Computational Information Games

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Main Question

Can we turn the process of discovery of a scalable numerical method into a UQ problem and, to some degree, solve it as such in an automated fashion?

Can we use a computer, not only to implement a numerical method but also to find the method itself?

Problem: Find a method for solving (1) as fast as possible to a given accuracy

(1)
$$\begin{cases} -\operatorname{div}(a\nabla u) = g, & x \in \Omega, \\ u = 0, & x \in \partial\Omega, \end{cases}$$
$$\Omega \subset \mathbb{R}^d \quad \partial\Omega \text{ is piec. Lip.} \\a \text{ unif. ell.} \\a_{i,j} \in L^{\infty}(\Omega) \end{cases}$$

Multigrid Methods

Multigrid: [Fedorenko, 1961, Brandt, 1973, Hackbusch, 1978]

Multiresolution/Wavelet based methods

[Brewster and Beylkin, 1995, Beylkin and Coult, 1998, Averbuch et al., 1998]

 \mathbb{R}^{m}

• Linear complexity with smooth coefficients

Problem Severely affected by lack of smoothness

Robust/Algebraic multigrid

[Mandel et al., 1999, Wan-Chan-Smith, 1999, Xu and Zikatanov, 2004, Xu and Zhu, 2008], [Ruge-Stüben, 1987] [Panayot - 2010]

Stabilized Hierarchical bases, Multilevel preconditioners

[Vassilevski - Wang, 1997, 1998] [Panayot - Vassilevski, 1997] [Chow - Vassilevski, 2003] [Aksoylu- Holst, 2010]

 Some degree of robustness but problem remains open with rough coefficients

Why? Interpolation operators are unknown Don't know how to bridge scales with rough coefficients!

Low Rank Matrix Decomposition methods

Fast Multipole Method: [Greengard and Rokhlin, 1987]Hierarchical Matrix Method: [Hackbusch et al., 2002][Bebendorf, 2008]:

$$N \ln^{d+3} N$$
 complexity

Common theme between these methods

Their process of discovery is based on intuition, brilliant insight, and guesswork



Can we turn this process of discovery into an algorithm?





[Owhadi 2015, Multi-grid with rough coefficients and Multiresolution PDE decomposition from Hierarchical Information Games, arXiv:1503.03467]

Resulting method:

$$N \ln^2 N$$
 complexity

This is a theorem

Resulting method:

$$\begin{cases} -\operatorname{div}(a\nabla u) = g \text{ in } \Omega, \\ u = 0 \text{ on } \partial\Omega, \end{cases}$$

$$H_0^1(\Omega) = \mathfrak{W}^{(1)} \oplus_a \mathfrak{W}^{(2)} \oplus_a \cdots \oplus_a \mathfrak{W}^{(k)} \oplus_a \cdots$$

$$\langle \psi, \chi \rangle_a := \int_{\Omega} (\nabla \psi)^T a \nabla \chi = 0 \text{ for } (\psi, \chi) \in \mathfrak{W}^{(i)} \times \mathfrak{W}^{(j)}, \, i \neq j$$



$$||v||_a^2 := \langle v, v \rangle_a = \int_{\Omega} (\nabla v)^T a \nabla v$$

Looks like an eigenspace decomposition

$$u = w^{(1)} + w^{(2)} + \dots + w^{(k)} + \dots$$

$w^{(k)} = F.E.$ sol. of PDE in $\mathfrak{W}^{(k)}$ Can be computed independently

 $B^{(k)}$: Stiffness matrix of PDE in $\mathfrak{W}^{(k)}$



Just relax in $\mathfrak{W}^{(k)}$ to find $w^{(k)}$

Quacks like an eigenspace decomposition

Multiresolution decomposition of solution space



Solve time-discretized wave equation (implicit time steps) with rough coefficients in $\mathcal{O}(N \ln^2 N)$ -complexity

Swims like an eigenspace decomposition

\mathfrak{V} : F.E. space of $H_0^1(\Omega)$ of dim. N

Theorem The decomposition $\mathfrak{V} = \mathfrak{W}^{(1)} \oplus_a \mathfrak{W}^{(2)} \oplus_a \cdots \oplus_a \mathfrak{W}^{(k)}$

