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Numerical Mountain Pass and its Applications

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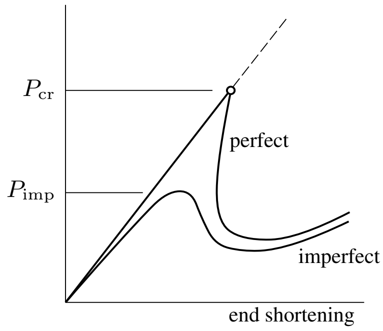
The mountain pass theorem is an important tool in the calculus of variations and in finding solutions to nonlinear PDEs in general. The mountain pass structure can be exploited numerically, as well. We explain the main ideas on an example of buckling of a cylindrical shell. First, we prove existence of an MP-solution for almost all values of a given load parameter. Then, we find a numerical approximation of such a solution. Finally, we compare the results of a numerical continuation in the load parameter with results of physical experiments and make a few comments about further numerical investigations of the problem.

1 Introduction to buckling of a cylindrical shell

A classical problem in structural engineering is the prediction of the load-carrying capacity of an axially-loaded cylinder. As well as being a commonly used structural element, the axially-loaded cylinder is also the archetype of unstable, imperfection-sensitive buckling, and this has led to a large body of theoretical and experimental research.

Viewed as a bifurcation problem, the buckling of the cylinder is a subcritical symmetry-breaking pitchfork bifurcation (Figure 1 left). Generically, imperfections in the structure eliminate the bifurcation and round off the branch of solutions, resulting in a turning-point at a load P_{imp} strictly below the critical (bifurcation) load P_{cr} of the perfect structure. In an experiment in which the load is slowly increased, the system will fail (*i.e.* make a large jump in state space) at load P_{imp}.



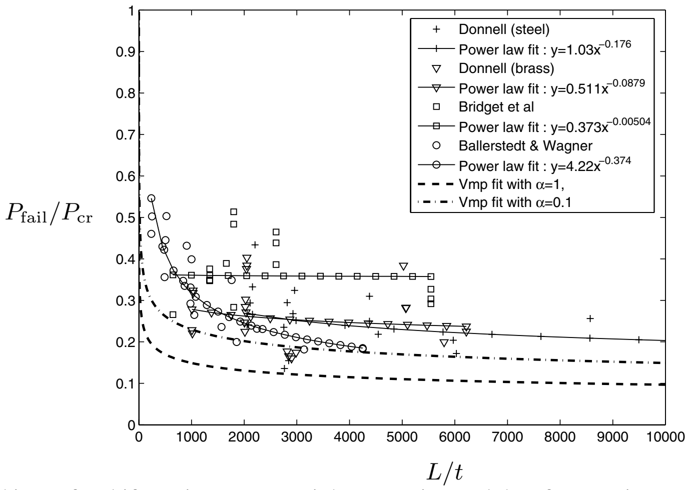


Fig. 1 Left: Illustration of perfect and imperfect bifurcation curves. Right: Experimental data from various research groups, all representing failure loads of axially-loaded cylinders. The horizontal axis is the ratio of cylinder length and wall thickness; the vertical axis is the ratio of the failure load and the theoretical critical load as predicted for perfect cylinders. Note that all tested cylinders fail at loads significantly lower than that predicted by theory; in some cases failure occurred at less than one-fifth of the theoretical load-carrying capacity. Power-law fitting lines are added to emphasize the dependence of failure load on geometry. The data are from [5, 3, 2].

Instead of studying actual behavior of imperfect cylinders, we deduce an estimate of the sensitivity to imperfections from the energy landscape of the perfect cylinder. The final result is a lower bound on the failure load, and the approach gives additional insight into the problem. The key result is the existence of a *mountain-pass point*, an equilibrium state that sits astraddle in the energy landscape between two valleys; one valley surrounds the unbuckled state, and the other contains many buckled, large-deformation states.

