KdV soliton solutions to a model of hepatitis C virus evolution

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Russell and the Wave of Translation

"<...> the boat suddenly stopped - not so the mass of water in the channel which it had put in motion; it accumulated round the prow of the vessel in a state of violent agitation, then suddenly leaving it behind, rolled forward with great velocity, assuming the form of a large solitary elevation <...> which continued its course along the channel apparently without change of form or diminution of speed. <...> was my first chance interview with that singular and beautiful phenomenon which I have called the **Wave of Translation**. (1834)"

Figure: John Scott Russell (1808 – 1882)

First Mathematical Model: KdV equation

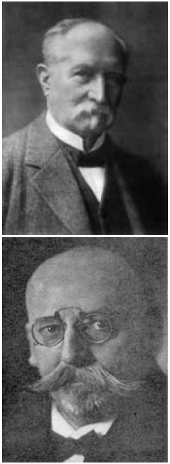


Figure: D. Korteweg (top), G. de Vries

The first actual mathematical model of solitary waves (solitons) was discovered by **Boussinesq** (1877) and later rediscovered and studied in detail by **Diederik Korteweg** and **Gustav de Vries**.

The KdV equation

$$\frac{\partial u}{\partial t} - \frac{\partial^3 u}{\partial x^3} + 6u\,\frac{\partial u}{\partial x} = 0.$$

It was shown that there exist solutions of the form:

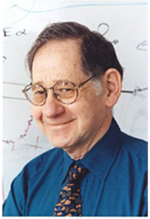
KdV soliton

$$u(t,x) = -\frac{c}{2}\mathrm{sech}^2\left(\frac{\sqrt{c}}{2}(x - ct - a)\right).$$

Zabusky and Kruskal: Rediscovery

The works of Russell, Boussinesq, Korteweg and de Vries fell into obscurity until 1965, when **Norman J. Zabusky** and **Martin Kruskal** made connections between the KdV equation and the Fermi-Pasta-Ulam experiment.

The word "soliton" was coined and extensive studies into the nature of soliton (solitary) processes were launched that are still continuing today. It has had a broad and far-reaching impact in myriad fields ranging from the purest mathematics to experimental science.



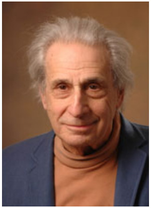


Figure: N. Zabusky (top), M. Kruskal

Rise to fame: the Schrödinger equation

A particular surge in interest of the analysis of solitary processes in physics came when **Vladimir Zakharov** and **Aleksei Shabat** demonstrated in 1972 that the nonlinear Schrödinger (NLS) equation has soliton solutions.

NLS equation

$$\mathrm{i}\,\frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial t^2} \pm 2\,|u|^2\,u = 0.$$

This discovery had enormous repercussions in physics, especially in nonlinear optics, Bose-Einstein condensates, where the NLS equation plays a very important role.

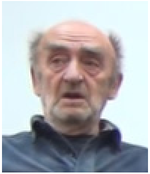



Figure: V. Zakharov (top), A. Shabat

Applications of Soliton Theory

Soliton theory has had a great impact on myriad fields of science, including:

- Nonlinear optics;
- Bose-Einstein condensates;
- Hydrodynamics;
- Biophysics;
- MEMs and NEMs;
- Plasmas;
- Population dynamics.

Physical Properties of Solitary Solutions

A nonlinear wave is called a soliton if:

- It maintains its shape as it propagates at a constant speed;
- If it collides with another soliton, it emerges from the collision unaltered, except for a phase shift.

The definition is not universally accepted – there are a few ways to define solitons in the physical sense (for example allowing a small loss of energy after collision ("light bullets")), however, from a mathematical perspective the definition given above is almost ubiquitous.

Solitary solutions – analytic expression

Solitary solution

The m-th order solitary solution reads:

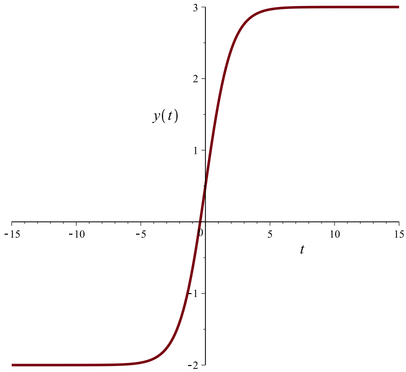
$$x(t) = \frac{\sum_{k=0}^{m} \alpha_k \exp\left(\eta k (t-c)\right)}{\prod_{k=1}^{m} \Big(\exp\left(\eta(t-c)\right) - t_k\Big)},$$

where $\eta, \alpha_k, t_k, c \in \mathbb{C}$ are fixed parameters.

