A multi-parameter singular perturbation analysis of the Robertson model

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The Robertson model (RM)

Chemical reaction

1.	X	$\xrightarrow{k_1}$	Y
2.	$Y+Y$	$\xrightarrow{k_2}$	$Y+Z$
3.	$Y+Z$	$\xrightarrow{k_3}$	$X+Z$

Robertson model (RM) [Robertson, 1966]

$$\dot{x} = -k_1 x + k_3 yz$$
$$\dot{y} = k_1 x - k_2 y^2 - k_3 yz$$
$$\dot{z} = k_2 y^2$$

- Reaction rates $k_1 = 4 \cdot 10^{-2}$, $k_2 = 3 \cdot 10^{7}$, $k_3 = 10^4$ and initial value $(x_0, y_0, z_0)^T = (1, 0, 0)^T$.

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- Conserved quantity $x + y + z = const.$ and forward invariant state space $\mathbb{R}^3_+$
  $\implies$ existence and uniqueness of solutions for all $t \geq 0$.
- Convergence to unique equilibrium $(0, 0, 1)^T$ by standard dynamical systems arguments.

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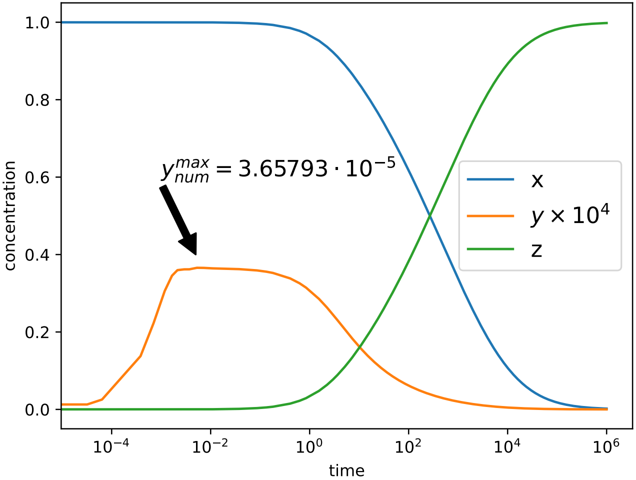
Why are we studying this model?

Numerical simulation shows clear multi-scale behaviour

- Note the logarithmic time scale!
- Essentially 3 phases of the reaction: Fast - intermediate - slow.
- Prototypical model for multi-scale solution structures observed in many biological and chemical systems.



Dynamics on widely different time scales observed for $k_1, k_3 \ll k_2$

- Define small parameters
  $\varepsilon_1 := k_1/k_2 \ll 1$ and
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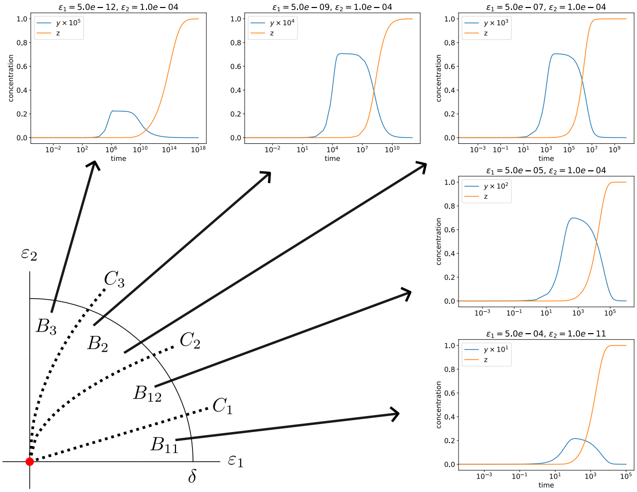
- Note the logarithmic time scale!

- Quantitative changes of solutions close to $(\varepsilon_1, \varepsilon_2) = (0, 0)$.



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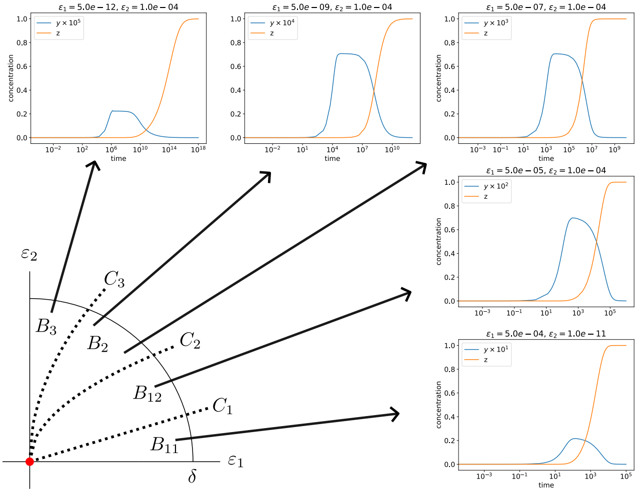
- Quantitative changes of solutions close to $(\varepsilon_1, \varepsilon_2) = (0, 0)$.
- **Today:** Asymptotic analysis based on geometric singular perturbation theory (GSPT).



