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

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Micro-to-Macroscale Reduction

Available A $\left\{ \dfrac{\text{microscopic}}{\text{mesoscopic}} \right\} \left\{ \dfrac{\text{analytic}}{\text{computer}} \right\}$ model

Desired All kinds of macroscopic information

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- Full-scale simulations prohibitive
- Macroscopic model unavailable

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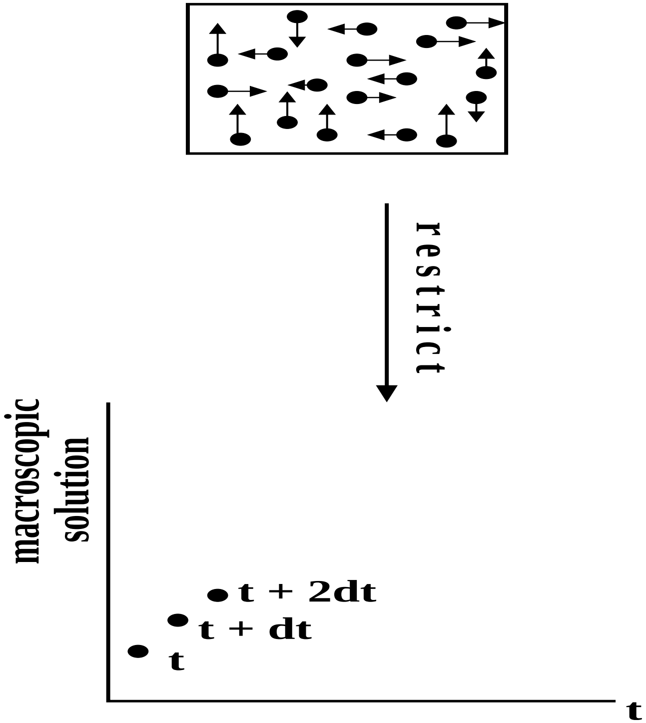
- Projective integration schemes

