A multi-parameter singular perturbation analysis of the Robertson model

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TECHNISCHE UNIVERSITÄT WIEN

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The Robertson model

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 [Robertson, 1966]

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

- 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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- Convergence to unique equilibrium $(0, 0, 1)^T$ by standard dynamical systems arguments.

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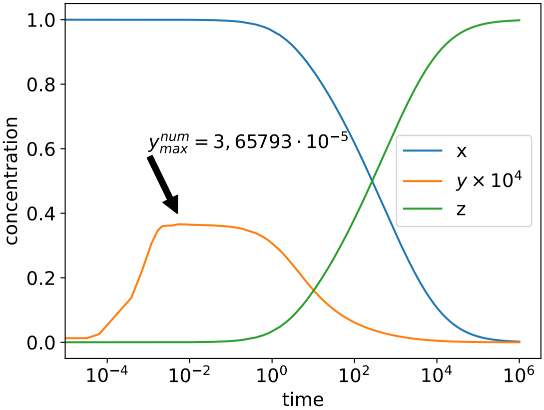
Why are we studying this model?

Numerical simulation shows multi-scale behaviour

- Dynamics on widely different time scales observed for $k_1, k_3 \ll k_2$.
- Note the logarithmic time scale!
- Essentially 3 phases of the reaction: Fast - intermediate - slow.
- Similar phenomena observed in many chemical and biological models.



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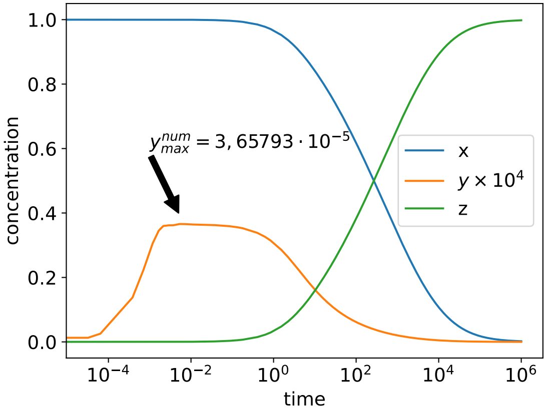
- Essentially 3 phases of the reaction: Fast - intermediate - slow.
- Similar phenomena observed in many chemical and biological models.
- **Today:** Asymptotic analysis based on geometric singular perturbation theory (GSPT).



Overview

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

A two-parameter singular perturbation problem

- Initial value $(x_0, y_0, z_0) = (c, 0, 0)$ with $c > 0$.
- Use constant of motion $x(t) = c - y(t) - z(t)$ for all $t \geq 0$.

- New initial value $(y, z) = (0, 0)$ and equilibrium $(y, z) = (0, c)$
- 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

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

Minimalistic overview of GSPT

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

Standard form

$$\dot{x} = f(x, y, \varepsilon)$$
$$\dot{y} = \varepsilon g(x, y, \varepsilon).$$

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

Non-standard form

$$\dot{z} = H(z, \varepsilon)$$

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- S normally hyperbolic $\implies \exists$ invariant slow manifold S_ε 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?

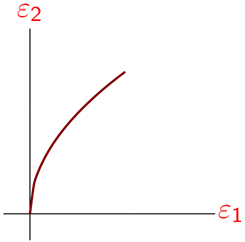
Singular perturbations for several small parameters

$$\dot{z} = H(z, \varepsilon_1, \ldots, \varepsilon_p),\ 0 < \varepsilon_i \ll 1,\ i = 1, \ldots, p.$$

- Common approach: Reduce to one-parameter case

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

  - Good numerical approximation of parameters needed, e.g., [Jelbart et al., 2022]
  - Valid only on a curve of the parameter space.
  - Inherent arbitrariness.



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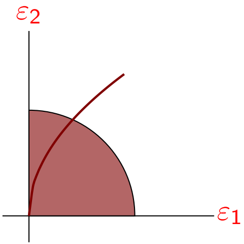


- Goal: Cover a neighbourhood of $(\varepsilon_1, \ldots, \varepsilon_p) = (0, \ldots, 0)$
  - Case studies are available, e.g., [De Maesschalck and Dumortier, 2011] and [Carter et al., 2023].
  - Recent review on singular double limits of differential equations [Kuehn et al., 2022].