Overview

- GSPT with one small parameter.
- Singular perturbations with several small parameters.
- Robertson model as two-parameter singular perturbation problem.
- Sketch proof of main result.
- Conclusion and Outlook.

Slow-fast systems in standard form

Fast variables $x \in \mathbb{R}^m$, slow variables $y \in \mathbb{R}^n$, $0 < \varepsilon \ll 1$.

Slow time scale t

$$\begin{cases} \varepsilon \dot{x} &= f(x, y, \varepsilon) \\ \dot{y} &= g(x, y, \varepsilon) \end{cases}$$

$$\xleftrightarrow{t = \tau\varepsilon}$$

Fast time scale τ

$$\begin{cases} x' &= f(x, y, \varepsilon) \\ y' &= \varepsilon g(x, y, \varepsilon) \end{cases}$$

- For $\varepsilon > 0$ the two systems are equivalent.
- Two limiting problems for $\varepsilon = 0$:

Reduced problem

$$\begin{cases} 0 &= f(x, y, 0) \\ \dot{y} &= g(x, y, 0) \end{cases}$$

Layer problem

$$\begin{cases} x' &= f(x, y, 0) \\ y' &= 0 \end{cases}$$

GSPT based on slow manifolds

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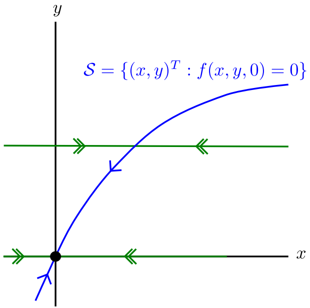
- Critical manifold $\mathcal{S} := \{(x,y)^T : f(x,y,0) = 0\}$.



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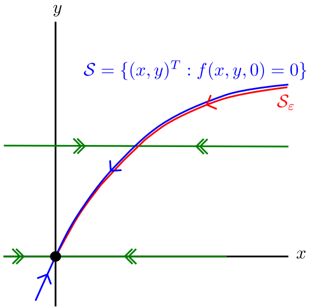
- Critical manifold $\mathcal{S} := \{(x,y)^T : f(x,y,0) = 0\}$.
- Fenichel Theory (1979):
  If $\mathcal{S}$ normally hyperbolic $\implies \exists$ invariant slow manifold $\mathcal{S}_\varepsilon$, $\mathcal{O}(\varepsilon)$-close to $\mathcal{S}$ with similar properties, for $\varepsilon \ll 1$.
- For attracting critical manifolds: Tikhonov's Theorem.



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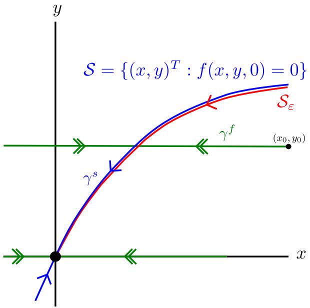

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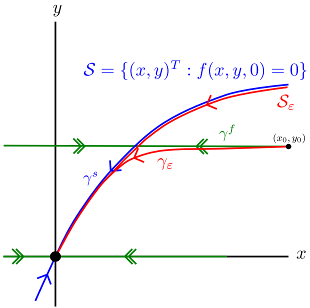

Today's GSPT = Fenichel Theory + Blow-up

Distinguished small parameter $0 < \varepsilon \ll 1$.

Standard form

$$x' = f(x, y, \varepsilon)$$
$$y' = \varepsilon g(x, y, \varepsilon).$$

Critical manifold $\mathcal{S} = \{f(x, y, 0) = 0\}$.

Non-standard form

$$z' = H(z, \varepsilon)$$

Layer problem: $z' = H(z, 0)$

Critical manifold $\mathcal{S} = \{H(z, 0) = 0\}$.

- $\mathcal{S}$ normally hyperbolic $\implies$ $\exists$ invariant slow manifold $\mathcal{S}_\varepsilon$ for $0 < \varepsilon \ll 1$ [Fenichel, 1979].
- Blow-up method for non-hyperbolic points [Dumortier and Roussarie, 1996] and [Krupa and Szmolyan, 2001].
- Very successful theory, many applications, vast literature with contributions from numerous authors.

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What about several small parameters?

Multi-parameter systems

$$\dot{z} = H(z, k_1, \dots, k_{p+1}), \quad k_i > 0,\ i = 1, \dots, p+1.$$

- Parameters k_i of different orders of magnitude.
- Common structure in biology and chemistry, e.g, mass action networks:

$$\dot{z} = \Gamma R(z, \kappa).$$

- In situations with $k_{p+1} \gg k_i \implies$ change to fast time scale $\tau = k_{p+1} t$
- Define $\varepsilon_i := \frac{k_i}{k_{p+1}}$ to obtain

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Can we still apply GSPT?