Resolution Micro-simulations + Time extrapolation $\Rightarrow$ Macro-info

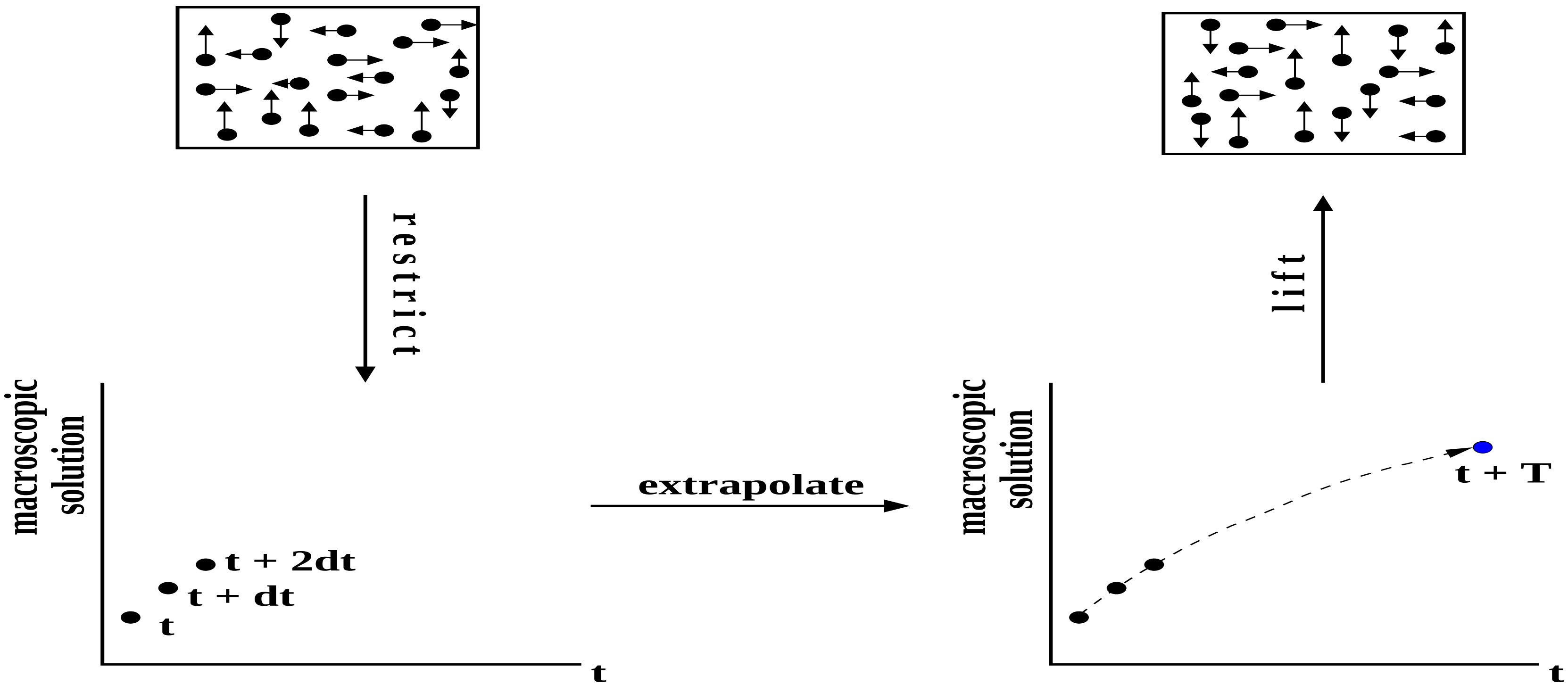
Micro-to-Macro Dynamics

Microscopic simulations



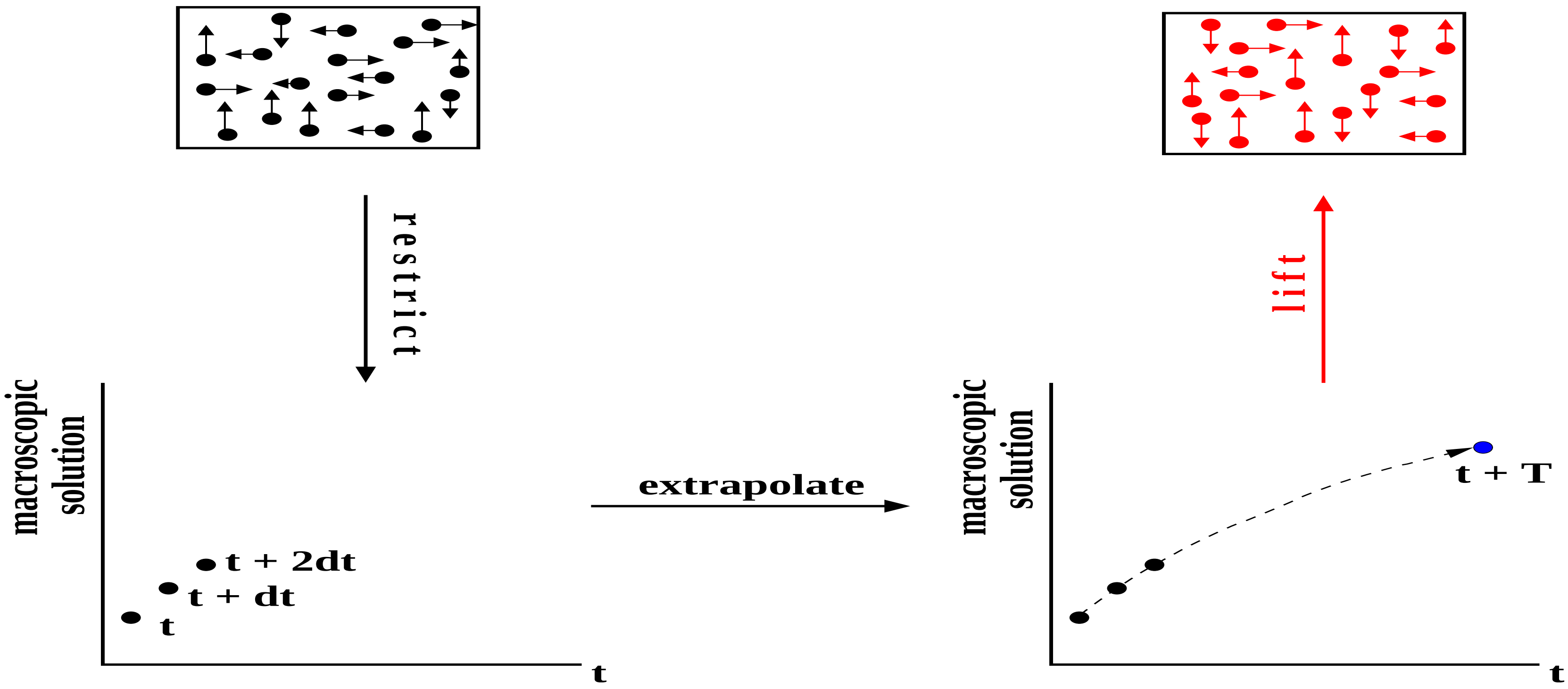
Micro-to-Macro Dynamics

Microscopic simulations $\Rightarrow$ Macroscopic information



Micro-to-Macro Dynamics

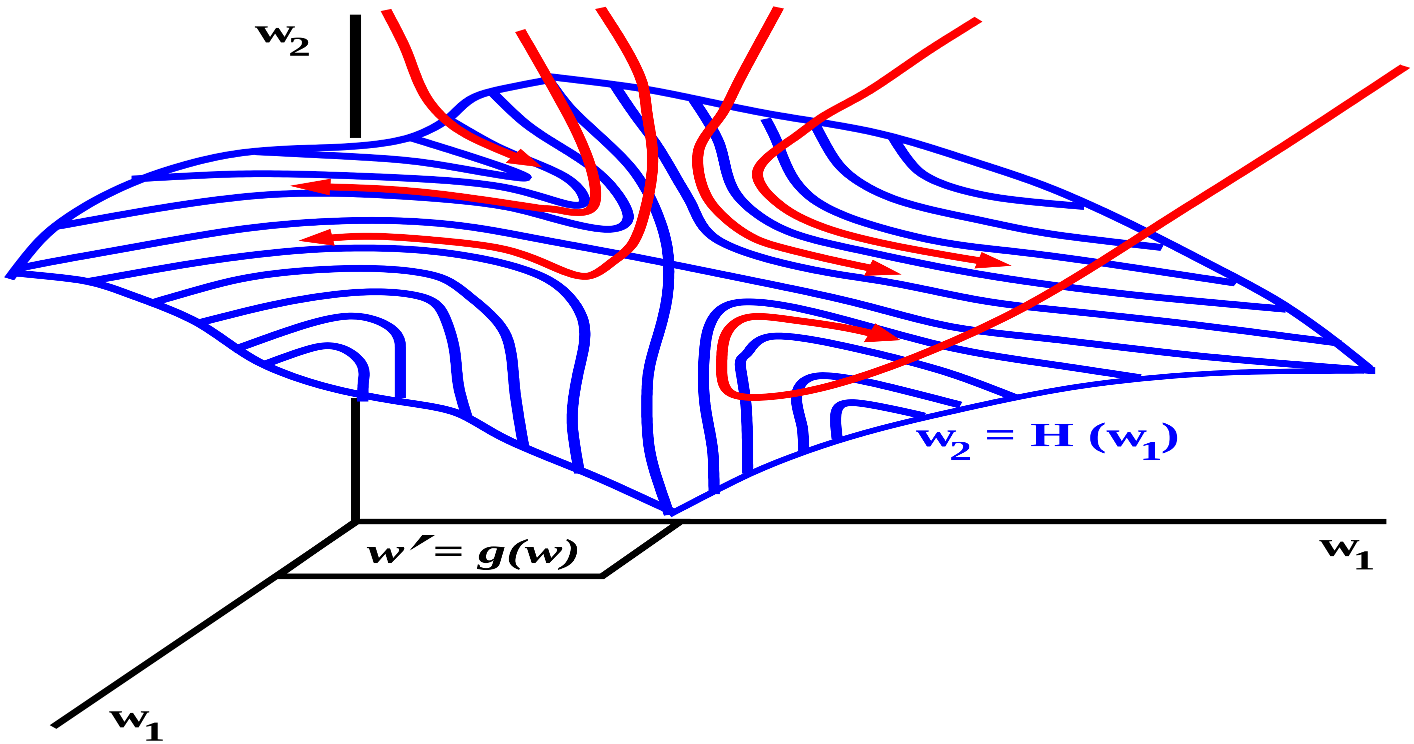
Microscopic simulations ⇒ Macroscopic information