Can be performed and stored in

$$\mathcal{O}(N\ln^2 N)$$
 operations

Doesn't have the complexity of an eigenspace decomposition

Basis functions look like and behave like wavelets: Localized and can be used to compress the operator and locally analyze the solution space

$$\begin{array}{c} H_0^1(\Omega) & \underbrace{\operatorname{div}(a\nabla \cdot)}_{\operatorname{Reduced operator}} H^{-1}(\Omega) \\ u & g \\ \uparrow & \downarrow \\ \mathbb{R}^m \ni u_m, \underbrace{\operatorname{Inverse Problem}}_{g_m} g_m \in \mathbb{R}^m \\ \text{Numerical implementation requires computation with partial information.} \\ \phi_1, \dots, \phi_m \in L^2(\Omega) \\ u_m = (\int_{\Omega} \phi_1 u, \dots, \int_{\Omega} \phi_m u) \\ u_m \in \mathbb{R}^m \underbrace{\operatorname{Missing information}}_{g_m} u \in H_0^1(\Omega) \end{array}$$

Player A & B both have a blue and a red marble At the same time, they show each other a marble

How should A & B play the (repeated) game?

A's expected payoff John Nash = 3pq + (1-p)(1-q) - 2p(1-q) - 2q(1-p)= $1 - 3q + p(8q - 3) = -\frac{1}{8}$ for $q = \frac{3}{8}$

Continuous game but as in decision theory under compactness it can be approximated by a finite game

Abraham Wald

The best strategy for A is to play at random

Player B's best strategy live in the Bayesian class of estimators

Player B's class of mixed strategies

Pretend that player A is choosing g at random $g \in L^2(\Omega)$ \longleftrightarrow ξ : Random field $\begin{cases} -\operatorname{div}(a\nabla u) = g \text{ in } \Omega, \\ u = 0 \text{ on } \partial\Omega, \end{cases}$ \longleftrightarrow $\begin{cases} -\operatorname{div}(a\nabla v) = \xi \text{ in } \Omega, \\ v = 0 \text{ on } \partial\Omega, \end{cases}$

Player B's bet

 $u^*(x) := \mathbb{E}\left[v(x) \left| \int_{\Omega} v(y) \phi_i(y) \, dy = \int_{\Omega} u(y) \phi_i(y) \, dy, \forall i \right]$

Player's B optimal strategy?

Player B's best bet? \longleftrightarrow min max problem over distribution of ξ

What are these gamblets?

Depend on

- Γ : Covariance function of ξ (Player B's decision)
- $(\phi_i)_{i=1}^m$: Measurements functions (rules of the game)

- $a = I_d \iff \psi_i$: Polyharmonic splines [Harder-Desmarais, 1972][Duchon 1976, 1977, 1978]
- $a_{i,j} \in L^{\infty}(\Omega) \iff \psi_i$: Rough Polyharmonic splines [Owhadi-Zhang-Berlyand 2013]

What is Player B's best strategy? What is Player B's best choice for $\Gamma(x, y) = \mathbb{E}[\xi(x)\xi(y)]$?

Why? See algebraic generalization

The recovery is optimal (Galerkin projection)

Theorem If $\Gamma = \mathcal{L}$ then

 $u^*(x)$ is the F.E. solution of (1) in span{ $\mathcal{L}^{-1}\phi_i | i = 1, ..., m$ }

$$||u - u^*||_a = \inf_{\psi \in \operatorname{span}\{\mathcal{L}^{-1}\phi_i : i \in \{1, \dots, m\}\}} ||u - \psi||_a$$

1)
$$\begin{cases} \mathcal{L} = -\operatorname{div}(a\nabla \cdot) \\ -\operatorname{div}(a\nabla u) = g, & x \in \Omega, \\ u = 0, & x \in \partial\Omega, \end{cases}$$

Optimal variational properties

Theorem

 $\sum_{i=1}^{m} w_i \psi_i \text{ minimizes } \|\psi\|_a$ over all ψ such that $\int_{\Omega} \phi_j \psi = w_j$ for $j = 1, \dots, m$

Variational characterization

Theorem ψ_i : Unique minimizer of $\begin{cases} \text{Minimize} & \|\psi\|_a \\ \text{Subject to} & \psi \in H^1_0(\Omega) \text{ and } \int_{\Omega} \phi_j \psi = \delta_{i,j}, \quad j = 1, \dots, m \end{cases}$

