

Battling bottlenecks:

Overcoming the computational complexity of reduced basis methods for high-d parameter spaces

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We consider the need to model physical systems of the form

$$\begin{split} \mathcal{L}(\mathbf{x},\mu) u(\mathbf{x},\mu) &= f(\mathbf{x},\mu) & \mathbf{x} \in \Omega \\ u(\mathbf{x},\mu) &= g(\mathbf{x},\mu) & \mathbf{x} \in \partial \Omega \end{split}$$

where the solutions are implicitly parameterized by

 $\mu \in \mathcal{D} \subset \mathsf{R}^M$

We focus on problems with special characteristics

- ✓ Real-time or near real time need
- Many query problems
- In situ needs/deployed system







What we need is an accurate way to evaluate the solution at new parameter values at reduced complexity.

Fast input-output procedure:

input: parameter value $\mu \in \mathcal{D}$





Let us define:

The exact solution: Find $u(\mu) \in X$ such that

 $a(u,\mu,v)=f(\mu,v), \ \forall v\in X$

The truth solution: Find $u_h(\mu) \in X_h$ such that $a_h(u_h, \mu, v_h) = f_h(\mu, v_h), \quad \forall v_h \in X_h \quad \dim(X_h) = \mathcal{N}$

The RB solution: Find $u_{RB}(\mu) \in X_N$ such that $a_h(u_{RB}, \mu, v_N) = f_h(\mu, v_N), \forall v_N \in X_N \quad \dim(X_N) = N$

We always assume that $\mathcal{N} \gg N$



Solving for the truth is expensive - but we need to be able to trust the RB solution

 $||u(\mu) - u_{RB}(\mu)|| \le ||u(\mu) - u_h(\mu)|| + ||u_h(\mu) - u_{RB}(\mu)||$

We assume that

$$\|u(\mu) - u_h(\mu)\| \le \varepsilon$$

This is <u>your favorite solver</u> and it is assumed it can be as accurate as you desire - the truth

So if we can bound we achieve two things

Certify the accuracy of the reduced basis method
 Use this estimate to build the basis



Let us define the residual in the dual norm

$$R_N(\mu, v) := f(v, \mu) - a(u_{RB}, \mu, v), \quad \forall v \in X$$
$$\varepsilon_N(\mu) := \sup_{v \in X} \frac{|R_N(\mu, v)|}{\|v\|_X}$$

and require stability as

$$\beta(\mu) := \inf_{v \in X} \sup_{w \in X} \frac{|a(v, \mu, w)|}{\|v\|_X \|w\|_X}$$

 $0 < \beta_{LB}(\mu) \leq \beta(\mu), \ \forall \mu \in \mathcal{D}$

then the error is obtained as

$$\Delta_N(\mu) := \frac{\varepsilon_N(\mu)}{\beta_{LB}(\mu)}$$



Defining the effectivity

$$\eta_N(\mu) := \frac{\Delta_N(\mu)}{\|u_h - u_{RB}\|_X}$$

One proves

$$1 \leq \eta_N(\mu), \ \forall \mu \in \mathcal{D}$$

So if the basis is known, we can estimate the error when using the reduced model

... but we have still to construct the reduced basis

We use the error estimator to construct the reduced basis in a greedy approach.



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Speed relies on the affine assumption

$$a(u, \mu, v) = \sum_{k=1}^{Q_a} \Theta_k(\mu) a_k(u, v)$$
$$f(\mu, v) = \sum_{k=1}^{Q_f} \Theta_k^f(\mu) f_k(v)$$

This pushes majority of work off-line, e.g.

$$\sum_{i=1}^{N} \left[\sum_{k=1}^{Q_a} \Theta_k(\mu) a_k(\xi_i, \xi_j) \right] u_N^j(\mu) = \sum_{k=1}^{Q_f} \Theta_k^f(\mu) f_k(\xi_j), \quad j \in [1, \dots, N]$$

All operations are now independent of ${\cal N}$ and depends solely on N and Q

Also possible for error estimator

One example - 2D Pacman problem



TM polarization

Scattering by 2D PEC Pacman

Backscatter depends very sensitively on cutout angle and frequency.

