Optimal Upscaling with Transport Maps

Chinedu Eleh and Hans-Werner van Wyk

Department of Mathematics and Statistics, Auburn University

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Introduction

Let

$$u = \mathcal{G}(x; \theta(\xi))$$

and consider the problem of finding θ, an input function to a mathematical model, given u an observation of solution to the model at point x [1].

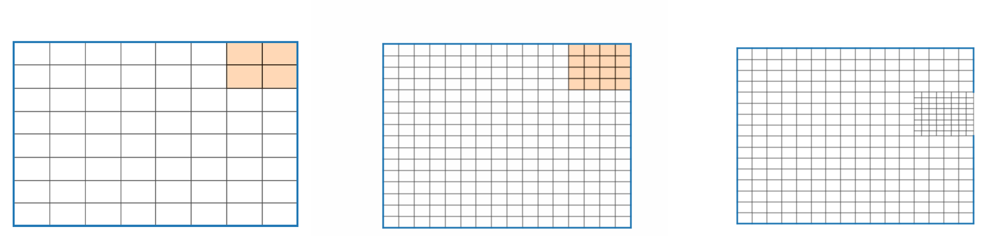
Goals

We aim to:

- Find a representation of $\theta(\xi)$ that captures the stochasticity in u.
- Learn a low dimensional representation of $\mathcal{G}$, the *observation operator* via *transport maps*.

Background

- When $\theta(\xi)$ is rough and $\mathcal{G}$ is a forward solver, FEM requires high resolution to capture fine details in u.



This leads to computational complications and intractability.

- Techniques such as midpoint (MP), spatial averaging (SA), shape function (SF) and series expansion (SE) are used to *homogenize* the random field [2].
- The method of moments approach easily leads to the long-standing well known unsolved *closure problem* [3].
- When $\theta(\xi)$ is a random variable and is $\ll 1$, u is also amenable to perturbation techniques.
- Monte Carlo sampling is great but we have to wrestle with *burn-out* and slow convergence.

If all existing methods are defied, what then is a way forward?

Transport Maps

- Transport maps are measure preserving transforms.
- Given measures μ and ν, find a map T s.t. $T_\sharp \mu = \nu$. i.e., find T s.t.

$$\min_T \mathbb{E}[||\xi - T(\xi)||] \quad \text{s. t.} \quad \nu = T_\sharp \mu \qquad (1)$$

- When the measure μ has no atoms, problem (1) has been shown to have a *unique* and *monotone* solution [4].

Karhunen-Loeve Expansion

- When the covariance kernel of a random field is known, the Kosambi-Karhunen-Loeve theorem guarantees the representation

$$\theta_t(\omega) = \mu_\theta(t) + \sum_{i=1}^{\infty} \sqrt{\lambda_i}\phi_i(t)\theta_i(\omega)$$

where ϕ_i's are the orthogonal eigenfunctions and λ_i's are the corresponding eigenvalues of the integral equation

$$\int_T C(t,s)\phi_i(s)ds = \lambda_i \phi_i(t), \qquad t \in T$$

Important Result

McCann [1995]:
Given that μ and ν are Borel probability meausres on $\mathbb{R}^n$ with μ vanishing on subsets of $\mathbb{R}^n$ having Hausdorff dimension less than or equal to $n-1$. Then the optimization problem (1) has a uniquely determined μ-almost everywhere solution. This map is the gradient of a convex function and is therefore monotone [5]

Generalized Polynomial Chaos Expansion

- Generalized polynomial chaos are *orthogonal* polynomials w.r.t to the standard probability distributions.

Distribution	polynomials	density
Gaussian	Hermite	$\rho(\xi) = \frac{1}{\sqrt{2\pi}} e^{-\xi^2/2}$
Gamma(α, λ)	Laguerre	$\rho(\xi) = \frac{\lambda}{\xi(\alpha)} (\lambda\xi)^{\alpha-1} e^{-\lambda\xi}$
Beta(α, β)	Jacobi	$\rho(\xi) = \frac{(1-\xi)^\alpha (1+\xi)^\beta}{2^{\alpha+\beta+1} B(\alpha+1, \beta+1)}$
Uniform(α, β)	Legendre	$\rho(\xi) = \frac{1}{\beta - \alpha}$
Arcsin	Chebyshev	$\rho(\xi) = \frac{1}{\sqrt{1-\xi^2}}$

Figure 1:Wiener-Askey Scheme

- Cameron & Martin [1947] first proved the space of the chaos polynomials is dense in L^2, for the case when the distribution is *Gaussian*.
- Ernst etal [2012] extended this result to an arbitrary distribution whose moment problem is uniquely solvable.

