Analysis of the Constrained Runs Algorithm(s)

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Outline

- setting of the problem
- the zero-derivative principle
- the constrained runs scheme
- summary
Outline

setting of the problem

the zero-derivative principle

the constrained runs scheme

summary
Micro-to-Macroscale Reduction

Available

\[ \begin{array}{c}
\text{microscopic} \\
\text{mesoscopic}
\end{array} \begin{array}{c}
\text{analytic} \\
\text{computer}
\end{array} \] model

Desired

All kinds of macroscopic information
Micro-to-Macroscopic Reduction

Available

\[ A \left\{ \begin{array}{c} \text{microscopic} \\ \text{mesoscopic} \end{array} \right\} \left\{ \begin{array}{c} \text{analytic} \\ \text{computer} \end{array} \right\} \text{model} \]

Desired

All kinds of \textit{macroscopic} information

Issues

- Full-scale simulations \textit{prohibitive}
- Macroscopic model \textit{unavailable}
Micro-to-Macroscale Reduction

Available

\[
\begin{align*}
\text{A} & \left\{ \begin{array}{c}
\text{microscopic} \\
\text{mesoscopic} \\
\text{analytic} \\
\text{computer}
\end{array} \right\} \text{ model}
\end{align*}
\]

Desired

All kinds of \textit{macroscopic} information

Issues

- Full-scale simulations \textit{prohibitive}
- Macroscopic model \textit{unavailable}

Resolution

- \textbf{Projective integration} schemes
- \textbf{Micro-simulations} + \textbf{Time extrapolation} \Rightarrow \textbf{Macro-info}
Micro-to-Macro Dynamics

Microscopic simulations

Micro-to-Macro Dynamics

Microscopic simulations $\Rightarrow$ Macroscopic information

```
restrict

{\text{macroscopic solution}}

{t + dt} \quad {t + 2dt} \quad t

e\text{extrapolate}

{\text{macroscopic solution}}

t

lift

t + T
```
Micro-to-Macro Dynamics

**Microscopic simulations** $\Rightarrow$ **Macroscopic information**

The lifting step is a **one-to-many** map.
Reduction of Multiscale Dynamics

\[
\begin{align*}
\mathbf{w}_1 &= \mathbf{w}_1(t) \quad \text{macroscopic variables (lower moments)} \\
\mathbf{w}_2 &= \mathbf{w}_2(t) \quad \text{slaved variables (higher moments)}
\end{align*}
\]

\[
\mathbf{w}_2 = H(\mathbf{w}_1)
\]

slaved dynamics

\[
\begin{align*}
\mathbf{w}_2 &= H(\mathbf{w}_1)
\end{align*}
\]

reduction

\[
\begin{align*}
\mathbf{w}'_1 &= g_1(\mathbf{w}_1, H(\mathbf{w}_1))
\end{align*}
\]

reduced dynamics
Lifting Scheme
Lifting Scheme

2-step Iterative Lifting

- Integrate until relaxation surface is reached
- Reset $w_1 = w_1^*$
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The Zero-derivative Principle

\[ w_1' = g_1(w) \quad \text{where } w_1 \begin{cases} \text{describe the macro-dynamics} \\ \text{parameterize the manifold} \end{cases} \]

- Fix \( w_1 = w_1^* \)
- Choose \( m \in \{0, 1, \ldots\} \)
- Approximate \( H(w_1^*) \) by \( w_2^* \) obtained via

\[
\left. \frac{d^{m+1}w_2}{dt^{m+1}} \right|_{(w_1^*, w_2^*)} = 0
\]

zero-derivative principle
The Zero-derivative Principle

\[ \begin{align*}
w'_1 &= g_1(w) \\
w'_2 &= g_2(w)
\end{align*} \]

where \( w_1 \) describes the macro-dynamics and \( w_2 \) parameterizes the manifold.

- Fix \( w_1 = w_1^* \)
- Choose \( m \in \{0, 1, \ldots\} \)
- Approximate \( H(w_1^*) \) by \( w_2^* \) obtained via

\[
\left. \frac{d^{m+1} w_2}{dt^{m+1}} \right|_{(w_1^*, w_2^*)} = 0
\]

zero-derivative principle

How close is \( w_2^* \) to \( H(w_1^*) \)? proximity
Singular Perturbation Setting

Original System

\[
\begin{align*}
    w'_1 &= g_1(w) \\
    w'_2 &= g_2(w)
\end{align*}
\]
Singular Perturbation Setting

Original System

\[
\begin{align*}
    w_1' &= g_1(w) \\
    w_2' &= g_2(w)
\end{align*}
\]

\[
\begin{align*}
    w_2 &= H(w_1) \quad \text{w}_{\rightarrow} \text{x} \quad \text{w}_{\leftarrow} \text{x}
\end{align*}
\]