The lifting step is a one-to-many map

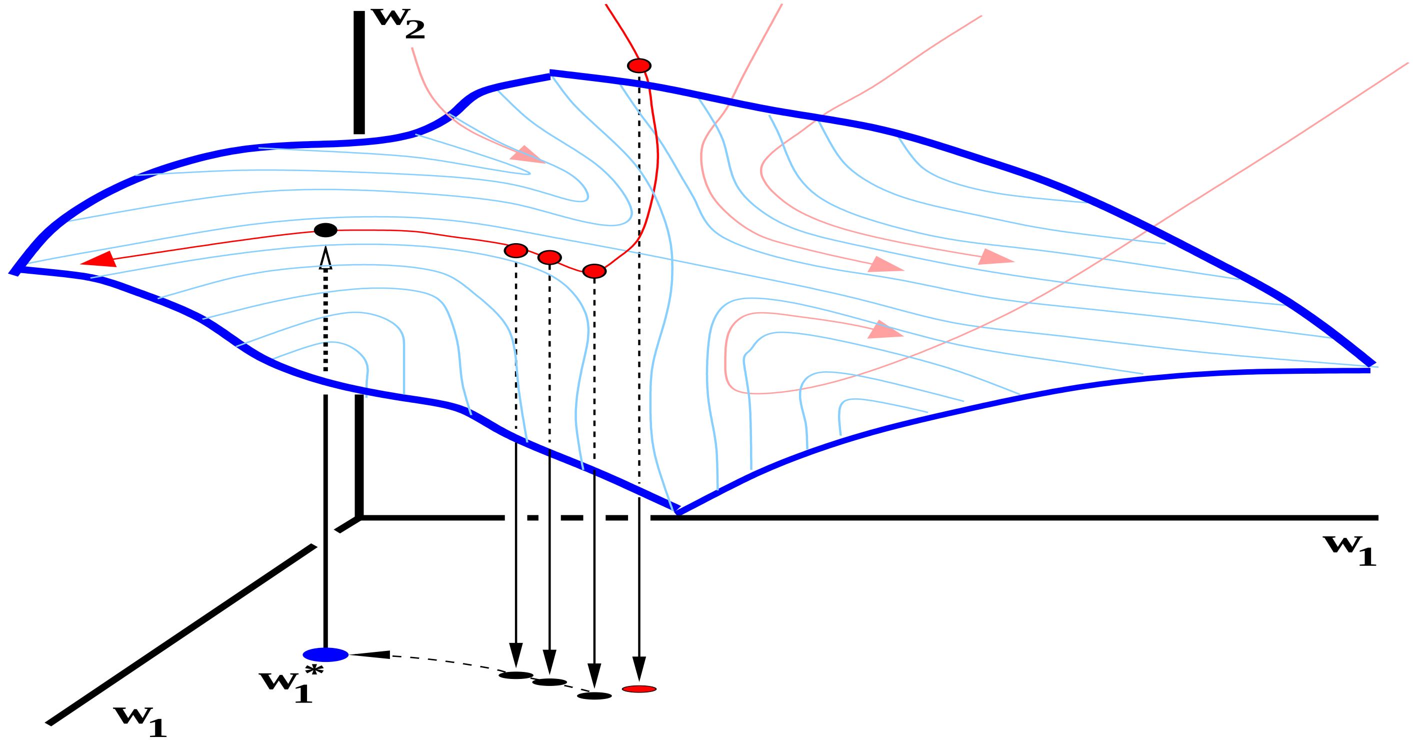
Reduction of Multiscale Dynamics

$w_1 = w_1(t)$	macroscopic variables (lower moments)
$w_2 = w_2(t)$	slaved variables (higher moments)

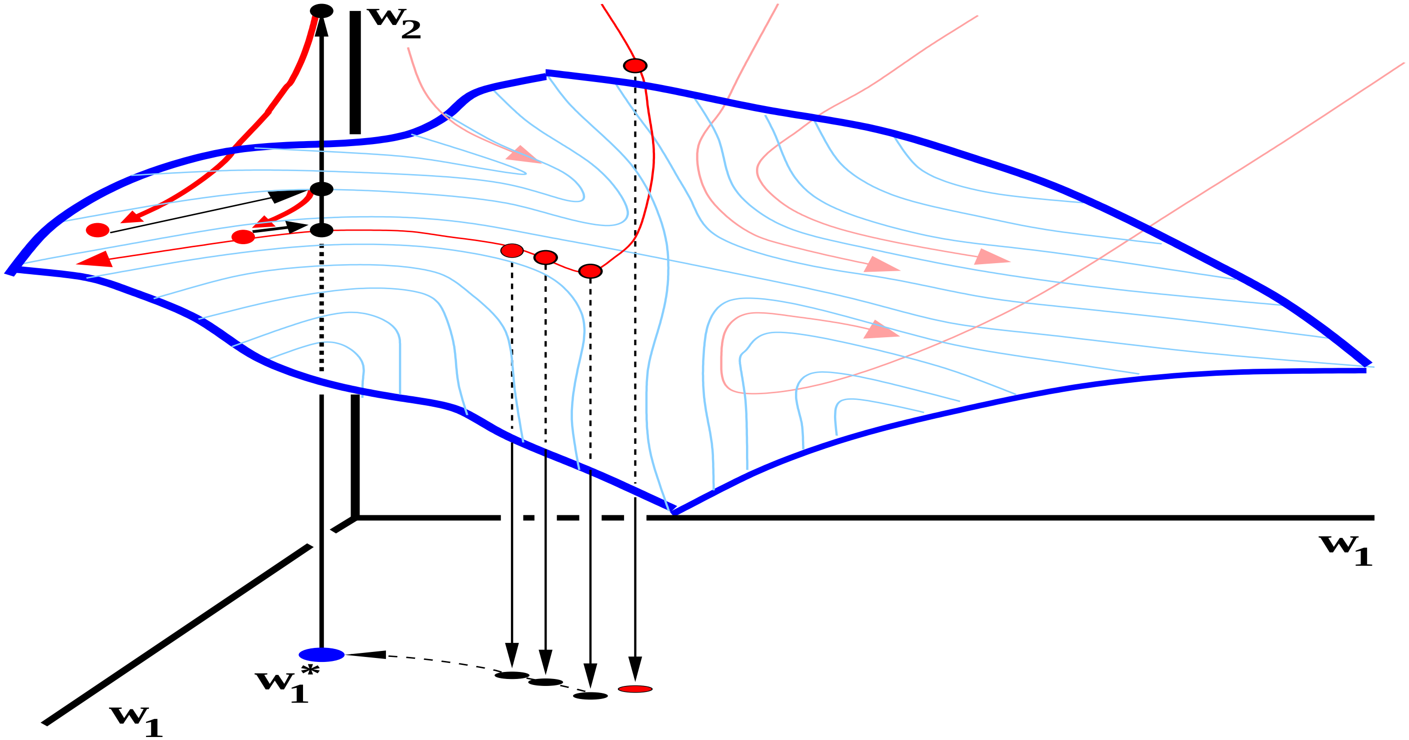


slaved dynamics		reduced dynamics
$w_2 = H(w_1)$	⟵ reduction ⟶	$w_1' = g_1(w_1, H(w_1))$

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

$$\begin{aligned} w_1' &= g_1(w) \\ w_2' &= g_2(w) \end{aligned}$$

where w_1 { describe the macro-dynamics / parameterize 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

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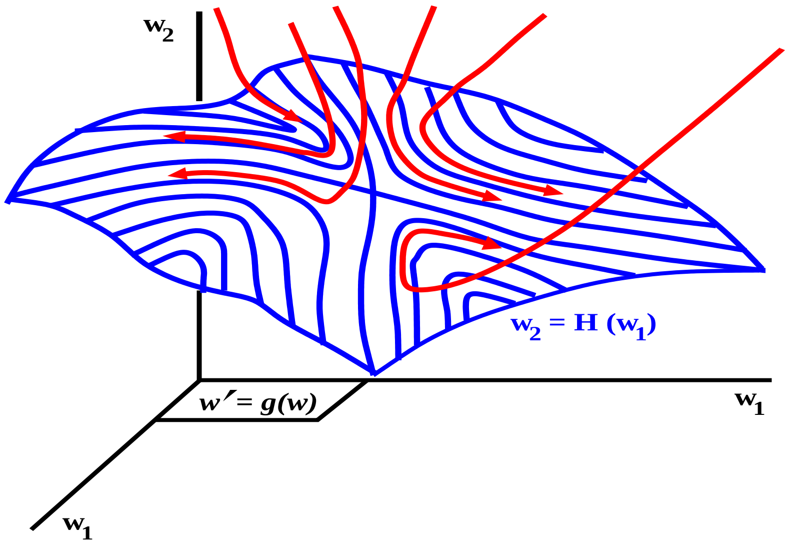
zero-derivative principle