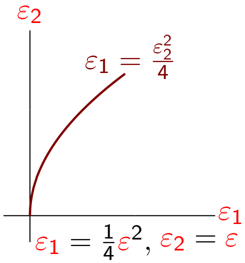
Singular perturbations for several small parameters

$$z' = H(z, \varepsilon_1, \dots, \varepsilon_p), \quad 0 < \varepsilon_i \ll 1,\ i = 1, \dots, p.$$

- Common approach: Reduce to one-parameter case

$$(\varepsilon_1, \dots, \varepsilon_p) \sim (\varepsilon^{\alpha_1}, \dots, \varepsilon^{\alpha_p}),\ \alpha_i \in \mathbb{Z},\ i = 1, \dots, p.$$

  - Need to know orders of magnitude of parameters.
  - Covers only a curve of parameter space.



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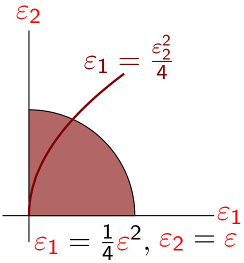


- Goal: Cover a neighbourhood of $(\varepsilon_1, \dots, \varepsilon_p) = (0, \dots, 0)$
  - Case studies are available, e.g., [De Maesschalck and Dumortier, 2011].
  - Recent review on singular double limits of differential equations [Kuehn et al., 2022].

Types of multi-parameter singular perturbations (non-exhaustive)

$$\dot{z} = H(z, \varepsilon_1, \varepsilon_2),\ 0 < \varepsilon_1, \varepsilon_2 \ll 1.$$

1) Nested sequence of time scales [Cardin and Teixeira, 2017] and [Krupa et al., 2008]:

$$\begin{aligned}\dot{x}_1 &= f_1(x, \varepsilon_1, \varepsilon_2)\\ \dot{x}_2 &= \varepsilon_1 f_2(x, \varepsilon_1, \varepsilon_2)\\ \dot{x}_3 &= \varepsilon_1 \varepsilon_2 f_3(x, \varepsilon_1, \varepsilon_2).\end{aligned}$$

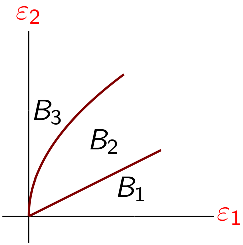
- Apply Fenichel theory iteratively.
- Nested sequence of critical manifolds.
- Well understood in the normally hyperbolic case.

2) Only ε_1 is a classical singular perturbation parameter:

- Critical manifold $\mathcal{S}(\varepsilon_2)$.
- $\mathcal{S}(\varepsilon_2)$ 'singular' as $\varepsilon_2 \to 0$.

3) ε_1 and ε_2 are classical singular perturbation parameters:

- Different slow-fast structures in different regions B_i, $i = 1, \ldots, m$, of parameter space.



RM viewed as a two-parameter singular perturbation problem

- Initial value $(x_0, y_0, z_0) = (c, 0, 0)$ with $c > 0$.
- Use conserved quantity $x(t) = c - y(t) - z(t)$ for all $t \geq 0$.
- Assume $k_1,\ k_3 \ll k_2$.
- Change to fast time scale $\tau = k_2 t$.
- Define new parameters:

$$\varepsilon_1 := k_1/k_2 \ll 1.$$
$$\varepsilon_2 := k_3/k_2 \ll 1.$$

Robertson model 3D

$$\dot{x} = -k_1 x + k_3 yz$$
$$\dot{y} = k_1 x - k_2 y^2 - k_3 yz$$
$$\dot{z} = k_2 y^2$$

$\downarrow$

Robertson model 2D

$$y' = \varepsilon_1 (c - y - z) - y^2 - \varepsilon_2 yz$$
$$z' = y^2$$

Degenerate layer problem of RM

Robertson model 2D

$$y' = \varepsilon_1(c - y - z) - y^2 - \varepsilon_2 yz$$
$$z' = y^2$$

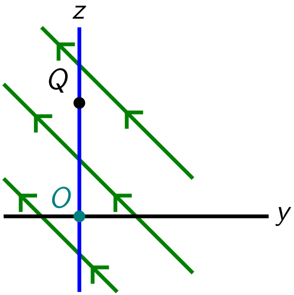
Layer problem

$$y' = -y^2$$
$$z' = y^2$$

- Detailed asymptotic structure depends sensitively on $(\varepsilon_1, \varepsilon_2) \approx (0, 0)$!

Layer problem $\varepsilon_1 = \varepsilon_2 = 0$:

- Non-hyperbolic critical manifold $y = 0$.
- Contains the **initial value** $O = (0, 0)$ and the **equilibrium** $Q = (0, c)$.

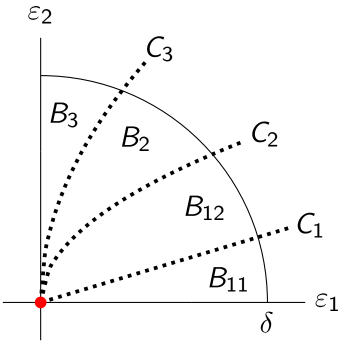


Main Result

Theorem

1. In ${\varepsilon_1}^2 + {\varepsilon_2}^2 < \delta$, with $\delta > 0$ there exist four regions B_{11}, B_{12}, B_2, B_3 corresponding to different slow-fast structures.
2. In B_{11}, B_{12}, B_2, B_3 there exists a different type of singular orbit γ_0 connecting $O = (0, 0)$ to $Q = (0, c)$, which perturbes to orbit γ_ε, $0 < \varepsilon \ll 1$.
3. Orbits γ_ε converge to γ_0 in Hausdorff distance as $(\varepsilon_1, \varepsilon_2) \to (0, 0)$ in B_{11}, B_{12}, B_2, B_3.

