Local Numerics

Problem

Parameter-dependent ODE

$$\dot{x} = f(x, \lambda),$$

$x \in \mathbb{R}^d$, $\lambda \in \mathbb{R}$, f "smooth" enough.

Goal: compute ("follow") equilibrium solutions as λ varies, i.e. compute solutions (x, λ) to

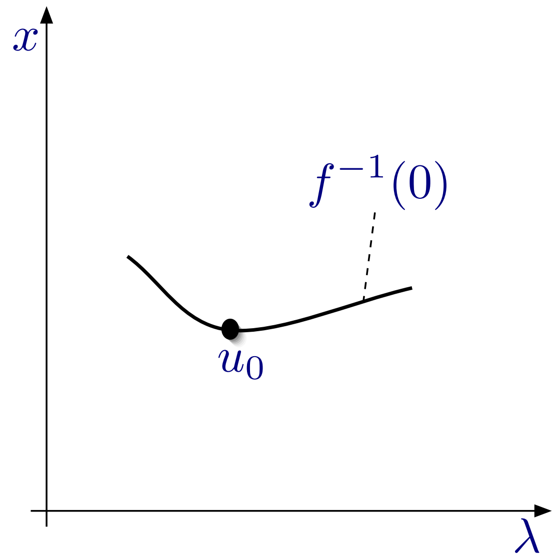
$$0 = f(x, \lambda).$$

Structure of the Solution

Let $u_0 = (x_0, \lambda_0)$ s.t.

$$f(u_0) = 0 \quad \text{and} \quad \text{rank}(f'(u_0)) = N.$$

Then locally $f^{-1}(0)$ is a one-dimensional manifold in $\mathbb{R}^{d+1}$.



Tangent vector

Let $c : (-1, 1) \to \mathbb{R}^{d+1}$ be a local parametrization of $f^{-1}(0)$. Then

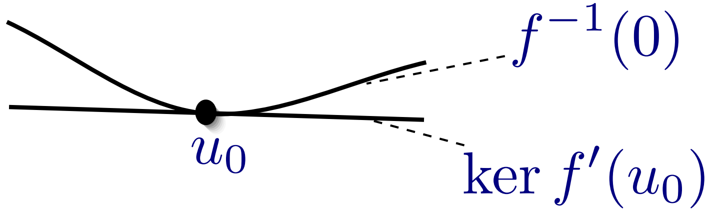
$$f(c(s)) = 0,$$

i.e.

$$f'(c(s))\, c'(s) = 0.$$

In other words

$$T_{c(s)} f^{-1}(0) = \ker f'(c(s)).$$



Fixing the orientation

We will use $\ker f'(c(s))$ to "move along c".

In order to fix a consistent direction, we require that

$$|c'(s)| = 1$$

and

$$\det \begin{bmatrix} f'(c(s)) \\ c'(s)^T \end{bmatrix} > 0.$$

Exercise 1 Show that $\begin{bmatrix} f'(c(s)) \\ c'(s)^T \end{bmatrix}$ is regular.

The induced tangent vector

For a $d \times d+1$-matrix A with $\operatorname{rank}(A) = d$ let $t = t(A) \in \mathbb{R}^{d+1}$ be the unique vector such that

(i) $At = 0$;

(ii) $|t| = 1$;

(iii) $\det \begin{bmatrix} A \\ t^T \end{bmatrix} > 0$.

We call $t(A)$ the tangent vector induced by A.

Exercise 2 Show that the set of all $d \times (d+1)$-matrices with full rank is open.

The associated differential equation

Consider the ODE

$$c' = t(f'(c)). \tag{1}$$

Since $\frac{d}{ds}f(c(s)) = f'(c(s))\, c'(s) = 0$, f is constant along solutions of (1).

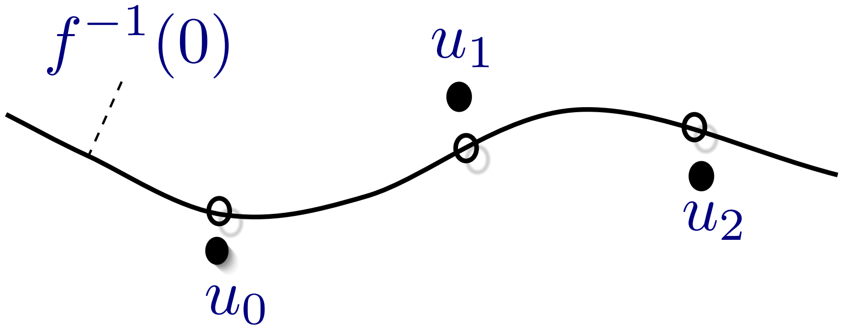
Idea: in order to compute the “path” c, solve (1).

Given data: vector field $t(f'(\cdot))$ and condition $f(c(s)) = 0$.

$\rightsquigarrow$ predictor-corrector methods.

Predictor-corrector scheme

Given u_0 with $|f(u_0)| < \varepsilon$, find sequence $u_1, u_2, \ldots$ of points such that $|f(u_i)| < \varepsilon$ for some prescribed accuracy $\varepsilon > 0$.