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

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

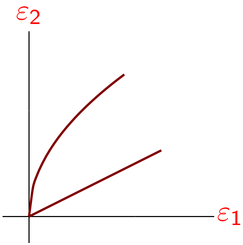
1) Nested sequence of time scales [Cardin and Teixeira, 2017] and [Krupa et al., 2008]:

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

- 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 $S(\varepsilon_2)$.
   - $S(\varepsilon_2)$ 'singular' as $\varepsilon_2 \to 0$.

3) ε_1 and ε_2 are classical singular perturbation parameters:
   - Different slow-fast structures in different regions of parameter space.



Robertson as a two-parameter singular perturbation problem

Robertson model 2D

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

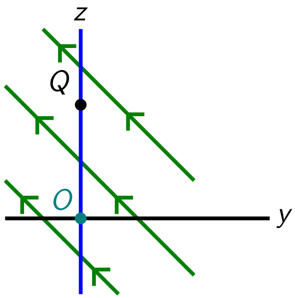
Limit problem ($\varepsilon_1 = \varepsilon_2 = 0$)

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

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

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

- Very degenerate (double zero eigenvalue) line of equilibria $y = 0$.
- Contains the **initial value** $O = (0, 0)$ and the **equilibrium** $Q = (0, c)$.

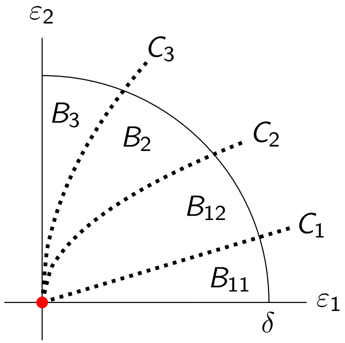


Main Result

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. For each B_{11}, B_{12}, B_2, B_3 there exists a different type of singular orbit γ_0 connecting $O = (0, 0)$ to $Q = (0, c)$.
3. Solutions 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'*. ArXiv preprint (June 2024)]



Scaling regimes in parameter space

- Three regions B_1, B_2 and B_3 corresponding to

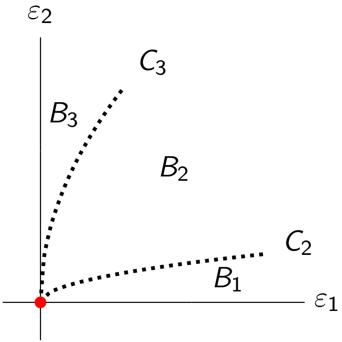
$$\varepsilon_2^2 \ll \varepsilon_1,\ \varepsilon_1 \approx \varepsilon_2^2,\ \varepsilon_1 \ll \varepsilon_2^2.$$

- 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.



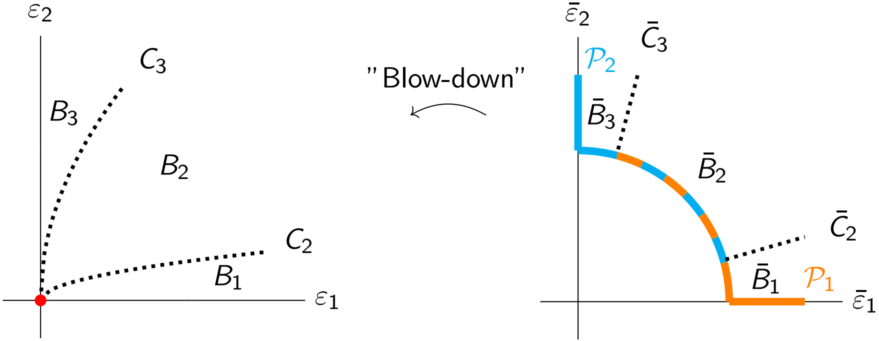
Blow-up of the origin in parameter space

- The blow-up transformation is given by:

$$\varepsilon_1 = r^2\bar{\varepsilon}_1 \qquad \varepsilon_2 = r\bar{\varepsilon}_2$$

with $r \in [0,\infty)$ and $(\bar{\varepsilon}_1, \bar{\varepsilon}_2) \in S^1$.

