Stochastic Dimension Reduction

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Computational and Theoretical Challenges in Interdisciplinary Predictive Modeling Over Random Fields
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Motivation

- Objective is to characterize solution, u, of equations with stochastic coefficients on (Ω, Σ, P)
- Coefficients serve to construct an adapted Hilbert space:
  $k = \sum_i k_i \xi_i \qquad \xi_i : (\Omega, \Sigma(\xi_i), P) \mapsto \mathbb{R}$ i.i.d
  $G = \text{span}\{\xi_1, \cdots, \xi_d\}, \quad L^2(\Omega) \equiv L^2(\Omega, \Sigma(G), P).$
- THEN $u(\xi) = u(\xi_1, \cdots, \xi_d) \in L^2(\Omega)$

  and $u(\xi) = \sum_i (u, \psi_i)_{L^2(\Omega)} \psi_i(\xi)$ is a unique representation of $u(\xi)$
- Sandard PC machinery tries to identify the unique $u(\xi)$ in $\mathbb{R}^d$.
- Number of terms in PC Expansion: $M = \frac{(P+d)!}{P!d!}$

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Pushing Uncertainty Through Model: Intrusive Stochastic Projection:

Consider governing equation of general form:

$$\mathcal{M}_{\boldsymbol{\xi}} u = f \ .$$

$$\sum_{j=0}^{P} \langle \Psi_k \Psi_j \mathcal{M}_{\boldsymbol{\xi}} \rangle u_j = \langle \Psi_k f \rangle \qquad 0 \leq k \leq P \ ,$$

If $\mathcal{M}_{\boldsymbol{\xi}} = \sum_i^L \Psi_i(\boldsymbol{\xi}) \mathcal{M}_i$, results in a coupled system of equations:

$$\sum_{j=0}^{P} \sum_{i=0}^{L} \langle \Psi_i \Psi_j \Psi_k \rangle \mathcal{M}_i u_j = \langle \Psi_k f \rangle \qquad 0 \leq k \leq P.$$

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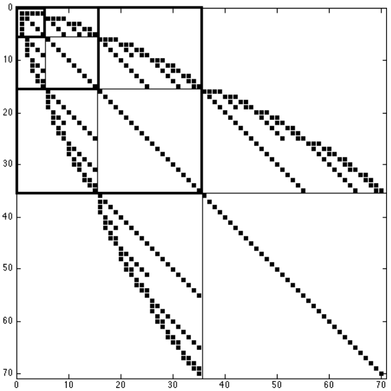
$$\boxed{\textstyle\sum_j M^{jk} u_j = f_k \quad \forall k}$$

Intrusive Stochastic Projection: Resulting System of Equations

$c_{ijk} = \langle \xi_i \psi_j \psi_k \rangle$:

$$A_\ell = \begin{bmatrix} A_{\ell-1} & B_\ell \\ C_\ell & D_\ell \end{bmatrix}$$



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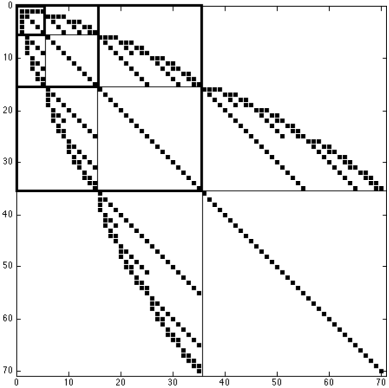

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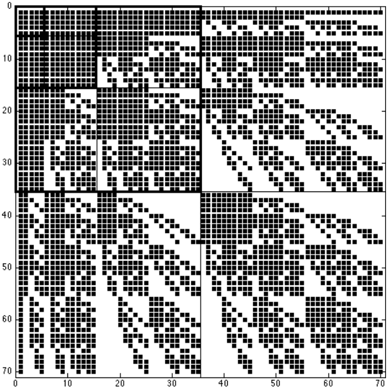