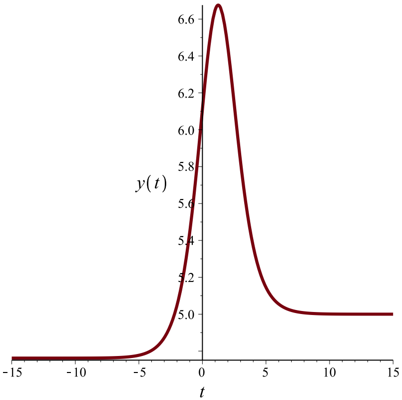
The shape is based on the **KdV soliton**, which is a special case of the above solution (hyperbolic secant):

$$\varphi(\xi) = -\frac{c}{2}\operatorname{sech}^2\left(\frac{\sqrt{c}}{2}(\xi - \xi_0)\right).$$

Solitary solutions

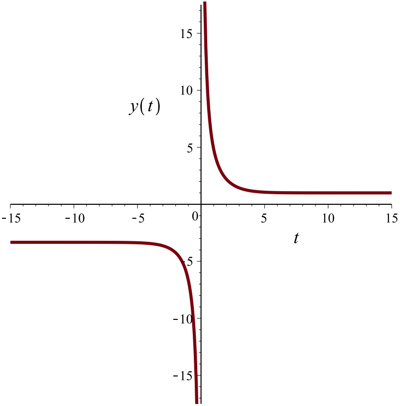


(a) Kink solitary solution

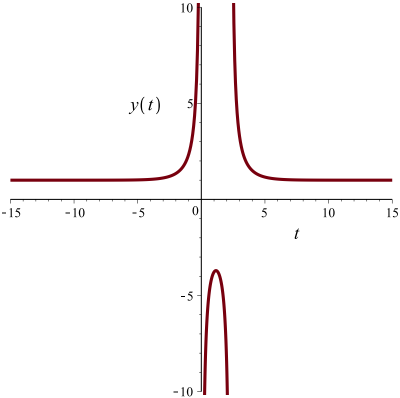


(b) Bright solitary solution

Solitary solutions



(c) Solitary solution with one singularity



(d) Solitary solution with two singularities

Coupled Riccati equations (1)

Regula et al (2009) introduced the following system for modeling Hepatitis C virus (HCV) evolution:

$$x'_t = x(1-x-y) - (1-\theta)\,bxy + qy + s;$$
$$y'_t = ry(1-x-y) + (1+\theta)\,bxy - (d+q)y,$$
$$\theta, b, q, s, r, d \in \mathbb{R}.$$

Simple generalization leads to:

$$x'_t = a_0 + a_1 x + a_2 x^2 + a_3 xy + a_4 y;$$
$$y'_t = b_0 + b_1 y + b_2 y^2 + b_3 xy + b_4 x,$$
$$a_j, b_j \in \mathbb{R}.$$

Coupled Riccati equations (2)

$$x'_t = a_0 + a_1 x + a_2 x^2 + a_3 xy + a_4 y;$$
$$y'_t = b_0 + b_1 y + b_2 y^2 + b_3 xy + b_4 x,$$
$$a_j, b_j \in \mathbb{R}.$$

- Standard diffusive coupling terms $a_4 y, b_4 x$;
- Multiplicative coupling terms $a_3 xy, b_3 xy$;
- **Conditions for existence of soliton solutions – ?**
- **Construction of soliton solutions – ?**

Inverse balancing technique

- The inverse idea of common ansatz methods;
- Insert known solution into DE;
- If DE depends linearly on equation parameters, solve for them;
- Application of technique is **not used to solve the DE**, but to obtain **necessary existence conditions** for the solitary solutions.