How close is w_2^* to $H(w_1^*)$? proximity

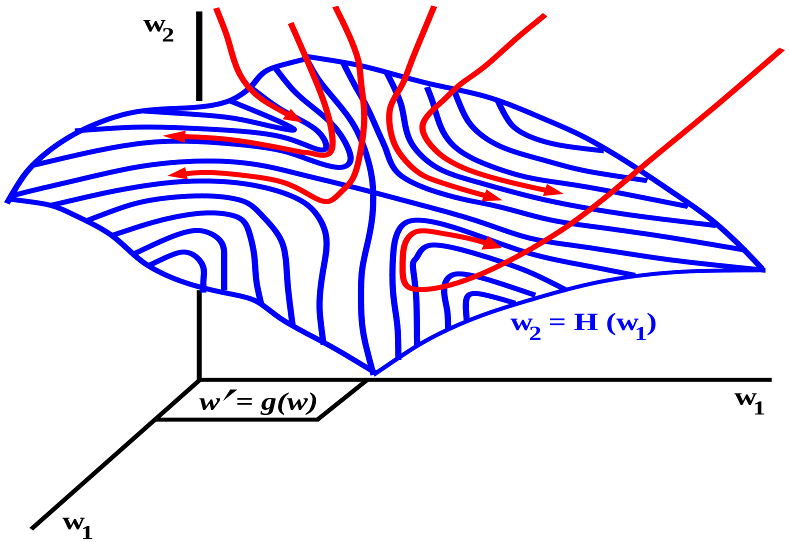
Singular Perturbation Setting

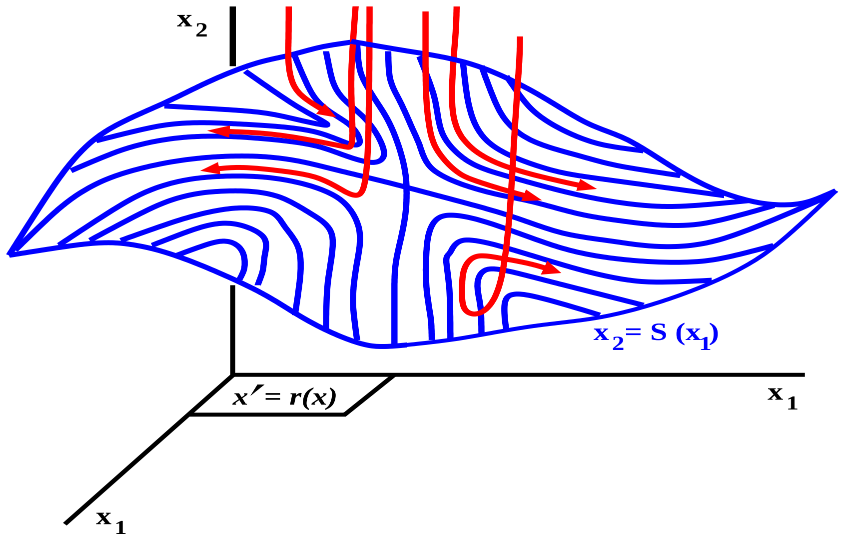
Original System	
$w_1' = g_1(w)$	
$w_2' = g_2(w)$	



Singular Perturbation Setting

Original System		Slow-Fast System
$w_1' = g_1(w)$	$w \longrightarrow x$	$x_1' = r_1(x, \varepsilon)$
$w_2' = g_2(w)$	$w \longleftarrow x$	$\varepsilon\, x_2' = r_2(x, \varepsilon)$





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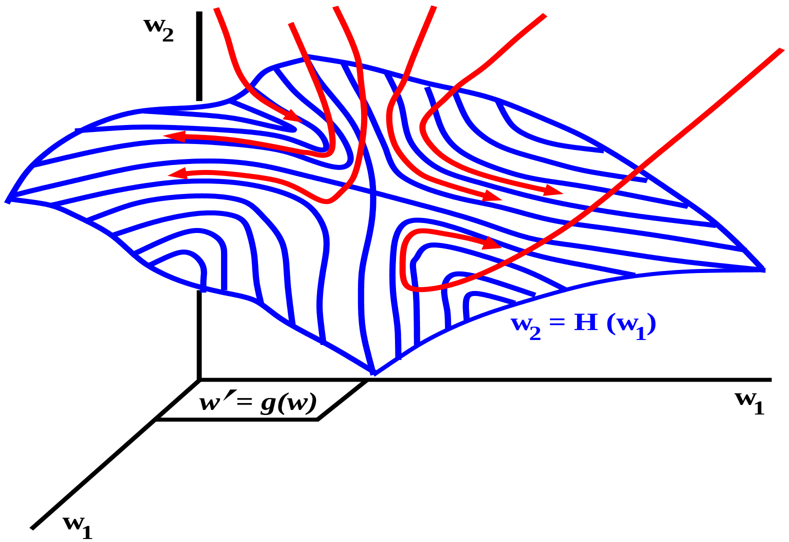

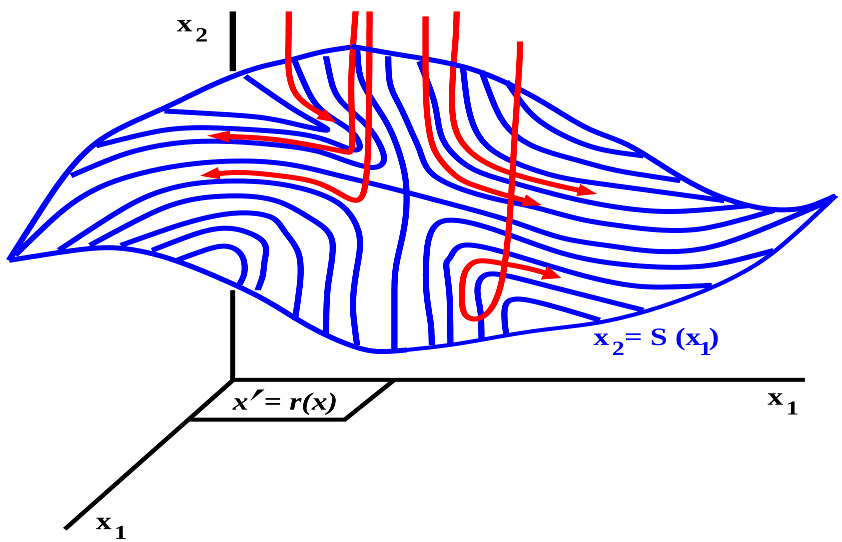

$$\mathrm{Re}\left(\sigma\ (\partial r_2/\partial x_2)|_S\right) \subset \mathbb{R}_-$$ normal hyperbolicity

Proximity Results

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

$\det\left(\partial w_2/\partial x_2\right) \neq 0$ — inclusion of fast directions

$\det\left(\partial g_2/\partial w_2\right) \neq 0$ — hyperbolicity in w_2–direction

in a neighborhood of the manifold. Then, the condition

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

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

$$w_2^* - H(w_1^*) = \mathcal{O}(\varepsilon^{m+1}), \qquad \varepsilon \downarrow 0.$$

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Constrained Runs Algorithms

- CHOOSE $\mathrm{m} \in \{0, 1, \ldots\}$ — order of the method
- FIX $\mathrm{w}_1 = \mathrm{w}_1^*$ & SEED with $\mathrm{w}_2^{(0)}$ — initial guess
- ITERATE using — fixed point iteration

$$\mathrm{w}_2^{(n+1)} = \mathrm{F}_\mathrm{m}\left(\mathrm{w}_2^{(n)}\right) = \mathrm{w}_2^{(n)} - (-\mathrm{h})^{\mathrm{m}+1} \left.\frac{\mathrm{d}^{\mathrm{m}+1}\mathrm{w}_2}{\mathrm{d}t^{\mathrm{m}+1}}\right|_{\left(\mathrm{w}_1^*,\mathrm{w}_2^{(n)}\right)}$$

- STOP when converged to $\mathrm{w}_2 = \mathrm{w}_2^{(\#)}$ — converged w_2
- SET $\mathrm{w}_2^{(\#)} \approx \mathrm{w}_2^* \approx \mathrm{H}(\mathrm{w}_1^*)$ — approximate slow manifold

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Does the iteration converge to w_2^*? — attractivity

The Jacobian $\partial F_m / \partial w_2$

- Calculate, to leading order in ε,

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

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

    not positive semidefinite, not a projection

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$\sigma\left(\partial F_m / \partial w_2\right)$ is unavailable — generalized eigenvalue problem

Vertical Fibration ($\mathrm{P} = \mathrm{I}$)

- Write the normal spectrum of the vector field as

$$\sigma \left(\left. \frac{\partial \mathrm{r}_2}{\partial \mathrm{x}_2} \right|_{\mathrm{w}^*} \right) = \{ \lambda_\ell = |\lambda_\ell| \mathrm{e}^{\mathrm{i}\theta_\ell} : 1 \leq \ell \leq \mathrm{N}_2 \}$$

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

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

Is the fixed point also stable if $\lambda_\ell \in \mathbb{C} - \mathbb{R}$ for some ℓ?