Non-Intrusive Characterization

We want:

$$u(\boldsymbol{\xi}) = \sum_i (u, \psi_i)_{L^2(\Omega)} \psi_i(\boldsymbol{\xi})$$

Orthogonality of $\{\psi_i\}$

$$\begin{aligned} u_i &= (u, \psi_i)_{L^2(\Omega)} \\ &= E\{u(\boldsymbol{\xi})\psi_i(\boldsymbol{\xi})\} \\ &= \int_{\Gamma_1} \cdots \int_{\Gamma_d} u(\boldsymbol{\xi})\psi_i(\boldsymbol{\xi}) d\mu(\boldsymbol{\xi}) \end{aligned}$$

If $\boldsymbol{\xi}$ are independent and have density functions:

$$u_i = \int_{\Gamma_1} \cdots \int_{\Gamma_d} u(\boldsymbol{\xi})\psi_i(\boldsymbol{\xi}) f_1(\xi_1) \cdots f_d(\xi_d) d\xi_1 \cdots d\xi_d$$

Challenges:

Intrusive

Very large system of equations; Constructing K_i and K^{jk}.

Non-Intrusive

High-dimensional integration.

Opportunities:

Intrusive

Linear Algebra, dimension reduction, adaptive refinement.

Non-Intrusive

Sparsity, anisotropy, dimension reduction.

First Idea: L^2 reduction

- replace the "generic" basis ψ_i by a basis that is adapted to $u \in H$

Karhunen-Loeve and PC:

Consider the polynomial chaos representation of the solution u:

$$u = \sum_{i=0}^{P} u_i \psi_i, \qquad u, u_i \in H$$

Covariance Operator is nuclear, $R_u : H' \mapsto H$

$$(R_u X, Y)_H = \sum_{i=1}^{P} (u_i, X)_H (u_i, Y)_H \qquad X, Y \in H'$$

Solve eigenproblem:

$$(R_u e, v)_H = \sum_{i=1}^{P} (u_i, e)_H (u_i, v)_H = \lambda (e, v)_H \quad \forall v \in H$$

Then we can represent PC coefficients on KL directions:

$$u_i = \sum_{j=1}^{KL} (u_i, e_j)\, e_j$$

But

$$u = \sum_{i=1}^{P} \sum_{j=1}^{KL} (u_i, e_j) e_j \psi_i = \sum_{j=1}^{KL} \sum_{i=1}^{P} (u_i, e_j) \psi_i e_j = \sum_{j=1}^{KL} \sqrt{\lambda_j} \eta_j e_j$$

Thus:

$$\eta_j = \frac{1}{\sqrt{\lambda_j}} \sum_{i=1}^{P} (u_i, e_j) \psi_i \qquad j = 1, \cdots, KL$$

(N, P)-discretization:

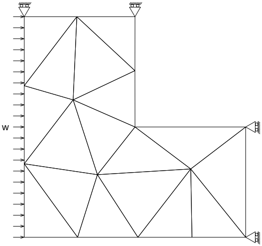
$$\eta_j^{(N,P)} = \frac{1}{\sqrt{\lambda_j}} \sum_{i=1}^{P} (u_i^N, e_j^P) \psi_i$$

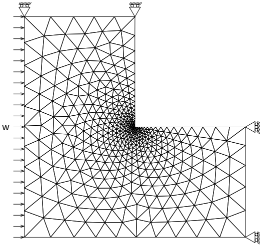
Error:

$$\epsilon_j = \|\eta_j^{(N,P)} - \eta_j\| \leq C_j \max_i \left| (u_i^N, e_j^P) - (u_i, e_j) \right|^2$$

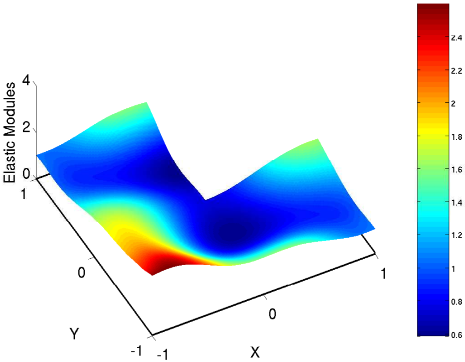
- P must be large enough to approximate R.
- N must be large enough to capture projection of u_i on e_j for the j that matter.
- Reduce global error - no control over local error.