PDEs with polynomial nonlinearity

Class of PDEs

$$\frac{\partial^m u}{\partial t^m} + A_{m-1,0}\frac{\partial^{m-1} u}{\partial t^{m-1}} + A_{0,m-1}\frac{\partial^{m-1} u}{\partial z^{m-1}} + \cdots + A_{10}\frac{\partial u}{\partial t} + A_{01}\frac{\partial u}{\partial z} = a_n u^n + \cdots + a_0.$$

When do the considered PDEs have solitary solutions (of any order l)?

$$u\left(t - \alpha z\right) = \frac{\sum_{k=0}^{l} \alpha_k \exp\left(\eta k \left(t - \alpha z\right)\right)}{\prod_{k=1}^{l}\left(\exp\left(\eta\left(t - \alpha z\right)\right) - t_k\right)}.$$

Necessary existence conditions (1)

Condition #1: derivative and nonlinear term balance

$$n = m + 1.$$

Condition #2: equation and solution order balance

$$\frac{(m+1)l}{2} \leq l + m + 1, \qquad l, m \in \mathbb{N}.$$

Necessary existence conditions (2)

Table of necessary existence conditions of solitary solutions to the considered PDEs. $\exists$ denotes existence with all parameter values, $\exists^*$ denotes existence with additional constraints on parameters, $\nexists$ denotes the nonexistence of solitary solutions.

l \ (n,m)	$(2,1)$	$(3,2)$	$(4,3)$	$(5,4)$	$(6,5)$	$(7,6)$	$(8,7)$
1	$\exists$	$\exists^*$	$\exists^*$	$\exists^*$	$\exists^*$	$\exists^*$	$\exists^*$
2	$\nexists$	$\exists^*$	$\exists^*$	$\exists^*$	$\exists^*$	$\exists^*$	$\exists^*$
3	$\nexists$	$\exists^*$	$\exists^*$	$\exists^*$	$\exists^*$	$\nexists$	$\nexists$
4	$\nexists$	$\nexists$	$\nexists$	$\nexists$	$\nexists$	$\nexists$	$\nexists$
5	$\nexists$	$\nexists$	$\nexists$	$\nexists$	$\nexists$	$\nexists$	$\nexists$

Generalized differential operator

The notation $\mathbf{D}_\alpha := \dfrac{\partial}{\partial \alpha}$ will be used.

Generalized differential operator (GDO)

$$\mathbf{D}_{csu} := R\left(c,s,u\right)\mathbf{D}_c + P\left(c,s,u\right)\mathbf{D}_s + Q\left(c,s,u\right)\mathbf{D}_u,$$

where R, P, Q are analytic.

Properties of GDO

- $\mathbf{D}_{csu}\left(f_1 + f_2\right) = \mathbf{D}_{csu} f_1 + \mathbf{D}_{csu} f_2;$
- $\mathbf{D}_{csu}\left(f_1 f_2\right) = \left(\mathbf{D}_{csu} f_1\right) f_2 + f_1 \mathbf{D}_{csu} f_2.$

Multiplicative operator

Suppose a GDO $\mathbf{D}_{csu}$ is given. The multiplicative operator reads:

$$\mathbf{G} := \sum_{j=0}^{+\infty} \frac{(t-c)^j}{j!} \mathbf{D}_{csu}^j.$$

Main property

$$\mathbf{G} f\left(c, s, u\right) = f\left(\mathbf{G}c, \mathbf{G}s, \mathbf{G}u\right).$$

Each ODE or ODE system has unique generalized differential and multiplicative operators.

First order ODE system

$$x'_t = P(t,x,y); \quad x = x(t;c,s,u), \quad x(c;c,s,u) = s;$$
$$y'_t = Q(t,x,y); \quad y = y(t;c,s,u), \quad y(c;c,s,u) = u.$$

System operators

$$\mathbf{D}_{csu} = \mathbf{D}_c + P(c,s,u)\,\mathbf{D}_s + Q(c,s,u)\,\mathbf{D}_u; \quad \mathbf{G} = \sum_{j=0}^{+\infty} \frac{(t-c)^j}{j!} \mathbf{D}_{csu}^j.$$

General solution

$$x(t) = \sum_{j=0}^{+\infty} \frac{(t-c)^j}{j!} \left(\mathbf{D}_{csu}^j s\right) = \mathbf{G}s, \quad y(t) = \sum_{j=0}^{+\infty} \frac{(t-c)^j}{j!} \left(\mathbf{D}_{csu}^j u\right) = \mathbf{G}u.$$

