High dimensional sparse polynomial approximation of parametric PDE's - Theory and algorithms

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Taipei, 28-05-2014

We are interested in PDE's of the general form

$$\mathcal{D}(u, y) = 0,$$

where $\mathcal{D}$ is a partial differential operator, u is the unknown and $y = (y_j)_{j=1,\dots,d}$ is a parameter vector of dimension $d >> 1$ or $d = \infty$.

For simplicity (up to a change of variable), we assume that all y_j range in $[-1, 1]$, and therefore

$$y \in U = [-1, 1]^d \text{ or } [-1, 1]^{\mathbb{N}}.$$

We also assume well-posedness of the solution in some Banach space V for every $y \in U$,

$$y \mapsto u(y)$$

is the solution map from U to V.

Solution manifold $\mathcal{M} := \{u(y) \ : \ y \in U\} \subset V$.

The parameters may be deterministic (control, optimization, inverse problems) or random (uncertainty modeling and propagation, risk assessment).

These applications often requires many queries of $u(y)$, and therefore in principle running many times a numerical solver.

Objective : economical numerical approximation of the map $y \mapsto u(y)$.

Motivation : parametric PDE's

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Agenda

1. Curse of dimensionality.. and how we could hope to fix it.

2. Linear-affine parametric PDE model.

3. Other models.

4. Adaptive numerical methods.

5. Sparse interpolation.

7. Conclusions

Curse of dimensionality

Standard methods (polynomials of fixed degree, meshes) are too costly for $d >> 1$.

Uniform approximation of C^m functions of d variable is at best $\mathcal{O}(N^{-m/d})$ accurate where N is the number of degrees of freedom.

Exponential growth with d of the complexity for a prescribed accuracy also occurs for infinitely smooth functions (Novak-Wozniakowski).

A possible way out : exploit anisotropic features in the function $y \mapsto u(y)$.

A typical situation : the PDE is parametrized by a function a (diffusion coefficient, velocity, domain boundary) and y_j are the coordinates of a in a certain basis representation $a = \overline{a} + \sum_{j \geq 1} y_j \psi_j$.

If the ψ_j decays as $j \to +\infty$ (for instance if a has some smoothness) then the variable y_j is less active for large j.

We showed that in certain relevant instances, this mechanism allows to break the curse of dimensionality by using suitable expansions : we obtain approximation rates $\mathcal{O}(N^{-s})$ that are independent of d in the sense that they hold when $d = \infty$.

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Sparse tensorized expansion $y \mapsto u(y)$

Approximation of $u(y)$ by truncated expansions of the form

$$u_N(y) = \sum_{\nu \in \Lambda_N} u_\nu \phi_\nu(y), .$$

with $\phi_\nu : U \to \mathbb{R}$ and $u_\nu \in V$, and $\#(\Lambda_N) = N$.

We are interested in establishing bounds of the form

$$\|u - u_N\|_{L^q(U,V)} \leq CN^{-s},$$

e.g. for $q = 2$ (for some probability measure) or $q = \infty$.

The case $q = \infty$ allows us to control the Kolmogorov width of the solution manifold : with $E_N := \mathrm{span}\{u_\nu \ : \ \nu \in \Lambda_N\}$, one has

$$d_N(\mathcal{M}) = \inf_{\dim(E)=N} \sup_{v \in \mathcal{M}} \mathrm{dist}(v, E)_V \leq \sup_{y \in U} \mathrm{dist}(u(y), E_N)_V \leq \|u - u_N\|_{L^\infty(U,V)},$$

This is of interest in the analysis of reduced basis methods.

The case $q = 2$ is of interest in the analysis of POD (principal component) methods.