Coarse and fine meshes used in analysis:

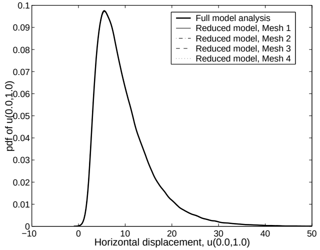


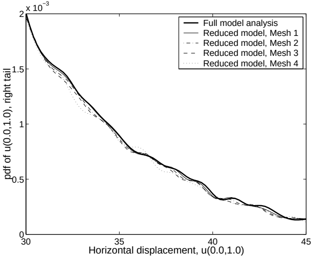


Realization of elasticity over L-shaped domain:

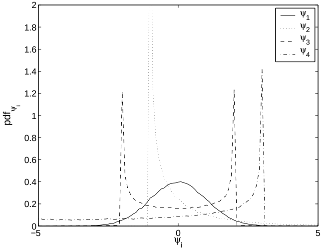


Comparison of pdf for fine model and reduced-model:

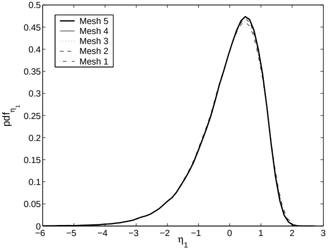




Comparison of Stochatsic bases:



PDF for 4 terms in PC basis

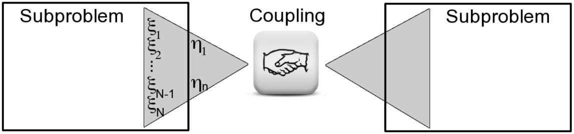


PDF for first term in adapted basis.

Muliscale Quadrature

Main Idea

- Develop UQ for coupled models in Nuclear Reactor Technology.
- Adapt measure of approximation at every handshaking.
- Mitigate mixing of uncertainty at handshaking.
- Develop multiscale quadrature rules.

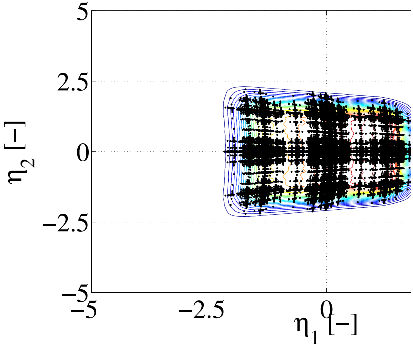


Reduction

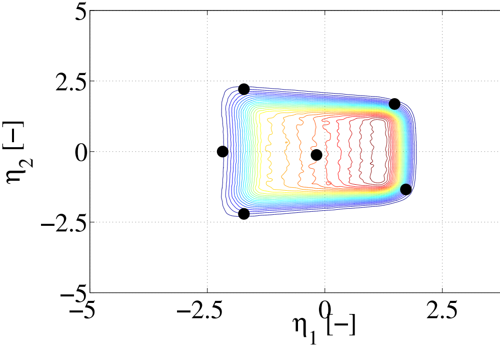
The output from Model I is reduced using Karhunen-Loeve expansion. The joint PDF of the dominant KL variables is estimated and a corresponding orthogonal polynomials constructed.

Multiscale Quadrature

Numerical quadrature in Model II can be developed relative to new measure:



Quadrature points relative to initial measure.



Quadrature points relative to adapted measure.

Some analysis

- New basis is adapted to the solution, and not to the parameters.
- Complexity is driven by physics - not by parameters.
- Solution is still a random process - very high-dimensional.
- In many cases, the QoI is a functional of the solution, that is much less complex than solution.
- We are still spinning our wheels a lot for more than we need.