(i) Predictor: solve the initial value problem $u' = t(f'(u))$, $u(0) = u_i$, by an explicit scheme, e.g. one Euler-step:

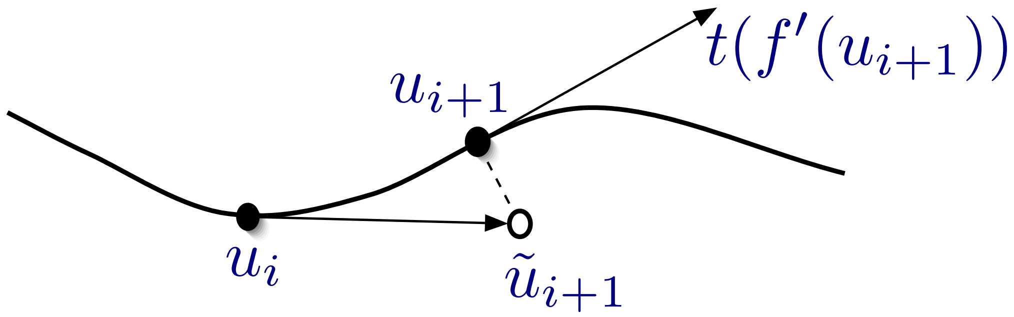
$$\tilde{u}_{i+1} = u_i + ht(f'(u_i)),$$

where h is the stepsize.

(ii) Corrector: compute

$$u_{i+1} = \operatorname{argmin}_{f(u)=0} |u - \tilde{u}_{i+1}|$$

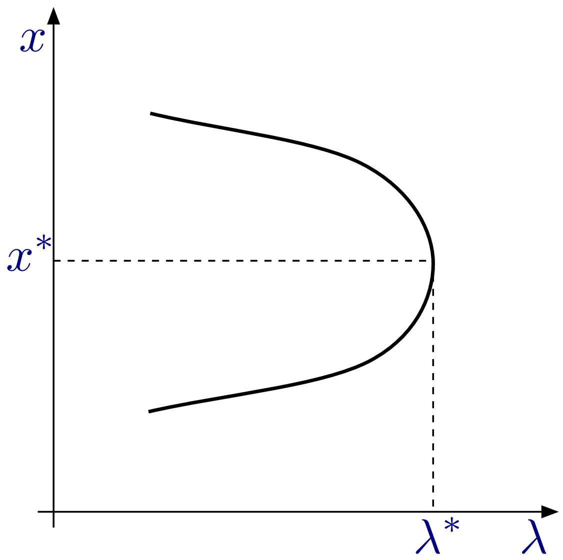
by some iteration scheme, e.g. Newton's method.



A necessary condition for u_{i+1} is

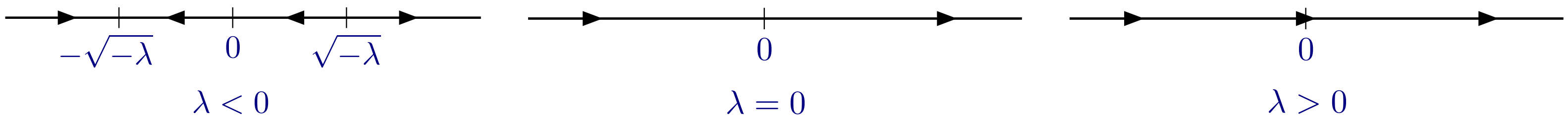
$$\begin{aligned} f(u_{i+1}) &= 0, \\ t(f'(u_{i+1}))(u_{i+1} - \tilde{u}_{i+1}) &= 0. \end{aligned}$$

Saddle-node bifurcation



Example 1

$$\dot{x} = \lambda + x^2$$



Saddle-node bifurcation

Condition:

$$\dim\ker f_x(x^*,\lambda^*) = 1$$

(but still $\operatorname{rank}(f'(x^*,\lambda^*)) = d$).

Detection: during path-following, check sign of

$$\det f_x(x(s),\lambda(s)).$$

Computation: Solve (Moore, Spence, 1980)

$$\begin{aligned} f(x,\lambda) &= 0 \\ f_x(x,\lambda)\phi &= 0 \\ \ell^T\phi - 1 &= 0, \quad \ell \in \mathbb{R}^d. \end{aligned}$$

Saddle-node bifurcation

Let

$$\psi^* f_x(x^*, \lambda^*) = 0.$$

Theorem 1 *If*

$$\dim\ker f'(x^*, \lambda^*) = d \qquad \textit{and} \qquad \dim\ker f_x(x^*, \lambda^*) = 1,$$

then (x^*, ϕ^*, λ^*) *is a regular zero of the extended system, if and only if*

$$\psi^* f_{xx}(x^*, \lambda^*)\phi^*\phi^* \neq 0.$$

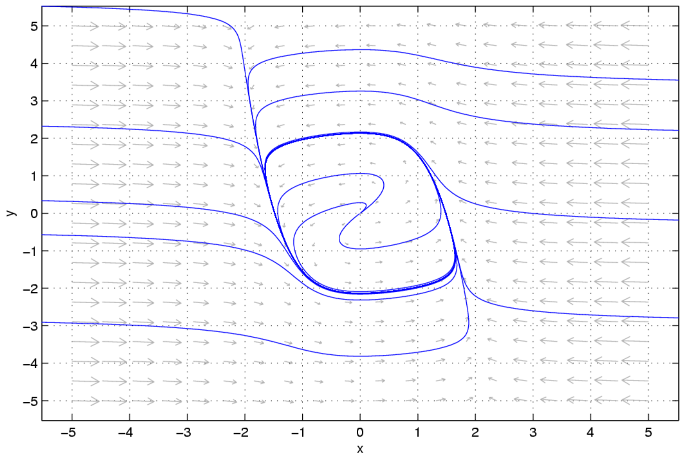
The point (x^*, λ^*) is a quadratic turning point.