Results

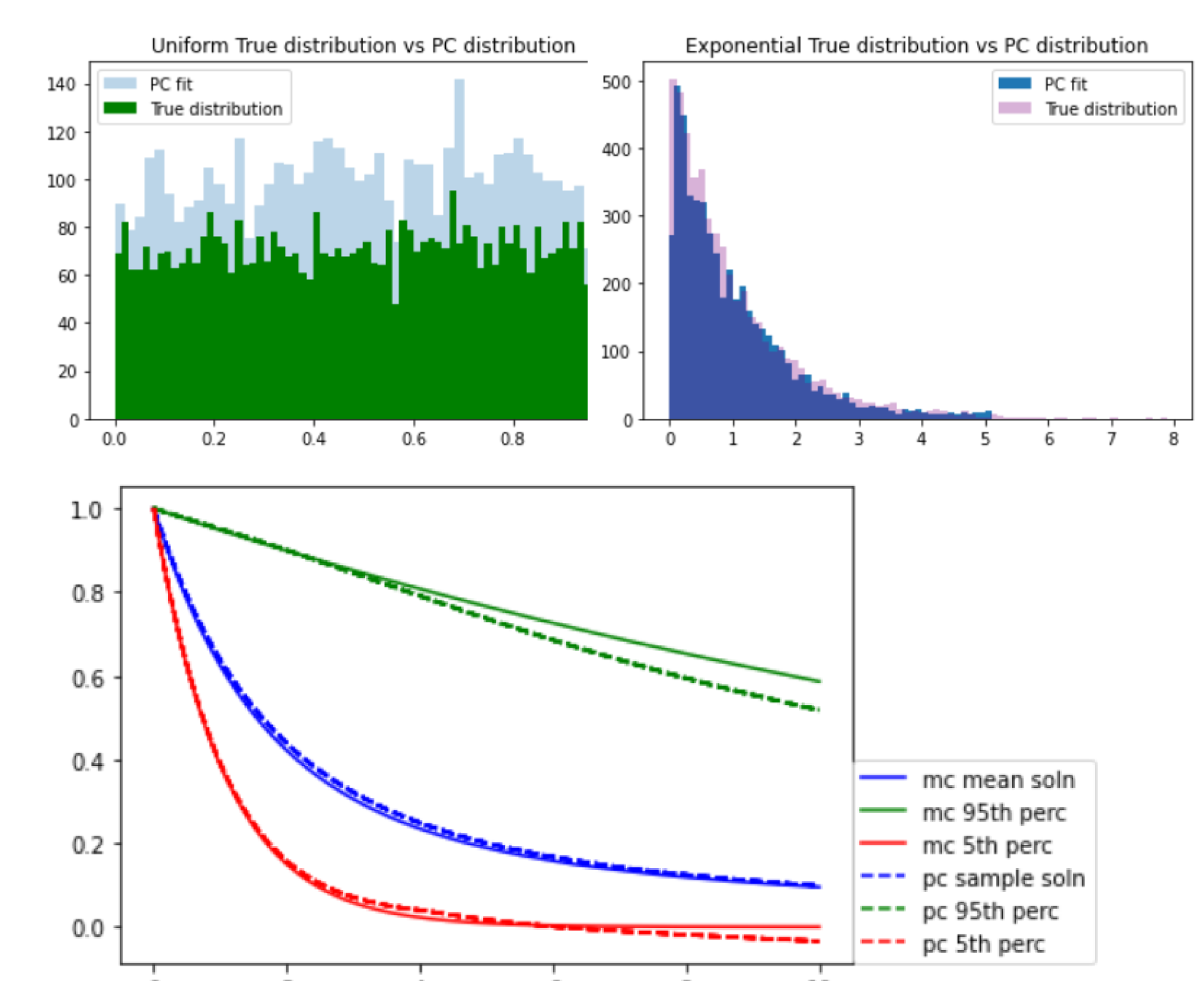


Figure 2:Soln of $u'(x) = -\theta u(x)$

Fig (2) compares a 5, 9 degrees chaos representation for the parameter θ & the solution u respectively with 10, 000 Monte Carlo samples [6].

Conclusion

- Most, if not all mathematical models depend on certain random parameter(s)
- Successes in making inference from or validating these models depend on how well the stochastic information from these parameters are propagated into the state variables
- We demonstrated that transport maps are powerful and handy in this regard
- In progress, we are looking to leverage the expressive power of Deep Neural Networks in constructing transport maps

Contact Information

- Web: `http://webhome.auburn.edu/~cae0027/`
- Email: cae0027@auburn.edu

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In Preparation.