Computing multiple solutions of nonlinear problems

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Can you conduct an experiment twice . . .

. . . and get two different answers?

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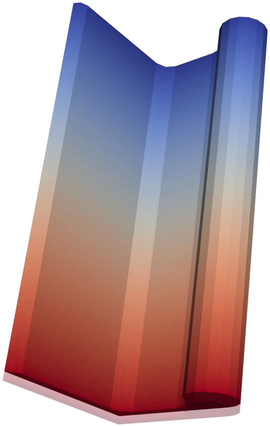
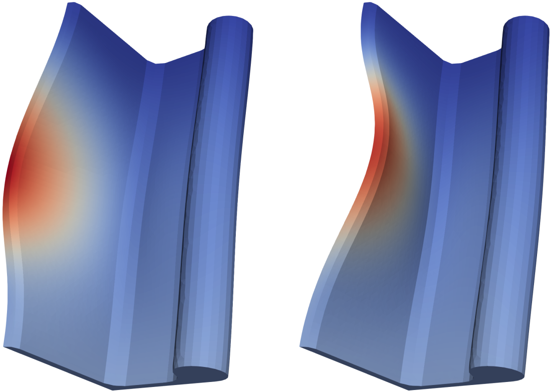


Axial displacement test of an Embraer aircraft stiffener.

Can you conduct an experiment twice . . .

. . . and get two different answers?



Two different, stable configurations.

When a problem has multiple solutions, it is usually crucial.

The AIAA/NASA high lift prediction test case (Kamenetskiy et al., 2013)

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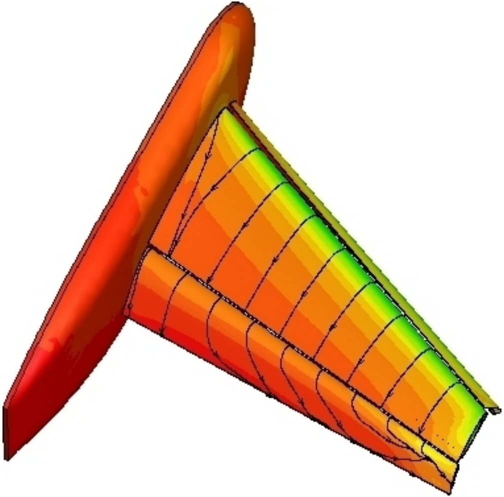

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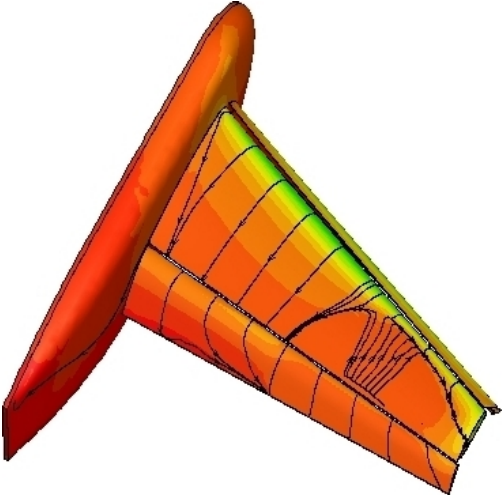

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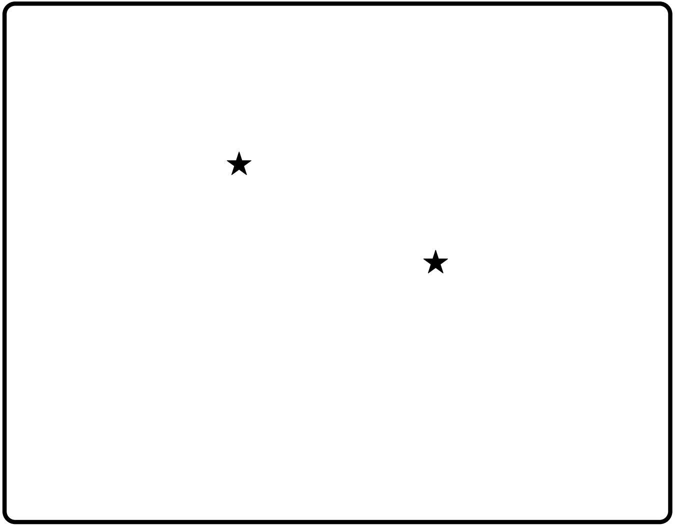
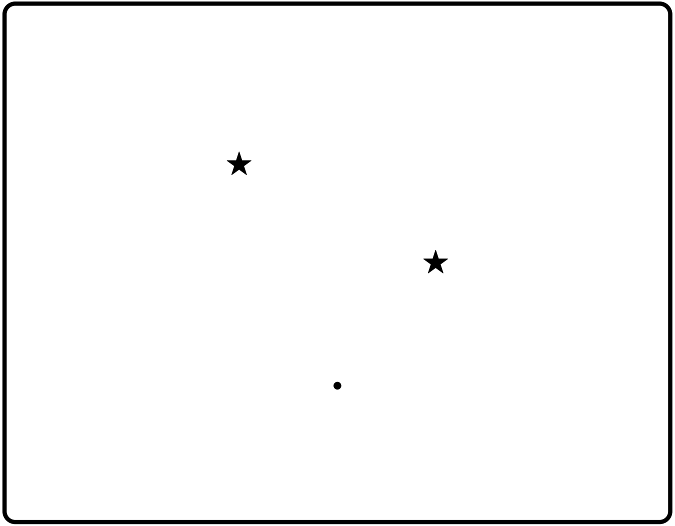


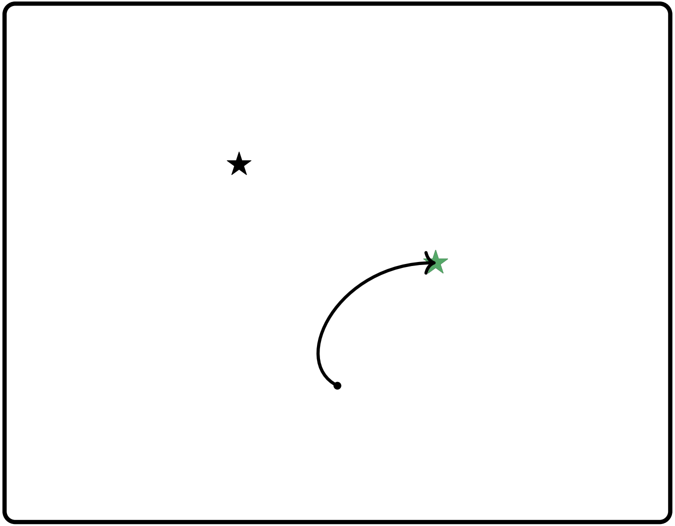
A PDE with two unknown solutions

When a problem has multiple solutions, it is usually crucial.



Start from some initial guess

When a problem has multiple solutions, it is usually crucial.



We converge to one solution, our prediction

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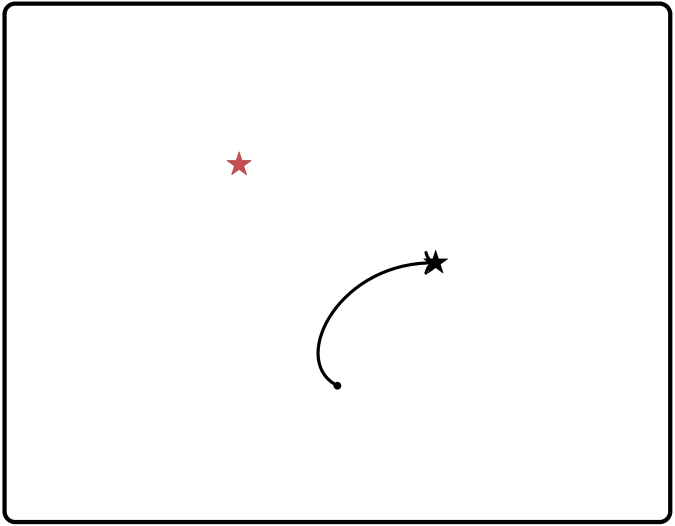

But nature has chosen another (unknown) solution!

When a problem has multiple solutions, it is usually crucial.

Warning

Your calculations can be correct, but still return the *wrong answer*.

Mathematical formulation

Compute the multiple *solutions* $u^\star$ of a stationary nonlinear equation

$$F(u^\star, \lambda) = 0$$
$$F \in C^1(X \times \mathbb{R}, Y)$$

as a function of a parameter $\lambda \in \mathbb{R}$. (X, Y Banach spaces.)

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Case #1: aircraft stiffener

$u^\star$ displacement (a vector field), λ loading, F hyperelasticity

Case #2: aircraft wing

$u^\star$ velocity and pressure, λ angle of attack, F Navier–Stokes

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Warning

We (usually) can't guarantee to find *all* solutions. But finding many is better than finding one.

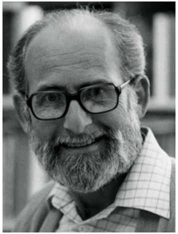
Section 2

Classical techniques

Basic idea of numerical bifurcation analysis:

procedure $\text{ANALYSE}(u_0, \lambda_0)$

end procedure

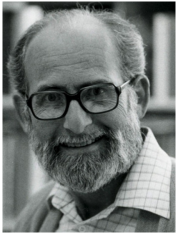


Herbert Keller

Basic idea of numerical bifurcation analysis:

procedure ANALYSE(u_0, λ_0)
    continue branch of solutions;

end procedure



Herbert Keller

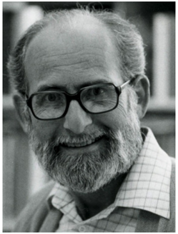
Continuation

Extending our knowledge of the branch to other values of λ.

Basic idea of numerical bifurcation analysis:

procedure ANALYSE(u_0, λ_0)
    continue branch of solutions;
    detect bifurcations on the branch;

end procedure



Herbert Keller

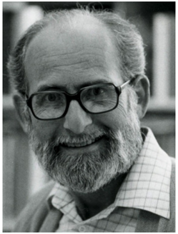
Bifurcation detection

Discovering when a bifurcation has occurred on the branch.

Basic idea of numerical bifurcation analysis:

procedure ANALYSE(u_0, λ_0)
    continue branch of solutions;
    detect bifurcations on the branch;
    localise bifurcations;

end procedure



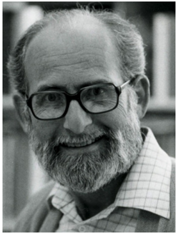
Herbert Keller

Bifurcation localisation

Identifying precisely the bifurcation point.

Basic idea of numerical bifurcation analysis:

procedure ANALYSE(u_0, λ_0)
continue branch of solutions;
detect bifurcations on the branch;
localise bifurcations;
switch branches at bifurcations, and recurse.
end procedure



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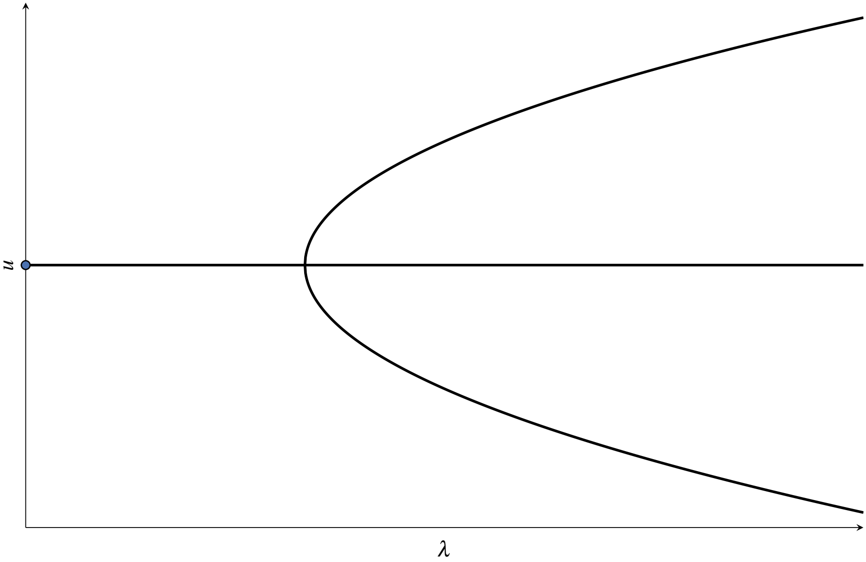
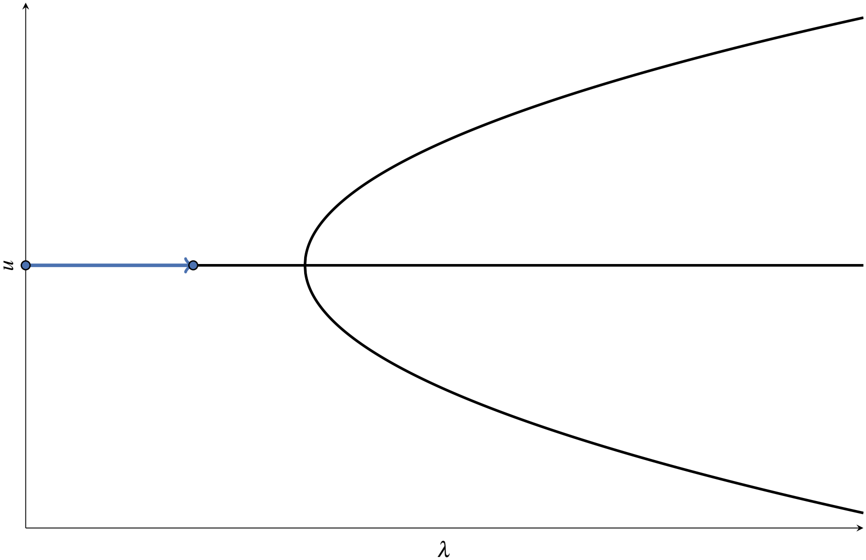
Branch switching

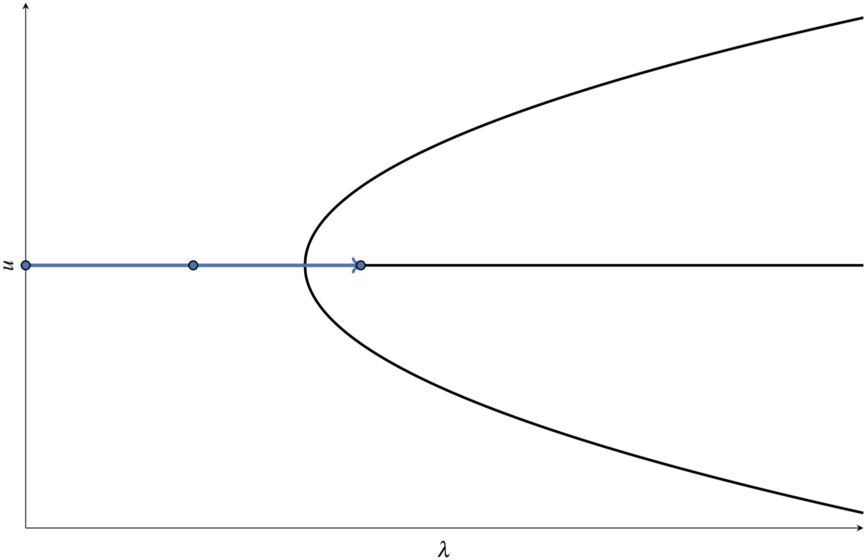
Constructing the emanating branches, and analysing them recursively.