[B. and Szmolyan. *'A multi-parameter singular perturbation analysis of the Robertson model'*. 2024. arXiv:2407.04008]



Scaling regimes in parameter space

- Three regions B_1, B_2 and B_3 corresponding to

$$\varepsilon_2^2 \ll \varepsilon_1,\ \varepsilon_1 \approx \varepsilon_2^2,\ \varepsilon_1 \ll \varepsilon_2^2.$$

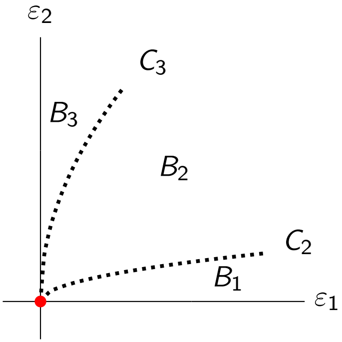
- Separated by the curves

$$C_2 := \{(\varepsilon_1, \varepsilon_2) \in \mathbb{R}^2 : \varepsilon_1 = \beta_2 \varepsilon_2^2\}$$

$$C_3 := \{(\varepsilon_1, \varepsilon_2) \in \mathbb{R}^2 : \varepsilon_1 = \beta_3 \varepsilon_2^2\}$$

with $0 < \beta_3 < \beta_2$.

- Describe neighbourhood of origin in blown-up parameter space.

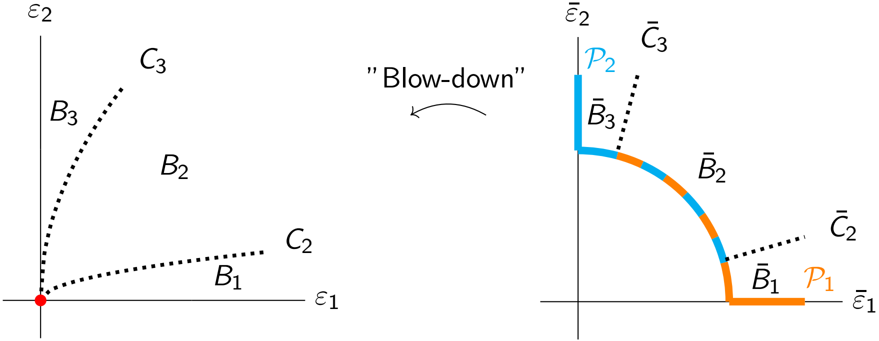


Blow-up of the origin in parameter space

- The blow-up transformation is given by:

$$\varepsilon_1 = r^2\bar{\varepsilon}_1 \qquad \varepsilon_2 = r\bar{\varepsilon}_2 \qquad \text{with } r \in [0,\infty) \text{ and } (\bar{\varepsilon}_1, \bar{\varepsilon}_2) \in \mathbb{S}^1.$$

- Analysis in directional charts $\mathcal{P}_1$ and $\mathcal{P}_2$ corresponding to $\bar{\varepsilon}_1 = 1$ and $\bar{\varepsilon}_2 = 1$.

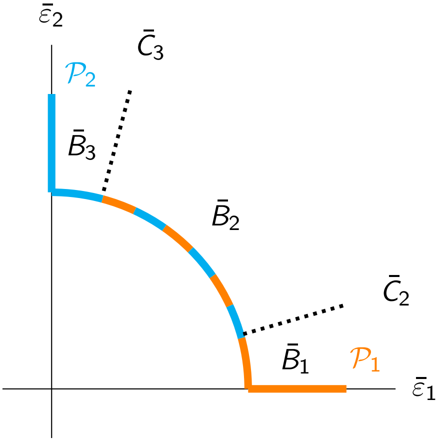


Analysis in region B_2 (easiest case)

Robertson model 2D

$$y' = \varepsilon_1(c - y - z) - y^2 - \varepsilon_2 yz$$
$$z' = y^2$$

- $\varepsilon_1 = r^2$, $\varepsilon_2 = r\tilde{\varepsilon}_2$



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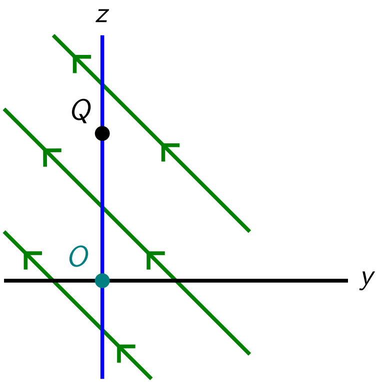
- Rescaling $y = r\tilde{y}$



Parameter blow-up and rescaling of y

Chart $\mathcal{P}_1$, Region B_2 $\left(\tilde{\varepsilon}_2^2 \geq \frac{1}{\beta_2}\right)$