Hopf bifurcation

Consider the system

$$\begin{aligned} \dot{x} &= \lambda x - y - x^3 \\ \dot{y} &= x \end{aligned}$$

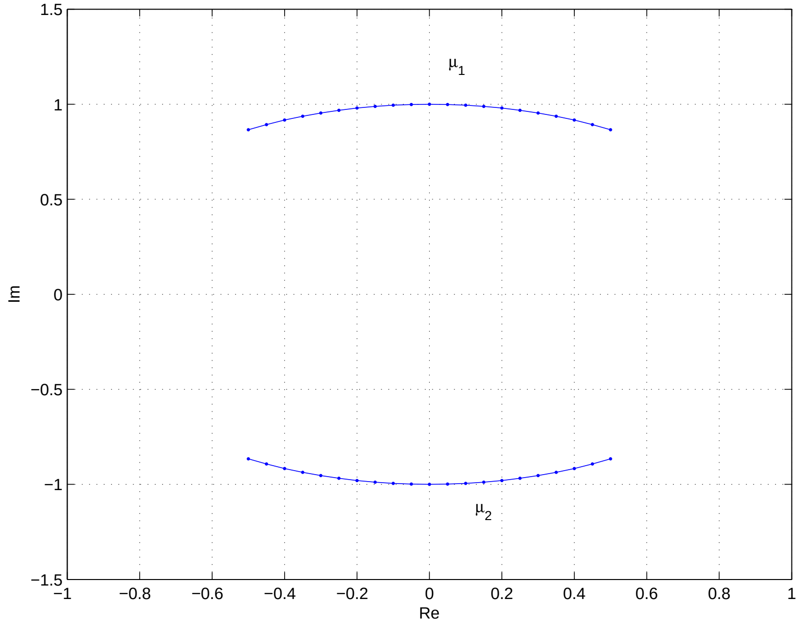
for various $\lambda \in \mathbb{R}$.



Eigenvalue movement

Linearization in 0, eigenvalues:

$$Df(0) = \begin{bmatrix} \lambda & -1 \\ 1 & 0 \end{bmatrix}, \quad \mu_{1,2} = \frac{\lambda}{2} \pm \sqrt{\frac{\lambda^2}{4} - 1}$$



The Theorem of Hopf

- (x_0, λ_0) equilibrium,
- $i\omega \neq 0$ simple eigenvalue of $f_x(x_0, \lambda_0)$,
- $i\mathbb{R} \cap \sigma(f_x(x_0, \lambda_0)) = \{i\omega, -i\omega\}$,
- $C = \{(x(\lambda), \lambda)\}$ local path of equilibria,
- $\mu(\lambda) + i\nu(\lambda)$ eigenvalue of $f_x(x(\lambda), \lambda)$ with $\mu(\lambda_0) + i\nu(\lambda_0) = i\omega$,

If

$$\frac{d\mu}{d\lambda}(\lambda_0) \neq 0,$$

then there exists a unique one-parameter family of periodic solutions (with positive period) in a neighborhood of (x_0, λ_0).

Computing Hopf points

Consider an eigenvector $v + iw$ at $i\omega$ of $D := d_x f(x_0, \lambda_0)$, i.e.

$$\begin{aligned} & D(v+iw) = i\omega(v+iw) \\ \Leftrightarrow \quad & Dv = -\omega w \quad \text{and} \quad Dw = \omega v. \end{aligned}$$

Exercise 3 Show that v and w are linearly independent.

Thus

$$D^2 v = -\omega^2 v \quad \text{and} \quad D^2 w = -\omega^2 w.$$

Computing Hopf points

Consider the extended system

$$F(x, \varphi, \lambda, \nu) = \begin{bmatrix} f(x, \lambda) \\ (d_x f(x, \lambda)^2 + \nu^2 I)\varphi \\ (\varphi, \varphi) - 1 \\ \ell^T \varphi \end{bmatrix} = 0.$$

If ℓ is not orthogonal to $\mathrm{span}\{v, w\}$, then there exists a unique (up to its sign) vector $\varphi_0 \in \mathrm{span}\{v, w\}$, such that $(x_0, \varphi_0, \lambda_0, \omega)$ is a regular[a] solution of this system.

[a]Roose,Hlavacek, 85

Computation of periodic solutions

Goal: compute periodic solution of

$$x' = f(x), \quad x \in \mathbb{R}^d,$$

i.e. a solution $\bar{x}(t)$ with $\bar{x}(t) = \bar{x}(t+T)$ for some unknown period $T = 2\pi/\omega$.