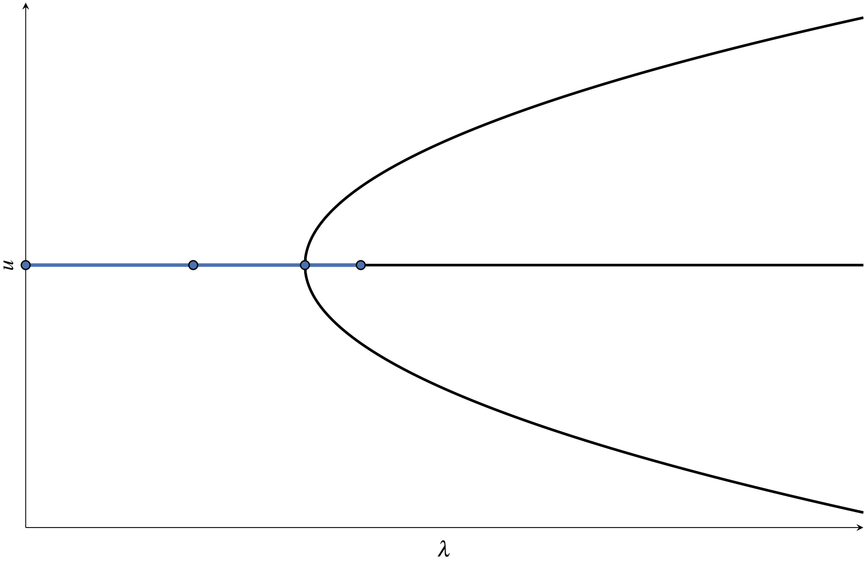
Start with one known solution (u_0, λ_0).



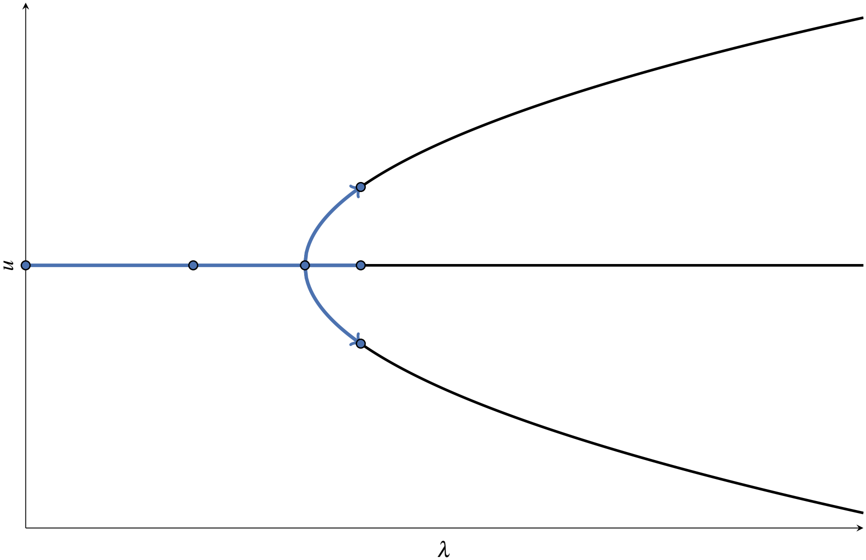
Continue the branch, finding a solution for the next parameter value.



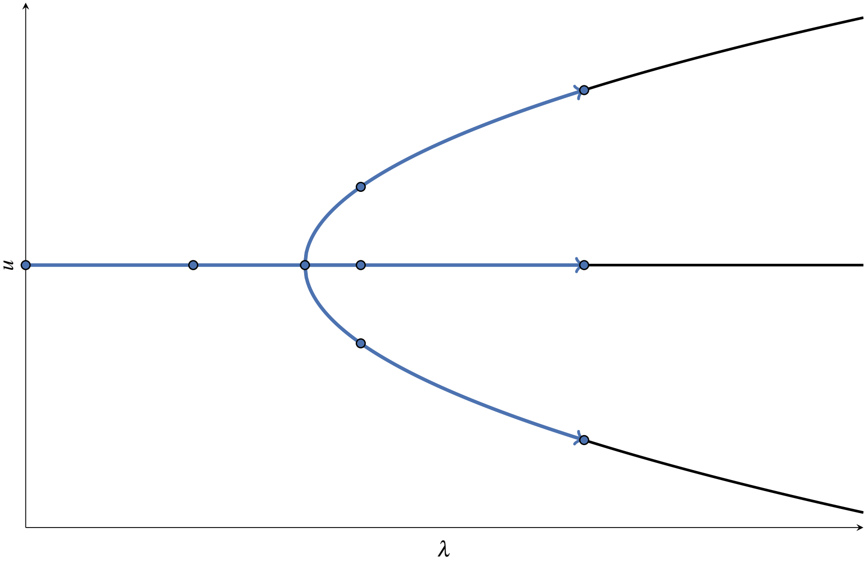
Detect we have passed a bifurcation, where the number of solutions varies.



Localise bifurcation point, by solving a system of equations.



Switch branches.



Apply recursively.

Good news

The combination of continuation and branch switching is very powerful.

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Bad news

However, it has some disadvantages and weaknesses, too.

Downside A

You have to solve a lot of different problems.

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$$\begin{bmatrix} F(u, \lambda) \\ p(u, \lambda, s) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad F_u(u, \lambda)v = \lambda v \qquad \begin{bmatrix} F(u, \lambda) \\ F_u(u, \lambda)v \\ \|v\|^2 - 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

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Finely-resolved simulations

This is OK when you can afford Gaussian elimination, but not at scale.

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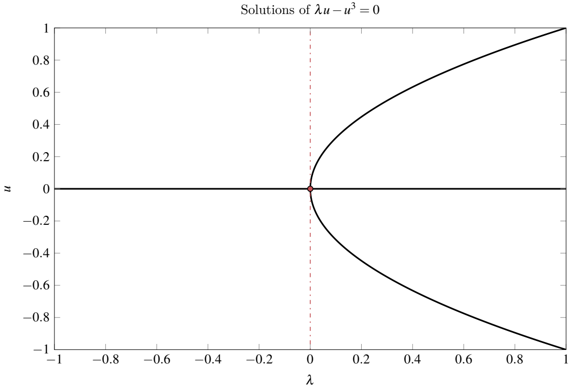

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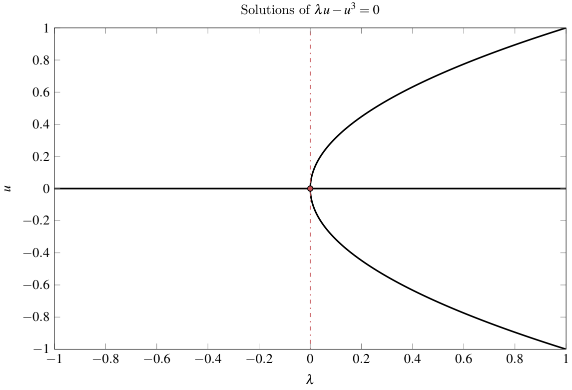
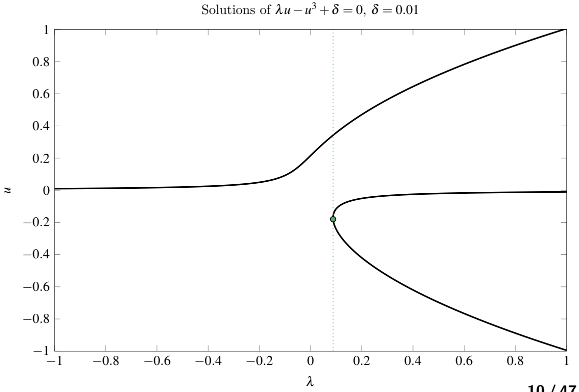


. . . but this does not.



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Problem B

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Problem B

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Problem C

Restoring connectedness is not always possible!

In this talk I describe a complementary approach.

Disconnected diagrams

An algorithm that can compute **disconnected bifurcation diagrams**.

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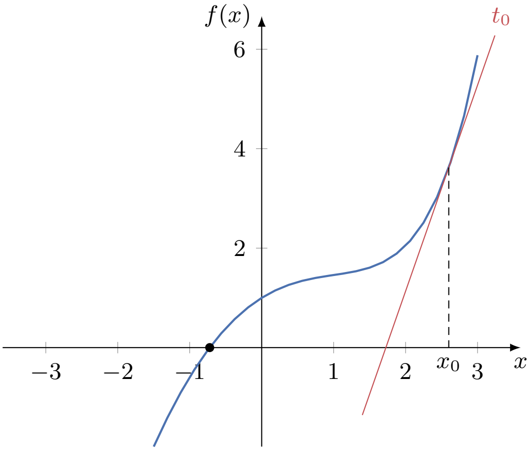
Simplicity & scaling

The computational kernel is exactly the same as Newton's method:
only one kind of problem to solve.

Section 3

Newton's method

Essential idea: solve a succession of *linearised* rootfinding problems.



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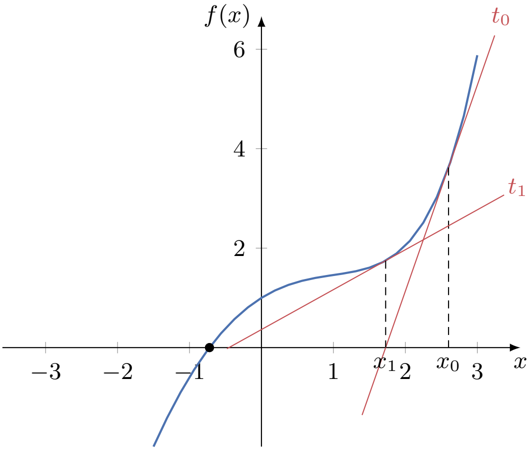

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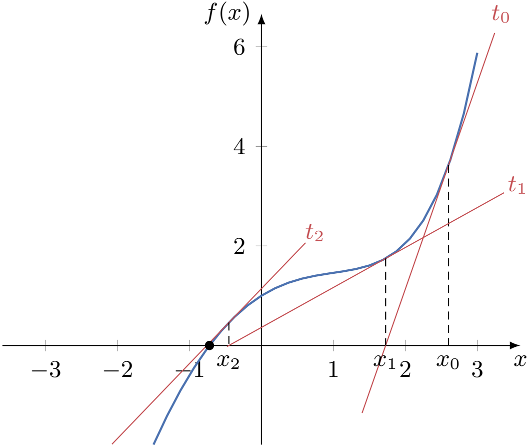

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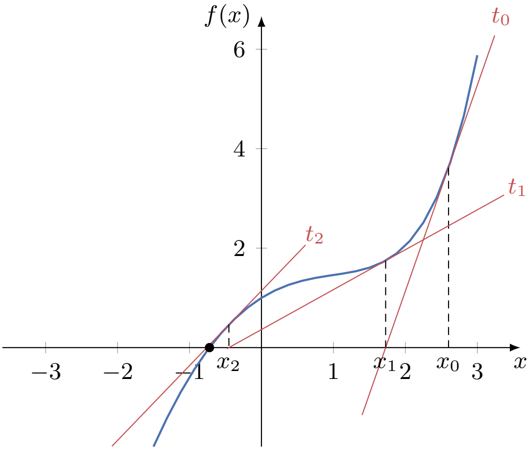

solve $f'(x_k)\delta x_k = -f(x_k)$; update $x_{k+1} = x_k + \delta x_k$.

This extends to $F \in C^1(X;Y)$. Given $u_0 \in X$, Newton's method is to

$$\text{solve } F_u(u_k)\delta u_k = -F(u_k); \text{ update } u_{k+1} = u_k + \delta u_k,$$

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Good news

This converges if u_0 is close to a root, and usually converges *quadratically*.