Difference in scattering is clear in fields



2D Pacman problem



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Note: Linear scale, not db scale

2D Pacman prototype for UQ

Fast evaluation over parameter space allows for rapid uncertainty quantification





Nymerical results: test I Scattering example Ults: test I





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Stability parameter 1 0.1 0.01 10 12 14 16 18 20 k 40 20 N±21 SOH -20 upper error bar lower error bar rcs(u_N) rcs(u_h) -40 12 14 16 18 20 10 k 40 20 N=22 RCS ° upper error bar lower error bar rcs(u_N) rcs(u_h) -20 -40 0.1 12 20 0.01 14 16 18 10 k 0.001 40 0.0001 20 N=2.3001 RCS 0 1 Upper error bar lower error bar rcs(u_N) rcs(u_h) -20 -40 M=5 M=10 12 14 18 20 10 16 M=15 k



So where are the bottlenecks?

In the online stage -

Large number of terms in the affine expansion

$$a(u,\mu,v) = \sum_{k=1}^{Q_a} \Theta_k(\mu) a_k(u,v)$$

Large number of terms in basis

$$N_d \propto N_1^{\alpha d}, \ 0 < \alpha \le 1$$

 $\mu \in \Pi_{train}$

In the offline stage -

The cost of greedy approach by evaluating the train space $\mu_{i+1} = \arg \sup \varepsilon_N(\mu)$ Also for SCM, EIM

Non-affine problems



Let us consider the extension of these techniques to problems described by integral equations

Electric field integral equation (EFIE)

$$ik \int_{\Gamma \times \Gamma} G_k(\boldsymbol{x}, \boldsymbol{y}) \left[\boldsymbol{j}(\boldsymbol{x}) \cdot \boldsymbol{j}^t(\boldsymbol{y}) - \frac{1}{k^2} \operatorname{div}_{\Gamma} \boldsymbol{j}(\boldsymbol{x}) \operatorname{div}_{\Gamma} \boldsymbol{j}^t(\boldsymbol{y}) \right] d\boldsymbol{x} d\boldsymbol{y} = \boldsymbol{F}(\boldsymbol{j}^t)$$

$$G_k(\boldsymbol{x}, \boldsymbol{y}) := rac{e^{ik|\boldsymbol{x}-\boldsymbol{y}|}}{|\boldsymbol{x}-\boldsymbol{y}|}.$$

Truth approximation is a standard MoM solver.

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$$M(f)(\mathbf{x}, \mu) = \sum_{m} a_m(\mu) f(\mathbf{x}, \mu_m)$$

Empirical Interpolation
 $\Omega_{\mathbf{x}} \in \mathcal{D}_{\mathbf{x}}$ by $f(\mathbf{x}, \mu)$ for all $(\mathbf{x}, \mu) \in \Omega$. The EIM is a
second approximation of $f(\mathbf{x}, \mu)$ for all $(\mathbf{x}, \mu) \in \Omega$. The EIM is a
lure that provides $\{\mu_m\}_{m=1}^M$ such that
 $\mathcal{I}_M(f)(\mathbf{x}; \mu) = \sum_{m=1}^M \alpha_m(\mu) f(\mathbf{x}; \mu_m)$
 $\mathcal{I}_M(f)(\mathbf{x}; \mu) = \sum_{m=1}^M \alpha_m(\mu) f(\mathbf{x}; \mu_m)$
d approximation of $f(\mathbf{x}, \mu)$ for $m = 1$ $(\mathbf{x}, \mu) \in \Omega$
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EFIE operators

$$G_k^{ns}(r) = G^{ns}(r;k) = \frac{e^{ikr} - 1}{r}, \quad r \in \mathbb{R}^+, k \in \mathbb{R}^+$$

$$\mathbf{E}^{i}(\boldsymbol{x};\boldsymbol{\mu}) = -\boldsymbol{p} e^{i\boldsymbol{k}\hat{\boldsymbol{s}}(\boldsymbol{\theta},\boldsymbol{\phi})\cdot\boldsymbol{x}}, \quad \boldsymbol{x}\in\Gamma,\boldsymbol{\mu}\in\mathcal{D}$$

EIM example Basic test case npirical Interpolation Method $f(x;k) = \frac{e^{ikx} - 1}{Numerical (results} k \in [1, k_{max}]$



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Results for EIM



Element based EIM direct computation. As solution, the *parameter* domain can adaptively be split into subel

the function is approximated by a different Magic point expansion.

