Rigorous global minimization of nonlinear integral functionals using finite element discretizations and polynomial optimization

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Minimum Residual & Least-Squares Finite Element Methods
October 6, 2022

Introduction

Find (global) minimizer of integral functional

$$\inf_{u \in \mathcal{U}} \int_\Omega E(x, u, \nabla u)\, \mathrm{d}x$$

where $u : \mathbb{R}^n \supseteq \Omega \to \mathbb{R}^m$ is a vector-valued function sought in an **infinite-dimensional** energy space $\mathcal{U}$ with gradient $\nabla u \in \mathbb{R}^{n\times m}$, and E is a real-valued energy functional.

Foundational question for many problems in (nonlinear) mechanics: nonlinear elasticity, pattern formation equations, etc.

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Goal: Find practical algorithm producing discretizations that rigorously converge to the *global* minimum, when E is polynomial in its inputs (and satisfies some technical conditions ensuring existence of solutions to original problem).

Introduction

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has a minimizer if $\mathcal{U} = W_0^{1,p}$ and E is p-coercive, exhibits p-growth and quasiconvex wrt ∇u in the sense of Morrey.

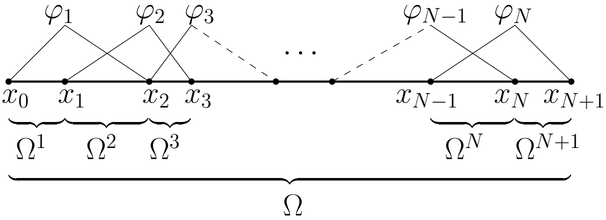
Approaches:

- Variational argument to produce Euler-Lagrange equations, discretize them, solve using ``Newton's method''. *Problem*: Only finds approximations to *local* stationary solutions, not *global*.
- Discretize minimization problem directly and solve resulting finite-dimensional minimization. *Problem*: Convergence to original infinite-dimensional problem only if the discrete *global* minimum is found, but this typically cannot be guaranteed (Bartels, 2017; Arada, 2002).

Insight: Take second approach and use recent results from multivariate polynomial optimization to rigorously compute the discrete *global* minimum by formulating as a sequence of convex relaxations.

Discretization

$$\inf_{u\in\mathcal{U}}\int_\Omega E(x,u,\nabla u)\,\mathrm{d}x \le \min_{u_h\in\mathcal{U}_h}\int_\Omega E(x,u_h,\nabla u_h)\,\mathrm{d}x$$



Use ``hat'' functions:

$$u_h(x) = \sum_{j=1}^{N} \xi_j \varphi_j(x)$$

$$\mathcal{U}_h = \operatorname{span}\{\varphi_j\}_{j=1}^{N}$$

Result is a **polynomial optimization problem (POP)** in the variables ξ_j representing the unknown DOF:

$$\min_{u_h\in\mathcal{U}_h}\int_\Omega E(x,u_h,\nabla u_h)\,\mathrm{d}x = \min_{\boldsymbol{\xi}\in\mathbb{R}^N} f(\boldsymbol{\xi}) \qquad \text{e.g. } E = \tfrac{1}{100}|\nabla u|^2 + (u+1)^2(u-2)^2$$

Here, f is *polynomial* in ξ_j, since E is polynomial (note the powers of $\varphi_j(x)$ can be integrated exactly).

Polynomial optimization

Lasserre (2001) -- using Putinar's positivstellensatz in real algebraic geometry -- noticed the non-convex global POP could be solved trough a series of convex relaxations involving sum-of-squares (SOS) polynomials that can be formulated as semidefinite programs (SDPs):

$$\min_{|\xi_j|\leq B} f(\boldsymbol{\xi}) = \lim_{\omega\to\infty} \underbrace{\max \lambda \quad \text{s.t. } f(\boldsymbol{\xi}) - \lambda = \sigma_0(\boldsymbol{\xi}) + \sum_{j=1}^{N}(B^2 - \xi_j^2)\sigma_j(\boldsymbol{\xi})}_{\text{(convex) moment-SOS relaxation of order } \omega \ (\mathrm{SDP}_\omega)}$$

relaxation order

where σ_0 and σ_j are SOS of order 2ω and $2\omega - 2$ respectively,...