Section 4

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- a solution $u \in X$, $F(u) = 0$, $F_u(u)$ nonsingular

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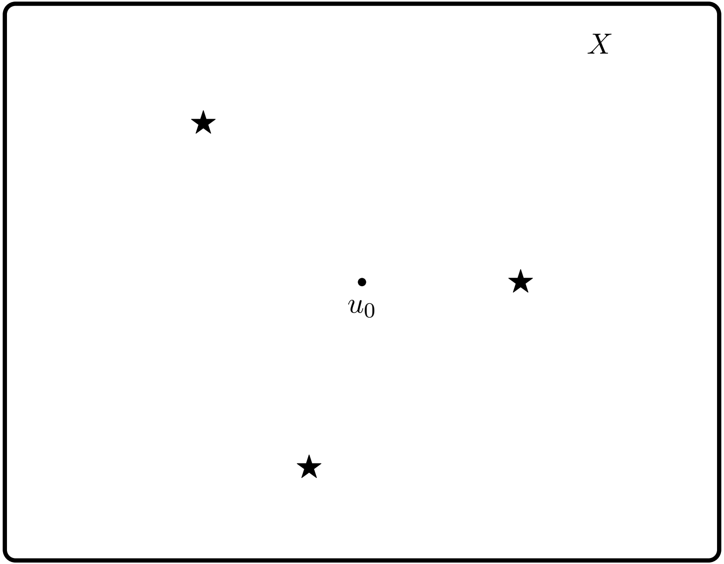
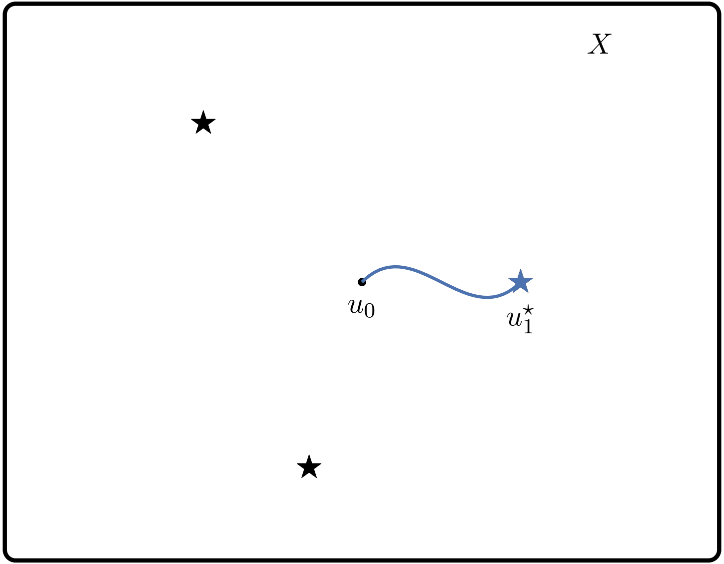
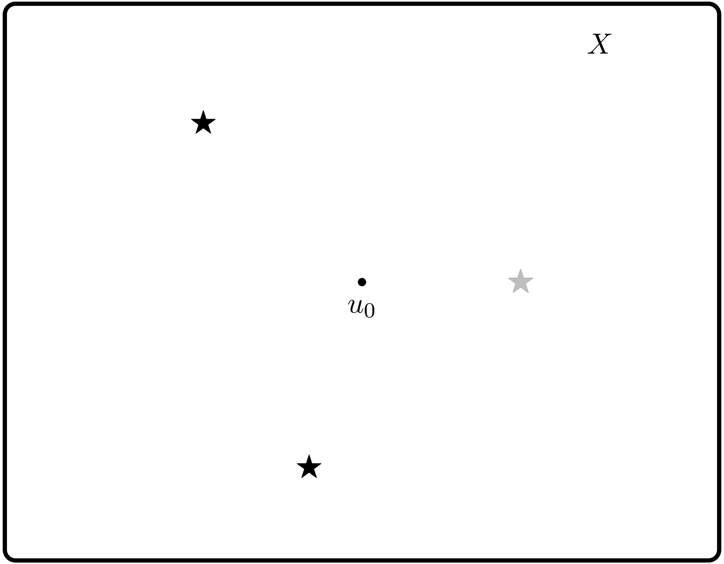
Find more solutions, starting from the same initial guess.

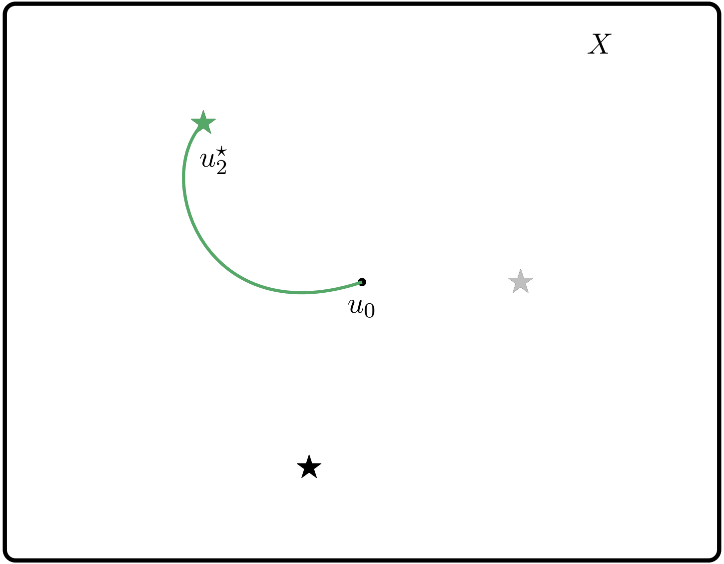

X
u_0



Newton from initial guess.



Deflate solution found.



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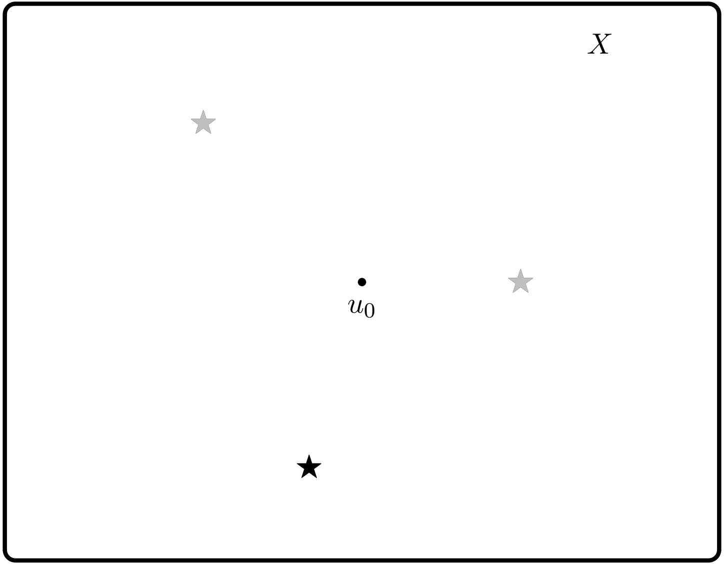

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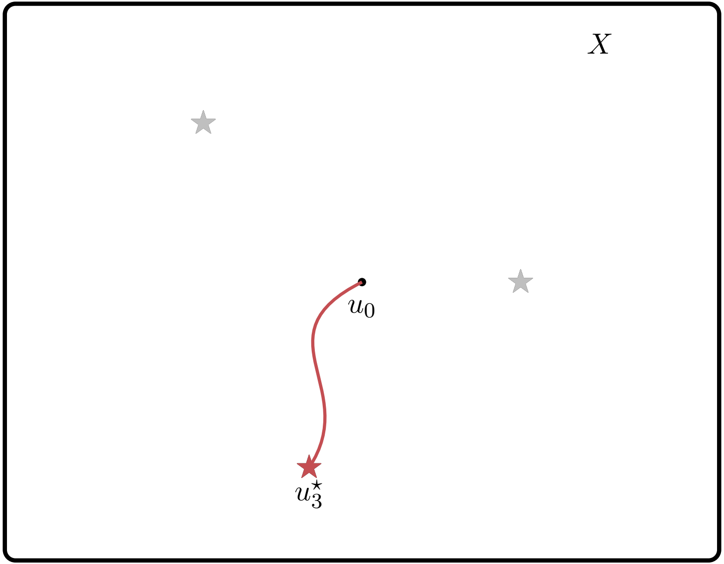

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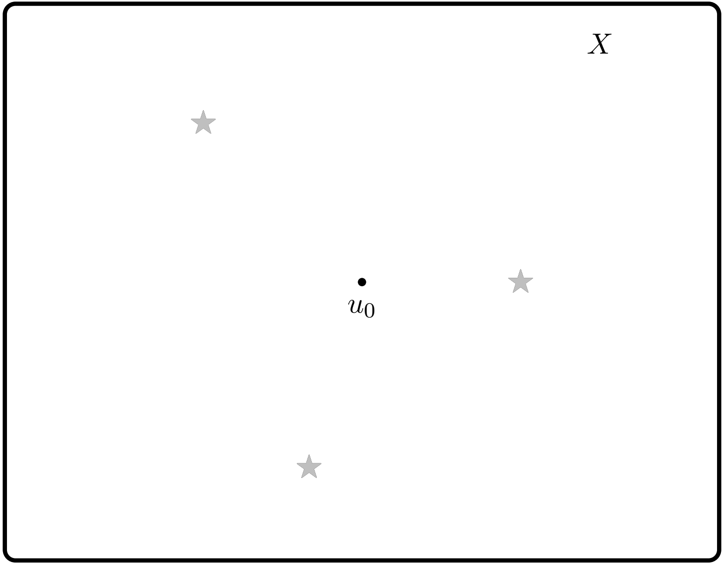

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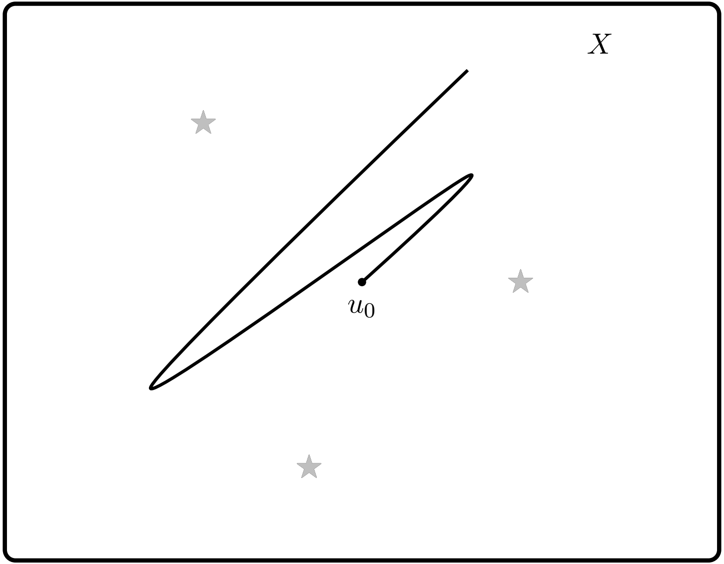
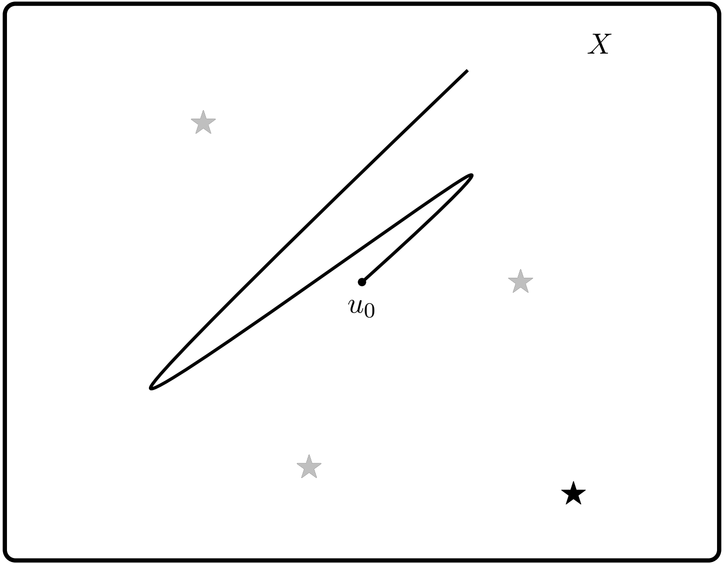


Terminate on nonconvergence.



Terminate on nonconvergence.

How can you do it?

Definition

We say that $M(u; u^\star) \in C^1(X, Y)$ is a *deflation operator* if

$$\liminf_{u \to u^\star} \|G(u)\| := \liminf_{u \to u^\star} \|M(u; u^\star) F(u)\| > 0.$$

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Newton's method is looking for sequences (u_k) that send $G(u_k) \to 0$. But a deflation operator hides the existence of the root as $u \to u^\star$.

The deflation operator we propose

$$M(u; u^\star) := \left(\frac{1}{\|u - u^\star\|^p} + 1 \right), \quad p \geq 1.$$

Ásgeir Birkisson, 1985–

Simon Funke, 1983–

The deflation operator we propose

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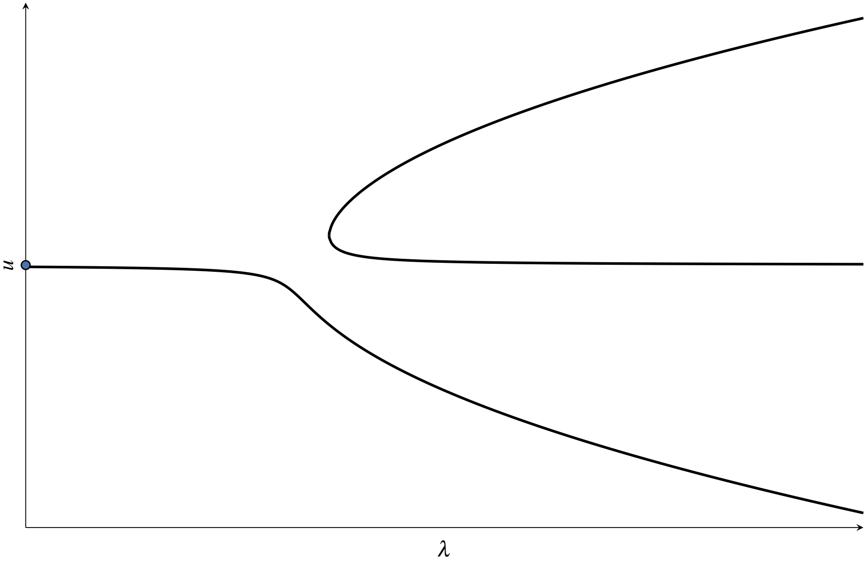
This has the right behaviour *both* as

$$\|u - u^\star\| \to 0,$$
$$\|u - u^\star\| \to \infty,$$

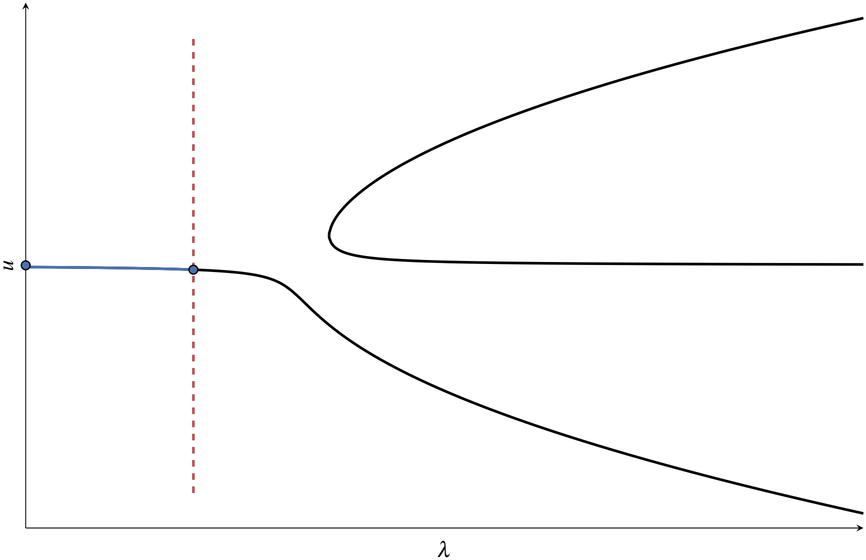
which makes deflation much more reliable.