The transformation $y(t) = x(t/\omega)$ yields the system

$$y' = \frac{1}{\omega} f(y),$$

for which $\bar{y}(t) = \bar{x}(t/\omega)$ is a 2π-periodic solution.

Boundary value problem:

$$\begin{aligned} y' &= \frac{1}{\omega} f(y) \\ y(0) &= y(2\pi). \end{aligned}$$

Let $\varphi^t(\cdot, \omega)$ denote the flow of this ode.

Shooting method: solve

$$S(\xi, \omega) = \varphi^{2\pi}(\xi, \omega) - \xi = 0.$$

Because of the S^1-symmetry of each periodic solution we need an additional phase condition. Simple choice:

$$\xi_1 = \bar{\xi}_1$$

The variational equation

In order to solve $S(\xi,\omega)=0, \xi_1=\bar{\xi}_1$ by Newton's method, we need to compute DS.

$D_\xi S(\xi,\omega) = D_\xi \varphi^{2\pi}(\xi,\omega) - I$ can be computed via the variational equation

$$\frac{\partial}{\partial t} D_\xi \varphi^t(\xi,\omega) = \frac{1}{\omega} Df(\varphi^t(\xi,\omega)) D_\xi \varphi^t(\xi,\omega), \quad D_\xi \varphi^0(\xi,\omega) = I.$$

For $\frac{\partial S}{\partial \omega}(\xi,\omega)$ we compute

$$\frac{\partial}{\partial \omega}\varphi^t = -\frac{t}{\omega^2}\dot{x}(t/\omega) = -\frac{t}{\omega^2} f(x(t/\omega)),$$

thus

$$\frac{\partial S}{\partial \omega}(\xi, \omega) = \frac{\partial}{\partial \omega}\varphi^{2\pi}(\xi, \omega) = -\frac{2\pi}{\omega^2} f(\varphi^{2\pi}(\xi, \omega)).$$

Advantage of shooting: stability of the periodic solution is directly given by the eigenvalues of

$$D_\xi \varphi^{2\pi}(\xi, \omega).$$

Galerkin approach

Let

$$C^r_{2\pi} \;=\; \{u \in C^r(\mathbb{R}, \mathbb{R}^d) : u(s+2\pi) = u(s)\}.$$

Consider the operator $F : C^1_{2\pi} \times \mathbb{R} \to C^0_{2\pi}$,

$$F(y, \omega) = \frac{dy}{dt} - \frac{1}{\omega} f(y).$$

A zero of this operator is a periodic solution of the boundary value problem.

Line of Reasoning

(i) Choose a suitable, countable basis of the underlying space $\rightsquigarrow$ countable system of equations;

(ii) using finitely many modes, numerically compute an approximate solution (Galerkin);

(iii) construct a restricted domain for F that isolates the numerical zero;

(iv) using topological arguments, show that there actually exists a zero in the restricted domain.

Setting

$$F(y, y', \dots, y^{(r)}) = 0, \quad y(t) \in \mathbb{R},$$

$F : \mathbb{R}^{r+1} \to \mathbb{R}$ smooth. We look for functions $y : \mathbb{R} \to \mathbb{R}, y \in C^r, y(t) = y(t + 2\pi/\omega)$ for some $\omega \in \mathbb{R}$ such that

$$F(y, y', \dots, y^{(r)}) = 0.$$

Rescaling time, $x(t) = y(t/\omega)$, yields the map

$$\hat{F} : \mathbb{R} \times C_1^r \to C_1^0$$
$$\hat{F} : (\omega, x) \mapsto F(x, \omega x', \dots, \omega^r x^{(r)})$$

$\hat{F}$ induces a map on the Fourier coefficients $(c_k)_{k\in\mathbb{Z}}$ of x. Note that

$$c_{-k} = \overline{c_k}, \quad k \in \mathbb{Z},$$

so it suffices to consider

$$\ell^2 = \left\{ (c_k)_{k=0}^{\infty} \in \mathbb{C}^{\mathbb{N}} : \sum_{k=0}^{\infty} |c_k|^2 < \infty \right\}.$$

Correspondingly

$$\ell_r^2 = \left\{ (c_k)_{k=0}^{\infty} \in \ell^2 \mid \exists u \in C_1^r : c_k \text{ is the } k\text{-th Fourier coefficient of } u \right\}.$$

Induced map

$$\tilde{F} : \mathbb{R} \times \ell_r^2 \to \ell_0^2.$$

Phase Condition

Since the original ODE is autonomous:

$$x \in C_1^r \text{ solution} \quad \Rightarrow \quad x(\cdot + t) \text{ solution} \forall t \in [0, 1].$$

Numerically more favorable: regularize by phase condition

$$\varphi(c) = 0.$$

Full system:

$$\Phi : \mathbb{R} \times \ell_r^2 \to \mathbb{R} \times \ell_0^2$$
$$\Phi(\omega, c) = (\varphi(c), \tilde{F}(\omega, c)).$$