BUT only applies for *bounded* DOF $|\xi_j| \leq B$. Thus,

Trick: To ensure boundedness, use $\mathcal{U}_h^B = \{u_h = \sum_{j=1}^N \xi_j \varphi_j(x) \mid |\xi_j| \leq B\}$ instead of $\mathcal{U}_h$ and choose $B = \frac{1}{h}$ so that $\mathcal{U}_h^B \to \mathcal{U}_h \to \mathcal{U}$ as $h \to 0$.

$$\inf_{u\in\mathcal{U}} \int_\Omega E(x, u, \nabla u)\,\mathrm{d}x \leq \min_{u_h\in\mathcal{U}_h^B} \int_\Omega E(x, u_h, \nabla u_h)\,\mathrm{d}x = \min_{|\xi_j|\leq B} f(\boldsymbol{\xi})$$

Sparse polynomial optimization

So it is possible to solve the finite-dimensional global POP.

Issue: for $\gtrapprox 10$ DOF, computational cost is prohibitive. Even in 2D we need $\gg 10$ DOF.

Solution: Sparsity. Waki *et al* (2006) noticed computational cost is reduced significantly when ``correlative sparsity'' is present in the problem, allowing for a sparse relaxation instead. Lasserre (2006) proved the sparse relaxations converge provided the ``sparsity graph'' is chordal*

$$\min_{u_h \in \mathcal{U}_h^B} \int_\Omega E(x, u_h, \nabla u_h)\,\mathrm{d}x = \min_{u_h \in \mathcal{U}_h^B} \sum_{e=1}^{n_{\mathrm{el}}} \int_{\Omega^e} E(x, u_h, \nabla u_h)\,\mathrm{d}x = \min_{|\xi_j| \le B} \sum_{e=1}^{n_{\mathrm{el}}} f^e(\xi^e)$$

where ξ^e are the DOF associated to element e, and are referred to as *cliques*.

*Actually assuming an implied condition called the ``running intersection property'' (RIP).

Example and sparsity graphs

In 1D, consider $E = \frac{1}{100}|\nabla u|^2 + (u+1)^2(u-2)^2$ and discretization with bounded-DOF hat functions, so that $\mathcal{U}_h^B = \{u_h = \sum_{j=1}^N \xi_j \varphi_j(x) \mid |\xi_j| \leq B\}$ and

$$\begin{aligned}\min_{u_h \in \mathcal{U}_h^B} \int_\Omega E \, \mathrm{d}x &= \min_{u_h \in \mathcal{U}_h^B} \sum_{e=1}^{N+1} \int_{\Omega^e} \frac{1}{100}|\nabla u_h|^2 + (u_h+1)^2(u_h-2)^2 \, \mathrm{d}x \\ &= \min_{u_h \in \mathcal{U}_h^B} \sum_{e=1}^{N+1} \underbrace{A_1\xi_e^2 + A_2\xi_e\xi_{e-1} + A_3\xi_{e-1}^2 + B_1\xi_e^4 + \cdots + B_5\xi_{e-1}^4}_{f^e(\xi_e,\xi_{e-1})}\end{aligned}$$

Thus, the objective is a sum of polynomials each depending on very few variables.

Among the DOF ξ_j, two variables are said to be connected if they appear in one of these polynomials. If each DOF is a node, then this leads to a graph referred to as a ``sparsity graph''. In 1D it is trivial:

$$\xi_1 \;\text{———}\; \xi_2 \;\text{———}\; \xi_3 \;\text{—}\; \cdots \;\text{—}\; \xi_{N-1} \;\text{———}\; \xi_N$$

Example and sparsity graphs

If the sparsity graph is chordal, then the sparse representation theorem mentioned before holds. A graph is chordal if all cycles of four or more vertices have an edge that is not part of the cycle that connects two vertices of the cycle.

A clique is a group of variables all connected to each other, and a maximal clique is a clique that cannot be extended by including one more adjacent vertex. If κ is the size of the largest maximal clique, then the cost of solving the optimization problem drops from $\mathcal{O}(N^{2\omega})$ to $\mathcal{O}(\kappa^{2\omega})$.