Ásgeir Birkisson, 1985–

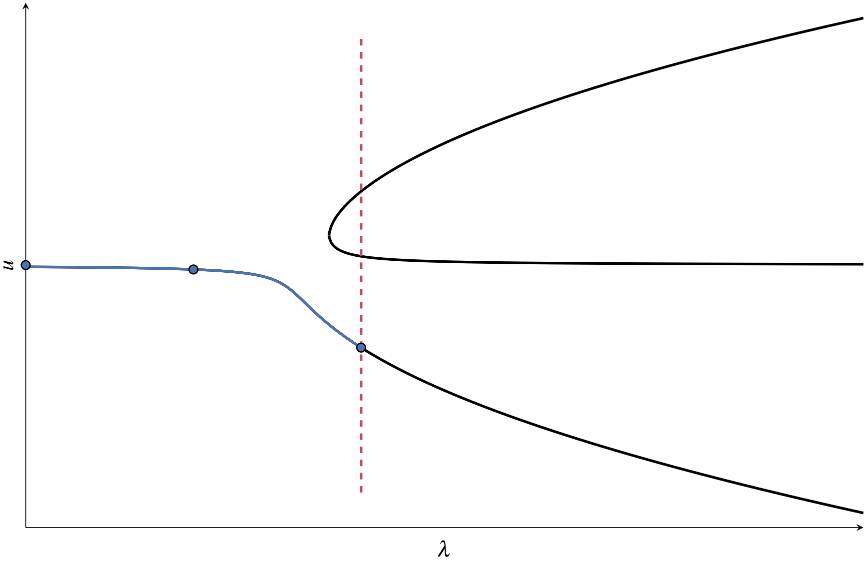
Simon Funke, 1983–



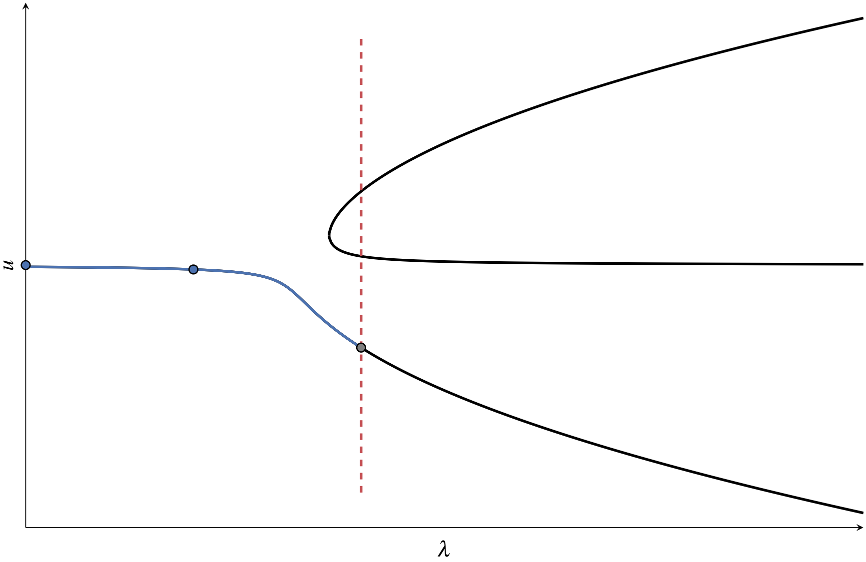
Start with (u_0, λ_0).



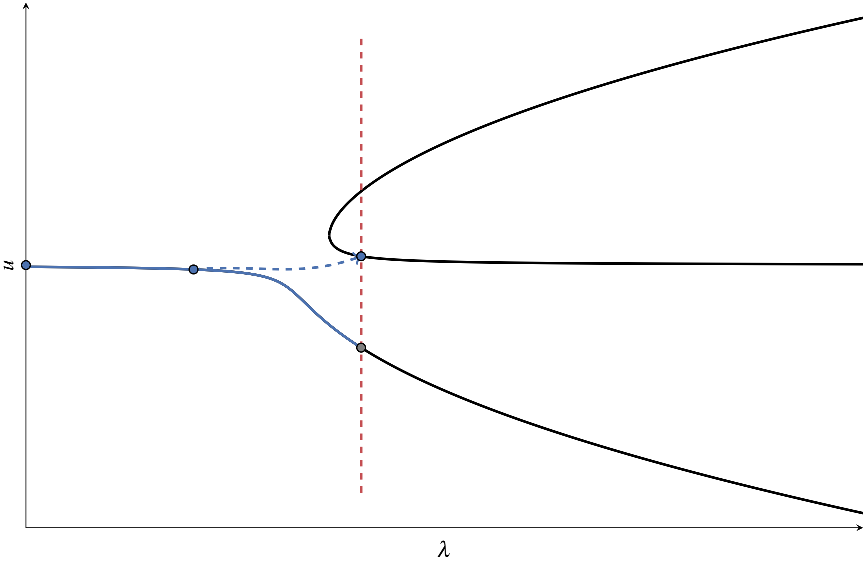
Perform a continuation step.



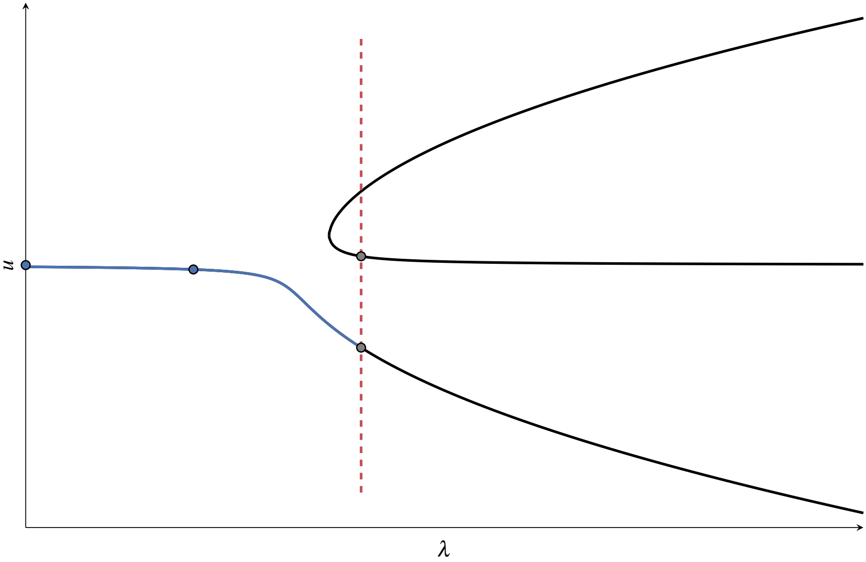
Perform another continuation step.



Deflate the solution found.



Solve again.



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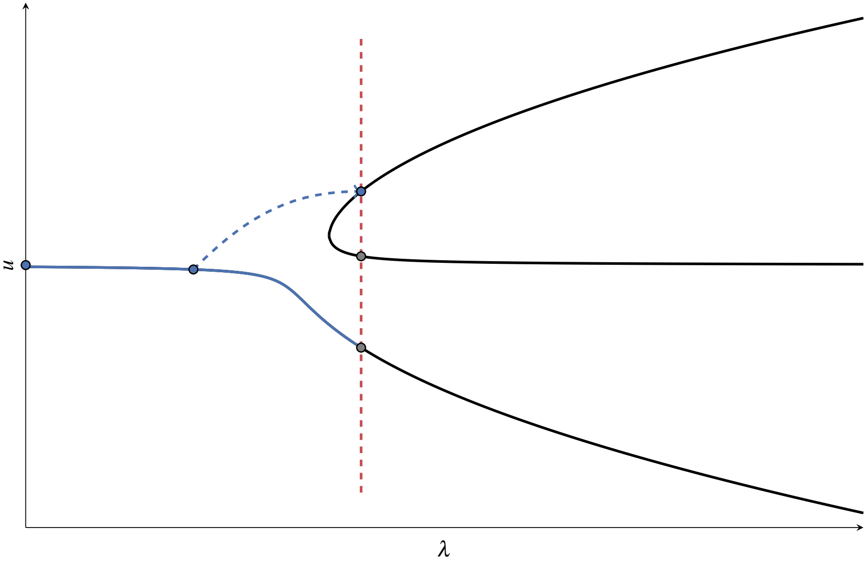

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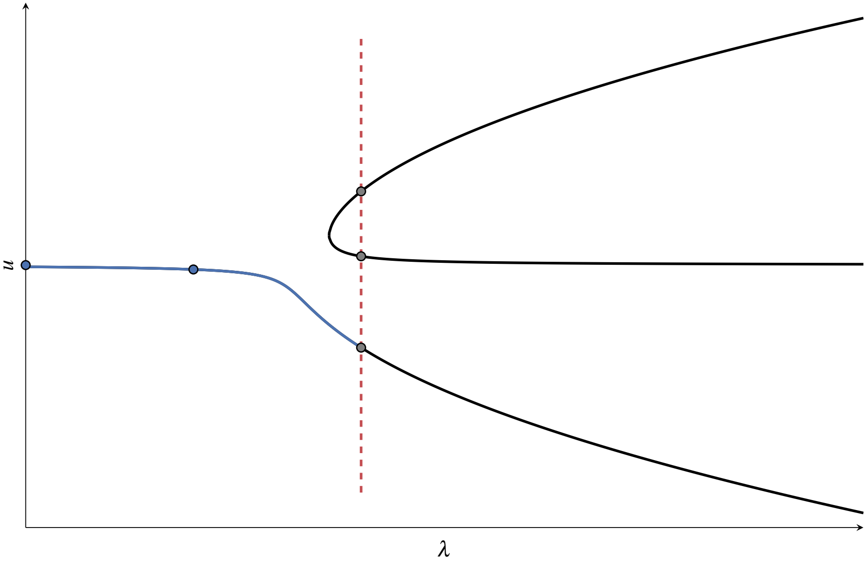

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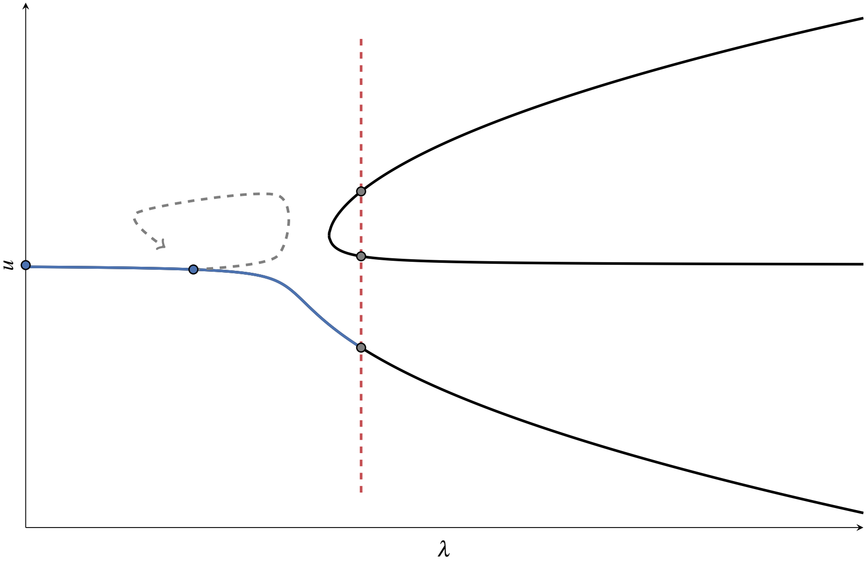
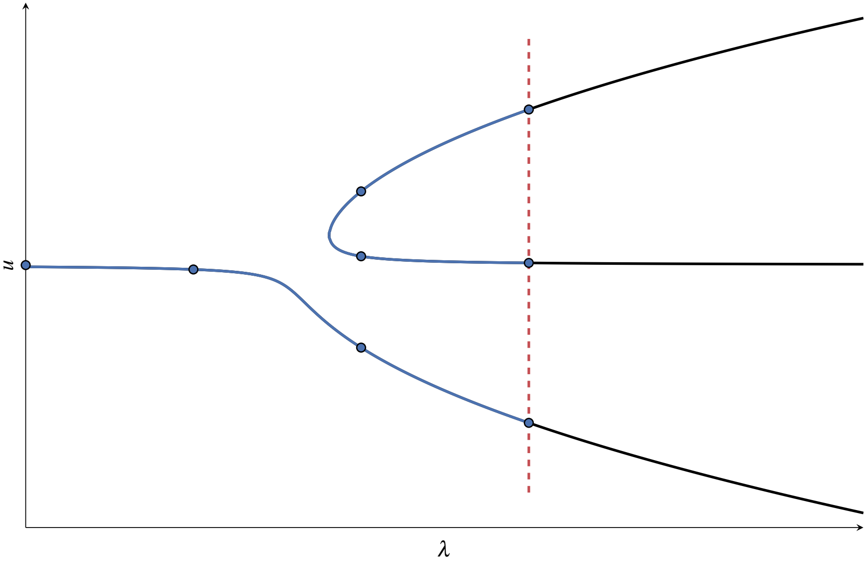


Search again, unsuccessfully.