Image of solution

Suppose an ODE is given:

$$x'_t = P\left(x\right), \quad x = x\left(t; c, s\right); \quad x\left(c; c, s\right) = s.$$

Variable substitution

$$\widehat{t} := \exp\left(\eta t\right), \quad \widehat{c} := \exp\left(\eta c\right); \ \eta \in \mathbb{R}\backslash\{0\}$$

Image of solution

$$x = x(t) = x\left(\frac{1}{\eta}\ln\widehat{t}\right) =: \widehat{x}\left(\widehat{t}\right) = \widehat{x};$$

$$x'_t = \eta\widehat{t}\widehat{x}'_{\widehat{t}}.$$

Image of ODE

Image of ODE

$$\eta\widehat{t}\widehat{x}'_{\widehat{t}} = P\left(\widehat{x}\right);$$

$$\widehat{x} = \widehat{x}\left(\widehat{t}; \widehat{c}, s\right), \quad \widehat{x}\left(\widehat{c}; \widehat{c}, s\right) = s.$$

Operators of transformed ODE

$$\widehat{\mathbf{D}}_{\widehat{c}s} := \mathbf{D}_{\widehat{c}} + \frac{1}{\eta\widehat{c}} P\left(s\right)\mathbf{D}_s;$$

$$\widehat{\mathbf{G}} := \sum_{j=0}^{+\infty} \frac{\left(\widehat{t} - \widehat{c}\right)^j}{j!} \widehat{\mathbf{D}}_{\widehat{c}s}^j.$$

Linear recurring sequences

Let $p_j := \mathbf{D}^j_{csu} s$. Solutions can be written in the closed form if the sequence $(p_j; j \in \mathbb{Z}_0)$ (or a sequence constructed from p_j in a known way) is linearly recurring.

$$d_k := \det \left(\begin{bmatrix} p_0 & p_1 & \dots & p_{k-1} \\ p_1 & p_2 & \dots & p_k \\ \vdots & \vdots & \ddots & \vdots \\ p_{k-1} & p_k & \dots & p_{2k-2} \end{bmatrix} \right).$$

Linear recurring sequence

$(p_j; j \in \mathbb{Z}_0)$ is an m-th order linear recurring sequence (LRS), if

$$d_m \neq 0, \quad d_{m+l} = 0; \quad l = 1, 2, \dots .$$

It is denoted as

$$\text{order}\, (p_j; j \in \mathbb{Z}_0) = m.$$

Canonical expression of LRS

The characteristic equation reads:

$$\begin{vmatrix} p_0 & p_1 & \dots & p_{m-1} & p_m \\ p_1 & p_2 & \dots & p_m & p_{m+1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ p_{m-1} & p_m & \dots & p_{2m-2} & p_{2m-1} \\ 1 & \rho & \dots & \rho^{m-1} & \rho^m \end{vmatrix} = 0.$$

Characteristic roots: $\rho_1, \dots, \rho_m; \quad \rho_k \neq \rho_j, \, k \neq j$.

Canonical expression

$$p_j = \sum_{k=1}^{m} \lambda_k \rho_k^j, \quad j = 0, 1, \dots .$$

Coefficients $\lambda_k, k = 1, \dots, m$ are determined from a system of linear equations.

Exponent sum solution

Suppose that

$$\operatorname{order}\left(\mathbf{D}_{csu}^{j}s; j \in \mathbb{Z}_0\right) = m;$$

$$\mathbf{D}_{csu}^{j}s = \sum_{k=1}^{m} \lambda_k \rho_k^j.$$

Form of solution

$$x\left(t; c, s, u\right) = \mathbf{G}s = \sum_{j=0}^{+\infty} \frac{(t-c)^j}{j!} \sum_{k=1}^{m} \lambda_k \rho_k^j$$

$$= \sum_{k=1}^{m} \lambda_k \exp\left(\rho_k\left(t-c\right)\right).$$

Solitary (soliton) solution (1)

Let

$$\operatorname{order}\left(\mathbf{D}_{csu}^{j} s; j \in \mathbb{Z}_0\right) = +\infty, \quad \text{but} \quad \operatorname{order}\left(\frac{1}{j!}\widehat{\mathbf{D}}_{\widehat{c}su}^{j} s; j \in \mathbb{Z}_0\right) = m.$$

Then $\frac{1}{j!}\widehat{\mathbf{D}}_{\widehat{c}su}^{j} s = \sum_{k=1}^{m} \lambda_k \rho_k^j$.