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Second Idea: Probabilistic reduction

- In many instances, the QoI is $h(u)$ where h is some nonlinear functional.
- if the QoI is a single random variable, describing it in terms of more than one random variables seems to be a waste of bandwidth.

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- Other representations in $\mathbb{R}^d$ that have the same distribution.
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Focus on QoI

Consider square-integrable nonlinear functionals $h : H \mapsto \mathbb{R}$:

$$h \stackrel{def}{=} h(u(\boldsymbol{\xi})) = h_0 + \sum_{|\boldsymbol{\alpha}|=1} h_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) + \sum_{|\boldsymbol{\alpha}|>1} h_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

Inverse CDF: A mapping from a Gaussian variable $\hat{\xi}$ to h can be constructed as follows:

$$h \stackrel{d}{=} \hat{h}(\hat{\xi}) \stackrel{def}{=} \mu^{-1}\left[\Phi\left(\hat{\xi}\right)\right]$$

Expand as: $\hat{h}(\hat{\xi}) = \hat{h}_0 + \hat{h}_1 \hat{\xi} + \sum_i \hat{h}_i \psi_i(\hat{\xi})$

Thus a one-dimensional expansion in terms of a Gaussian variable exists. It only matches probability measure of h.

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Focus on QoI

Introduce a new Gaussian rv η_1:

$$\hat{h}_1\eta_1 = \sum_{|\boldsymbol{\alpha}|=1} h_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}} = \sum_{i=1}^{d} h_i\xi_i$$

Then:

$$h = h_0 + \hat{h}_1\eta_1 + \sum_{|\boldsymbol{\alpha}|>1} h_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

Let: A be an isometry and ξ be Gaussian. Then $u(A\xi)$ has the same probability measure as $u(\xi)$.

If: ξ is Gaussian, then $\eta = A\xi$ has the same probability measure as ξ. Thus η is a basis for the Gaussian Hilbert space spanned by ξ.

Then: Hermite Polynomials in η span the same space as Hermite polynomials in ξ - namely: $L^2(\Omega, \Sigma(\xi), P) = L^2(\Omega, \Sigma(\eta), P)$.

Choose: A so that $\hat{h}_1\eta_1 = \sum_{|\alpha|=1} h_\alpha \psi_\alpha$

Then in L^2:

$$\begin{aligned} h(\xi) &= h_0 + \hat{h}_1\eta_1 + \sum_{|\alpha|>1} h_\alpha \psi_\alpha(\eta) \\ &= h_0 + \hat{h}_1\eta_1 + \sum_{\substack{|\alpha|>1 \\ \alpha=(|\alpha|,0,\cdots,0)}} h_\alpha \psi_\alpha(\eta_1) \\ &\quad + \sum_{\substack{|\alpha|>1 \\ \alpha\neq(|\alpha|,0,\cdots,0)}} h_\alpha \psi_\alpha(\eta) \end{aligned}$$

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Then in L^2:

$$\begin{aligned} h(\xi) &= h_0 + \hat{h}_1\eta_1 + \sum_{|\alpha|>1} h_\alpha \psi_\alpha(\eta) \\ &= h_0 + \hat{h}_1\eta_1 + \sum_{\substack{|\alpha|>1 \\ \alpha=(|\alpha|,0,\cdots,0)}} h_\alpha \psi_\alpha(\eta_1) \\ &\quad + \sum_{\substack{|\alpha|>1 \\ \alpha\neq(|\alpha|,0,\cdots,0)}} h_\alpha \psi_\alpha(\eta) \end{aligned}$$

Let: A be an isometry and $\boldsymbol{\xi}$ be Gaussian. Then $u(A\boldsymbol{\xi})$ has the same probability measure as $u(\boldsymbol{\xi})$.

If: $\boldsymbol{\xi}$ is Gaussian, then $\boldsymbol{\eta} = A\boldsymbol{\xi}$ has the same probability measure as $\boldsymbol{\xi}$. Thus $\boldsymbol{\eta}$ is a basis for the Gaussian Hilbert space spanned by $\boldsymbol{\xi}$.