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Linear-affine model

Consider the steady state diffusion equation

$$-\mathrm{div}(a\nabla u) = f \quad \text{on} \quad D \subset \mathbb{R}^m \quad \text{and} \quad u_{|\partial D} = 0,$$

where $f = f(x) \in L^2(D)$ and the diffusion coefficients are given by

$$a = a(x,y) = \bar{a}(x) + \sum_{j\geq 1} y_j \psi_j(x),$$

where (ψ_j) is a given family of functions. Uniform ellipticity assumption :

$$(UEA) \qquad 0 < r \leq a(x,y) \leq R, \quad x \in D, \ y \in U.$$

or equivalently $\bar{a} \in L^\infty(D)$ and $\sum_j |\psi_j(x)| \leq \bar{a}(x) - r, \quad x \in D$.

Then the solution map is bounded from U to $V := H_0^1(\Omega)$:

$$\|u(y)\|_V \leq C_r := \frac{\|f\|_{V^*}}{r}, \quad y \in U, \quad \text{where} \quad \|v\|_V := \|\nabla v\|_{L^2}.$$

More generally, we could consider linear equations of the form

$$A(y)u = f,$$

where $A(y) := \overline{A} + \sum y_j A_j$ is boundedly invertible in suitable spaces uniformly in y.

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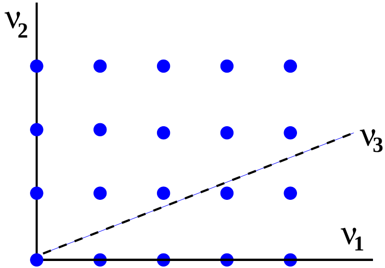
We consider the expansion of $u(y) = \sum_{\nu\in\mathcal{F}} t_\nu y^\nu$, where

$$y^\nu := \prod_{j\geq 1} y_j^{\nu_j} \text{ and } t_\nu := \frac{1}{\nu!}\partial^\nu u_{|y=0} \in V \text{ with } \nu! := \prod_{j\geq 1} \nu_j! \text{ and } 0! := 1.$$

where $\mathcal{F}$ is the set of all finitely supported sequences of integers (finitely many $\nu_j \neq 0$). The sequence $(t_\nu)_{\nu\in\mathcal{F}}$ is indexed by countably many integers.



Objective : identify a set $\Lambda_N \subset \mathcal{F}$ with $\#(\Lambda_N) = N$ such that u is well approximated by the partial expansion

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Sparse Taylor approximations

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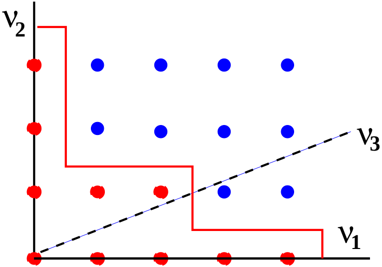

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Best N-term approximation

For all $y \in U = [-1,1]^{\mathbb{N}}$ we have

$$\|u(y) - u_N(y)\|_V \leq \|\sum_{\nu \notin \Lambda_N} t_\nu y^\nu\|_V \leq \sum_{\nu \notin \Lambda_N} \|t_\nu\|_V$$

Best N-term approximation in the $\ell^1(\mathcal{F})$ norm : use for Λ_N the N largest $\|t_\nu\|_V$.

Observation (Stechkin) : if $(\|t_\nu\|_V)_{\nu\in\mathcal{F}} \in \ell^p(\mathcal{F})$ for some $p < 1$, then for this Λ_N,

$$\sum_{\nu \notin \Lambda_N} \|t_\nu\|_V \leq CN^{-s}, \quad s := \frac{1}{p} - 1, \quad C := \|(\|t_\nu\|_V)\|_p.$$

Proof : with $(t_n)_{n>0}$ the decreasing rearrangement, we combine

$$\sum_{\nu \notin \Lambda_N} \|t_\nu\|_V = \sum_{n>N} t_n = \sum_{n>N} t_n^{1-p} t_n^p \leq t_N^{1-p} C^p \quad \text{and} \quad N t_N^p \leq \sum_{n=1}^{N} t_n^p \leq C^p.$$

Question : do we have $(\|t_\nu\|_V)_{\nu\in\mathcal{F}} \in \ell^p(\mathcal{F})$ for some $p < 1$?