Repeat.

Good news

Deflation lets us discover disconnected branches!

Section 5

Solving the deflated problem

We assume we have a good solver for our discretised Newton step

$$F_u(u, \lambda)\delta u_F = -F(u, \lambda), \quad F \in C^1(\mathbb{R}^N \times \mathbb{R}, \mathbb{R}^N).$$

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We now want to solve

$$G_u(u,\lambda)\delta u_G = -G(u,\lambda)$$

where

$$G(u,\lambda) = M(u;u_1)M(u;u_2)\cdots M(u;u_n)F(u,\lambda) =: M(u)F(u,\lambda).$$

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Good news

You can compute δu_G easily from δu_F! (Sherman–Morrison)

By the product rule,

$$G_u(u, \lambda) = M(u)F_u(u, \lambda) + F(u, \lambda)M_u^\top.$$

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Sherman–Morrison–Woodbury formula

$$\left(A + uv^\top\right)^{-1} = A^{-1} - \left(\frac{A^{-1} u v^\top A^{-1}}{1 + v^\top A^{-1} u}\right).$$

Maurice Bartlett

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Maurice Bartlett

At first it looks like applying this to a vector w requires two solves with A: $A^{-1}u$ and $A^{-1}w$. But something magical happens . . .

Applying the Sherman–Morrison–Woodbury formula, we have

$$\delta u_G = -[G_u]^{-1} G = -\left(M F_u + F M_u^\top \right)^{-1} (MF)$$

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\end{aligned}$$

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&= -F_u^{-1} F + \frac{F_u^{-1} F M_u^\top M^{-1} F_u^{-1} F}{1 + M_u^\top M^{-1} F_u^{-1} F}
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&= \left(1 - \frac{M^{-1}M_u^\top F_u^{-1}F}{1 + M_u^\top M^{-1}F_u^{-1}F}\right)\left(-F_u^{-1}F\right)
\end{aligned}
$$

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\end{aligned}
$$

So we only need to solve one system with F_u!

Solving the deflated problem

To solve

$$G_u \delta u_G = -G,$$

do the following:

Solving the deflated problem

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$$p = M_u^\top \delta u_F.$$

Solving the deflated problem

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2. Evaluate
$$p = M_u^\top \delta u_F.$$
3. Evaluate
$$\tau = 1 + \frac{M^{-1} p}{1 - M^{-1} p}.$$
4. Return
$$\delta u_G = \tau \delta u_F.$$

Section 6

Convergence of deflation

It is possible to give sufficient conditions for deflation to find two roots.

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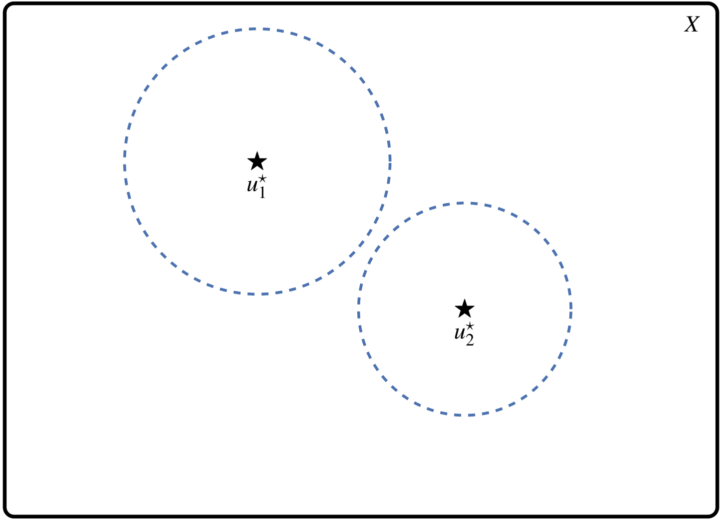
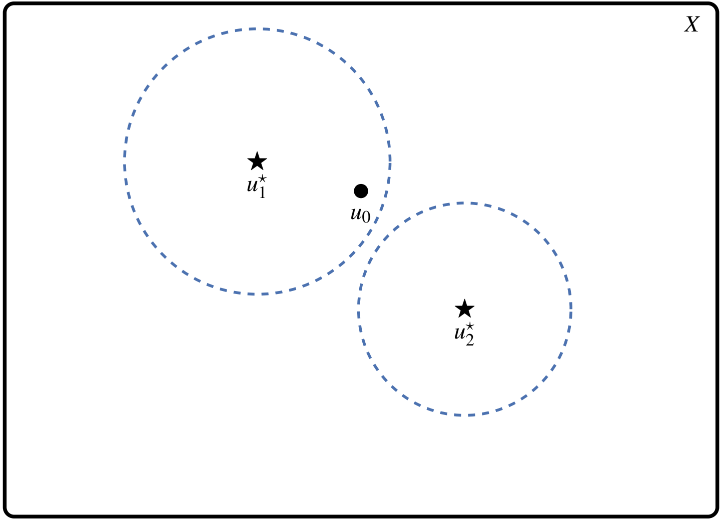


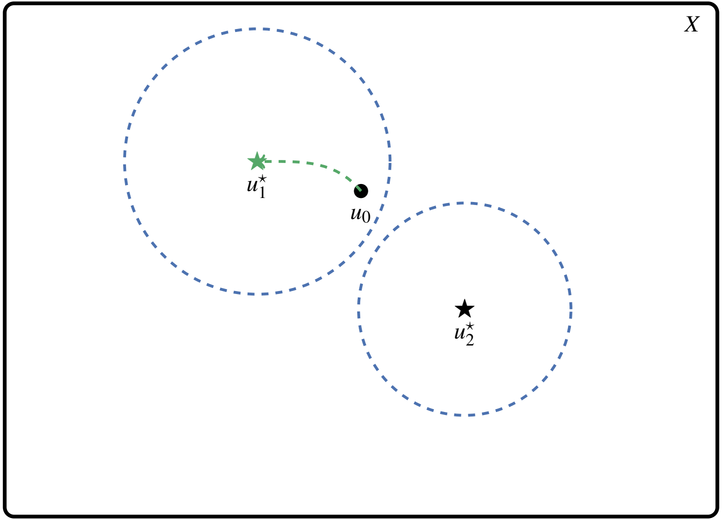
Two solutions, with Rall–Rheinboldt balls.

It is possible to give sufficient conditions for deflation to find two roots.



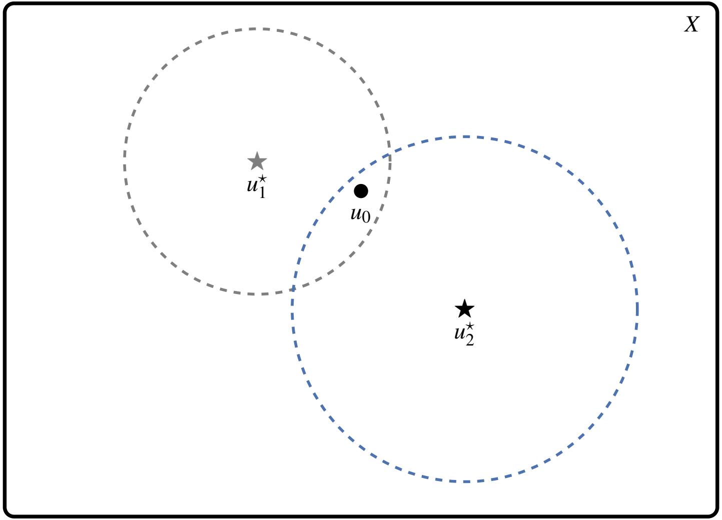
Start with an initial guess within a ball.

It is possible to give sufficient conditions for deflation to find two roots.



Converge to that solution.

It is possible to give sufficient conditions for deflation to find two roots.



Deflate that solution; the other Rall–Rheinboldt ball expands.

Section 7

Examples

Allen–Cahn equation

$$F(u, \lambda) = -\lambda^2 \nabla^2 u + u^3 - u = 0, \quad u = g \text{ on } \partial\Omega.$$

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Solutions found starting from $u = 0$ for $\lambda = 0.04$.

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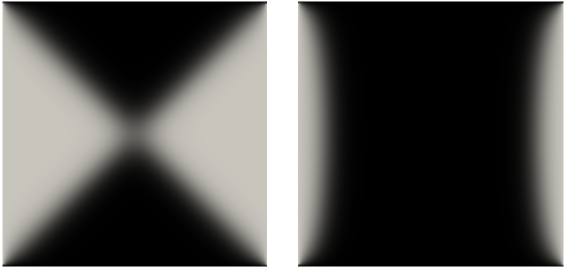

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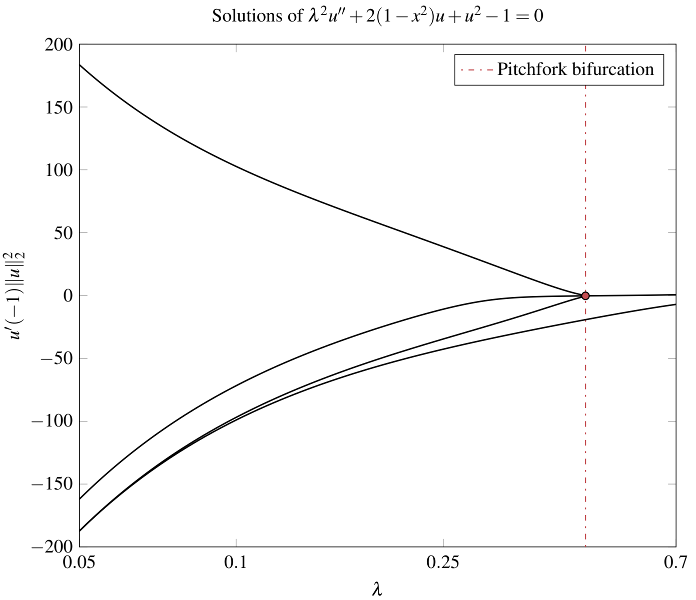
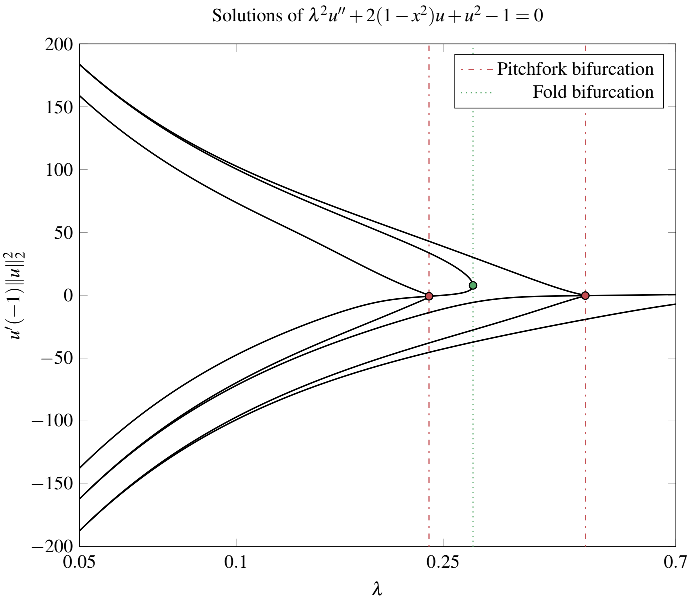
Solutions found starting from $u = 0$ for $\lambda = 0.04$.

Carrier's equation

$$F(u,\lambda) = \lambda^2 u'' + 2(1-x^2)u + u^2 - 1 = 0, \quad u(-1) = 0 = u(1).$$


Solutions of $\lambda^2 u'' + 2(1-x^2)u + u^2 - 1 = 0$
Pitchfork bifurcation
$u'(-1)\|u\|_2^2$
200
150
100
50
0
-50
-100
-150
-200
0.05
0.1
0.25
0.7
λ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Fold bifurcation

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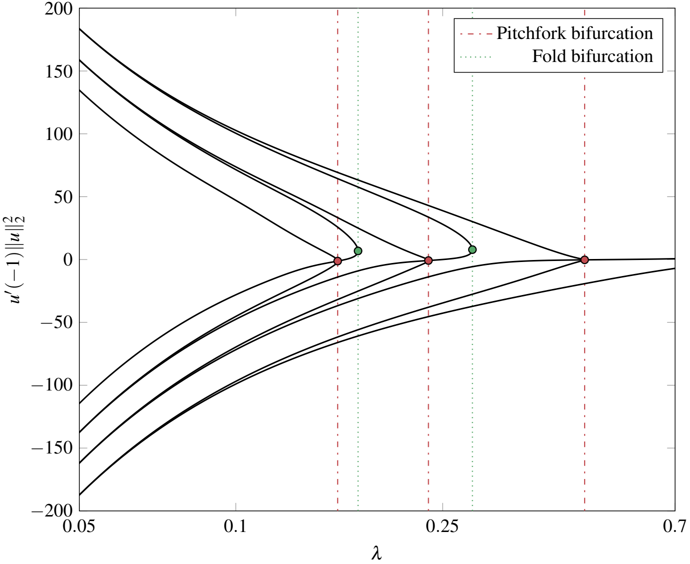

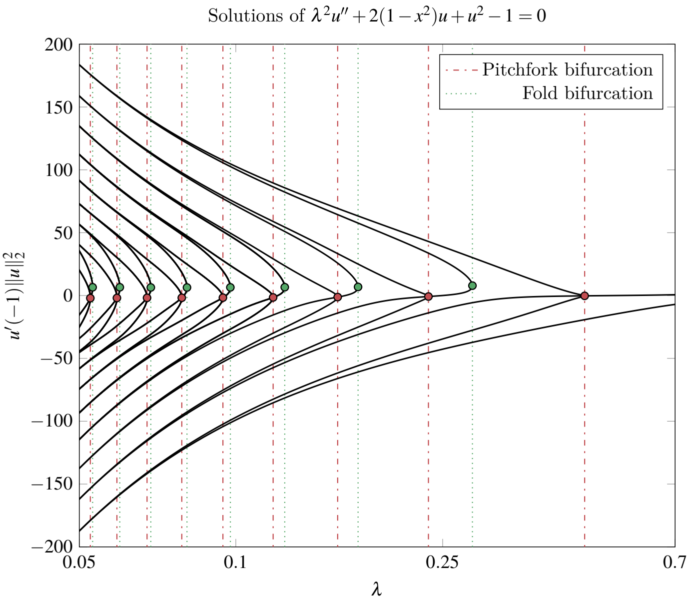
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Section 8

Symmetries

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Philosophy

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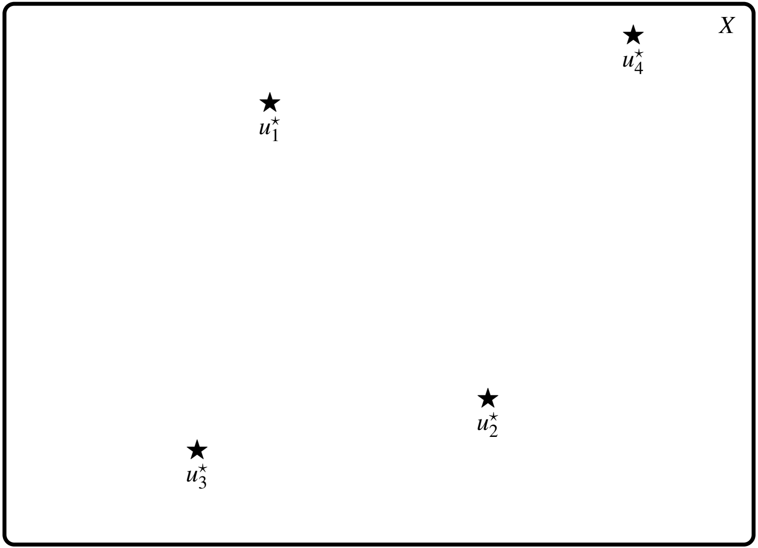
What if the equation has a continuous symmetry group?