Theorem

The soliton solution exists, if the following relations hold true:

$$\widehat{\mathbf{D}}_{\widehat{c}su} \rho_k = \rho_k^2, \quad \widehat{\mathbf{D}}_{\widehat{c}su} \lambda_k = \lambda_k \rho_k; \quad k = 1, \ldots, m.$$

Solitary (soliton) solution (2)

Form of solution

$$\widehat{x}\left(\widehat{t};\widehat{c},s,u\right)=\widehat{\mathbf{G}}s=\sum_{j=0}^{+\infty}\left(\widehat{t}-\widehat{c}\right)^{j}\sum_{k=1}^{m}\lambda_k\rho_k^{j}=\sum_{k=1}^{m}\frac{\lambda_k}{1-\rho_k\left(\widehat{t}-\widehat{c}\right)};$$

$$x\left(t;c,s,u\right)=\frac{\sum_{k=0}^{m}\alpha_k\exp\left(\eta k(t-c)\right)}{\prod_{k=1}^{m}\left(\exp\left(\eta(t-c)\right)-t_k\right)}.$$

General case

Suppose that $f\left(\xi\right)=\sum_{j=0}^{+\infty}\frac{q_j}{j!}\xi^j;\quad q_0=1,\, q_j=\prod_{k=0}^{j-1}(a+bk)\neq 0, j=1,2,\ldots.$

Let order $\left(\frac{1}{q_j}\widehat{\mathbf{D}}_{\widehat{c}su}^{j}s; j\in\mathbb{Z}_0\right)=m,\quad \frac{1}{q_j}\widehat{\mathbf{D}}_{\widehat{c}su}^{j}s=\sum_{k=1}^{m}\lambda_k\rho_k^j.$

Form of solution

$$\widehat{y}\left(\widehat{t};\widehat{c},s,u\right)=\widehat{\mathbf{G}}s=\sum_{j=0}^{+\infty}\frac{q_j}{j!}\left(\widehat{t}-\widehat{c}\right)^j\sum_{k=1}^{m}\lambda_k\rho_k^j=\sum_{k=1}^{m}\lambda_k f\left(\rho_k\left(\widehat{t}-\widehat{c}\right)\right);$$

$$x\left(t;c,s,u\right)=\sum_{k=1}^{m}\lambda_k f\left(\alpha_k-\beta_k\exp\left(\eta(t-c)\right)\right).$$

Hepatitis C model (Coupled Riccati equations)

$$
\begin{aligned}
&x_t' = a_0 + a_1 x + a_2 x^2 + a_3 xy + a_4 y; \quad x(c) = s;\\
&y_t' = b_0 + b_1 y + b_2 y^2 + b_3 xy + b_4 x; \quad y(c) = u,\\
&a_j, b_j \in \mathbb{R}.
\end{aligned}
$$

- Kink solutions (order = 1);
- Bright/dark and singular solutions (order = 2);

Bright/dark solutions

Analytical expression

$$x(t) = \sigma \frac{\Big(\exp\left(\eta(t-c)\right) - x_1\Big)\Big(\exp\left(\eta(t-c)\right) - x_2\Big)}{\Big(\exp\left(\eta(t-c)\right) - t_1\Big)\Big(\exp\left(\eta(t-c)\right) - t_2\Big)}; \quad (1)$$

$$y(t) = \gamma \frac{\Big(\exp\left(\eta(t-c)\right) - y_1\Big)\Big(\exp\left(\eta(t-c)\right) - y_2\Big)}{\Big(\exp\left(\eta(t-c)\right) - t_1\Big)\Big(\exp\left(\eta(t-c)\right) - t_2\Big)}. \quad (2)$$

- σ, γ, η are constants;
- $x_1, x_2, y_1, y_2, t_1, t_2$ depend on initial conditions s, u;
- Solutions which hold for **all initial conditions** are constructed.