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The main result

Theorem 1 (Cohen-DeVore-Schwab, 2011) : under the uniform ellipticity assumption (UAE), then for any $p < 1$,

$$(\|\psi_j\|_{L^\infty})_{j>0} \in \ell^p(\mathbb{N}) \Rightarrow (\|t_\nu\|_V)_{\nu\in\mathcal{F}} \in \ell^p(\mathcal{F}).$$

Interpretations :

(i) The Taylor expansion of u inherits the sparsity properties of the expansion of $a(y)$ into the ψ_j.

(ii) We approximate u in $L^\infty(U, V)$ with algebraic rate N^{-s} despite the curse of (infinite) dimensionality, due to the fact that y_j is less influencial as j gets large.

Such approximation rates cannot be proved for the usual a-priori choices of Λ.

Key idea in the proof : holomorphic extension $z \mapsto u(z)$ with $z = (z_j) \in \mathbb{C}^{\mathbb{N}}$. Diffusion PDE with complex coefficients $a(x, z) = \bar{a}(x) + \sum_{j\geq 1} z_j\psi_j$: Lax-Milgram theorem applies with $\Re(a(x, z)) \geq \delta > 0$

Domains of holomorphy : if $\rho = (\rho_j)_{j\geq 0}$ is any positive sequence such that

$$\sum_{j>0} \rho_j|\psi_j(x)| \leq \bar{a}(x) - \delta, \quad x \in D,$$

for some $\delta > 0$, then u is holomorphic, with bound $\|u(z)\|_V \leq C_\delta$, in the polydisc

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Estimate on the Taylor coefficients

Use Cauchy formula. In 1 complex variable if $z \mapsto u(z)$ is holomorphic and bounded in a neighbourhood of disc $\{|z| \leq b\}$, then for all z in this disc

$$u(z) = \frac{1}{2i\pi} \int_{|z'|=b} \frac{u(z')}{z - z'} dz',$$

which leads by n differentiation at $z = 0$ to $|u^{(n)}(0)| \leq n! b^{-n} \max_{|z| \leq b} |u(z)|$.

Recursive application of this to all variables z_j such that $\nu_j \neq 0$, with $b = \rho_j$, for a δ-admissible sequence ρ gives

$$\|\partial^\nu u_{|z=0}\|_V \leq C_\delta \nu! \prod_{j>0} \rho_j^{-\nu_j}.$$

and therefore

$$\|t_\nu\|_V \leq C_\delta \prod_{j>0} \rho_j^{-\nu_j} = C_\delta \rho^{-\nu}.$$

Since ρ is not fixed we have

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Estimate on the Taylor coefficients

Use Cauchy formula. In 1 complex variable if $z \mapsto u(z)$ is holomorphic and bounded in a neighbourhood of disc $\{|z| \leq b\}$, then for all z in this disc

$$u(z) = \frac{1}{2i\pi} \int_{|z'|=b} \frac{u(z')}{z - z'} dz',$$

which leads by n differentiation at $z = 0$ to $|u^{(n)}(0)| \leq n! b^{-n} \max_{|z| \leq b} |u(z)|$.

Recursive application of this to all variables z_j such that $\nu_j \neq 0$, with $b = \rho_j$, for a δ-admissible sequence ρ gives

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Other models

Parametric PDE's $\mathcal{D}(u,y)=0$ of the general form

$$\mathcal{P}(u,a)=0,$$

with $a=a(y)=\overline{a}+\sum_{j\geq 1} y_j\psi_j$, where

$$\mathcal{P}: V\times L \to W,$$

with V,L,W a triplet of complex Banach spaces, and $\overline{a}$ and ψ_j are functions in L.

The operator $\mathcal{P}$ could be nonlinear in u and in a.

Example : same problem with non-linearity, e.g.

$$u^3-\mathrm{div}(\exp(a)\nabla u)=f \;\text{ on }\; D=D(y)\;\; u_{|\partial D}=0,$$

well posed in $V=H_0^1(D)$ in dimension $m=3$ ($V\subset L^4$).