Complex Eigenvalues

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

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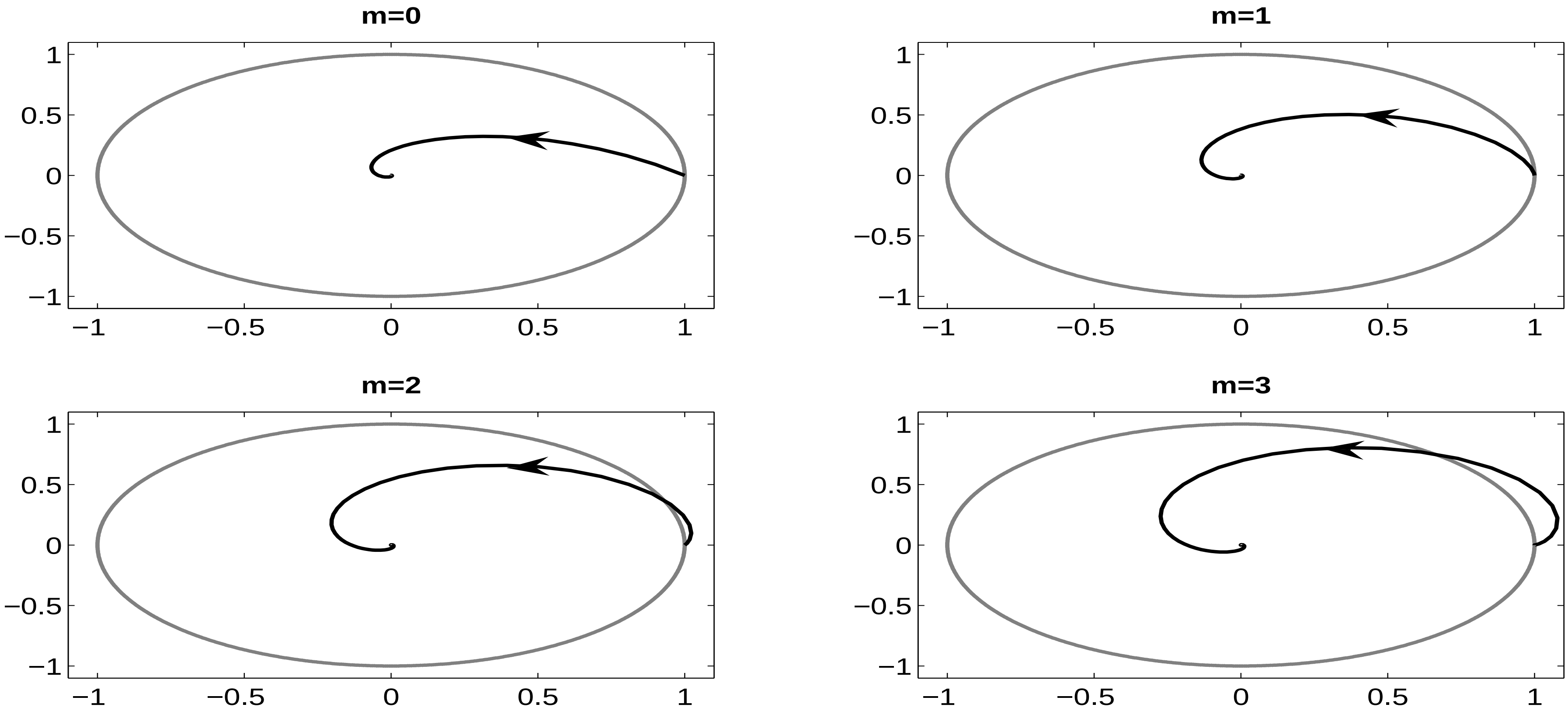