In 1D, the graph is trivially chordal, and $\kappa = 2$. In 2D, it is not usually chordal. However, it is always possible to add redundant connectivities to satisfy chordality at the cost of increasing κ.

Summary

Mevissen et al. had already considered similar discretization using finite differences for constrained problems, but had been unable to prove convergence to infinite-dimensional problem.

$$\begin{tikzcd}[column sep=huge]
\inf\limits_{u\in\mathcal{U}}\int_\Omega E(x,u,\nabla u)\,\mathrm{d}x \arrow[r, shift right, "\text{FD/finite elements}"'] \arrow[rr, bend right, dashed, "\text{Mevissen et al. (2008)}"'] & \min\limits_{|\xi_j|\le 1/h} \sum_{e=1}^{n_{\mathrm{el}}} f^e(\boldsymbol{\xi}^e) \arrow[l, shift right, red, "{\substack{\Gamma\text{-convergence}\\ h\to 0}}"'] \arrow[r, shift right, "{\substack{\text{sparse relaxation}\\ +\text{compactness}\\ \text{Waki et al. (2006)}}}"'] & (\mathrm{sSPD}_\omega) \arrow[l, shift right, "{\substack{\text{Lasserre (2006)}\\ +\text{chordality \& compactness}\\ \omega\to\infty}}"']
\end{tikzcd}$$

Missing: Proof that global finite-dimensional optimizers (POP solutions) converge to global optimizer of infinite-dimensional problem.

Solution: Γ-convergence (with compactness).

Γ-convergence

$$\Psi(u) = \int_{\Omega} E(x, u, \nabla u)\,\mathrm{d}x$$

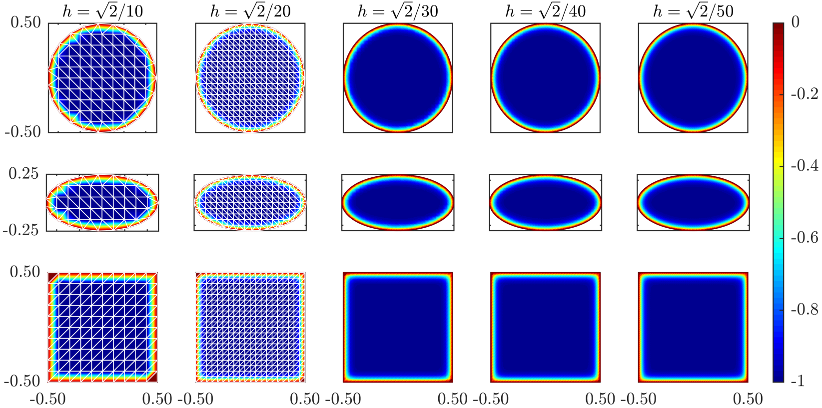
- Equicoercivity:
  - A uniform bound $\Psi(u_h) \leq C$ for a sequence $u_h \in \mathcal{U}_h^B$ implies $\|u_h\|_{\mathcal{U}}$ are also bounded uniformly.
  - This follows easily from the growth and coercivity conditions on E.
- Existence of recovery sequence:
  - For every $u \in \mathcal{U}$, there exists a sequence $\{u_h\}_h \subseteq \mathcal{U}_h^B$ such that $u_h \to u$ in $\|\cdot\|_{\mathcal{U}}$ and $\Psi(u_h) \to \Psi(u)$.
  - This follows from finite element approximation properties under the technical condition $p_{\mathrm{FE}} > k - 1 + \frac{n}{p}$ where p_{FE} is the FE order of discretization, k is the global regularity C^k of the discretization, with n and p coming from $W^{1,p}(\Omega)$ and $\Omega \subseteq \mathbb{R}^n$.
- Sequential weak lower semicontinuity:
  - If $u_h \rightharpoonup u$ then $\liminf_h \Psi(u_h) \geq \Psi(u)$.
  - Follows from ``standard'' arguments in calculus of variations (Morrey).