In contrast to the linear-affine model, bounded holomorphic extension is generally not feasible in a complex domain containing the polydisc $\mathcal{U}=\otimes\{|z_j|\leq 1\}$. For this reason,Taylor series are not expected to converge. Instead we consider the tensorized Legendre expansion

$$u(y)=\sum_{\nu\in\mathcal{F}} u_\nu L_\nu(y),$$

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Polynomial approximation results

Many of these models can be treated by the following result.

Theorem 2 (Chkifa-Cohen-Schwab, 2013) : assume that

(i) The problem is well posed for all $a = a(y)$ with $y \in U$ with solution $u(y) = u(a(y)) \in V$.

(ii) The map $\mathcal{P}$ is differentiable (holomorphic) from $L \times V$ to W.

(iii) For any $y \in U$, the differential $d_u\mathcal{P}(u(y), a(y))$ is an isomorphism from $V \to W$

(iv) One has $(\|\psi_j\|_L)_{j\geq 1}$ in $\ell^p(\mathbb{N})$ for some $0 < p < 1$,

Then $(\|u_\nu\|_V)_{\nu\in\mathcal{F}} \in \ell^p(\mathcal{F})$

Therefore, there exists approximations $u_N = \sum_{\nu\in\Lambda_N} u_\nu L_\nu$ converging with rate $\mathcal{O}(N^{-s})$ in $L^q(U, V)$ with $s = \frac{1}{p} - 1$ for $q = \infty$ and $s = \frac{1}{p} - \frac{1}{2}$ for $q = 2$.

Key ingredients in the proof : (i) estimates of Legendre coefficients for holomorphic functions in a "small" complex neighbourhood of U and (ii) holomorphic Banach valued version of the implicit function theorem.

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Taylor vs Legendre expansions

In one variable :

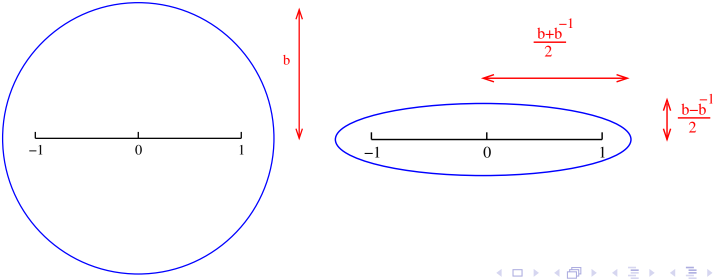
- If u is holomorphic in an open neighbourhood of the disc $\{|z| \le b\}$ and bounded by M on this disc, then the n-th Taylor coefficient of u is bounded by

$$|t_n| := \left| \frac{u^{(n)}(0)}{n!} \right| \le M b^{-n}$$

- If u is holomorphic in an open neighbourhood of the domain $\mathcal{E}_b$ limited by the ellipse of semi axes of length $(b + b^{-1})/2$ and $(b - b^{-1})/2$, for some $b > 1$, and bounded by M on this domain, then the n-th Legendre coefficent of u is bounded by

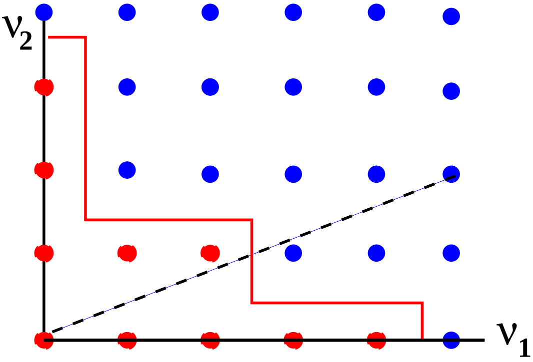
$$|u_n| := |\langle u, L_n \rangle| \le M b^{-n} \phi(n)$$

where ϕ has algebraic growth.