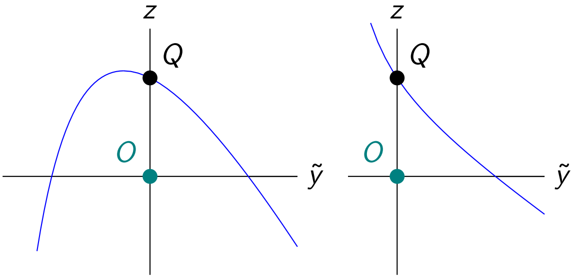
$$\tilde{y}' = c - r\tilde{y} - z - \tilde{y}^2 - \tilde{\varepsilon}_2 \tilde{y} z$$
$$z' = r\tilde{y}^2$$

Layer problem

$$\tilde{y}' = c - z - \tilde{y}^2 - \tilde{\varepsilon}_2 \tilde{y} z$$
$$z' = 0$$

- Critical manifold:

$$\mathcal{S} = \left\{ (\tilde{y}, z)^T \in \mathbb{R}^2 : z = \frac{c - \tilde{y}^2}{1 + \tilde{\varepsilon}_2 \tilde{y}} \right\}$$



(a) $\frac{1}{\tilde{\varepsilon}_2^2} > c$. (b) $\frac{1}{\tilde{\varepsilon}_2^2} < c$.

Singular orbit γ_0

Chart $\mathcal{P}_1$, Region B_2 ($\tilde{\varepsilon}_2^2 \geq \frac{1}{\beta_2}$)

$$\tilde{y}' = c - r\tilde{y} - z - \tilde{y}^2 - \tilde{\varepsilon}_2\tilde{y}z$$
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Layer problem

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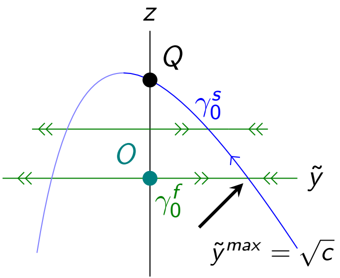
$$\mathcal{S} = \left\{(\tilde{y}, z)^T \in \mathbb{R}^2 : z = \frac{c-\tilde{y}^2}{1+\tilde{\varepsilon}_2\tilde{y}}\right\}$$

- Right branch of $\mathcal{S}$ is normally attracting.
- Singular orbit $\gamma_0 := \gamma_0^f \cup \gamma_0^s$.



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$$z' = r\tilde{y}^2$$

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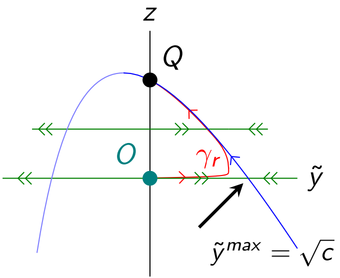
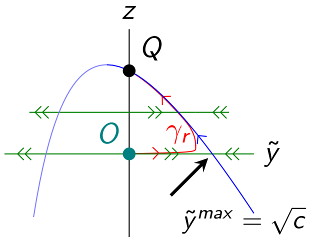
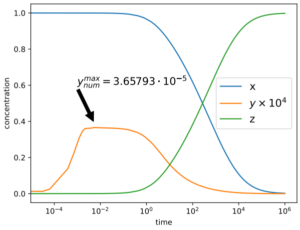
- Right branch of $\mathcal{S}$ is normally attracting.
- Singular orbit $\gamma_0 := \gamma_0^f \cup \gamma_0^s$.
- Fenichel: $\exists\, r_0 > 0\, \forall\, r \in (0, r_0]$ $\exists$ orbit γ_r, $\mathcal{O}(r)$-close to γ_0.



Asymptotic analysis fits well with the numerics

- Focus on the maximum of y along γ_r.
- Undoing all the rescalings:
  $y^{max} = \sqrt{\varepsilon_1}(\sqrt{c} + \mathcal{O}(\sqrt{\varepsilon_1})) = \sqrt{\varepsilon_1 c} + \mathcal{O}(\varepsilon_1)$.
- Inserting parameter values of the Robertson model:
  $y^{max} = 3.651 \cdot 10^{-5} + \mathcal{O}(10^{-9})$.
- Compare with $y_{max}^{num} = 3.65793 \cdot 10^{-5}$.



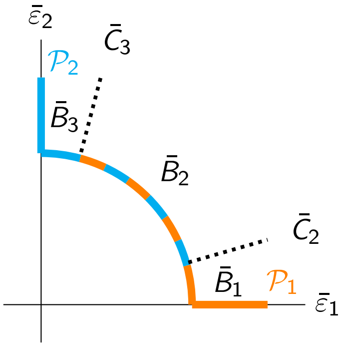


Analysis of region B_3

Robertson model 2D

$$y' = \varepsilon_1(c - y - z) - y^2 - \varepsilon_2 yz$$
$$z' = y^2$$

- Switch to chart $\mathcal{P}_2$:
  $\varepsilon_1 = r^2\tilde{\varepsilon}_1,\ \varepsilon_2 = r$