Extension to an element based EIM



Adaptive EIM Gravity point splitting: numerical results Extension to multilevel EIM









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A typical greedy approach

Input: A train set $\Xi_{train} \subset \mathcal{D}$, a tolerance tol > 0**Output**: S_N and W_N 1: Initialization: Choose an initial parameter value $\mu^1 \in \Xi_{train}$, set $S_1 = \{\mu^1\}$, compute $v(\mu^1)$, set $W_1 = \{v(\mu^1)\}$, and N = 1; 2: while $\max_{\mu \in \Xi} \eta(\mu; W_N) > tol$ do For all $\boldsymbol{\mu} \in \Xi_{train}$, compute $\eta(\boldsymbol{\mu}; W_N)$; 3: 4: Choose $\boldsymbol{\mu}^{N+1} = \operatorname{argmax}_{\boldsymbol{\mu} \in \Xi_{train}} \eta(\boldsymbol{\mu}; W_N);$ 5: Set $S_{N+1} = S_N \cup \{\boldsymbol{\mu}^{N+1}\};$ 6: Compute $v(\boldsymbol{\mu}^{N+1})$, and set $W_{N+1} = W_N \cup \{v(\boldsymbol{\mu}^{N+1})\};$ 7: $N \leftarrow N + 1;$ 8: end while

For a high-d problem with a large training set, this is expensive

Strategy for high-d sampling



We introduce the saturation assumption

 $\eta(\boldsymbol{\mu}; W_M) \leq C_{sa} \eta(\boldsymbol{\mu}; W_N)$ for some $C_{sa} > 0$ for all 0 < N < M

Different interpretations

For $C_{sa} < 1$ - error is strictly decreasing For $C_{sa} \ge 1$ - error is allowed to increase (intermittently)

We shall use this approach to propose two different sampling

An approach using just this saturation assumption
 An adaptive sampling with additional benefits



Strategy I -

When looking for the max error over the training set, recompute estimator only for those points where

 $C_{sa}\eta(\mu, W_N) \ge error_{tmpmax}$

3: while
$$\max_{\mu \in \Xi_{train}} \eta_{saved}(\mu) \ge tol \operatorname{do}$$

4:
$$error_{tmpmax} = 0;$$

5: for all
$$\mu \in \Xi_{train}$$
 do

6: **if**
$$C_{sa}\eta_{saved}(\boldsymbol{\mu}) > error_{tmpmax}$$
 then
7: Compute $\eta(\boldsymbol{\mu}; W_N)$, and let $\eta_{saved}(\boldsymbol{\mu}) = \eta(\boldsymbol{\mu}, W_N)$;
8: **if** $\eta_{saved}(\boldsymbol{\mu}) > error_{tmpmax}$ **then**
9: $error_{tmpmax} = \eta_{saved}(\boldsymbol{\mu})$, and let $\boldsymbol{\mu}_{max} = \boldsymbol{\mu}$;
10: **end if**
11: **end if**
12: **end for**







Strategy for high-d sampling

Percentage of full cost (%)







10¹

10⁻² L

Strategy for high-d sampling

Dependence on safety factor



Observations -

- Easy modification of standard greedy
- Relies on a reasonable assumption of convergence
- Potential offline saving of close to an order of magnitude
- Still requires a fixed (large) training set



Strategy II -

Choose training set size as can be afforded and sample randomly
 Resample #points for which η(μ, W_N) < tol
 Perform a safety check

14: if $\eta_{saved}(\boldsymbol{\mu}) < tol$ then

15: flag μ ; // all flagged parameters will be removed 16: end if

- 22: Discard all flagged parameters from Ξ_{train} and their corresponding saved error estimation in η_{saved} ;
- 23: Generate M sizeof(Ξ_{train}) new samples, add them into Ξ_{train} such that sizeof(Ξ_{train}) = M; set η_{saved} of all new points to ∞ ;
- 28: Discard Ξ_{train} , generate M new parameters to form Ξ_{train}