Philosophy

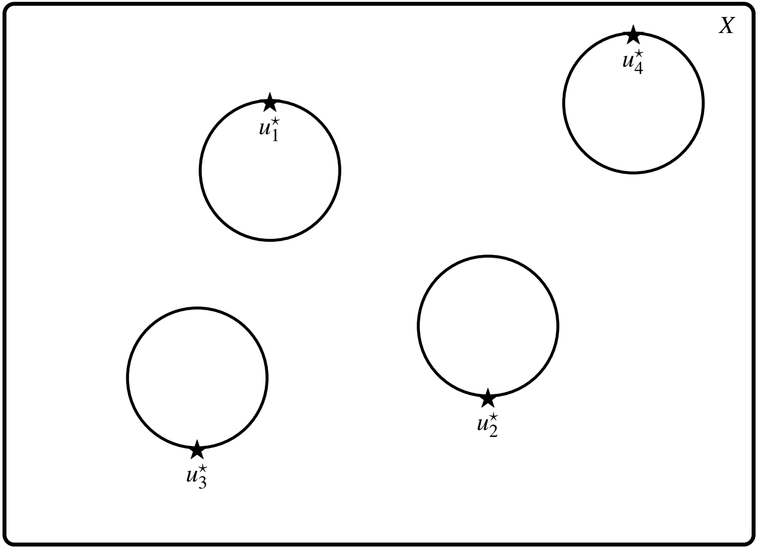
The fundamental structures are the distinct **orbits** of solutions.

Key idea

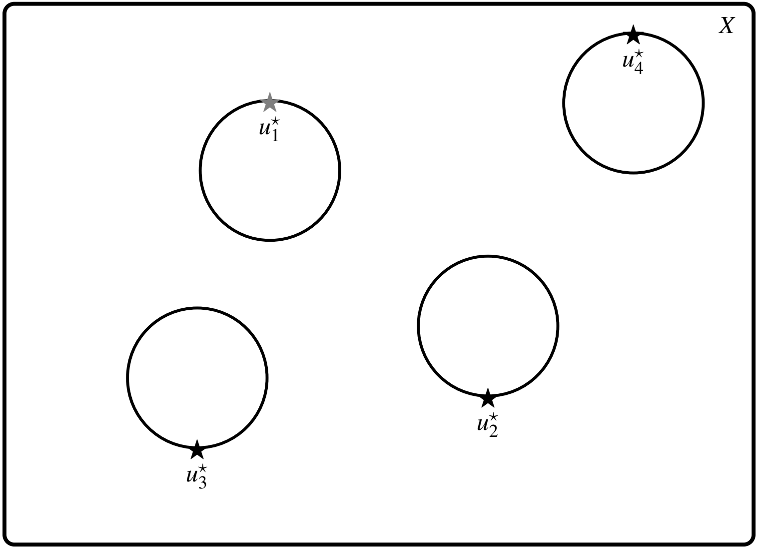
Construct a deflation operator invariant under the action of the Lie group.



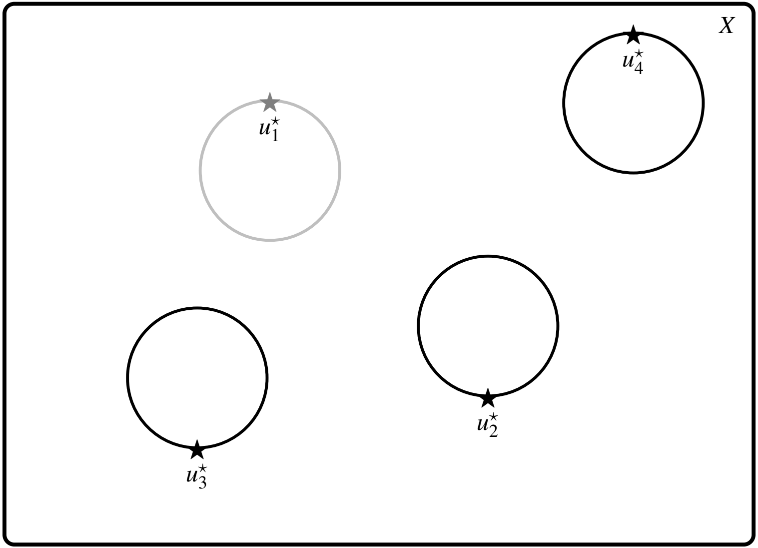
Four solutions, not related by the symmetry group.



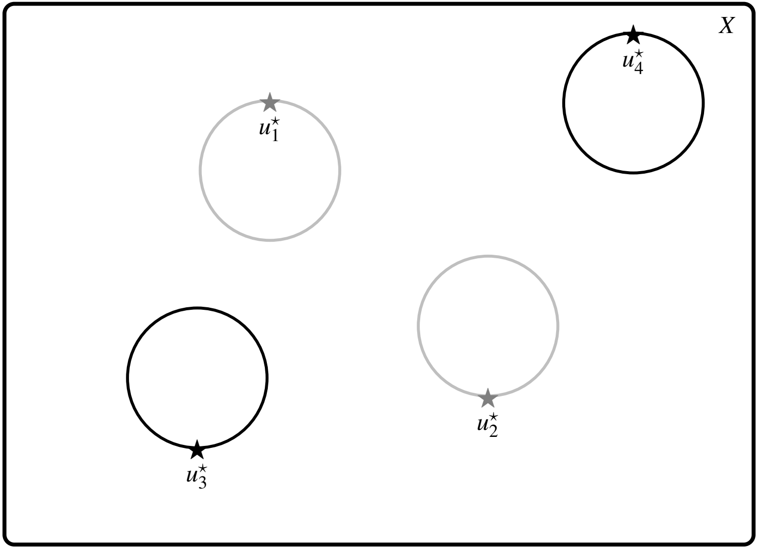
Each solution induces a *group orbit* of solutions, related by symmetry.



Not enough to deflate the solution—must deflate the entire orbit.



Design a deflation operator that deflates the entire orbit.



Design a deflation operator that deflates the entire orbit.

Gross–Pitaevskii equation

$$-\frac{1}{2}\Delta u + \frac{x^2+y^2+z^2}{2}u - \mu u + |u|^2 u = 0, \qquad u|_{\partial\Omega} = 0.$$

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First symmetry group $\mathrm{SO}(2)$: phase shifts

$$u(\vec{x}) \mapsto e^{i\theta}u(\vec{x}), \quad \theta \in \mathbb{R}.$$

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Invariant deflation operator

$$M(u;r) = \left\| |u|^2 - |r|^2 \right\|^{-2} + 1.$$

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Second symmetry group $\mathrm{SO}(3)$: spatial rotations

$$u(\vec{x}) \mapsto u(R\vec{x}), \quad R^{-1} = R^T, \ \det(R) = 1.$$

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Invariant deflation operator

$$M(u; r) = \|\bar{u} - \bar{r}\|^{-2} + 1,$$

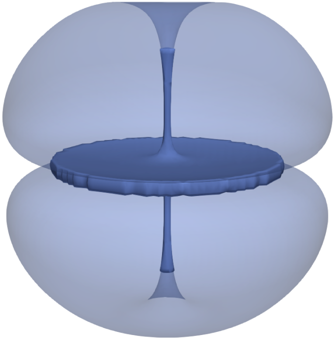
where

$\bar{u}(r, \theta, \psi)$ averages u over the sphere of radius r.

Gross–Pitaevskii equation

$$-\frac{1}{2}\Delta u + \frac{x^2+y^2+z^2}{2}u - \mu u + |u|^2 u = 0, \qquad u|_{\partial\Omega} = 0.$$

Solutions for $\mu = 6$.



A vortex line and a planar dark soliton.

Gross–Pitaevskii equation

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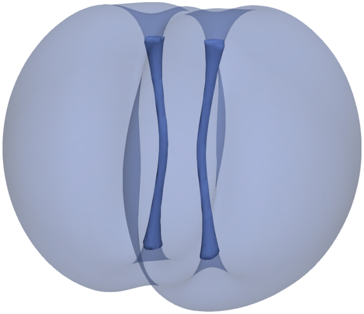

A pair of vortex lines.

Gross–Pitaevskii equation

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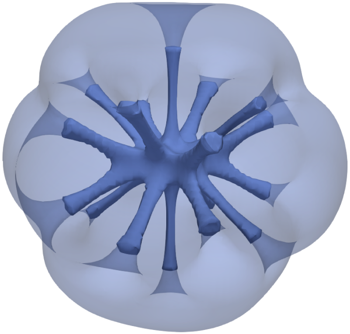

A vortex star.

Gross–Pitaevskii equation

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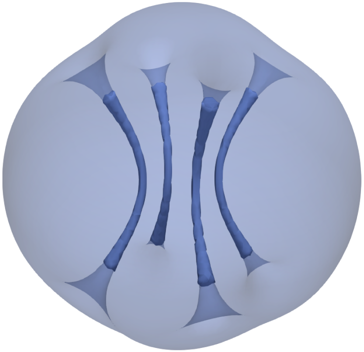

Four vortex lines of alternating charge.

Gross–Pitaevskii equation

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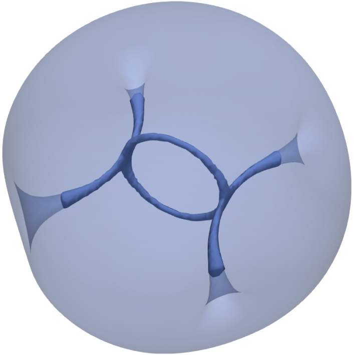

A vortex ring with two “handles”.

Gross–Pitaevskii equation

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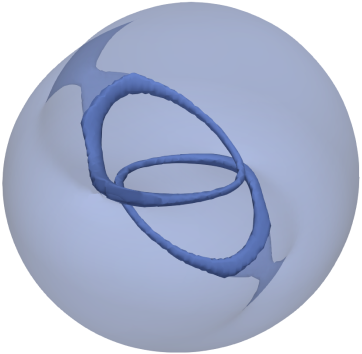

Two bent vortex rings?

Gross–Pitaevskii equation

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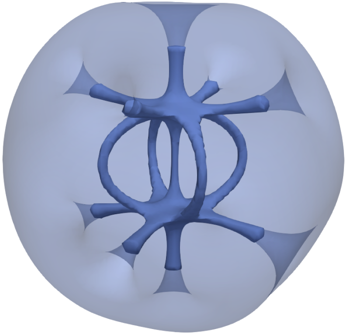

Two vortex rings and five lines?

Gross–Pitaevskii equation

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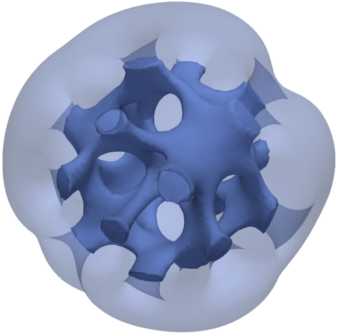

A vortex ring cage?

Section 9

Semismooth problems

Many problems feature inequality constraints.

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The natural language for formulating these is as a *variational inequality*.