Slow-Fast System

\[
\begin{align*}
    x_1' &= r_1(x, \varepsilon) \\
    \varepsilon x_2' &= r_2(x, \varepsilon)
\end{align*}
\]
Singular Perturbation Setting

Original System

\[
\begin{align*}
    w_1' &= g_1(w) \\
    w_2' &= g_2(w)
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\[
\begin{array}{c}
\text{w} \rightarrow \text{x} \\
\text{w} \leftarrow \text{x}
\end{array}
\]

Slow-Fast System

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\begin{align*}
    x_1' &= r_1(x, \varepsilon) \\
    \varepsilon x_2' &= r_2(x, \varepsilon)
\end{align*}
\]

\[
\text{Re } (\sigma (\partial r_2 / \partial x_2) \mid_S) \subset \mathbb{R}^-
\]

normal hyperbolicity
Proximity Results

**Theorem (GKKZ 2005).** Let \( m \in \{0, 1, \ldots\} \) and assume that

\[
\begin{align*}
\det (\partial w_2 / \partial x_2) &\neq 0 \\
\det (\partial g_2 / \partial w_2) &\neq 0
\end{align*}
\]

inclusion of fast directions
hyperbolicity in \( w_2 \)-direction

in a neighborhood of the manifold. Then, the condition

\[
\frac{d^{m+1} w_2}{dt^{m+1}} \bigg|_{(w_1^*, w_2)} = 0
\]

has an isolated solution \( w_2^* \) asymptotically close to \( H(w_1^*) \),

\[
w_2^* - H(w_1^*) = O(\varepsilon^{m+1}), \quad \varepsilon \downarrow 0.
\]
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Constrained Runs Algorithms

- **CHOOSE** \( m \in \{0, 1, \ldots\} \) order of the method
- **FIX** \( w_1 = w_1^* \) & **SEED** with \( w_2^{(0)} \) initial guess
- **ITERATE** using

\[
w_2^{(n+1)} = F_m \left( w_2^{(n)} \right) = w_2^{(n)} - ( -h )^{m+1} \left. \frac{d^{m+1} w_2}{d t^{m+1}} \right|_{(w_1^*, w_2^{(n)})}
\]

- **STOP** when converged to \( w_2 = w_2^{(#)} \) converged \( w_2 \)
- **SET** \( w_2^{(#)} \approx w_2^* \approx H(w_1^*) \) approximate slow manifold
Constrained Runs Algorithms

- **CHOOSE** \( m \in \{0, 1, \ldots\} \) order of the method
- **FIX** \( w_1 = w_1^* \) & **SEED** with \( w_2^{(0)} \) initial guess
- **ITERATE** using fixed point iteration
  \[
  w_2^{(n+1)} = F_m \left( w_2^{(n)} \right) = w_2^{(n)} - (\mathbf{-h})^{m+1} \frac{d^{m+1}w_2}{dt^{m+1}} \bigg|_{(w_1^*, w_2^{(n)})}
  \]
- **STOP** when converged to \( w_2 = w_2^{(#)} \) converged \( w_2 \)
- **SET** \( w_2^{(#)} \approx w_2^* \approx H(w_1^*) \) approximate slow manifold

**Does the iteration converge to** \( w_2^* \)? attractivity
The Jacobian $\frac{\partial F_m}{\partial w_2}$

Calculate, to leading order in $\varepsilon$,

$$\left. \frac{\partial F_m}{\partial w_2} \right|_{w^*} = I - C \left( I - e^{\frac{h}{\varepsilon} \frac{\partial r_2}{\partial x_2}} \right)^{m+1} C^{-1} P^{-1}$$
The Jacobian $\frac{\partial F_m}{\partial w_2}$

- Calculate, to leading order in $\epsilon$,

$$\left. \frac{\partial F_m}{\partial w_2} \right|_{w^*} = I - C \left( I - e^{\frac{\hbar}{\epsilon} \left. \frac{\partial r_2}{\partial x_2} \right|_{w^*}} \right)^{m+1} C^{-1} P^{-1}$$

- Here,

- $C = \left. \frac{\partial w_2}{\partial x_2} \right|_{w^*}$ non-degenerate

- $\text{Re} \left( \sigma \left( \left. \frac{\partial r_2}{\partial x_2} \right|_{w^*} \right) \right) \subset \mathbb{R}_-$ not self adjoint, not normal

- $P$ is the product of two non-commuting projections not positive semidefinite, not a projection
The Jacobian $\frac{\partial F_m}{\partial w_2}$

1. Calculate, to leading order in $\varepsilon$,

$$\frac{\partial F_m}{\partial w_2} \bigg|_{w^*} = I - C \left( I - e^{\frac{h}{\varepsilon} \frac{\partial r_2}{\partial x_2}} \bigg|_{w^*} \right)^{m+1} C^{-1} P^{-1}$$