We look for (ω, c) such that $\Phi(\omega, c) = 0$. Equivalently: look for fixed points of

$$G = id + \Phi.$$

Define

$$\begin{aligned} A_k(\omega, c) &= c_k \\ P_k(\omega, c) &= (\omega, c_0, \ldots, c_k) \\ Q_k(\omega, c) &= (c_{k+1}, c_{k+2}, \ldots) \end{aligned}$$

and consider the sets

$$\begin{aligned} Z_k &= \{(\omega, c) : P_k G(\omega, c) = P_k(\omega, c)\} \\ Z &= \bigcap_{k \geq 0} Z_k \end{aligned}$$

Proposition 1 *If G is continuous, Z_M is compact for some M and $Z_k \neq \emptyset$ for $k \geq M$, then Z is nonempty and all points in Z are fixed points of G.*

Proof of Existence

(i) Find compact restricted domain for G;

(ii) Show that Z_M is nonempty for some (**small**) M;

(iii) Show that Z_k is nonempty for $k > M$.

(i) Construction of the Restricted Domain

(i) Use Newton's method on a Galerkin projection of G in order to estimate a fixed point;

(ii) $F \in C^r \Rightarrow x \in C^r \Rightarrow$

$$|c_k| = \mathcal{O}(k^{-r}) \quad \text{as } k \to \infty.$$

Restricted domain: compact set $\Omega \times D \subset \mathbb{R} \times \ell^2_r$, where

$$D = D_0 \times \cdots \times D_{M-1} \times \prod_{k=M}^{\infty} \{c_k \in \mathbb{C} : |c_k| \leq r_k\},$$

where $D_0 \times \cdots \times D_{M-1} \subset \mathbb{C}^M$ contains the numerically computed fixed point.

(ii) Z_M is nonempty

Define the multivalued map

$$\mathcal{G}_M : P_M(\Omega \times D) \rightrightarrows P_M(\mathbb{R} \times \ell^2)$$
$$(\omega, \bar{c}) \mapsto \{P_M \circ G(\omega, c) : P_M(\omega, c) = (\omega, \bar{c}) \text{ and } (\omega, c) \in \Omega \times D\}.$$

We will show that every continuous selector of $\mathcal{G}_M$ has a fixed point.

Note that the set

$$Q_M(\Omega \times D)$$

determines the size of the images of $\mathcal{G}_M$.

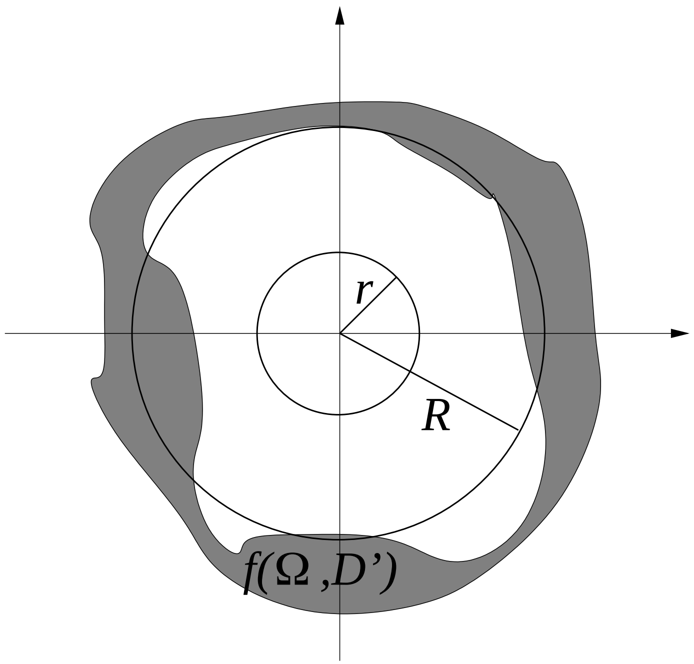
(iii) Z_k is nonempty for $k \geq M$

Definition 1 *A map $f : \Omega \times D \to \mathbb{C}$ is linearly dominated on the ball $B_0(r) \subset A_k(\Omega \times D)$ if*

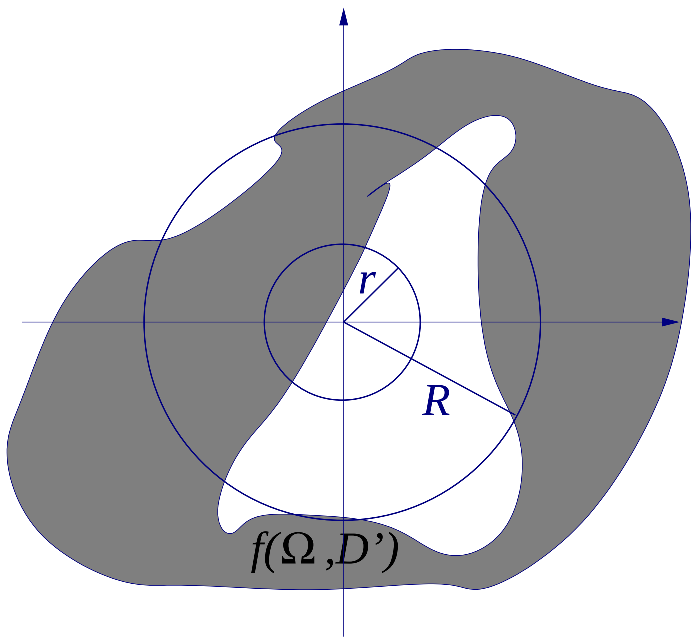
$$f(\omega, c) = L(\omega)c_k + g(\omega, c),$$

for all $(\omega, c) \in \Omega \times D$, $|c_k| \leq r$, where $L : I \to \mathbb{C}$, $\Omega \subset I$, and g are continuous functions, such that

$$\sup_{\Omega \times D} |g(\omega, c)| < r \inf_{\omega \in I} |L(\omega)| - r. \tag{2}$$



(a) Linearly dominated.