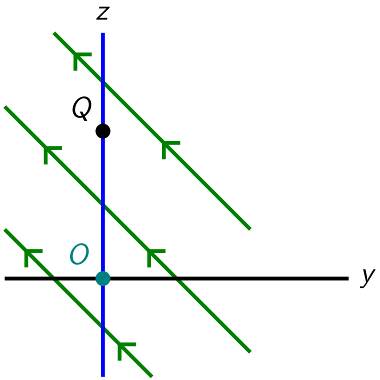


Analysis of region B_3

Robertson model 2D

$$y' = \varepsilon_1(c - y - z) - y^2 - \varepsilon_2 yz$$
$$z' = y^2$$

- Switch to chart $\mathcal{P}_2$:
  $\varepsilon_1 = r^2\tilde{\varepsilon}_1,\ \varepsilon_2 = r$
- Rescaling $y = r\tilde{y}$



For $\tilde{\varepsilon}_1 > \mu > 0$ identical to B_2

Chart $\mathcal{P}_2$, Region B_3 $(\tilde{\varepsilon}_1 \leq \beta_3)$

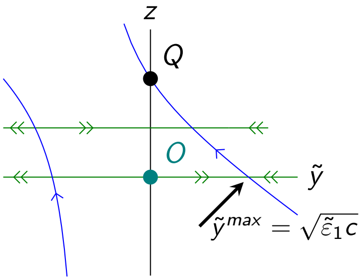
$$\tilde{y}' = \tilde{\varepsilon}_1(c - r\tilde{y} - z) - \tilde{y}^2 - \tilde{y}z$$
$$z' = r\tilde{y}^2$$

Layer problem

$$\tilde{y}' = \tilde{\varepsilon}_1(c - z) - \tilde{y}^2 - \tilde{y}z$$
$$z' = 0$$

Critical manifold:

$$\mathcal{S} = \left\{ (\tilde{y}, z)^T \in \mathbb{R}^2 : z = \frac{\tilde{\varepsilon}_1 c - \tilde{y}^2}{\tilde{\varepsilon}_1 + \tilde{y}} \right\}$$



(a) $\tilde{\varepsilon}_1 > 0$.

For $\tilde{\varepsilon}_1 > \mu > 0$ identical to B_2, then degenerates for $\tilde{\varepsilon}_1 = 0$

Chart $\mathcal{P}_2$, Region B_3 ($\tilde{\varepsilon}_1 \leq \beta_3$)

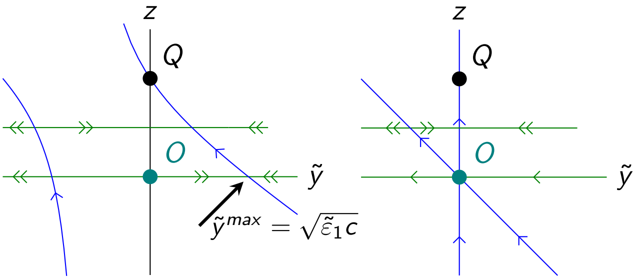
$$\tilde{y}' = \tilde{\varepsilon}_1(c - r\tilde{y} - z) - \tilde{y}^2 - \tilde{y}z$$
$$z' = r\tilde{y}^2$$

Layer problem

$$\tilde{y}' = \tilde{\varepsilon}_1(c - z) - \tilde{y}^2 - \tilde{y}z$$
$$z' = 0$$

Critical manifold:

$$\mathcal{S} = \left\{(\tilde{y}, z)^T \in \mathbb{R}^2 : z = \frac{\tilde{\varepsilon}_1 c - \tilde{y}^2}{\tilde{\varepsilon}_1 + \tilde{y}}\right\}$$



(a) $\tilde{\varepsilon}_1 > 0$. (b) $\tilde{\varepsilon}_1 = 0$.

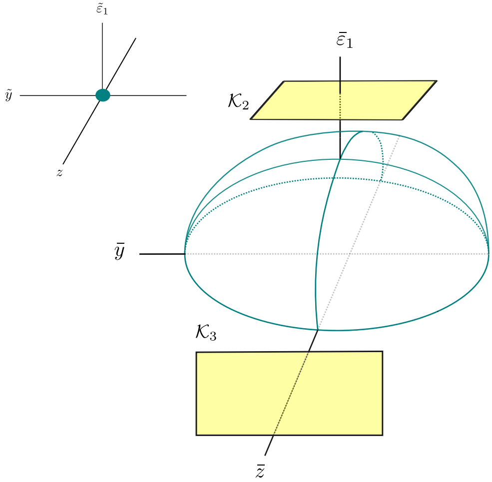
$\mathcal{S}$ not normally hyperbolic at the origin for $\tilde{\varepsilon}_1 = 0$.
$\Longrightarrow$ Blow-up the point $(\tilde{y}, z, \tilde{\varepsilon}_1) = (0, 0, 0)$ to a sphere.