Strategy for high-d sampling







N (M=1000)



While these tricks remain valuable, both offline and online cost typically scales with

$$M \propto (QN)^{\alpha d}, \ 0 < \alpha \le 1$$

For d>>1 this quickly becomes very expensive

Goal

Reduce the dimensionality of the problem without impacting the predictive accuracy

Compression by ANOVA expansions
 Problem segmentation



In many cases we need to evaluate

$$f(\mathbf{X}(x))$$
 $\int f(\mathbf{X}(x)) dx$ $\mathbf{X} = (X_1, \dots, X_d), \ d \gg 1$

which quickly becomes an expensive exercise.

DEF: The ANOVA expansion (exact)

$$f(\mathbf{X}) = f_0 + \sum_{t \subseteq \mathcal{D}} f_t(\mathbf{X}^t) \qquad \qquad \mathcal{D} = \{1, \dots, d\} \\ \Omega = [0, 1]^d$$

$$f_t(\mathbf{X}^t) = \int_{A^{d-|t|}} f(\mathbf{X}) d\mathbf{X}_{\mathcal{D}/t} - \sum_{w \in t} f_w(\mathbf{X}^w) - f_0 \qquad \qquad A^{|t|}$$

$$f_0 = \int_{A^d} f(\mathbf{X}) d\mathbf{X}, \quad \int_{A^0} f(\mathbf{X}) d\mathbf{X}^0 = f(\mathbf{X}) \qquad \qquad \mathbf{X}^t$$

t indexed sub-vector

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A few characteristics -

- The ANOVA expansion is unique and exact
- It is a finite expansion with 2^d terms
- All terms are mutually orthogonal

Example:

$$f(\alpha_1, \alpha_2, \alpha_3) = f_0 + \sum_{i=1}^3 \hat{f}_i(\alpha_i) + \sum_{1=i < j < d} \hat{f}_{ij}(\alpha_i, \alpha_j)$$

We have not achieved much yet.

Now consider the truncated expansion

$$f(\mathbf{X}, s) = f_0 + \sum_{t \subseteq \mathcal{D}; |t| \le s} f_t(\mathbf{X}^t)$$
 S = truncation dimension



Let us first introduce

$$V_t(f) = \int_{A^d} (f_t(\mathbf{X}^t))^2 \, d\mathbf{X}, \quad V(f) = \sum_{|t|>0} V_t(f)$$

... dimension-specific variances

Define the effective dimension through

$$\sum_{0 < |t| \le p_s} V_t(f) \ge qV(f) \qquad q \le 1$$

Then one can prove $Err(\mathbf{X}, p_s) \le 1 - q$

Sobol'90

$$\operatorname{Err}(\mathbf{X}, p_s) = \frac{1}{V(f)} \int_{A^d} [f\mathbf{X} - f(\mathbf{X}, p_s)]^2 \, d\mathbf{X}$$

NOTE: If p<<d there is hope!



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$$V_t(f) = \int_{A^d} (f_t(\mathbf{X}^t))^2 d\mathbf{X}, \quad V(f) = \sum_{|t|>0} V_t(f)$$

and introduce Sensitivities $\frac{V_t}{|t|>0} = \frac{V_t}{V} = \frac{1}{S(t)} = \frac{V_t}{V},$

We can now estimate sensitivity of output on specific parameter through $\sum_{t=1}^{\infty} V_t(f) \ge qV(f)$ $q \le 1$

 $\sum_{i \in t} S(t) + \sum_{i \notin t} S(i) = 1, \quad i = 1, \dots, d$ Compute approximate ANOVA expansion - learn $\sum_{i \in t} S(t) + \sum_{i \notin t} S(i) = 1, \dots, d$ Compute approximate ANOVA expansion - learn $\sum_{i \in t} S(t) + \sum_{i \notin t} S(i) = 1, \dots, d$ And the second se

reflect all interactions not involving α^i .