(b) Not linearly dominated.

$R = r \inf_{\omega \in I} |L(\omega)|$, $D' = D \cap \{|c_k| = r\}$.

Existence Theorem

Theorem 2 *Let $\Omega \times D$ be compact. Suppose that there exists a star-shaped enclosure $\hat{\mathcal{G}}_M$ for $\mathcal{G}_M$ such that (N, L) is an index pair for $\hat{\mathcal{G}}_M$ and*

$$\Lambda((N, L), \hat{\mathcal{G}}_M) \neq 0,$$

where Λ is the Lefschetz number of the index pair (N, L). Assume furthermore that the maps $A_k G$ are linearly dominated for all $k > M$, then there exists a fixed point for the map G.

Example

Consider

$$y''' + y'' + \sigma y' - \delta y + y^2 = 0,$$

$\sigma = 2, \delta = 3.$

Induced map on Fourier coefficients

$$A_k \tilde{F} : (\omega, c) \mapsto (-i\omega^3 k^3 - \omega^2 k^2 + \sigma\omega i k - \delta)c_k + \sum_{\ell \in \mathbb{Z}} c_l c_{k-l},$$

$k \geq 0.$ Computations: real version.

Phase condition

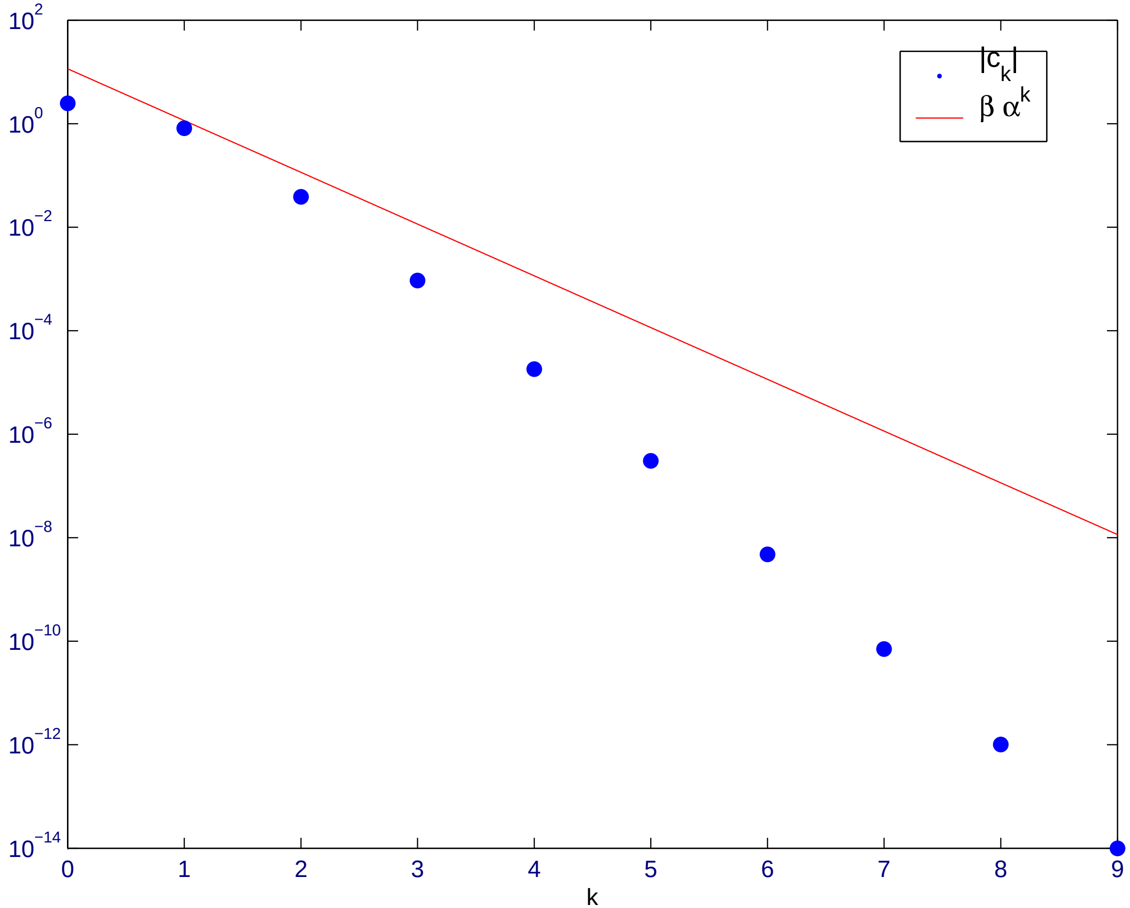
$$\varphi(c) = \mathrm{imag}(c_1) = 0.$$

$\rightsquigarrow G(\omega, c) = (\omega, c) + (\varphi(c), \tilde{F}(\omega, c))$ as above.