(i) Non-adaptive, based on the available a-priori estimates for the $\|t_\nu\|_V$ or $\|u_\nu\|_V$. Take Λ_N to be the set corresponding to the N largest such estimates.

(ii) Adaptive, based on a-posteriori information gained in the computation $\Lambda_1 \subset \Lambda_2 \subset \cdots \subset \Lambda_N \cdots$.



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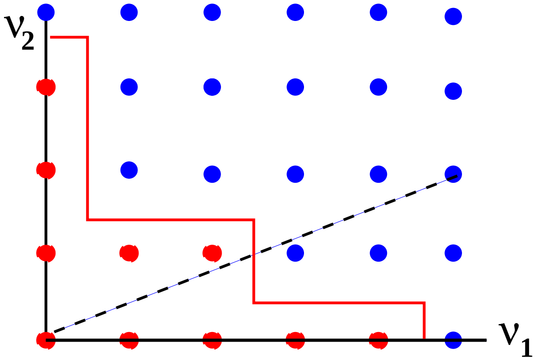

Numerical methods : strategies to build the sets Λ_N

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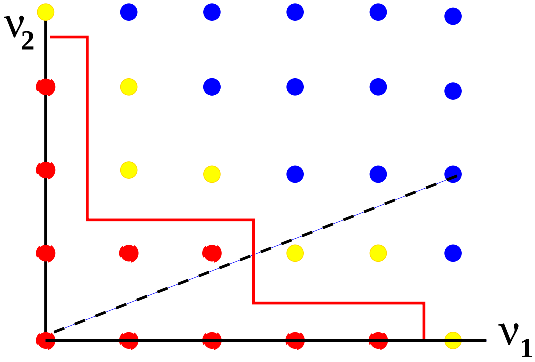

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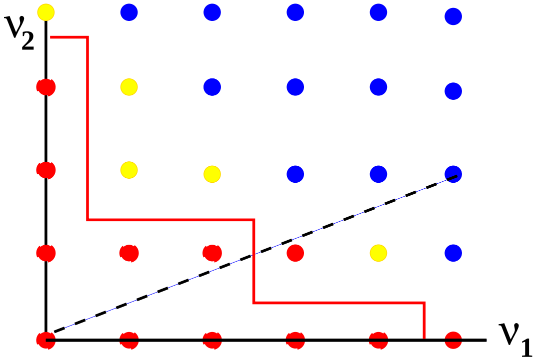

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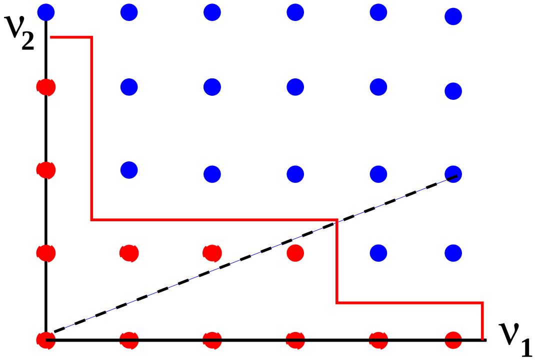
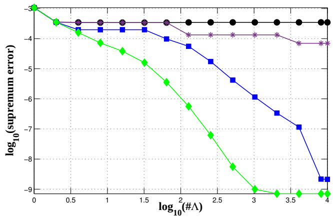


For adaptive algorithms it is critical that the index chosen sets are downward closed

$$\nu \in \Lambda \text{ and } \mu \leq \nu \Rightarrow \mu \in \Lambda.$$

Such sets are also called lower sets. This does not generally for the sets corresponding to the N largest estimates, however the same convergence rates as in Theorem 1 and 2, can be proved when imposing such a structure.

A test case for linear-affine model in dimension $d = 64$: comparison between the approximation performance with Λ_N given by standard choices $\{\sup \nu_j \leq k\}$ (black) or $\{\sum \nu_j \leq k\}$ (purple) and by anisotropic choices based on a-priori bounds (blue) or adaptively generated (green).