Existence conditions

Bright/dark solitary solutions exist if:

$$a_3 = b_2; \quad a_2 = b_3,$$

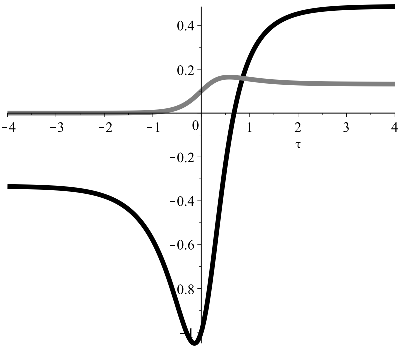
and

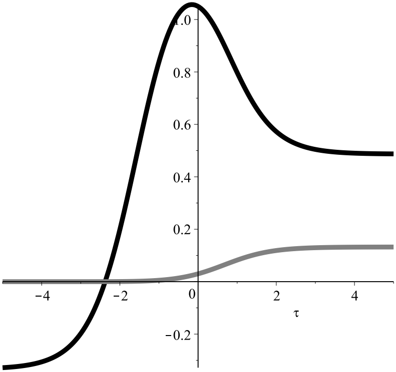
$$9a_0a_1a_2 + 9b_0b_1b_2 - 18a_0a_2b_1 - 18b_0b_2a_1 + 3a_1b_1^2 + 3b_1a_1^2 - 2a_1^3 - 2b_1^3 \\ - 9a_1a_4b_4 - 9b_1b_4a_4 + 27a_0b_2b_4 + 27b_0a_2a_4 = 0.$$

In the phase plane, bright/dark solution trajectories are conic sections:

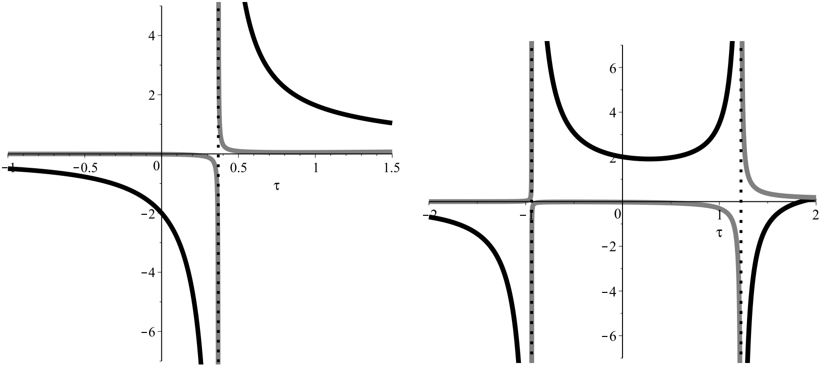
$$Ax^2(t) + By^2(t) + Cx(t)y(t) + Ex(t) + Fy(t) = G; \quad A, B, C, E, F, G \in \mathbb{R}.$$

Time evolution of solutions (1)

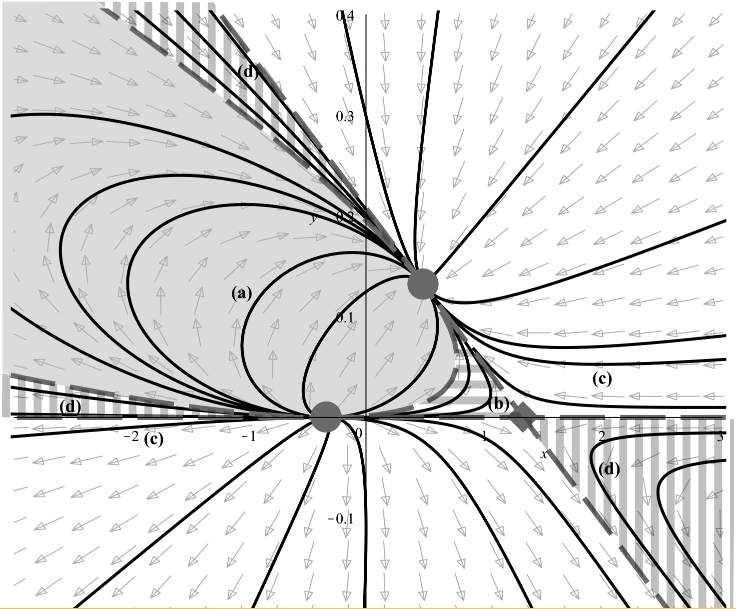




Time evolution of solutions (2)



Phase portrait



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Thank You For Your Attention