR	TLAI	EFLX_LH_TOT	FSH
1	r_mort	q10_mr	leafcn	k_s4	froot_leaf	leafcn	rholnir
2	q10_mr	leafcn	k_s4	froot_leaf	q10_mr	q10_mr	q10_mr
3	froot_leaf	froot_leaf	froot_leaf	q10_hr	q10_hr	froot_leaf	leafcn
4	br_mr	br_mr	flnr	fflnr	leaf_long	k_s4	br_mr
5	q10_mr	fflnr	q10_mr	q10_mr	k_s4	br_mr	flnr
6	leafcn	dnp	q10_hr	dnp	br_mr	flnr	k_s4
7	k_s4	q10_hr	dnp	rf_s3s4	dnp	leaf_long	taulnir
8	stem_leaf	leaf_long	rf_s3s4	leaf_long	stem_leaf	q10_hr	froot_leaf
9	flnr	k_s4	leaf_long	mp	r_mort	rf_s3s4	frootcn
10	dnp	frootcn	br_mr	bdnr	rf_s3s4	stem_leaf	f_frag

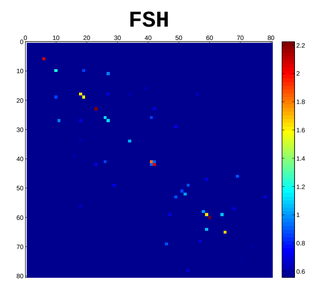
Second order BCS: most influential input parameter couplings for each output

- Each axis corresponds to the input parameter list. (i,j) element corresponds to the $\lambda_i \lambda_j$ basis term
- While full second order basis has $\sim$ 3000 terms, the iterative BCS algorithm picks only $\sim$ 100 of them that are able to capture the data well
- Higher order results leads to more accurate surrogate models. However, strong output non-linearities and smooth bases make input domain decomposition methods necessary









Conclusions

- Surrogate models are necessary for complex climate models
- Polynomial Chaos surrogate model is constructed using Bayesian techniques
- Constrained/dependent input parameters are mapped to an unconstrained input set via Rosenblatt transformation
- High-dimensionality is tackled by iterative Bayesian compressive sensing algorithm

Future work

- Targeted sampling for relevant basis terms to build a more accurate surrogate
- Clustering techniques for efficient domain decomposition to relieve the non-linear effects
- Spatially distributed input parameters, global CLM

References

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