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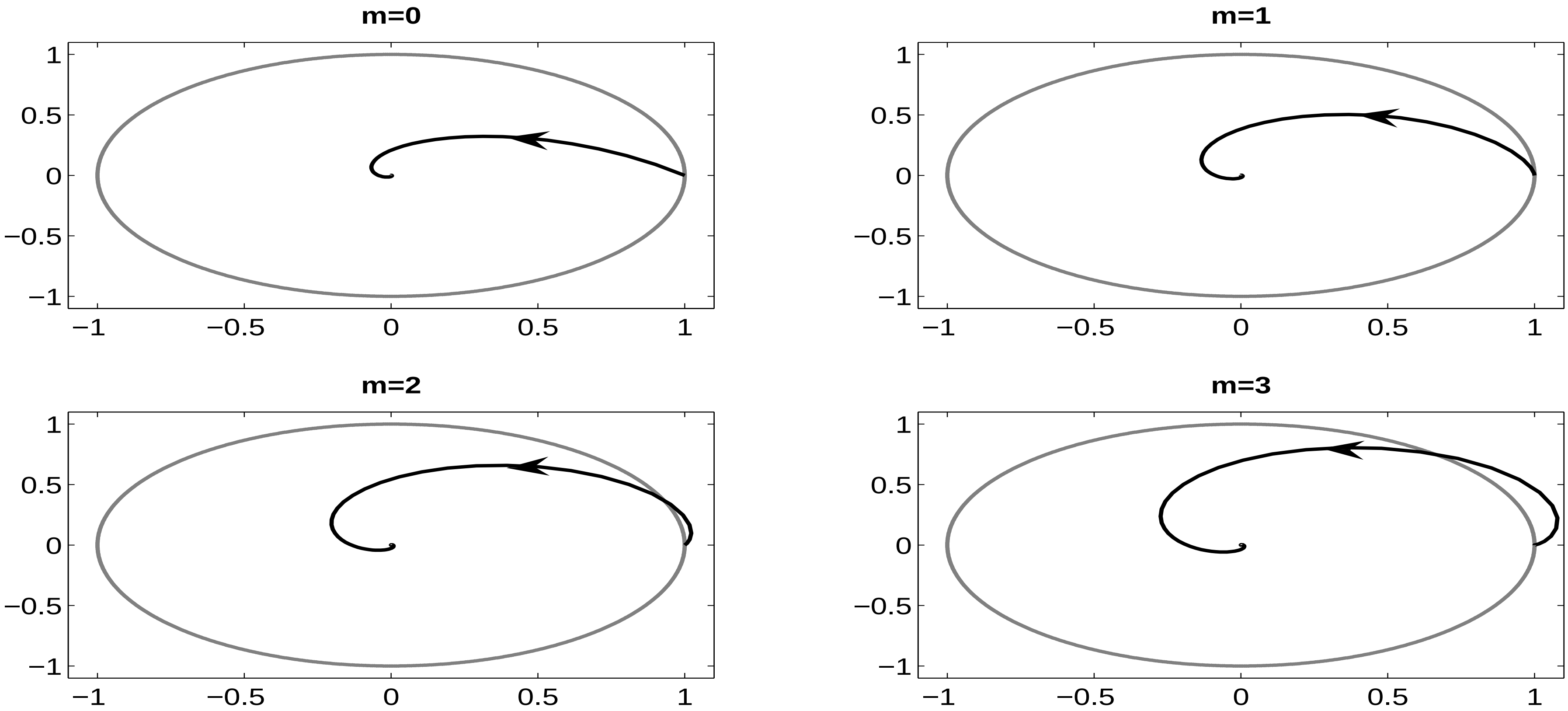
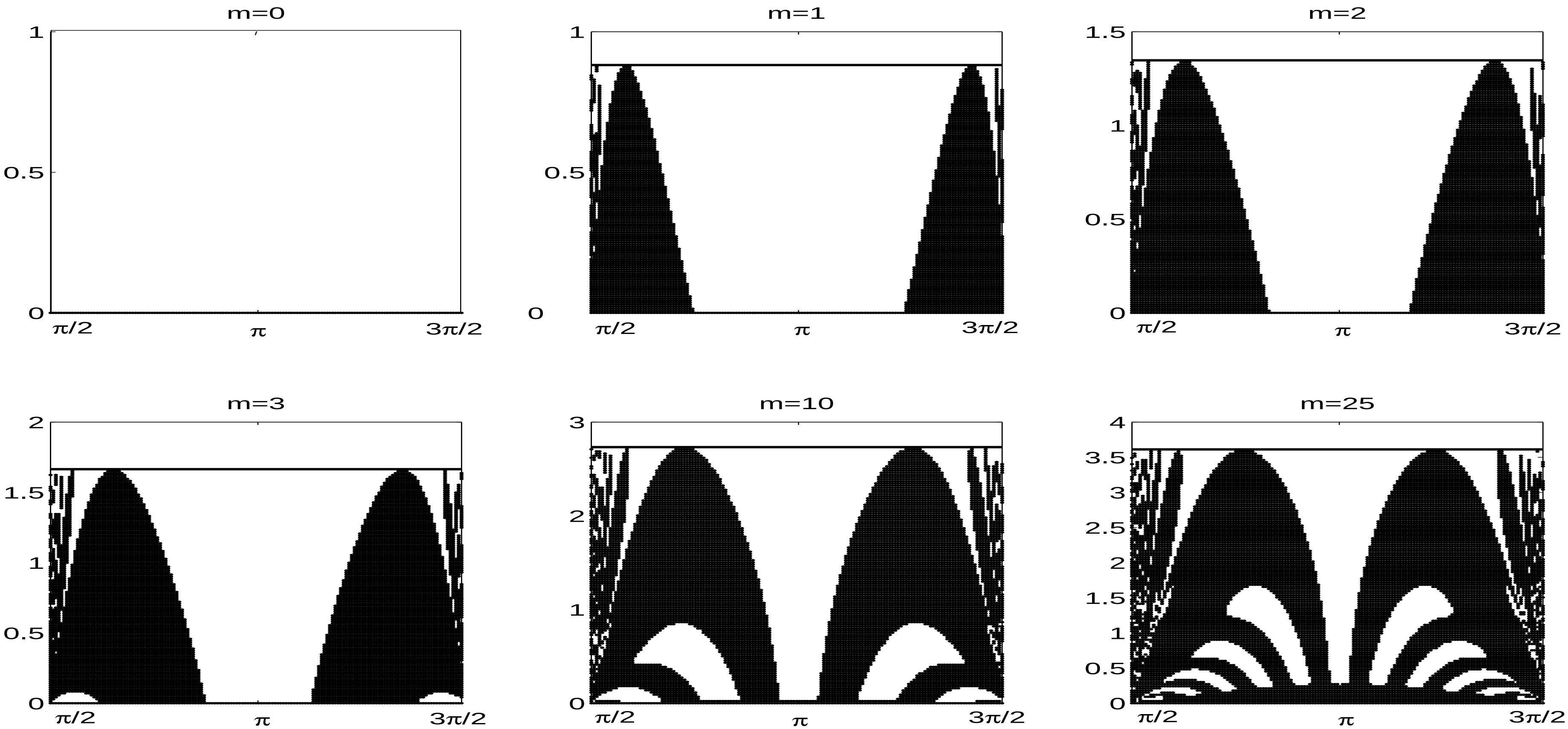