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

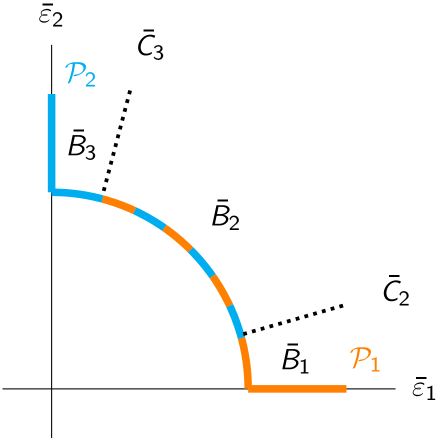


Analysis in region B_2

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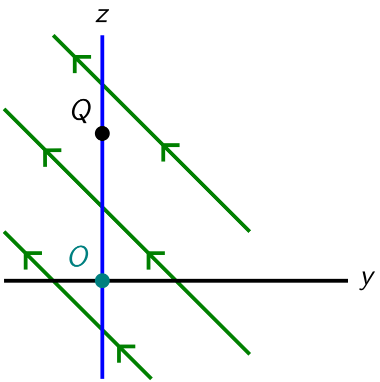
- Rescaling $y = r\tilde{y}$



Parameter blow-up and rescaling of y

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

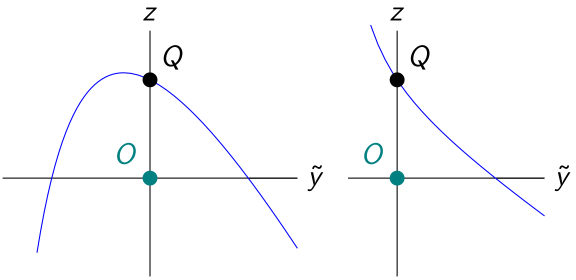
$$\tilde{y}' = c - r\tilde{y} - z - \tilde{y}^2 - \tilde{\varepsilon}_2 \tilde{y} z$$
$$z' = r\tilde{y}^2$$

Layer problem ($r=0$)

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

- 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

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

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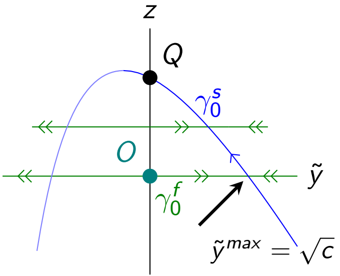
- $\mathcal{S}$ is normally attracting if $\tilde{y} > -\frac{1}{\tilde{\varepsilon}_2} + \sqrt{\frac{1}{\tilde{\varepsilon}_2^2} - c}$.
- Singular orbit $\gamma_0 := \gamma_0^f \cup \gamma_0^s$.



Singular orbit

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

$$\tilde{y}' = c - r\tilde{y} - z - \tilde{y}^2 - \tilde{\varepsilon}_2 \tilde{y} z$$
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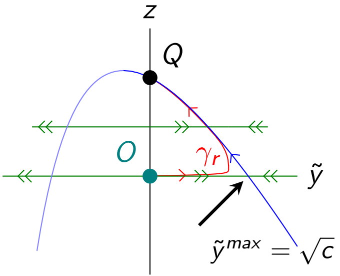
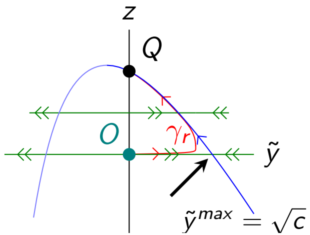
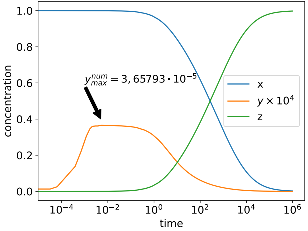
- $\mathcal{S}$ is normally attracting if $\tilde{y} > -\frac{1}{\tilde{\varepsilon}_2} + \sqrt{\frac{1}{\tilde{\varepsilon}_2^2} - c}$.
- Singular orbit $\gamma_0 := \gamma_0^f \cup \gamma_0^s$.
- Fenichel: $\exists\, r_0 > 0\, \forall\, r \in (0, r_0]$ $\exists$ orbit γ_r, $\mathcal{O}(r)$-close to 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 $y^{num}_{max} = 3,65793 \cdot 10^{-5}$.