Blow-up of the origin

- Blow-up transformation:

$$\begin{aligned}\tilde{y} &= \sigma \bar{y} \\ z &= \sigma \bar{z} \\ \tilde{\varepsilon}_1 &= \sigma^2 \bar{\varepsilon}_1\end{aligned}$$

  with $\sigma \in [0, \infty)$ and $(\bar{y}, \bar{z}, \bar{\varepsilon}_1) \in \mathbb{S}^2$.
- Pre-image of origin is a sphere.
- Think of weighted spherical coordinates.
- Analysis done in directional charts $\mathcal{K}_2$ and $\mathcal{K}_3$ corresponding to $\bar{\varepsilon}_1 = 1$ and $\bar{z} = 1$.



Blow-up analysis in two charts $\mathcal{K}_2$ and $\mathcal{K}_3$

$$\mathcal{K}_2 : \tilde{y} = \sigma_2 y_2, \quad z = \sigma_2 z_2, \quad \tilde{\varepsilon}_1 = \sigma_2^2$$

Dynamics in $\mathcal{K}_2$

$$\begin{aligned} y_2' &= c - \sigma_2 z_2 - y_2^2 - y_2 z_2 - r\sigma_2 y_2 \\ z_2' &= r y_2^2 \\ \sigma_2' &= 0. \end{aligned}$$

- Standard slow-fast with parameter r.
- Attracting 2D critical manifold $\mathcal{S}_2^a : \ y_2 = y_2(z_2, \sigma_2)$.

$$\mathcal{K}_3 : \tilde{y} = \sigma_3 y_3, \quad z = \sigma_3, \quad \tilde{\varepsilon}_1 = \sigma_3^2 \varepsilon_{13}$$

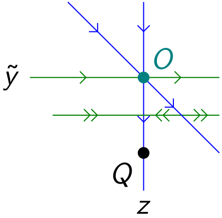
Dynamics in $\mathcal{K}_3$

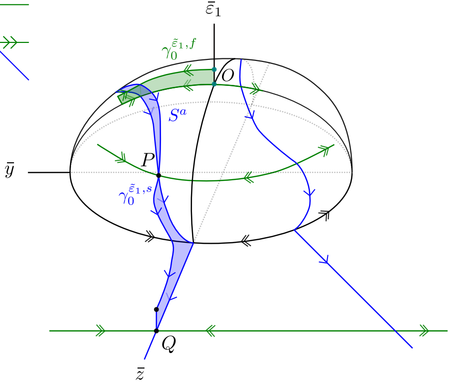
$$\begin{aligned} y_3' &= \varepsilon_{13}(c - r\sigma_3 y_3 - \sigma_3) - y_3^2 - y_3 - r y_3^3 \\ \sigma_3' &= r\sigma_3 y_3^2 \\ \varepsilon_{13}' &= -2r\varepsilon_{13} y_3^2. \end{aligned}$$

- Standard slow-fast with parameter r.
- Attracting 2D critical manifold $\mathcal{S}_3^a : \ y_3 = y_3(\sigma_3, \varepsilon_{13})$.

Details of dynamics in blown-up space

- For $\tilde{\varepsilon}_1 \in (0, \beta_3]$, identify singular orbit $\gamma_0^{\tilde{\varepsilon}_1} = \gamma_0^{\tilde{\varepsilon}_1, f} \cup \gamma_0^{\tilde{\varepsilon}_1, s}$, connecting initial value $O = (0, 0, \tilde{\varepsilon}_1)^T$ with true equilibrium $Q = (0, c, \tilde{\varepsilon}_1)^T$.

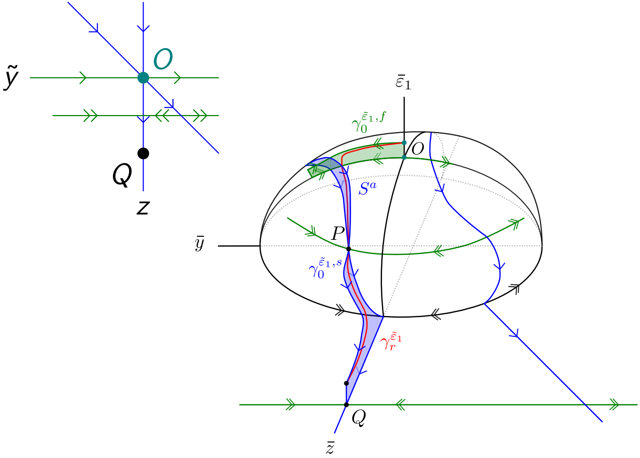




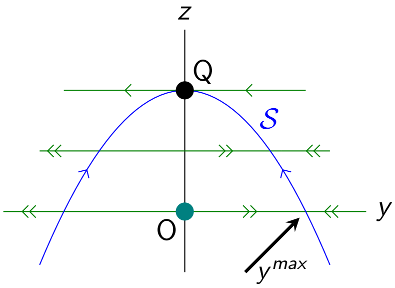
Details of dynamics in blown-up space

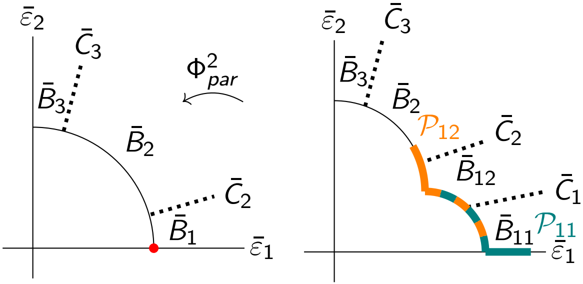
- For $\tilde{\varepsilon}_1 \in (0, \beta_3]$, identify singular orbit $\gamma_0^{\tilde{\varepsilon}_1} = \gamma_0^{\tilde{\varepsilon}_1,f} \cup \gamma_0^{\tilde{\varepsilon}_1,s}$, connecting initial value $O = (0, 0, \tilde{\varepsilon}_1)^T$ with true equilibrium $Q = (0, c, \tilde{\varepsilon}_1)^T$.