Complex eigenvalues may cause divergence

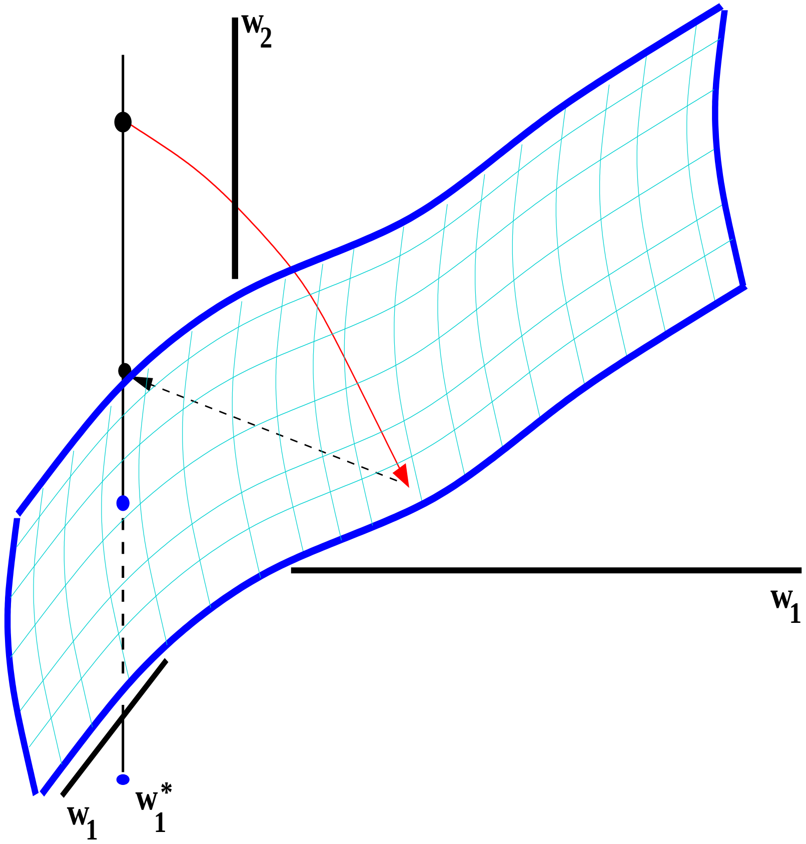
h **versus** θ

Stability

Instability



Geometric Configuration



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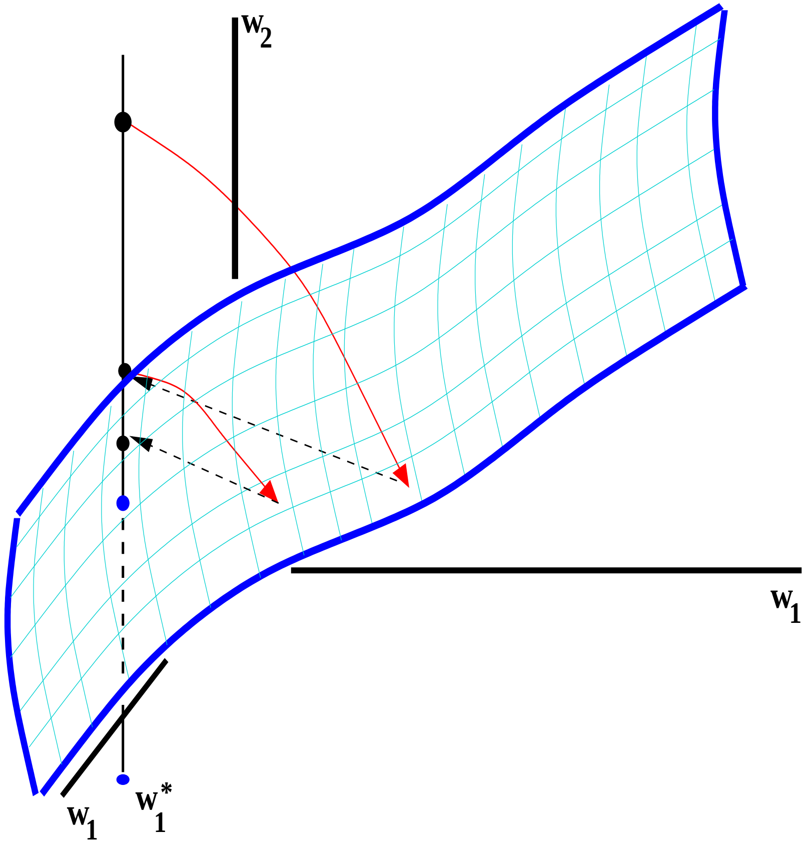

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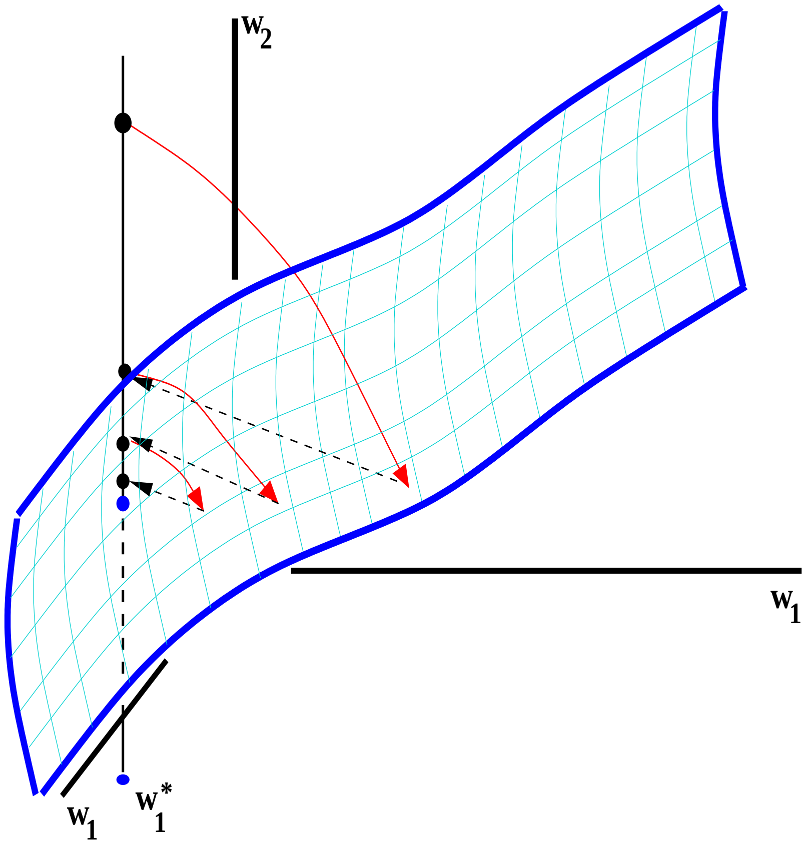

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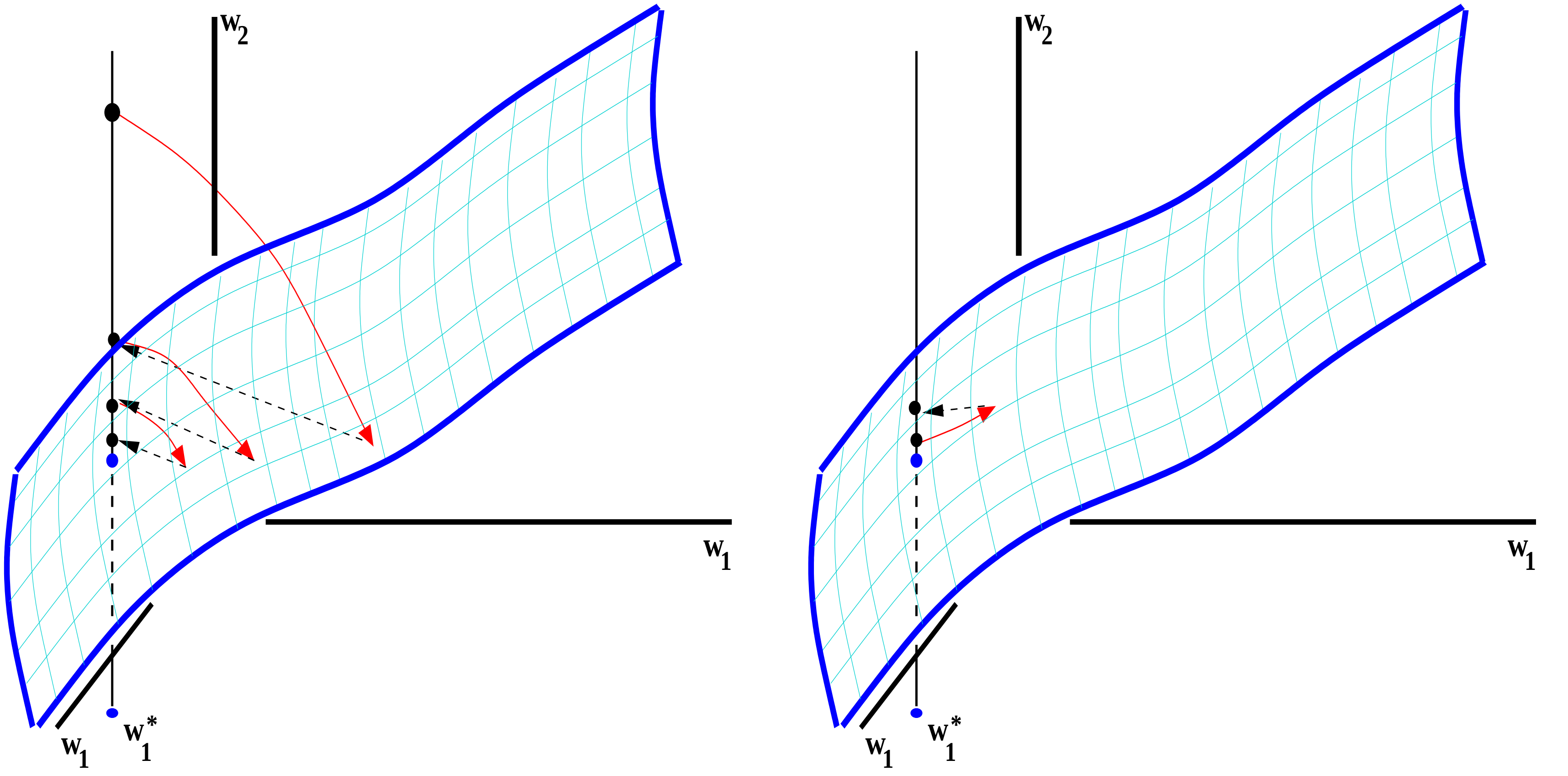