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Example: 25 planets of uncertain mass pull in a unit mass space-ship

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$$\ddot{\mathbf{x}}(t) = \sum_{i=1}^{p} m_i \hat{\mathbf{r}}_i / r_i^2, \qquad \mathbf{x}(\mathbf{t}_0) = \mathbf{x}_0. \qquad m_i = \frac{1}{p+1} [1+0.1 * U(-1,1)]$$
Full ANOVA based on Stroud-3
$$\int_{u=1}^{u=1} \int_{u=1}^{u=1} \int_{u=1}^{u=1}$$

Parameter compression for RBM



When extending this to PDEs and RBMs, key issue is

How to evaluate sensitivity at small cost ?

With the ability to build RB models, the following approach appears interesting

- Build a very coarse RBM over all parameters.
- Use RBM to build crude response surface
- Explore this very coarse model to estimate sensitivities
- Compress and develop RBM for important parameters





Output of interest - $s(\boldsymbol{\mu}) = \int_{\Gamma_{base}} u(\boldsymbol{\mu}) ds$,



We proceed with the following

- Build a coarse RBM over 16 parameters tol = one Need 33 elements
- Perform sensitivity analysis on output using RBM Reveals the 1,5,9,13 controls 99% variation
- Build new RBM over 4 parameters
- Compress and develop RBM for important parameters

$$e_i^{rel} = \frac{|\bar{s}_i^{fe} - \bar{s}_i^{rb}|}{|\bar{s}_i^{fe}|}, \quad i = 1, \dots, 100$$

16-d test space

tol	Number of RB	e_{max}	e_{ave}
100	16	5.091×10^{-2}	7.732×10^{-3}
10	21	3.912×10^{-2}	7.177×10^{-3}
1	24	3.900×10^{-2}	7.192×10^{-3}
10^{-1}	30	3.893×10^{-2}	7.190×10^{-3}
10^{-2}	32	3.892×10^{-2}	7.190×10^{-3}



Acoustic horn test



We consider a similar approach for the acoustic horn



8 parameters, describing wall impedance in horn

Combining RB and ANOVA



The model is

$$\begin{cases} \Delta u + 4u &= 0 \quad \text{in} \quad \Omega, \\ (2i + \frac{1}{25})u + \frac{\partial u}{\partial n} &= 0 \quad \text{on} \quad \Gamma_{out}, \\ 2iu + \frac{\partial u}{\partial n} &= 4i \quad \text{on} \quad \Gamma_{in}, \\ i\mu_j u + \frac{\partial u}{\partial n} &= 0 \quad \text{on} \quad \Gamma_j, j = 1, \cdots, 8, \\ \frac{\partial u}{\partial n} &= 0 \quad \text{on} \quad \text{other boundaries.} \end{cases}$$

Total of 8 parameters - boundary impedance

$$\boldsymbol{\mu} = (\mu_1, \mu_2, \cdots, \mu_8) \in [0, 1]^8.$$

Functional output -

$$s(\boldsymbol{\mu}) = \ell(u) = \operatorname{real}(\int_{\Gamma_{in}} u ds).$$

Combining RB and ANOVA



The approach is as follows

- Build coarse RB with high tolerance
- Tolerance of IOE-3 leads to 31 RB for 8 parameter problem.
- Use this coarse RB to compute ANOVA expansion of output and compute sensitivity.

Results are

$$S_3 = 0.4321, S_5 = 0.4314, S_{35} = 0.1256$$

 $S_3 + S_5 + S_{35} = 0.9891$

Similar results with tolerance of IE-2 - 22 RB

Combining RB and ANOVA





Exploring related ideas for many body scattering

- Build an RB for each element
- Build an RB for the interaction operation
- Combine through iteration to enable rapid modeling of complex scatterer configurations
- This is not a reduced basis method is the classic sense
- .. but using RB ideas allows us to solve problems that are otherwise very hard to approach
- .. and dramatically reduces number of parameters





warde multiple scattering





A1 AA

Multiple scattering problems





Multiple scattering problem







A few ideas on how to deal with the high-d problem

- Multi element EIM for improved online performance
- Sampling techniques to reduce offline cost
- Parametric compression through ANOVA expansions
- Problem splitting and iteration

Combining these techniques allows for the practical use of RBM for high-dimensional problems





Thank you