Selection of measurement functions

Example Indicator functions of a Partition of Ω of resolution H

Elementary gamble

Your best bet on the value of u given the information that

$$\int_{\tau_i} u = 1$$
 and $\int_{\tau_j} u = 0$ for $j \neq i$

Theorem

$$\int_{\Omega \cap (B(\tau_i, r))^c} (\nabla \psi_i)^T a \nabla \psi_i \le e^{-\frac{r}{\tau_H}} \|\psi_i\|_a^2$$

Formulation of the hierarchical game

Hierarchy of nested Measurement functions

$$\phi_{i_1,...,i_k}^{(k)}$$
 with $k \in \{1,..., \phi_{i_1,...,i_k}^{(k)} = \sum_j c_{i,j} \phi_{i,j}^{(k+1)}$

Example

 $\phi_i^{(k)}$: Indicator functions of a

 $\phi_{i_1,j_2,k_1}^{(3)}\phi_{i_1,j_2,k_2}^{(3)}\phi_{i_1,j_2,k_3}^{(3)}\phi_{i_1,j_2,k_4}^{(3)}$

 $\phi_{i_1,j_1}^{(2)} \phi_{i_1,j_2}^{(2)} \phi_{i_1,j_3}^{(2)} \phi_{i_1,j_4}^{(2)}$

 $\phi_{i_1}^{(1)}$

hierarchical nested partition of Ω of resolution $H_k = 2^{-k}$

q

In the discrete setting simply aggregate elements (as in algebraic multigrid)

Player B's best strategy
$$\xi \sim \mathcal{N}(0, \mathcal{L})$$
 $\left\{ -\operatorname{div}(a\nabla u) = g \text{ in } \Omega, \\ u = 0 \text{ on } \partial\Omega, \end{array} \right\}$ $\left\{ -\operatorname{div}(a\nabla v) = \xi \text{ in } \Omega, \\ v = 0 \text{ on } \partial\Omega, \end{array} \right.$

Player B's bets

$$u^{(k)}(x) := \mathbb{E}\left[v(x) \left| \int_{\Omega} v(y) \phi_i^{(k)}(y) \, dy = \int_{\Omega} u(y) \phi_i^{(k)}(y) \, dy, \, i \in \mathcal{I}_k \right]$$

The sequence of approximations forms a martingale under the mixed strategy emerging from the game

$$\mathcal{F}_k = \sigma(\int_{\Omega} v \phi_i^{(k)}, i \in \mathcal{I}_k) \quad v^{(k)}(x) := \mathbb{E}[v(x)|\mathcal{F}_k]$$

Theorem

$$\mathcal{F}_k \subset \mathcal{F}_{k+1}$$

$$v^{(k)}(x) := \mathbb{E}\left[v^{(k+1)}(x)\big|\mathcal{F}_k\right]$$

Accuracy of the recovery

In a discrete setting the last step of the game recovers the solution to numerical precision

Gamblets Elementary gambles form a hierarchy of deterministic basis functions for player B's hierarchy of bets

Theorem
$$u^{(k)}(x) = \sum_i \psi_i^{(k)}(x) \int_{\Omega} u(y) \phi_i^{(k)}(y) \, dy$$

 $\psi_i^{(k)}$: Elementary gambles/bets at resolution $H_k = 2^{-k}$

$$\psi_i^{(k)}(x) := \mathbb{E}\left[v(x) \middle| \int_{\Omega} v(y) \phi_j^{(k)}(y) \, dy = \delta_{i,j}, \, j \in \mathcal{I}_k\right]$$

Gamblets are nested

$$\begin{split} \mathfrak{V}^{(k)} &:= \operatorname{span}\{\psi_{i}^{(k)}, i \in \mathcal{I}_{k}\} \begin{array}{c} \psi_{i_{1}}^{(1)} \\ \psi_{i_{1}}^{(1)} \\ \psi_{i_{1},j_{1}}^{(2)} & \psi_{i_{1},j_{2}}^{(2)} & \psi_{i_{1},j_{3}}^{(2)} \\ \psi_{i_{1},j_{1}}^{(2)} & \psi_{i_{1},j_{2}}^{(2)} & \psi_{i_{1},j_{3}}^{(2)} \\ \psi_{i_{1},j_{1}}^{(3)} & \psi_{i_{1},j_{2},k_{3}}^{(3)} \\ \psi_{i_{1},j_{2},k_{1}}^{(3)} & \psi_{i_{1},j_{2},k_{3}}^{(3)} \\ \psi_{i_{1},j_{2},k_{1}}^{(3)} & \psi_{i_{1},j_{2},k_{3}}^{(3)} \\ \psi_{i_{1},j_{2},k_{3}}^{(3)} & \psi_{i_{1},j_{2},k_{3}}^{(3)} \\ \psi_{i_{1},j_{2$$

$$\psi_i^{(k)}(x) = \sum_{j \in \mathcal{I}_{k+1}} R_{i,j}^{(k)} \psi_j^{(k+1)}(x)$$