Highest polynomial degree for Λ_{1000} with different choices : 1, 2, 162 and 114.

Numerical methods : strategies to build the polynomial approximation

(i) Intrusive : exact computation of the Taylor coefficients $\|t_\nu\|_V$ for the linear-affine model (Chkifa-Cohen-DeVore-Schwab) or Galerkin approximation of the Legendre coefficients (Gittelson-Schwab). Adaptive algorithms with optimal theoretical guarantees.

(ii) Non-intrusive : based on snapshots $u_i := u(y^i)$ for $i = 1, \dots, m$. Interpolation (Chkifa-Cohen-Schwab) or Least Squares (Chkifa-Cohen-Migliorati-Nobile-Tempone). Adaptive algorithms seem to work well, however with no theoretical guarantees.

Additional prescriptions for non-intrusive methods :

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Sparse interpolation

Let $\{t_0, t_1, t_2 \dots\}$, be an infinite sequence of pairwise distinct points in $[-1, 1]$ and let I_k be the univariate interpolation operator on $\mathbb{P}_k$ associated to the section $\{t_0, \dots, t_k\}$.

Hierarchical (Newton) form : $I_k = \sum_{l=0}^{k} \Delta_l$, with $\Delta_l := I_l - I_{l-1}$ and $I_{-1} := 0$.

Tensorization and sparsification : for $\nu \in \mathcal{F}$, we define the point

$$z_\nu := (t_{\nu_1}, t_{\nu_2}, \dots) \in U.$$

Then (Kuntzmann 1959), if Λ is downward closed, the set

$$\Gamma_\Lambda := \{z_\nu \; : \; \nu \in \Lambda\},$$

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A straightforward adaptive algorithm : given Λ_N, define $\Lambda_{N+1} := \Lambda_N \cup \{\nu^*\}$ with $\nu^* \notin \Lambda_N$ such that Λ_{N+1} is downward closed and maximizing $\|\Delta_\nu u\|_{L^\infty}$.

Remark : the same principles apply to the tensorization of other systems, such as hierarchical piecewise linear finite elements.

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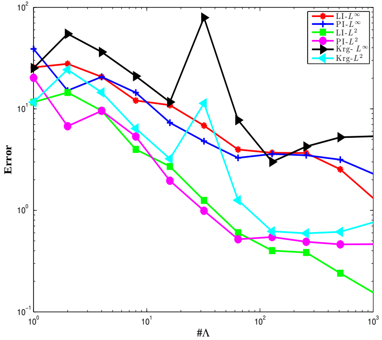
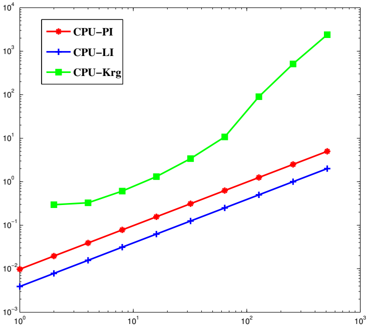
Comparison with Kriging interpolation algorithms

Test case : $y = (y_1, y_2, y_3, y_4)$ shape parameters in the design of an airfoil and $u(y)$ is the lift to drag ratio (scalar quantity of interest) obtained by ONERA numerical solver.





Error curves in terms of number of points are comparable.

The CPU cost for sparse interpolation scales linearly with the number of points.

This contrasts with Kriging methods which require solving ill-conditionned linear systems of growing size + optimization of the parameters of a Gaussian kernel.

Conclusion

The curse of dimensionality can be "defeated" by exploiting both the smoothness and anisotropy in the different variables.

For certain models, this can be achieved by sparse polynomial approximations.

Adaptive algorithms with optimal theoretical guarantees are still to be developed, in particular for non-intrusive approaches (interpolation, collocation, least-squares).

The choice of parametrization and representation of the solution are critical in this analysis since it affects the properties of the map $y \mapsto u(y)$.

Other approaches to evaluate Kolmogorov width of solution manifold ?

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