Numerical fixed point

$$
\begin{aligned}
\omega &= && 1.39, && && \\
c_0 &= && 2.46, && && \\
c_1 &= && 0.813, && && \\
c_2 &= && 0.0130 && - i && 0.0361, \\
c_3 &= -&& 7.79 \cdot 10^{-4} && - i && 5.13 \cdot 10^{-4}, \\
c_4 &= -&& 1.31 \cdot 10^{-5} && + i && 1.23 \cdot 10^{-5}, \\
c_5 &= && 1.55 \cdot 10^{-7} && + i && 2.64 \cdot 10^{-7}, \\
c_6 &= && 4.55 \cdot 10^{-9} && - i && 1.46 \cdot 10^{-9}, \\
c_7 &= -&& 6.51 \cdot 10^{-12} && - i && 7.04 \cdot 10^{-11}, \\
c_8 &= -&& 9.95 \cdot 10^{-13} && - i && 1.25 \cdot 10^{-13}, \\
c_9 &= -&& 4.65 \cdot 10^{-15} && + i && 1.29 \cdot 10^{-14}.
\end{aligned}
$$

Numerical fixed point: decay of coefficients



Restricted domain

$$\begin{aligned}
\Omega &= [1.36, 1.44], \\
D &= D_0 \times D_1 \times D_2 \times \prod_{k=3}^{\infty} B_0(\beta\alpha^k), \\
\text{with } \alpha &= 0.1, \quad \beta = 11.5, \\
\text{and } D_0 &= [2.43, 2.49], \\
D_1 &= [0.8, 0.8285], \\
D_2 &= [-0.003, 0.04] - [0.005, 0.06]i,
\end{aligned}$$

$\mathrm{imag}(D_0) = 0$, since the Fourier series is real valued.

$\mathrm{imag}(D_1) = 0$ due to the phase condition.

Linear domiation for $k > 2$

- **Lemma:**
$$\left|\sum_{l\in\mathbb{Z}} c_l c_{k-l}\right| \le \beta^2\alpha^k\left[\frac{2}{1-\alpha^2}+k-1\right].$$

- **Lemma:** The map $A_k G$ is linearly dominated on the ball $B_0(\beta\alpha^k)$ for $k > 2$.

- *Proof:* By the estimate we need to verify that
$$\beta^2\alpha^k\left[\frac{2}{1-\alpha^2}+k-1\right] < \beta\alpha^k \min_{\omega\in\Omega}\left(|-i\omega^3k^3-\omega^2k^2+\sigma\omega ik-\delta+1|-1\right).$$

- Rewrite the rhs, use $\Omega = [\underline{\omega}, \overline{\omega}]$, plug in $\underline{\omega}$ and $\overline{\omega}$ where appropriate,

- $\rightsquigarrow$ function $k \mapsto e(k, \underline{\omega}, \overline{\omega}, \delta, \sigma)$ such that A_k is linearly dominated, if $e(k) > 0$.

- Result: $e(k)$ is increasing and $e(3) > 0$. $\square$

Index pair for lower modes

- We need to numerically construct an index pair for $\hat{\mathcal{G}}_2$ (with, hopefully, a non-zero Lefschetz number).
- $7d \rightarrow 3d$ by exploiting the structure of the map;