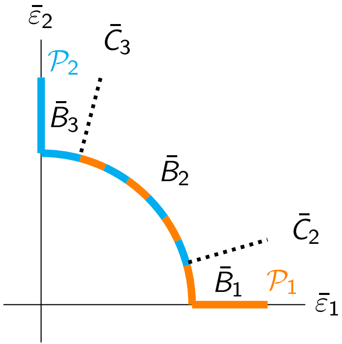


Analysis of region B_3

Robertson model 2D

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

- $\varepsilon_1 = r^2\tilde{\varepsilon}_1,\ \varepsilon_2 = r$



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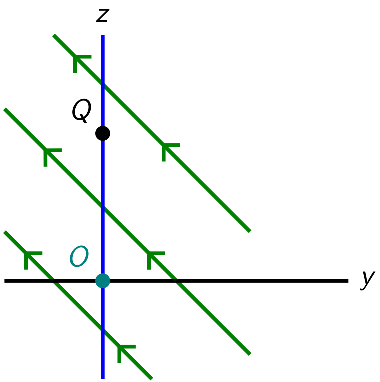


Problem degenerates for $\tilde{\varepsilon}_1 = 0$

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

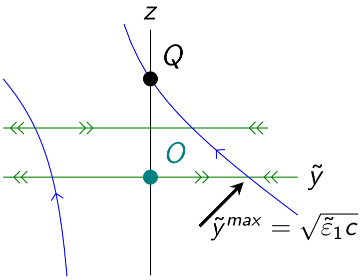
$$\tilde{y}' = \tilde{\varepsilon}_1(c - r\tilde{y} - z) - \tilde{y}^2 - \tilde{y}z$$
$$z' = r\tilde{y}^2$$

Layer problem (r=0)

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

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

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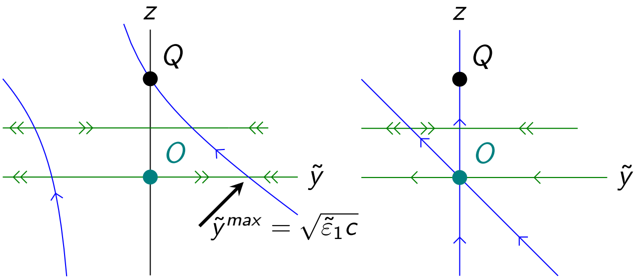


(a) $\tilde{\varepsilon}_1 > 0$. (b) $\tilde{\varepsilon}_1 = 0$.

$\mathcal{S}$ not normally hyperbolic at the origin for $\tilde{\varepsilon}_1 = 0$.

$\implies$ Blow-up the point $(\tilde{y}, z, \tilde{\varepsilon}_1) = (0, 0, 0)$ to a sphere.

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

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

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
  $S_2^a : \ y_2 = y_2(z_2, \sigma_2)$.

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

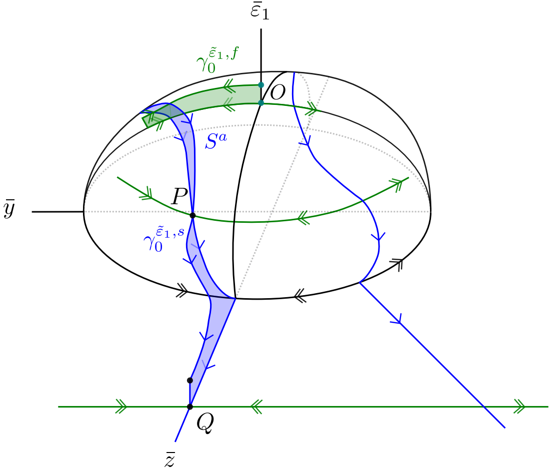
Dynamics in $\mathcal{K}_3$

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

- Standard slow-fast with parameter r.
- Attracting 2D critical manifold
  $S_3^a : \ y_3 = y_3(\sigma_3, \varepsilon_{13})$.