2D Example: two-well problem

$$\min_{u\in H_0^1(\Omega)} \int_\Omega \frac{1}{100}|\nabla u|^2 + (u+1)^2(u-2)^2\,\mathrm{d}x$$

Fix an h, then iterate over ω until achieving convergence to the finite-dimensional global minimum. Refine h and repeat.

In all meshes considered $\omega = 2$ was sufficient. No chordality was enforced. The bound used was $B = \sqrt{2}/h$. At least two possible local minima, only one global.



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$$\min_{u\in H_0^1(\Omega)} \int_\Omega \tfrac{1}{100}|\nabla u|^2 + (u+1)^2(u-2)^2\,\mathrm{d}x$$

No running intersection

h	# cliques	max sz	avg sz	time (s)
$\sqrt{2}/10$	128	3	3	0.47
$\sqrt{2}/20$	648	3	3	2.65
$\sqrt{2}/30$	1568	3	3	7.61
$\sqrt{2}/40$	2888	3	3	16.3
$\sqrt{2}/50$	4608	3	3	29.3

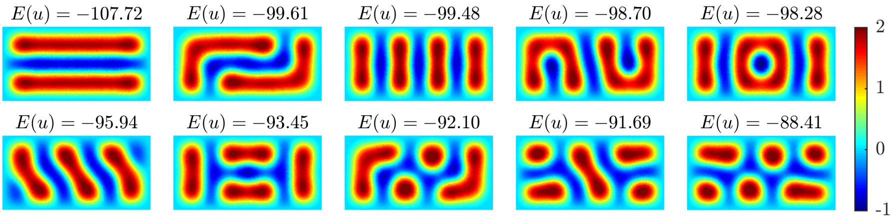
With running intersection

h	# cliques	max sz	avg sz	time (s)
$\sqrt{2}/10$	72	10	7.7	**21.9**
$\sqrt{2}/20$	342	20	14.3	**15 545**
$\sqrt{2}/30$	812	30	21	N/A
$\sqrt{2}/40$	1482	40	27.7	N/A
$\sqrt{2}/50$	2352	50	34.3	N/A

2D Example: Swift-Hohenberg

$$\min_{u \in H_0^2(\Omega)} \int_\Omega (\Delta u + u)^2 - \tfrac{3}{10}u^2 - \tfrac{6}{5}u^3 + \tfrac{1}{2}u^4 \, \mathrm{d}x \qquad \Omega = [-12, 12] \times [-6, 6]$$

Solution space is very rich: gradient descent from random initial conditions yielded a list of local solutions.



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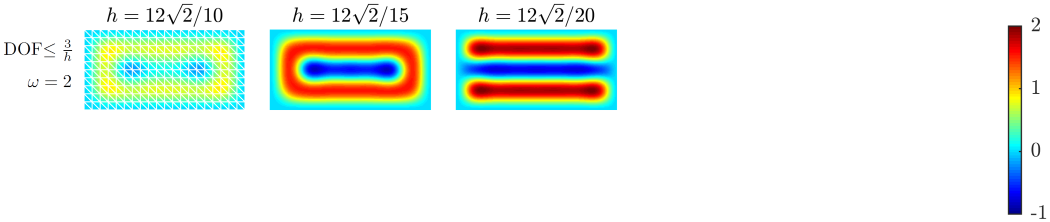

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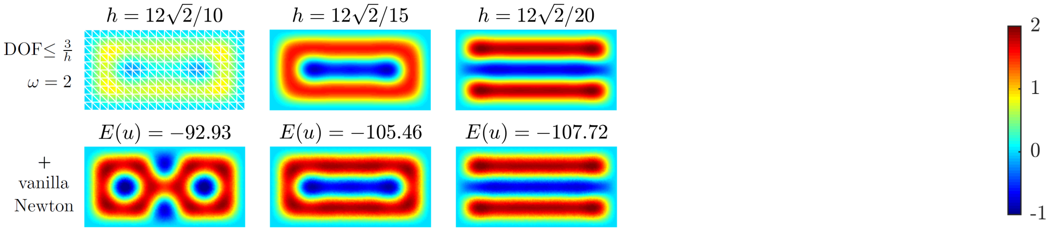