$\mathrm{VI}(Q, K)$

Let X be a real reflexive Banach space, $K \subset X$ a closed convex subset, and $Q : K \to X^*$. The task is to

$$\text{find } u^\star \in K \text{ such that } \langle Q(u^\star), v - u^\star \rangle \geq 0 \text{ for all } v \in K.$$

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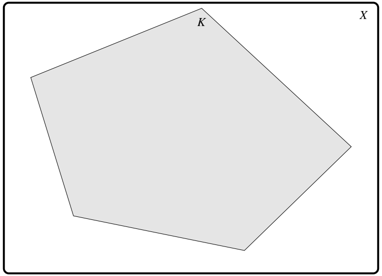

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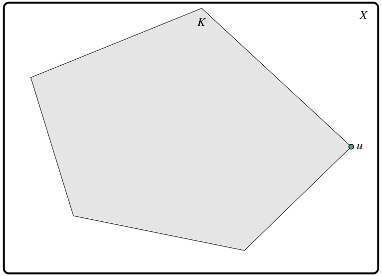

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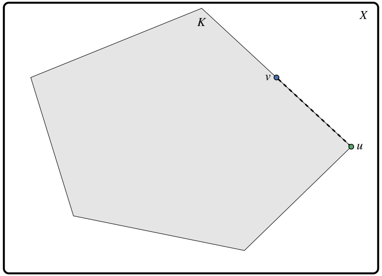

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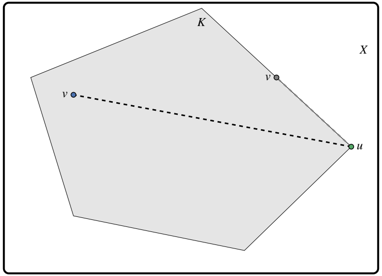

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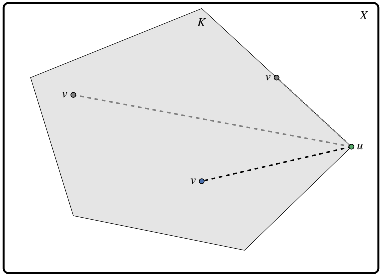

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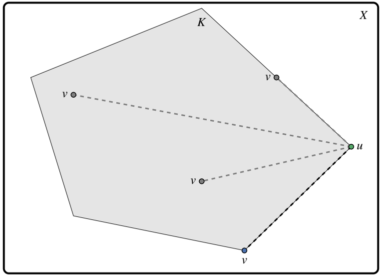

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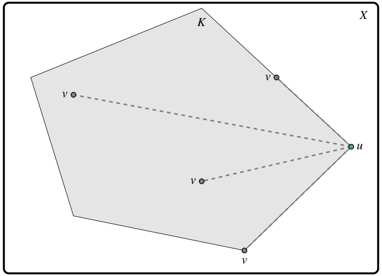

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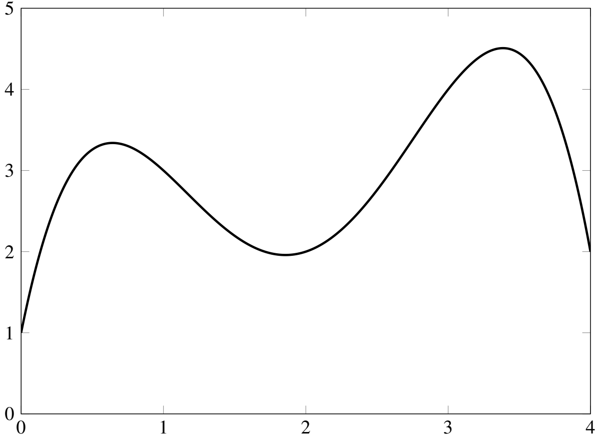

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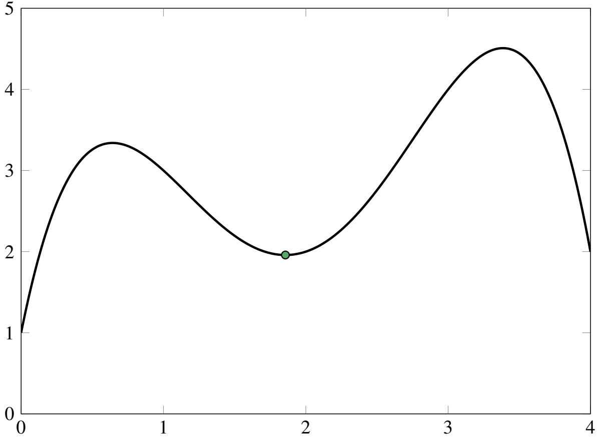

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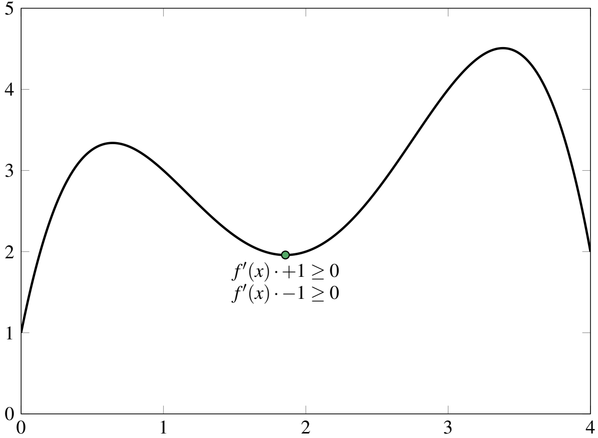

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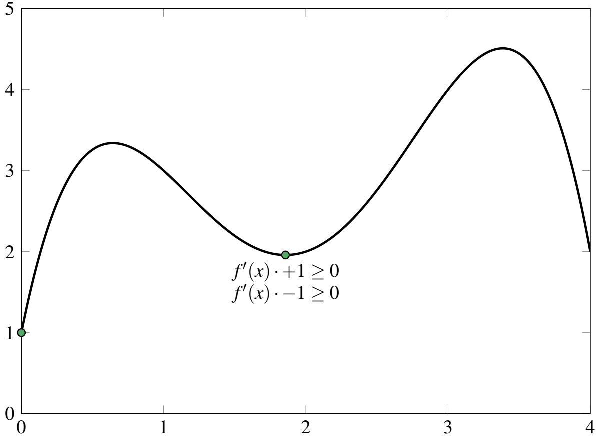

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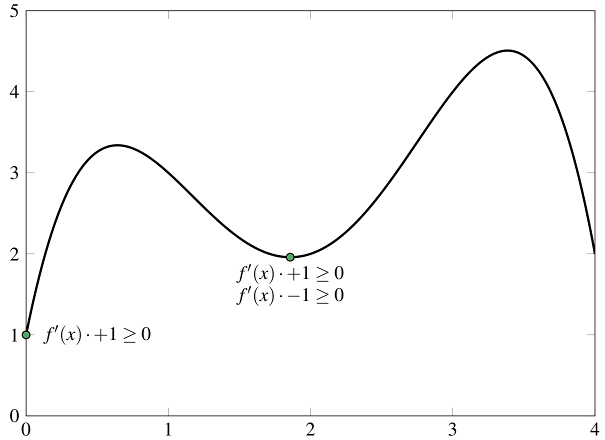

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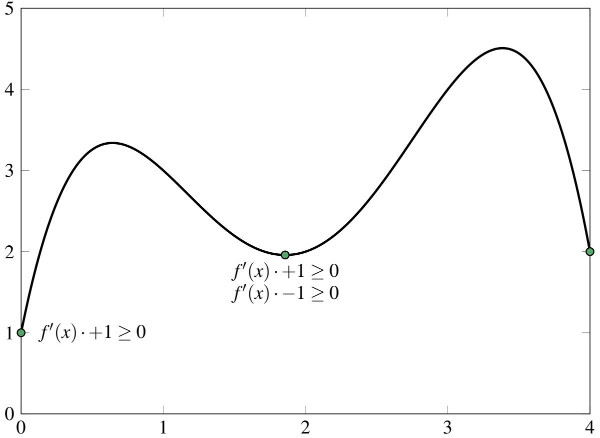

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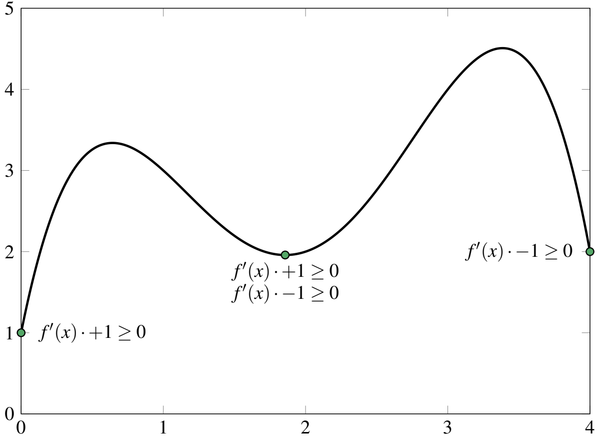

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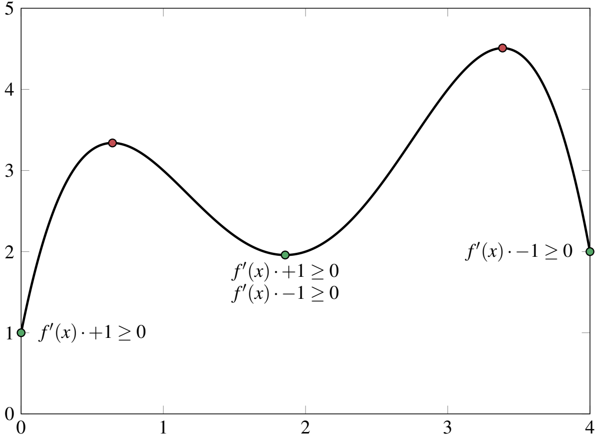

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The price we pay . . .

. . . is that S is not smooth.

Good news

S is *just smooth enough* to define a Newton-type method with superlinear convergence.

Michael Hintermüller

Michael Ulbrich

Good news

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Semismooth Newton works just like normal:

$$u_{i+1} = u_i - [H(u_i)]^{-1} S(u_i),$$

where H is the so-called Newton derivative.

This algorithm usually converges superlinearly.

Michael Hintermüller

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Good news

Deflation works for semismooth problems.

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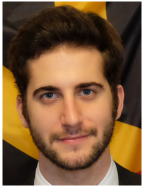
Theorem (F., Croci, Surowiec, 2020)

Under the same assumptions that are required for superlinear convergence of semismooth Newton, deflation works the same.



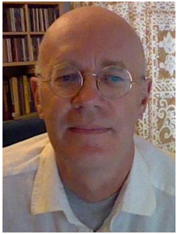
Matteo Croci

Thomas Surowiec

Gould gives an example where the central path is ill-behaved:

Nonconvex quadratic programming problem

$$
\begin{aligned}
\underset{x\in\mathbb{R}^2}{\text{minimise}} \quad & -2(x_1-0.25)^2+2(x_2-0.5)^2 \\
\text{subject to} \quad & x_1+x_2 \le 1 \\
& 3x_1+x_2 \le 1.5 \\
& x_1 \ge 0 \\
& x_2 \ge 0
\end{aligned}
$$



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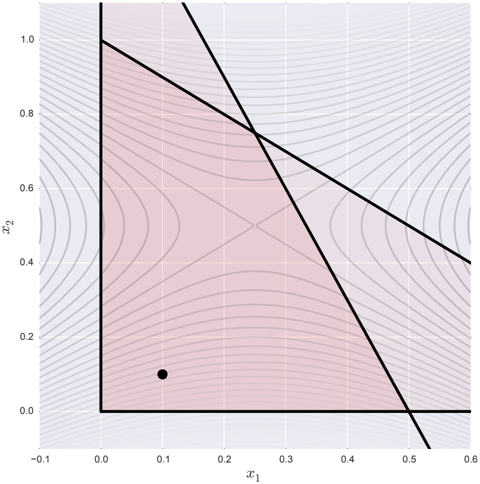

Deflation finds both minima and the saddle point.

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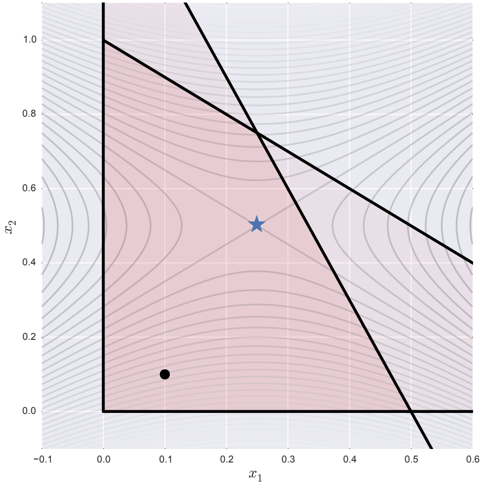

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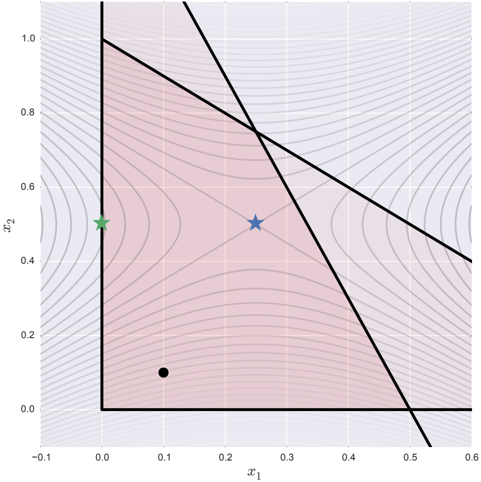

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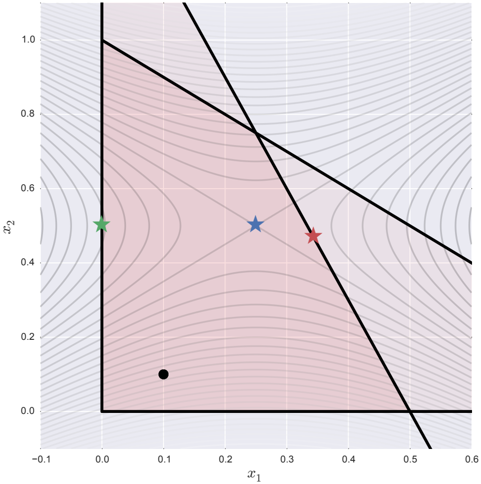

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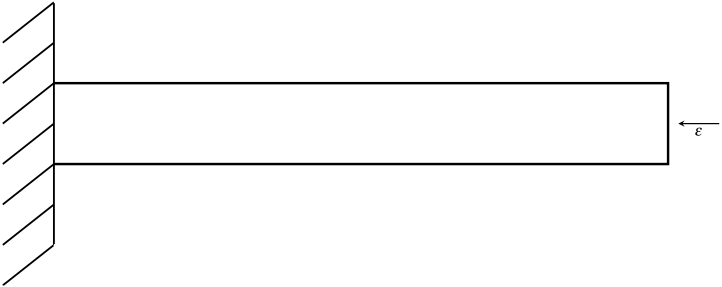
Buckling of a hyperelastic beam with contact constraints

$$\begin{aligned}\underset{u \in H^1(\Omega;\mathbb{R}^2)}{\text{minimise}} \quad & \Pi(u) = \int_\Omega \psi(u)\ \mathrm{d}x - \int_\Omega B \cdot u\ \mathrm{d}x \\ \text{subject to} \quad & u|_{\text{left}} = (0,0),\ \ u|_{\text{right}} = (-\varepsilon, 0), \\ & \operatorname{tr}(u_y) \in [a,b] \text{ a.e. in } \Gamma_{\text{top}}, \Gamma_{\text{bottom}}.\end{aligned}$$