$\exists$ a family of singular orbits $\gamma_0^{\tilde{\varepsilon}_1}$

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



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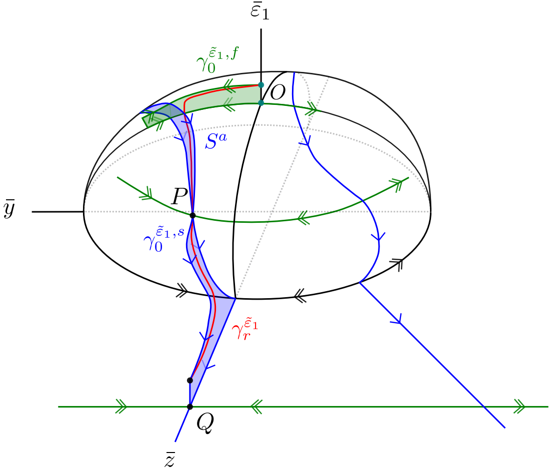
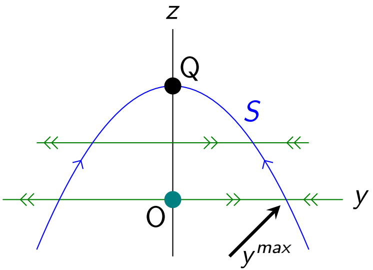
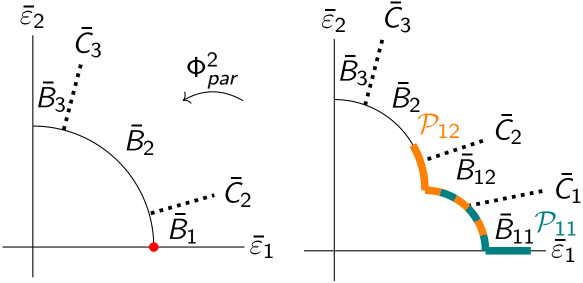
- S^a is normally attracting $\implies$ $\exists$ perturbed orbit $\gamma_r^{\tilde{\varepsilon}_1}$ for $r > 0$ small enough.



Analysis in region B_1



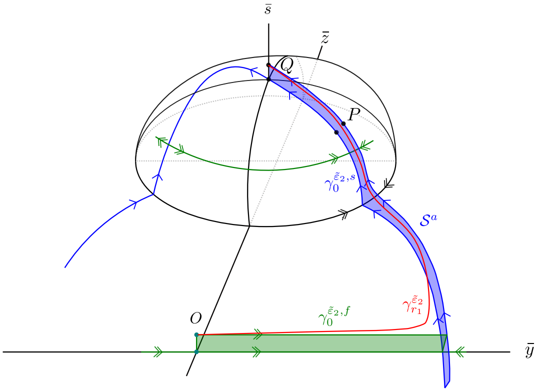
- Equilibrium Q is a fold point for $\tilde{\varepsilon}_2 = 0$.



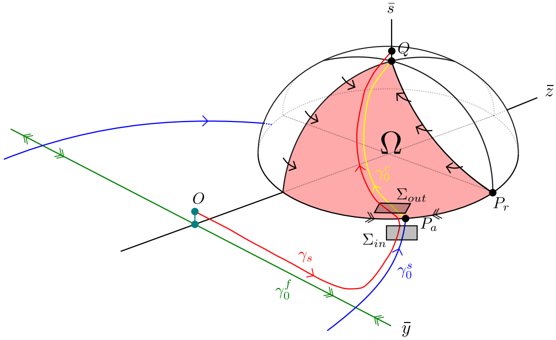
- Second parameter blow-up needed.
- Separate region $\bar{B}_1$ into two regions $\bar{B}_{11}$ and $\bar{B}_{12}$.
- Perform blow-up of fold point.

Identify singular orbits and apply GSPT

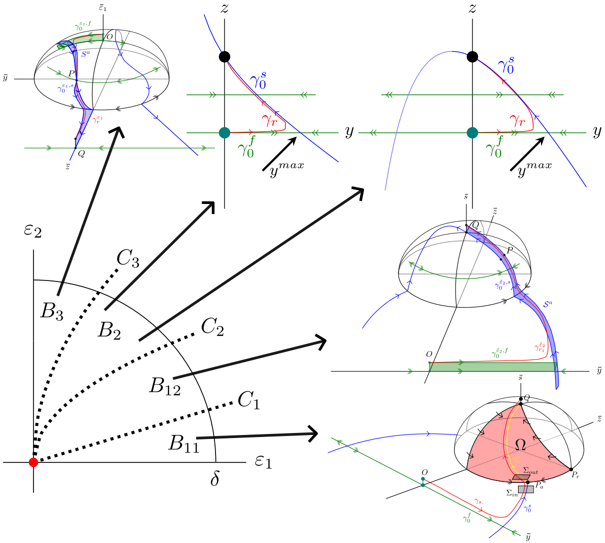
Region B_{12}



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.