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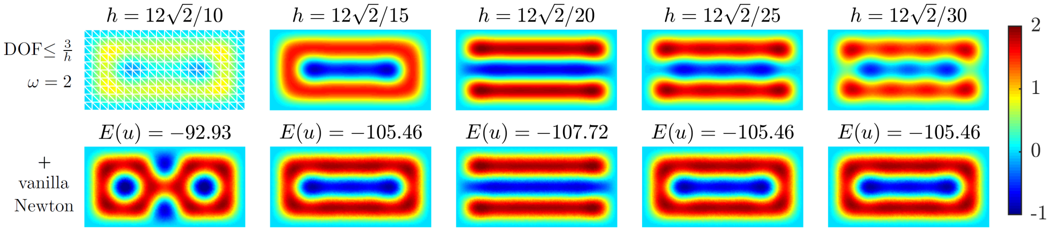

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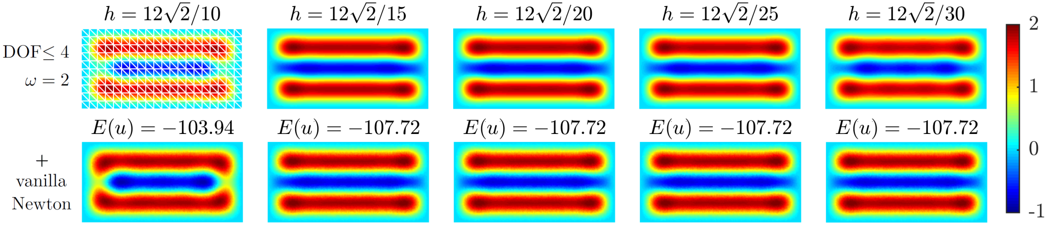

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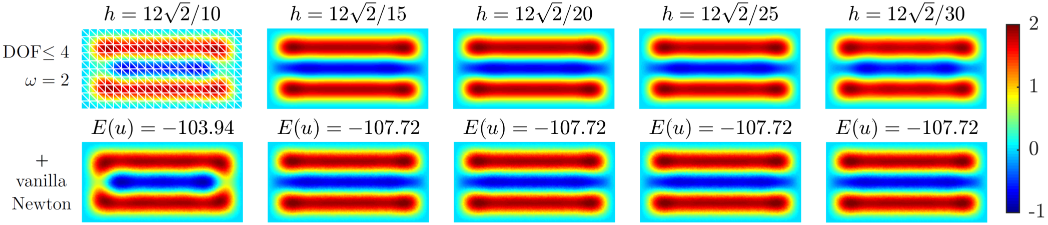

Lesson: Always try to converge in ω first. If bound $B = \frac{3}{h}$ is too large (thus needing higher ω), choose a fixed bound instead.

Extensions

Find (global) minimizer of integral functional

$$\inf_{\substack{u\in\mathcal{U} \\ \mathcal{N}(u,v)=0\ \forall v\in\mathcal{V}}} \int_\Omega E(x,u,\nabla u)\,\mathrm{d}x$$

so that the optimization is now PDE-constrained: $\mathcal{N}(u,v)$ is a PDE enforced variationally. Extra assumptions needed to ensure existence of solutions.

$\mathcal{N}(u,v)$ could be nonlinear. In fact it can be proved in the case it is monotonic.

Note that in this case the definition of connectivity in the sparsity graph is more complicated as it is dependent on the constraints, which typically implies the relevant maximal clique size is larger (which increases the cost).

Γ-convergence is now more difficult to establish with the PDE constraints.

Conclusions

To the authors' knowledge: First algorithm producing approximations that rigorously converge to a *global* optima of nonlinear integral functionals.

Combines finite element methods and polynomial optimization. The latter requires of compactness, and in theory a technical condition chordality, which does not appear to be necessary for the method to work in practice.

As long as the solution has ``converged'' in ω, it can be used as an initial guess for a Newton solver that is closer to the global optimum.

Numerous future applications where global optimality (as opposed to local) is relevant.

Preprint coming soon.

Thank you!

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