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A cylindrical shell is modeled by the Von Kármán-Donnell equations which can be rescaled [7] to the form

$$\Delta^2 w + \lambda w_{xx} - \phi_{xx} - 2\,[w,\phi] = 0, \tag{1}$$

$$\Delta^2 \phi + w_{xx} + [w,w] = 0, \tag{2}$$

where the bracket is defined as

$$[u,v] = \frac{1}{2}u_{xx}v_{yy} + \frac{1}{2}u_{yy}v_{xx} - u_{xy}v_{xy}. \tag{3}$$

The function w is a scaled inward radial displacement measured from the unbuckled (fundamental) state, ϕ is the Airy stress function, and $\lambda \in (0,2)$ is a load parameter. The unknowns w and ϕ are defined on a two-dimensional spatial domain $\Omega = (-a,a) \times (-b,b)$, where $x \in (-a,a)$ is the axial and $y \in (-b,b)$ is the tangential coordinate. Since the y-domain $(-b,b)$ represents the circumference of the cylinder, the following boundary conditions are prescribed:

$$w \text{ is periodic in } y, \quad \text{and} \quad w_x = (\Delta w)_x = 0 \text{ at } x = \pm a, \tag{4a}$$

$$\phi \text{ is periodic in } y, \quad \text{and} \quad \phi_x = (\Delta \phi)_x = 0 \text{ at } x = \pm a. \tag{4b}$$

1.1 Functional setting

We search for weak solutions w, ϕ of (1–4) in the space

$$X = \left\{ \psi \in H^2(\Omega) : \psi_x(\pm a, \cdot) = 0,\ \psi \text{ is periodic in } y, \text{ and } \int_\Omega \psi = 0 \right\}$$

with norm

$$\|w\|_{X,\lambda} = \left[\int_\Omega \left(\Delta w^2 + \Delta\phi_1^2 - \lambda w_x^2 \right) \right]^{1/2}$$

where the load parameter $\lambda \in (0,2)$ is fixed and $\phi_1 \in H^2(\Omega)$ is the unique solution of

$$\Delta^2 \phi_1 = -w_{xx}, \qquad \phi_1 \text{ satisfies (4b)}, \qquad \text{and} \qquad \int_\Omega \phi_1 = 0. \tag{5}$$

This norm is equivalent to the H^2-norm on the set X, and with the appropriate inner product $\langle \cdot, \cdot \rangle_{X,\lambda}$ the space X is a Hilbert space.

Equations (1–2) are related to the stored energy E, the average axial shortening S, and the total potential given by

$$E(w) := \frac{1}{2}\int_\Omega \left(\Delta w^2 + \Delta \phi^2 \right), \qquad S(w) := \frac{1}{2}\int_\Omega w_x^2, \qquad F_\lambda = E - \lambda S. \tag{6}$$

Note that the function ϕ in (6) is determined from w by solving (2) with boundary conditions (4b). All E, S, and F_λ belong to $C^1(X)$, *i.e.*, are continuously Fréchet differentiable.

2 The mountain pass

We briefly recall the general context of the Mountain-Pass Theorem of Ambrosetti and Rabinowitz [1]. Let I be a functional defined on a Banach space X, and let w_1, w_2 be two distinct points in X. Consider the family Γ of all paths in X connecting w_1 and w_2 and define

$$c = \inf_{\gamma \in \Gamma} \max_{w \in \gamma} I(w)\ , \tag{7}$$

that is the infimum of the maxima of the functional I along paths in Γ. If $c > \max\{I(w_1), I(w_2)\}$, then the paths have to cross a "mountain range" and one may conjecture that there exists a critical point w_{MP} of I at the level c, called a mountain pass point.

This idea is applied to the Von Kármán-Donnell-equations in the following way. We take for I the total potential F_λ at some fixed value of λ, and for the end point w_1 the origin. We will obtain a mountain-pass solution by the following steps:

- It can be shown that $w_1 = 0$ is a local minimizer; in particular there are $\varrho, \alpha > 0$ such that $F_\lambda(w) \geq \alpha$ for all w with $\|w\|_X = \varrho$.
- If the domain Ω is large enough, it can be shown that there exists w_2 with $F_\lambda(w_2) \leq 0$.
- Given a sequence of paths γ_n that approximates the infimum in (7), we extract a (Palais-Smale) sequence of points $w_n \in \gamma_n$, each one close to the maximum along γ_n, and show that this sequence converges in an appropriate manner.

In this way it follows that there exists a mountain-pass critical point w with $F_\lambda(w) = c$, provided that the domain is sufficiently large. For technical reasons (lack of coerciveness of the functional F_λ) this procedure can be performed only for almost all $0 < \lambda < 2$ (cf. [7] for details).