Explicit multivalued map

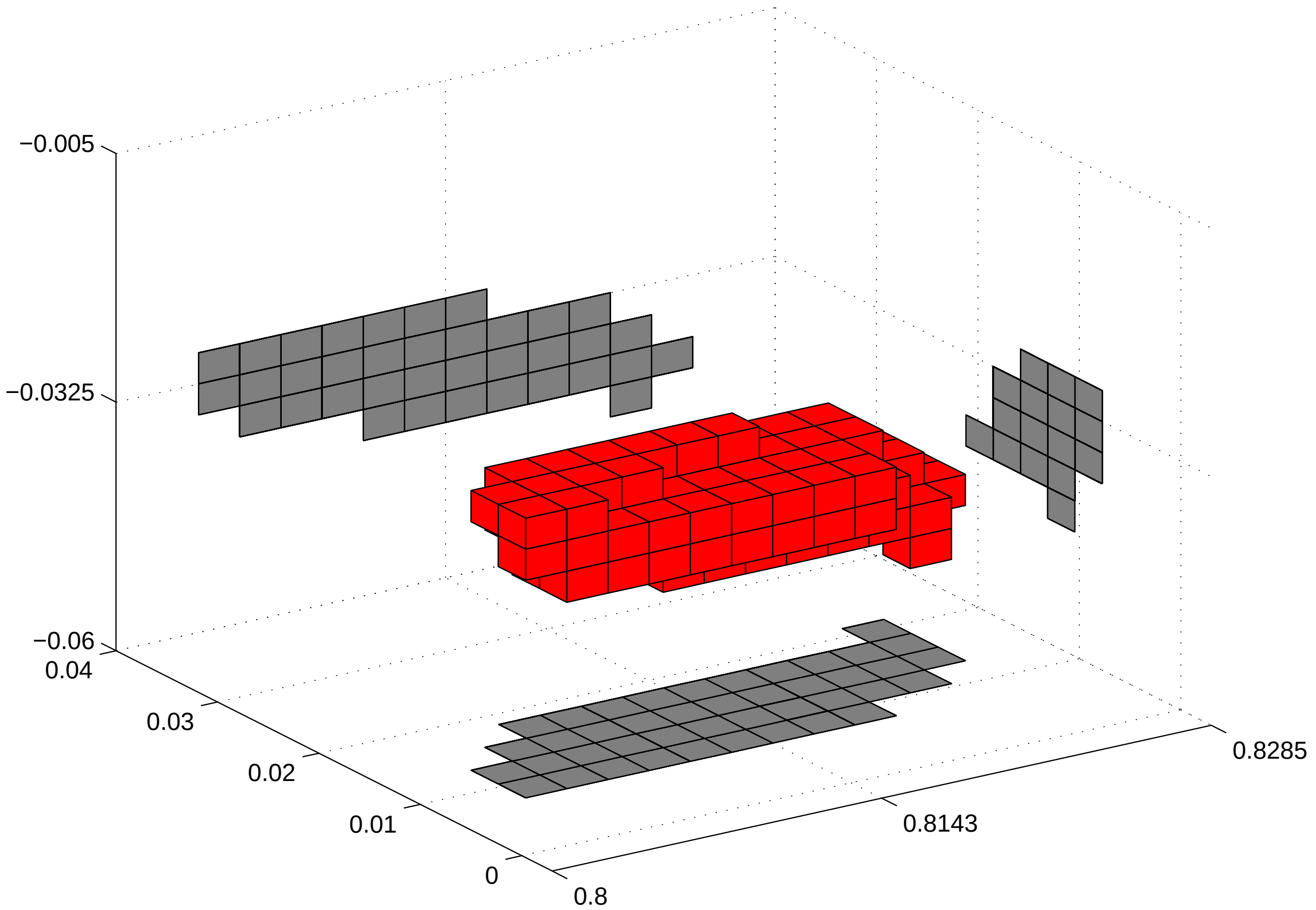
$$
\begin{aligned}
a_1 &\mapsto (-\bar{\omega}^2 - \delta + 1)a_1 + 2a_1a_2 + 2\bar{a}_0a_1 + |c_2|\ I_0 + 0.01\ I_1 \\
a_2 &\mapsto (-4\bar{\omega}^2 - \delta + 1)a_2 + (8\bar{\omega}^3 - 2\sigma\bar{\omega})b_2 + 2\bar{a}_0a_2 + a_1^2 \\
&\qquad + (|c_2|\ 0.1 + |c_1|)I_0 + 10^{-3}\ I_1 \\
b_2 &\mapsto (-8\bar{\omega}^3 + 2\sigma\bar{\omega})a_2 + (-4\bar{\omega}^2 - \delta + 1)b_2 + 2\bar{a}_0b_2 \\
&\qquad + |c_2|0.1\ I_0 + |c_1|I_0 + 10^{-3}\ I_1,
\end{aligned}
$$

where

$$
I_0 = 0.023 \cdot [-1, 1], \quad I_1 = 2.67172 \cdot 10^{-4} \cdot [-1, 1],
$$

and $\bar{a}_0 = \bar{a}_0(a_1, a_2, b_2)$ and $\bar{\omega} = \bar{\omega}(a_1, a_2, b_2)$ are intervals.

Isolating neighborhood



Index pair

$$(N, L) := (|\mathbf{G}_M(\mathcal{I})|, |\mathbf{G}_M(\mathcal{I})\backslash\mathcal{I}|),$$

where $\mathbf{G}_M : \mathcal{P} \rightrightarrows \mathcal{P}$ ($\mathcal{P}$ a partition of the "search box") such that for $C \in \mathcal{P}$ we have $\hat{\mathcal{G}}_2(C) \subset |\mathbf{G}_M(C)|$.

Induced homology map:

$$f_k = \begin{cases} 1 & k = 3, \\ 0 & else. \end{cases}$$

$\Rightarrow \Lambda((N, L), \hat{\mathcal{G}}_2) = 1.$

Theorem 3 *The differential equation with parameters $\sigma = 2$ and $\delta = 3$ possesses a periodic orbit*

$$y(t) = \sum_{k \in \mathbb{Z}} c_k e^{ik\omega t}$$

with $c_{-k} = \overline{c_k}$ and

$$\begin{aligned}
\omega &\in [1.36, 1.44] \\
c_0 &\in [2.43, 2.49] \\
c_1 &\in [0.8, 0.8285] \\
c_2 &\in [-0.003, 0.04] - [0.005, 0.06]i \\
c_k &\in \{z \in \mathbb{C} \mid |z| \leq \beta \cdot \alpha^k\}, \quad \beta = 11.5, \quad \alpha = 0.1, \quad k > 2.
\end{aligned}$$