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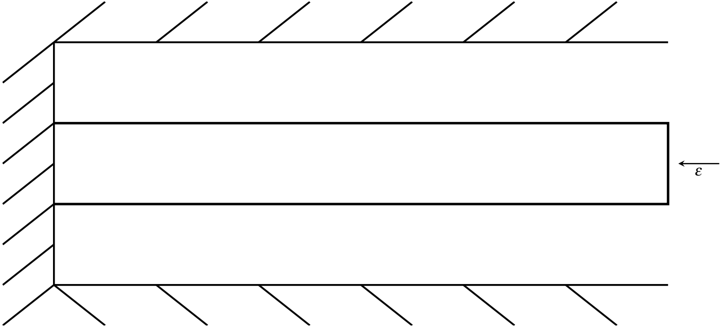

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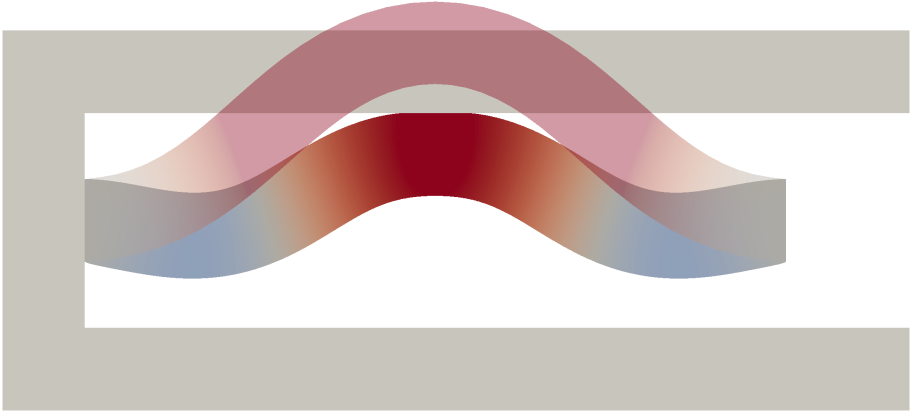
\end{aligned}
$$

Neo–Hookean strain energy density

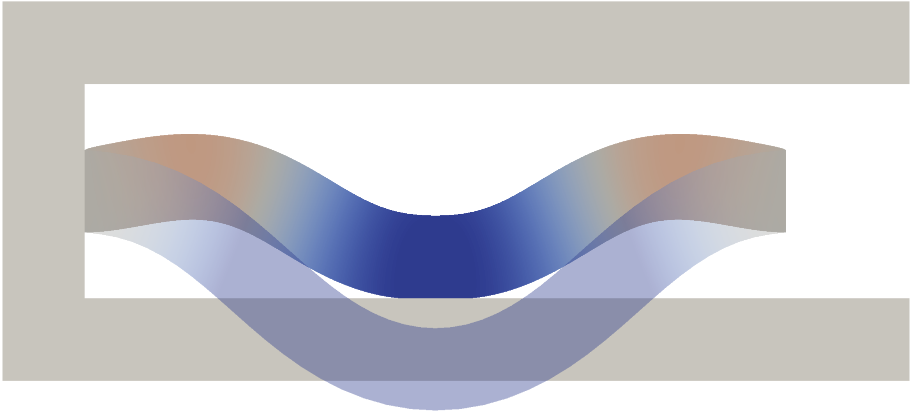
$$
\psi(u) = \frac{\mu}{2}(\operatorname{tr}(C) - 2) - \mu \log(\det(C)) + \frac{\lambda}{2}\log(\det(C))^2,
$$

where

$$
C = (I + \nabla u)^\top (I + \nabla u).
$$



Multiple solutions of the beam with contact constraints.



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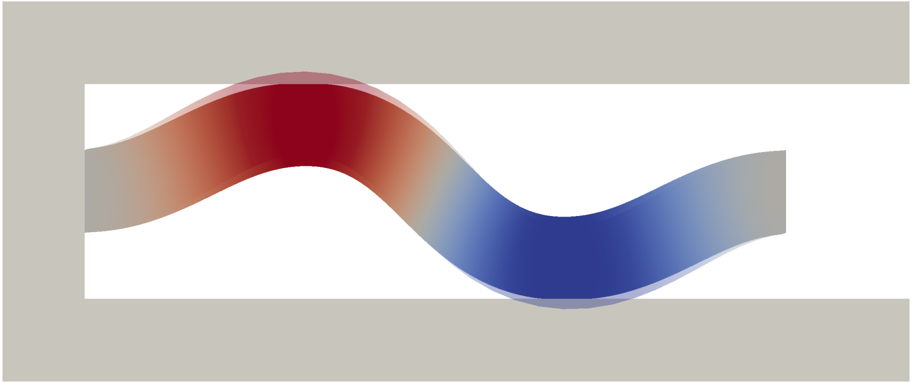

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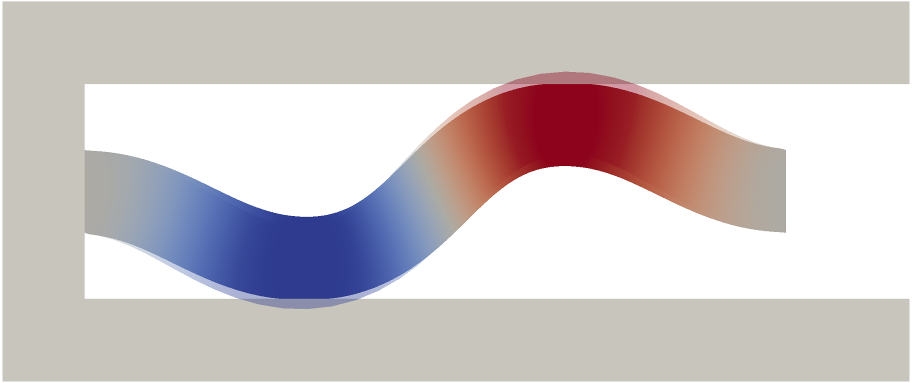

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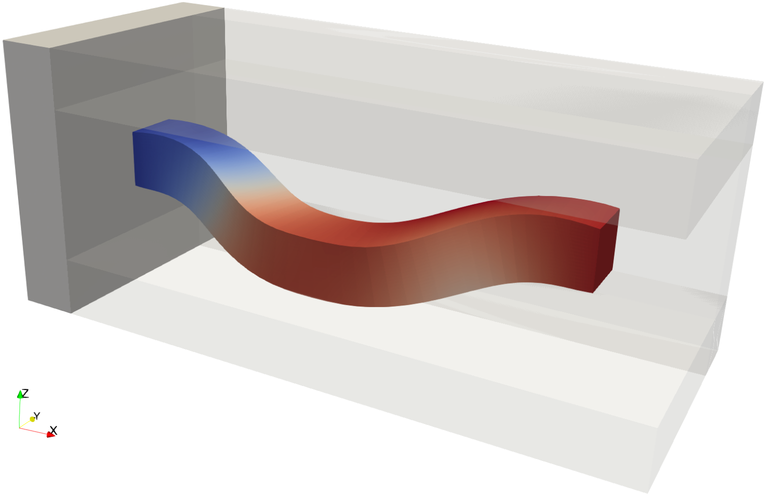

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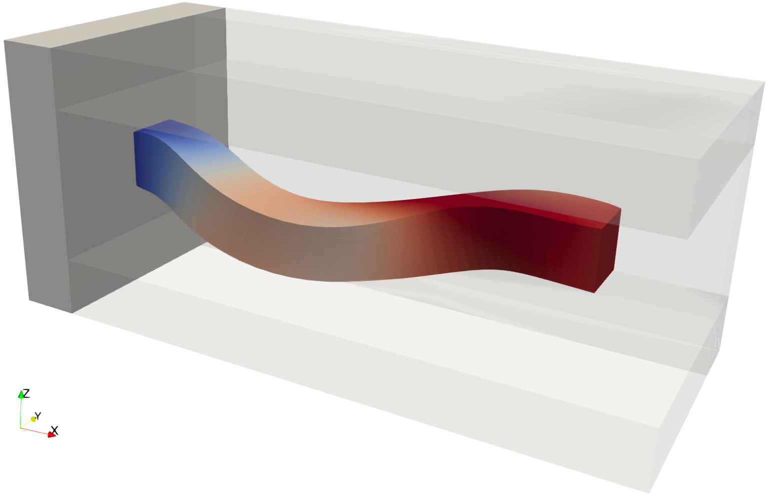

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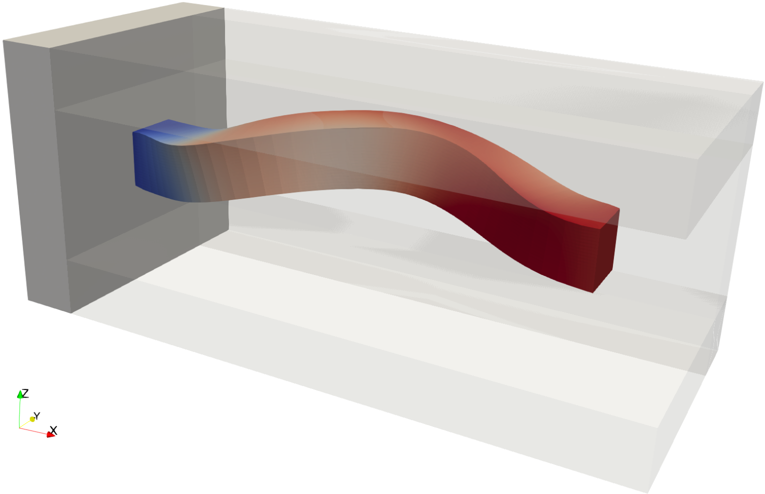

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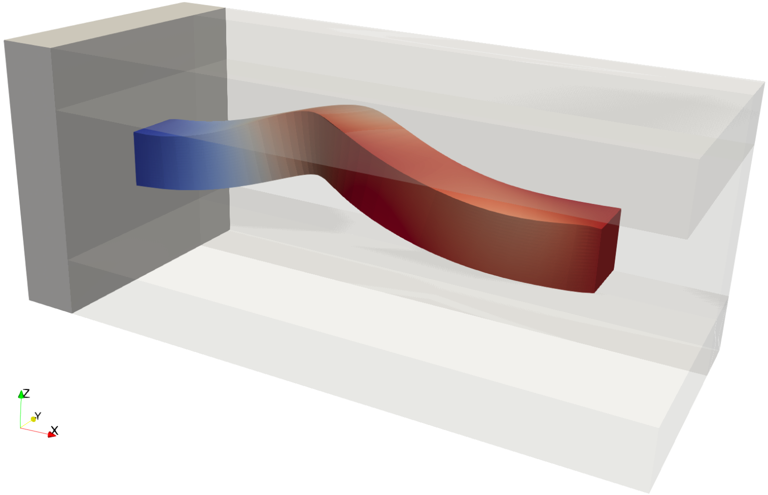

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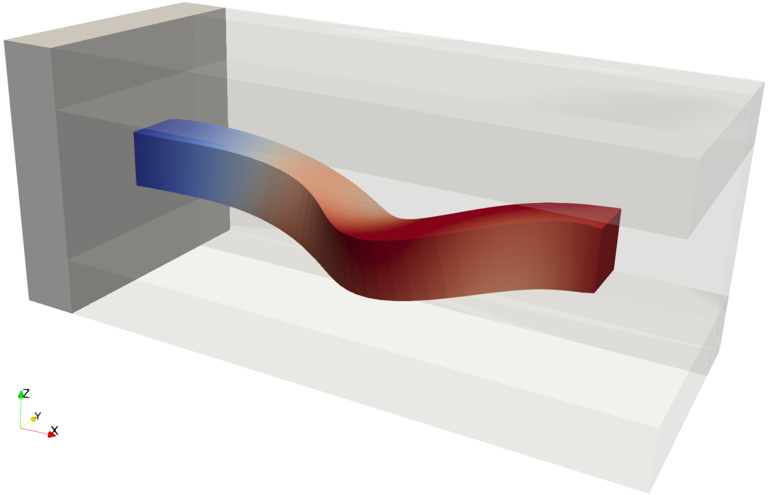

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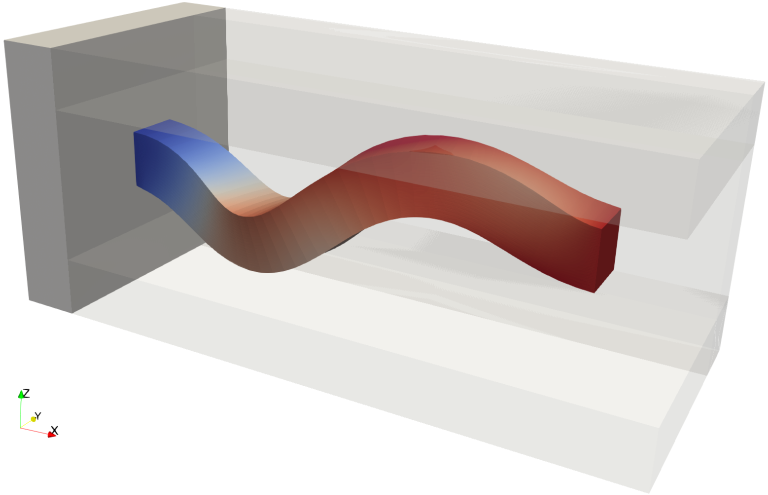

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Conclusions!

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Algorithms

Deflation is a very powerful technique for computing multiple solutions.