Then: Hermite Polynomials in $\boldsymbol{\eta}$ span the same space as Hermite polynomials in $\boldsymbol{\xi}$ - namely: $L^2(\Omega, \Sigma(\boldsymbol{\xi}), P) = L^2(\Omega, \Sigma(\boldsymbol{\eta}), P)$.

Choose: A so that $\hat{h}_1\eta_1 = \sum_{|\boldsymbol{\alpha}|=1} h_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}$

Then in L^2:

$$\begin{aligned} h(\boldsymbol{\xi}) &= h_0 + \hat{h}_1\eta_1 + \sum_{|\boldsymbol{\alpha}|>1} h_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{\eta}) \\ &= h_0 + \hat{h}_1\eta_1 + \sum_{\substack{|\boldsymbol{\alpha}|>1 \\ \boldsymbol{\alpha}=(|\boldsymbol{\alpha}|,0,\cdots,0)}} h_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\eta_1) \\ &\quad + \sum_{\substack{|\boldsymbol{\alpha}|>1 \\ \boldsymbol{\alpha}\neq(|\boldsymbol{\alpha}|,0,\cdots,0)}} h_{\boldsymbol{\alpha}}\psi_{\boldsymbol{\alpha}}(\boldsymbol{\eta}) \end{aligned}$$

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One-Dimensional Approximation of Solution

Projection of the solution on $L^2(\Omega, \Sigma(\eta_1), P)$:

$$h(\boldsymbol{\xi}) = h_0 + \hat{h}_1 \eta_1 + \sum_{|\boldsymbol{\alpha}|>1} h_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\eta_1)$$

Implementation

Recipe

- Compute linear components in expansion of QoI: $\eta_1 = \sum_i w_i \xi_i$.
- Construct isometry A with η_1 as leading direction.
- Construct projection operators for $\boldsymbol{\eta} = A\boldsymbol{\xi}$: $\langle f(\boldsymbol{\xi})\psi(\boldsymbol{\eta})\rangle$.
- Solve for the representation of solution with respect to η_1.
- If an L^2 characterization is required, then evaluate components with respect to full η basis.

Implementation

Numerical Effort:

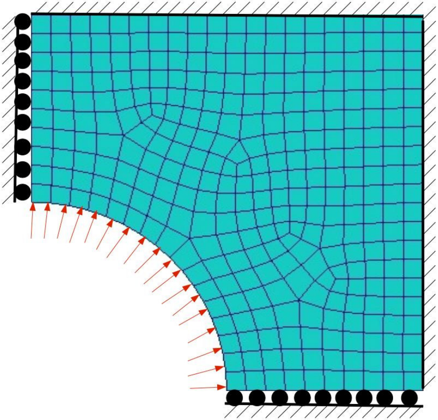
1. Evaluate:

$$\langle \psi_i(\boldsymbol{\xi})\psi_j(\boldsymbol{\eta})\psi_k(\boldsymbol{\eta})\rangle = \langle \psi_i(\boldsymbol{\xi})\psi_j(A\boldsymbol{\xi})\psi_k(A\boldsymbol{\xi})\rangle$$

   - This is the multi-dimensional integral of a scalar polynomial function. Function evaluations are very inexpensive.
   - These evaluations are massively parallelizable

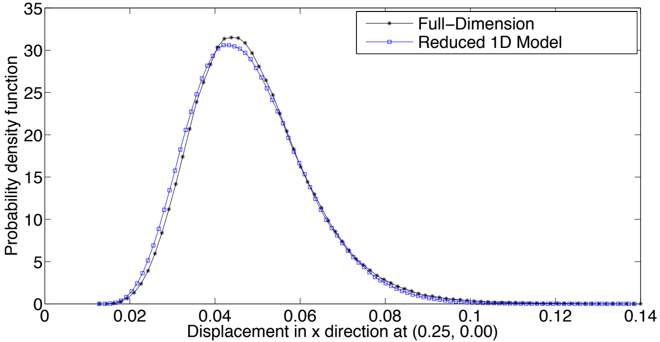
2. Discover the linear terms of the QoI in a non-intrusive fashion.