2. Here,
   - $C = \frac{\partial w_2}{\partial x_2} \bigg|_{w^*}$
     - non-degenerate
   - $\text{Re} \left( \sigma \left( \frac{\partial r_2}{\partial x_2} \bigg|_{w^*} \right) \right) \subset \mathbb{R}_-$
     - not self adjoint, not normal
   - $P$ is the product of two non-commuting projections
     - not positive semidefinite, not a projection

$\sigma \left( \frac{\partial F_m}{\partial w_2} \right)$ is unavailable

\[\text{generalized eigenvalue problem}\]
Vertical Fibration ($\mathcal{P} = I$)

Write the normal spectrum of the vector field as

$$\sigma \left( \left. \frac{\partial r_2}{\partial x_2} \right|_{w^*} \right) = \{ \lambda_{\ell} = |\lambda_{\ell}| e^{i\theta_{\ell}} : 1 \leq \ell \leq N_2 \}$$
Write the normal spectrum of the vector field as

$$\sigma \left( \frac{\partial r_2}{\partial x_2} \bigg|_{w^*} \right) = \{ \lambda_\ell = |\lambda_\ell|e^{i\theta_\ell} : 1 \leq \ell \leq N_2 \}$$

Calculate, to leading order in $\varepsilon$,

$$\sigma \left( \frac{\partial F_m}{\partial w_2} \bigg|_{w^*} \right) = \left\{ \mu_\ell = 1 - \left( 1 - e^{h\lambda_\ell/\varepsilon} \right)^{m+1} : 1 \leq \ell \leq N_2 \right\}$$
Vertical Fibration \((\mathcal{P} = I)\)

- Write the **normal** spectrum of the vector field as

  \[
  \sigma \left( \left. \frac{\partial r_2}{\partial x_2} \right|_{w^*} \right) = \{ \lambda_\ell = |\lambda_\ell|e^{i\theta_\ell} : 1 \leq \ell \leq N_2 \}
  \]

- Calculate, to leading order in \(\varepsilon\),

  \[
  \sigma \left( \left. \frac{\partial F_m}{\partial w_2} \right|_{w^*} \right) = \left\{ \mu_\ell = 1 - \left( 1 - e^{h|\lambda_\ell|/\varepsilon} \right)^{m+1} : 1 \leq \ell \leq N_2 \right\}
  \]

- If **all** \(\lambda_\ell \in \mathbb{R}\), the fixed point is **unconditionally stable**, 

  \[
  \mu_\ell = 1 - \left( 1 - e^{-h|\lambda_\ell|/\varepsilon} \right)^{m+1} < 1, \quad \text{for all } h > 0
  \]

  **Is the fixed point also stable if** \(\lambda_\ell \in \mathbb{C} - \mathbb{R}\) **for some** \(\ell\)?
Complex Eigenvalues

\[ \mu \sim 1 - (-\lambda h/\varepsilon)^{m+1} \sim 1 - (|\lambda| h/\varepsilon)^{m+1} e^{i(m+1)(\theta - \pi)}, \quad h \downarrow 0 \]
Complex Eigenvalues

\[ \mu \sim 1 - (-\lambda h/\varepsilon)^{m+1} \sim 1 - (|\lambda| h/\varepsilon)^{m+1} e^{i(m+1)(\theta - \pi)}, \quad h \downarrow 0 \]
Complex Eigenvalues

\[ \mu \sim 1 - (-\lambda h/\varepsilon)^{m+1} \sim 1 - (|\lambda| h/\varepsilon)^{m+1} e^{i(m+1)(\theta-\pi)}, \quad h \downarrow 0 \]

Complex eigenvalues may cause divergence
$h$ versus $\theta$

Stability

Instability
Geometric Configuration
Geometric Configuration

\[ w_1 \]

\[ w_2 \]

\[ w_1^* \]
Geometric Configuration
Geometric Configuration
Geometric Configuration
Geometric Configuration
Geometric Configuration

The relative orientation of the slow manifold and the fast fibers affects algorithm convergence.
Outline

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Summary

- $(m + 1)\text{st derivative condition} \rightarrow \mathcal{O}(\varepsilon^m) \text{ approximation}$

- functional iteration solver

<table>
<thead>
<tr>
<th>vertical fibration</th>
<th>non-vertical fibration</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m = 0$</td>
<td>$m \geq 1$</td>
</tr>
<tr>
<td>$\mathbb{R} \rightarrow \text{stable}$</td>
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</tr>
<tr>
<td>$\mathbb{C} \rightarrow \text{stable}$</td>
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- stabilization possible
  - Krylov subspace methods
  - implicit functional iteration
  - more intelligent resetting $w_1 = w_1^*$