- $\mathcal{S}^a$ is normally attracting $\implies \exists$ perturbed orbit $\gamma_r^{\tilde{\varepsilon}_1}$ for $r > 0$ small enough.



Analysis in region B_1 needs additional parameter blow-up



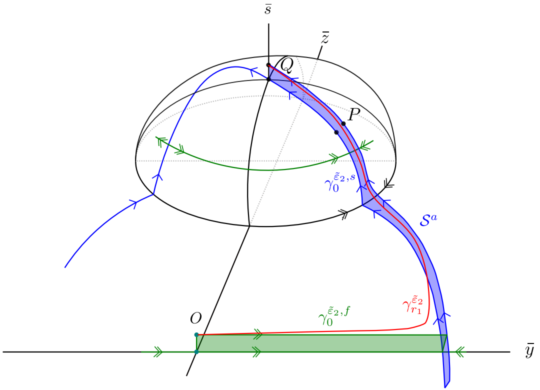


- Equilibrium Q coincides with the fold of $\mathcal{S}$ for $\tilde{\varepsilon}_2 = 0$ $\implies$ Q not normally hyperbolic.

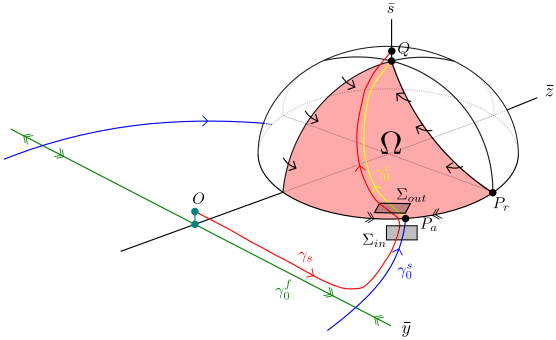
- Separate region $\bar{B}_1$ into two regions $\bar{B}_{11}$ and $\bar{B}_{12}$.
- Perform blow-up of fold point Q.

Identify singular orbits and apply GSPT

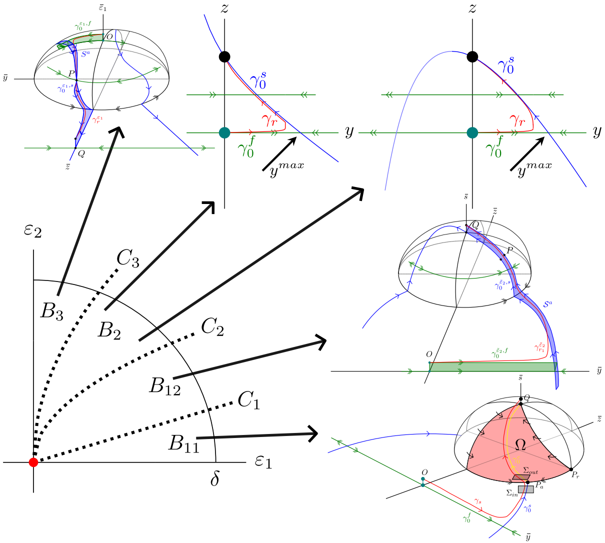
Region B_{12}



Region B_{11}



This analysis covers a neighbourhood of the origin



Summary and Outlook

- Asymptotic analysis of the Robertson model with $0 < k_1, k_3 \ll k_2$.
- A combination of blow-ups in parameter- and variable space makes GSPT applicable also in multi-parameter singular perturbations.
- Good qualitative and quantitative agreement with the numerics.
- Study more complicated problems towards a general framework for multi-parameter singular perturbations.
- Ongoing work on a cell cycle model and a gene regulatory network.

Comparing numerics with analytical results

Region	y_{num}^{max}	y^{max}
B_{11}	$2.16 \cdot 10^{-2}$	$2.2 \cdot 10^{-2} + \mathcal{O}(10^{-4})$
B_{12}	$6.98 \cdot 10^{-3}$	$7.0 \cdot 10^{-3} + \mathcal{O}(10^{-5})$
B_2 (lower)	$7.05 \cdot 10^{-4}$	$7.07 \cdot 10^{-4} + \mathcal{O}(10^{-7})$
B_2 (upper)	$7.07 \cdot 10^{-5}$	$7.071 \cdot 10^{-5} + \mathcal{O}(10^{-9})$
B_3	$2.26 \cdot 10^{-6}$	$2.236 \cdot 10^{-6} + \mathcal{O}(10^{-10})$