Numerical Example



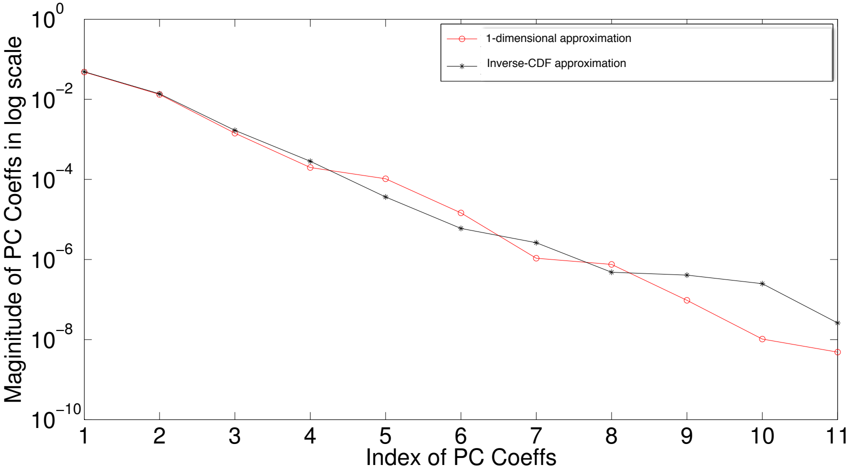
Plane Stress; Random Young's Modulus.
Quantity of Interest: X-Displacement at location (0.25,0).

Using leading dimension of new basis.

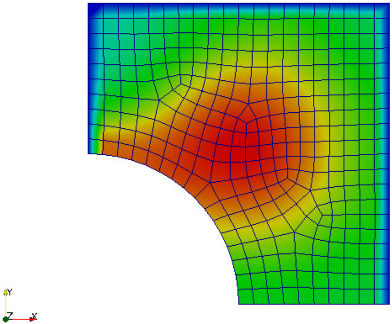


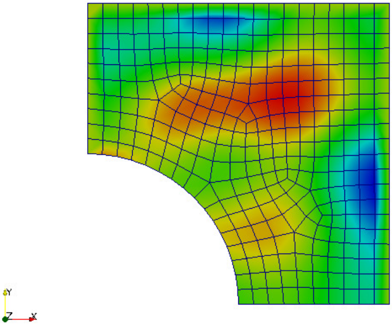
Behavior in L^2

PC Coefficients of the Solution Projected in L^2 on η_1 vs.
PC Coefficients of the Inverse CDF Operator.



Optimal Dimension Varies over the Domain

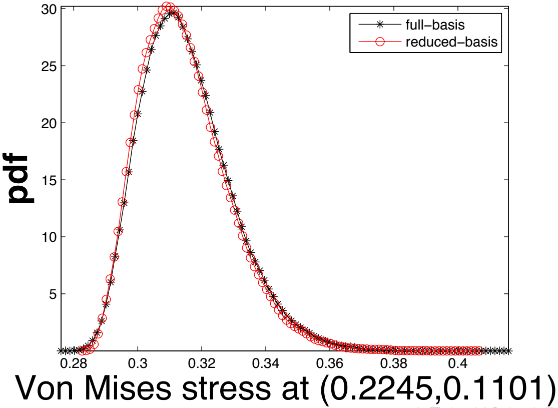




Nonlinear QoI

Von Mises Stress at a Point:

$$\sigma_v = \sqrt{\sigma_1^2 - \sigma_1\sigma_2 + \sigma_2^2}$$



Conclusions

- The geometric structure provides a very rich context to describe complicated objects (stochastic processes and white noise).
- Some quantities of interest are simple, and that simplicity can be discovered within the richer mathematical structure.
- If the QoI are scalars, and if we merely care about an L_1 characterization, then 1-d representations exist and the question can be reformulated as to discover them.
- Additional physical/empirical constraints can be reflected in the construction of A.