3 Mountain-pass algorithm

We now describe one of the variational methods used to find numerical approximations of critical points of the total potential F_λ. In our numerical experiments these methods are accompanied by the Newton method and continuation. The advantage of this approach is that it combines the knowledge of a part of the energy landscape with that of a small neighborhood of a solution.

The mountain-pass algorithm was first proposed in [4] for a second order elliptic problem in 1D. It was later used in [9] for a fourth-order problem in 2D.

Let the load parameter $\lambda \in (0, 2)$ be fixed, we work in a discretized version of $(X, \langle\cdot,\cdot\rangle_{X,\lambda})$. We denote $w_1 = 0$ the local minimum of F_λ and take a point w_2 such that $F_\lambda(w_2) < 0$. We find such a point by a steepest descent method—by numerical solution of the initial value problem

$$\frac{d}{dt} w(t) = -\nabla_\lambda F_\lambda(w(t)) , \qquad w(0) = w_0$$

on a sufficiently large interval $(0, T]$ for a suitable starting point w_0 ($\nabla_\lambda F_\lambda(w)$ denotes the gradient of F_λ at w).

We take a discretized path $\{z_m\}_{m=0}^{p}$ connecting $z_0 = w_1$ with $z_p = w_2$. After finding the point z_m at which F_λ is maximal along the path, this point is moved a small distance in the direction $-\nabla_\lambda F_\lambda(z_m)$. Thus the path has been deformed and the maximum of F_λ lowered. This deforming of the path is repeated until the maximum along the path cannot be lowered any more: a critical point $w_{\rm MP}$ has been reached. Figure 2 shows the main idea of the method.

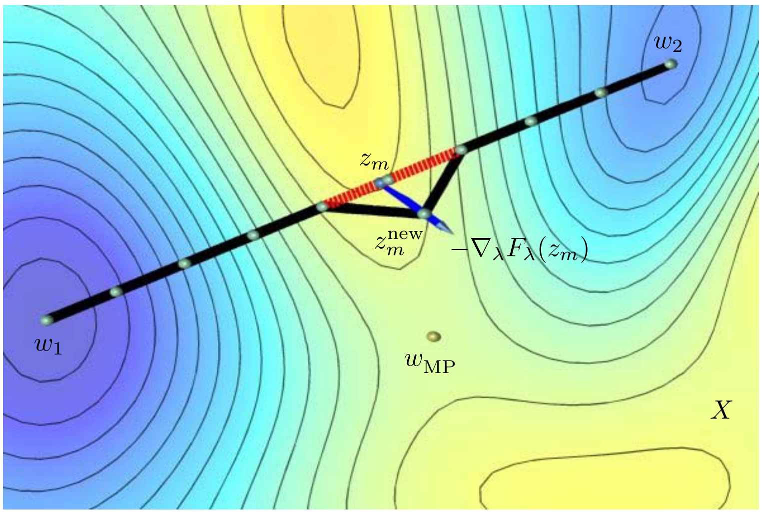

Fig. 2 Deforming the path in the main loop of the mountain pass algorithm: point z_m is moved a small distance in the direction $-\nabla_\lambda F_\lambda(z_m)$ and becomes $z_m^{\rm new}$. This step is repeated until the mountain pass point $w_{\rm MP}$ is reached.

The mountain pass algorithm is local in its nature. The numerical solution $w_{\rm MP}$ it finds has the mountain-pass property in a certain neighborhood only. The choice of the path endpoint w_2 may influence to which critical point the algorithm converges. Different choices of w_2 are in turn achieved by choosing different initial points w_0.

4 Numerical experiments

A numerical mountain-pass solution (with the smallest energy) for $\lambda = 1.4$ and $\Omega = (-100, 100)^2$ is shown in Fig. 3. In our numerical computations we have observed that for large domains the size of the domain has a small influence on the energy $F_\lambda(w_{\rm MP})$ at a fixed value of load λ [8]. Hence we can define numerically a function $V(\lambda) := F_\lambda(w_{\rm MP})$, the mountain-pass energy level at a given load λ (independent of the computational domain size).