Interpolation/Prolongation operator

$$R_{i,j}^{(k)} = \mathbb{E}\left[\int_{\Omega} v(y)\phi_{j}^{(k+1)}(y) \, dy \left| \int_{\Omega} v(y)\phi_{l}^{(k)}(y) \, dy = \delta_{i,l}, \, l \in \mathcal{I}_{k}\right]\right]$$

$$R_{i,j}^{(k)}$$
Your best bet on the value of $\int_{\tau_{j}^{(k+1)}} u$
given the information that
 $\int_{\tau_{i}^{(k)}} u = 1$ and $\int_{\tau_{l}} u = 0$ for $l \neq i$
 $(k+1)$

At this stage you can finish with classical multigrid

But we want multiresolution decomposition

Elementary gamble

Your best bet on the value of u given the information that

 $\int_{\tau_i^{(k)}} u = 1, \int_{\tau_i^{(k)}} u = -1 \text{ and } \int_{\tau_j^{(k)}} u = 0 \text{ for } j \neq i$

$$\chi_{i}^{(k)} = \psi_{i}^{(k)} - \psi_{i^{-}}^{(k)}$$

Multiresolution decomposition of the solution space

$$\mathfrak{V}^{(k)} := \operatorname{span}\{\psi_i^{(k)}, i \in \mathcal{I}_k\}$$

 $\mathfrak{W}^{(k)} := \operatorname{span}\{\chi_i^{(k)}, i\}$

 $\mathfrak{W}^{(k+1)}: \text{ Orthogonal complement of } \mathfrak{V}^{(k)} \text{ in } \mathfrak{V}^{(k+1)}$ with respect to $\langle \psi, \chi \rangle_a := \int_{\Omega} (\nabla \psi)^T a \nabla \chi$

Theorem

$$H_0^1(\Omega) = \mathfrak{V}^{(1)} \oplus_a \mathfrak{W}^{(2)} \oplus_a \cdots \oplus_a \mathfrak{W}^{(k)} \oplus_a \cdots$$

Multiresolution decomposition of the solution

Theorem

 $u^{(k+1)} - u^{(k)} =$ F.E. sol. of PDE in $\mathfrak{W}^{(k+1)}$

Subband solutions $u^{(k+1)} - u^{(k)}$ can be computed independently

Uniformly bounded condition numbers

$$A_{i,j}^{(k)} := \left\langle \psi_i^{(k)}, \psi_j^{(k)} \right\rangle_a$$

$$B_{i,j}^{(k)} := \left\langle \chi_i^{(k)}, \chi_j^{(k)} \right\rangle_a$$

Coefficients of the solution in the gamblet basis

Operator Compression

Gamblets behave like wavelets but they are adapted to the PDE and can compress its solution space

Throw 99% of the coefficients

Fast gamblet transform

 $\mathcal{O}(N \ln^2 N)$ complexity

Nesting
$$A^{(k)} = (R^{(k,k+1)})^T A^{(k+1)} R^{(k,k+1)}$$

Level(k) gamblets and stiffness matrices can be computed from level(k+1) gamblets and stiffness matrices

Well conditioned linear systems

Underlying linear systems have uniformly bounded condition numbers

$$\psi_i^{(k)} = \psi_{(i,1)}^{(k+1)} + \sum_j C_{i,j}^{(k+1),\chi} \chi_j^{(k+1)}$$

$$C^{(k+1),\chi} = (B^{(k+1)})^{-1} Z^{(k+1)}$$

Localization

$$Z_{j,i}^{(k+1)} := -(e_j^{(k+1)} - e_{j^-}^{(k+1)})^T A^{(k+1)} e_{(i,1)}^{(k+1)}$$

The nested computation can be localized without compromising accuracy or condition numbers