By definition, $V(\lambda)$ is the lowest energy level at which it is possible to move between the basins of attraction of w_1 and w_2 (path end points). If the loading imperfection is interpreted as a mechanism capable of maintaining the system at a higher energy level than that of the neighboring fundamental minimizer, then the number $V(\lambda)$ is critical: as long as the imperfection is so small that the energy is never raised by more than $V(\lambda)$, the new stationary point will be part of the same basin of attraction as w_1. For larger imperfections, however, it becomes possible to leave the fundamental basin of attraction, resulting in a large jump in state space.

Comparing cylinders of varying geometry requires a common measure of imperfection sensitivity. Here we choose to rescale the mountain-pass energy level by the other energy level present in the loaded cylinder: the energy that is stored in homogeneous compression of the unbuckled shell. The most straightforward calculation is to rescale the dimensional

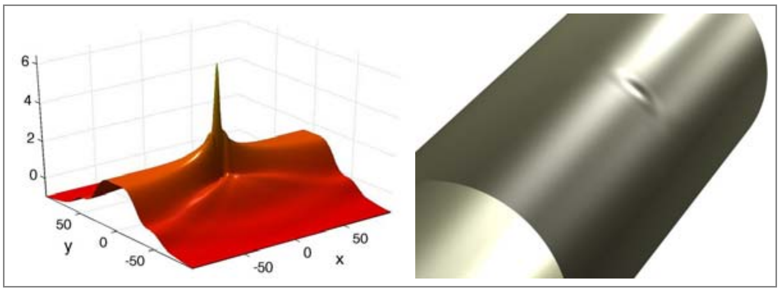

Fig. 3 MP-solution for $\lambda = 1.4$ found using the MP-algorithm. Left: graph of $w_{\mathrm{MP}}(x, y)$, right: rendering on a cylinder.

mountain-pass energy by the elastic strain energy stored in the full length of the compressed cylinder of length L to give an energy ratio α (or a rescaled mountain-pass energy level),

$$\alpha = \frac{1}{2\pi\sqrt{3(1-\nu^2)}} \frac{t}{L} \frac{V(\lambda)}{\lambda^2}, \tag{8}$$

where t denotes the thickness of the shell and ν is the Poisson's ratio. From this expression and the numerically obtained function $V(\lambda)$ curves may be drawn in a plot of load versus the ratio L/t (Figure 1 right). Note that to obtain this figure the curve $V(\lambda)$ was fitted to extend the range of λ. This figure shows two remarkable features:

1. The general trend of the constant-α curves is very similar to the trend of the experimental data;
2. The $\alpha = 1$ curve, which indicates the load at which the mountain-pass energy equals the stored energy in the prebuckled cylinder, appears to be a lower bound to the data.

It is possible to see the problem of finding critical points of F_λ from another perspective—find critical points of the stored energy E under a fixed shortening S. The load λ is a Lagrange multiplier in this case. Numerically, these points are searched for as local constrained minimizers or constrained mountain-pass points. A large number of solutions can be found under a fixed value of S [8], three of them are shown in Fig. 4.

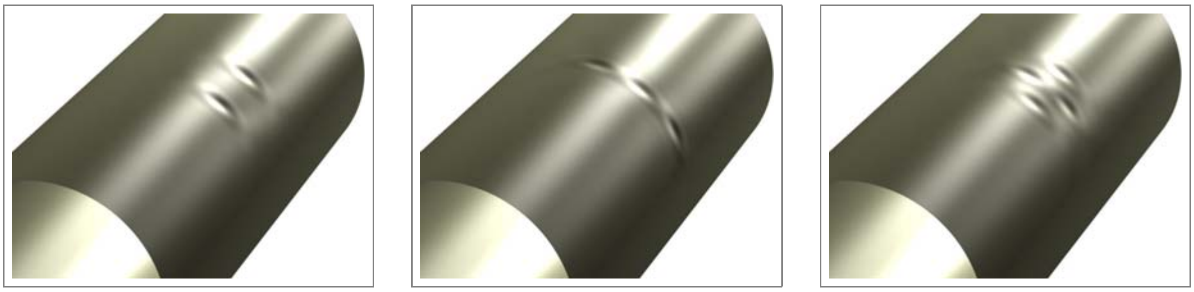

Fig. 4 Some numerical solutions for fixed shortening $S = 40$ found using the constrained descent method and the constrained mountain pass algorithm.

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