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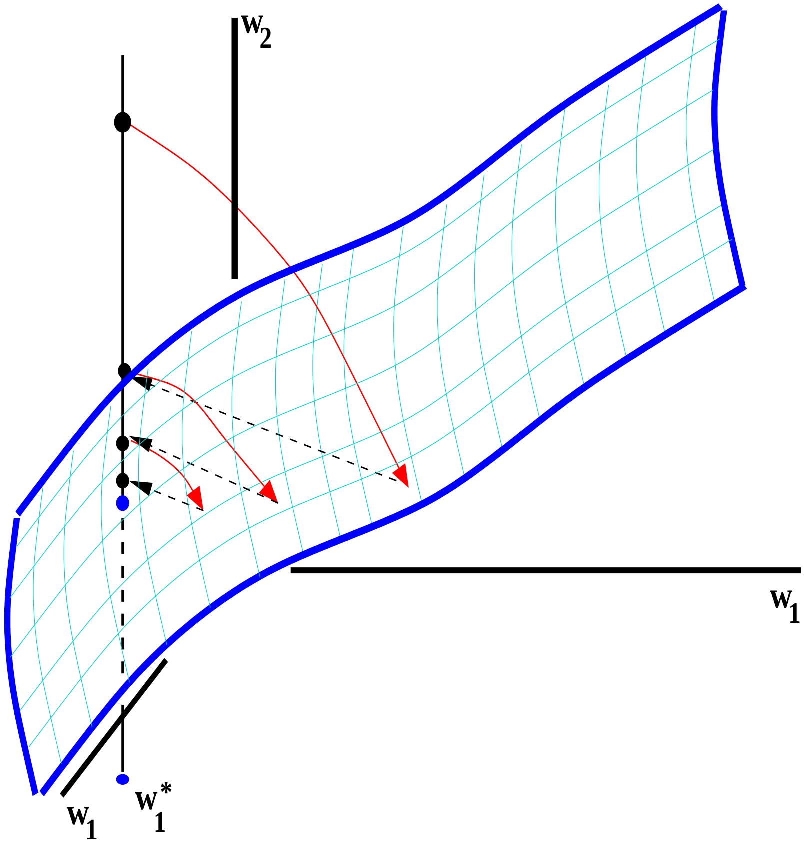

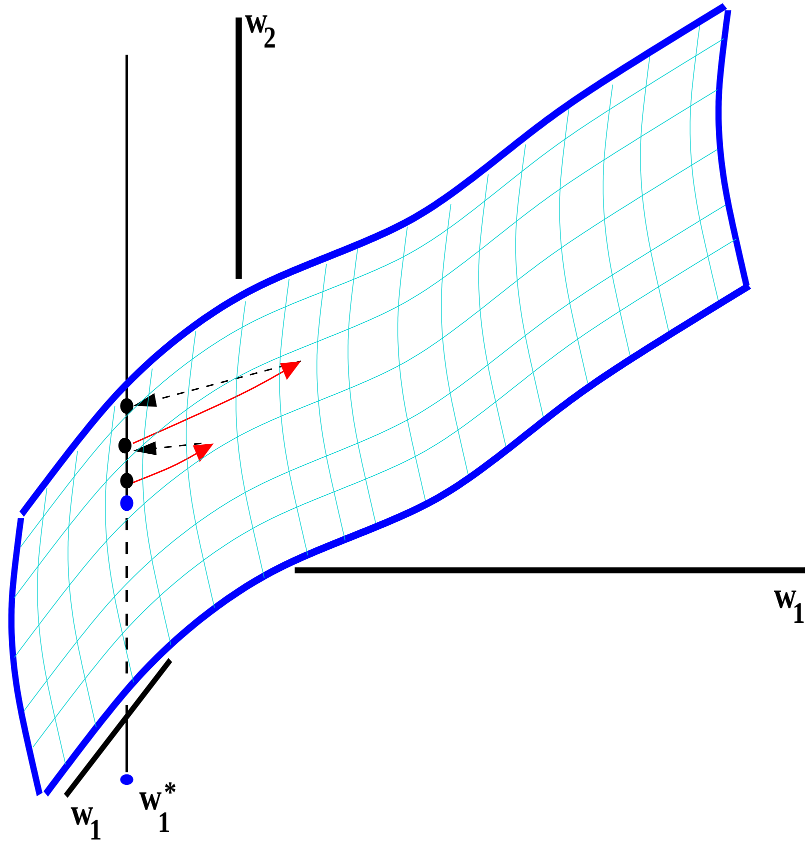

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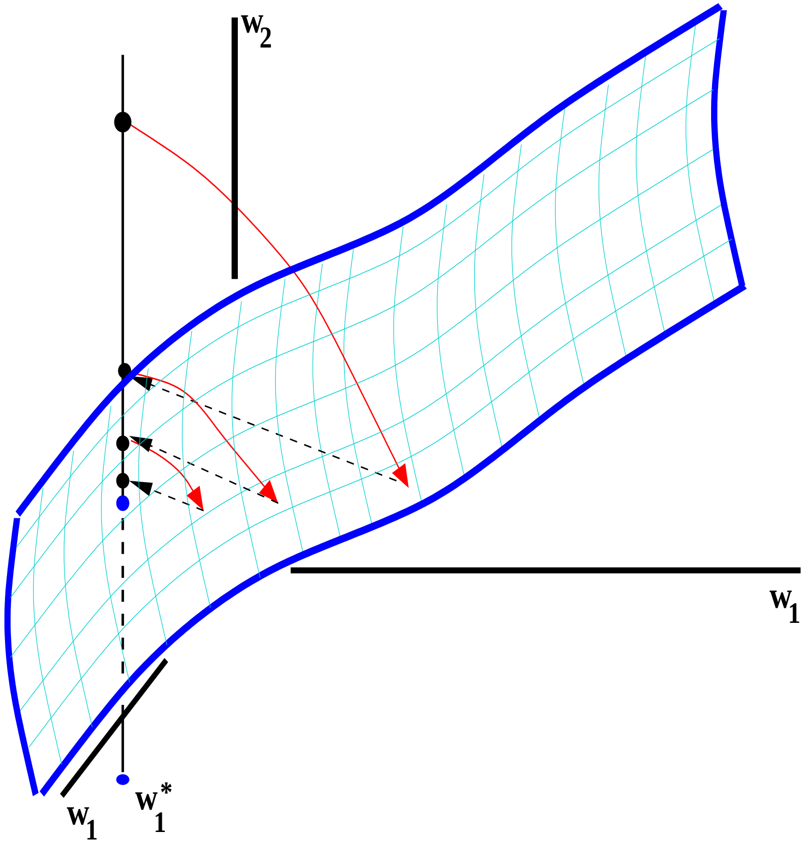

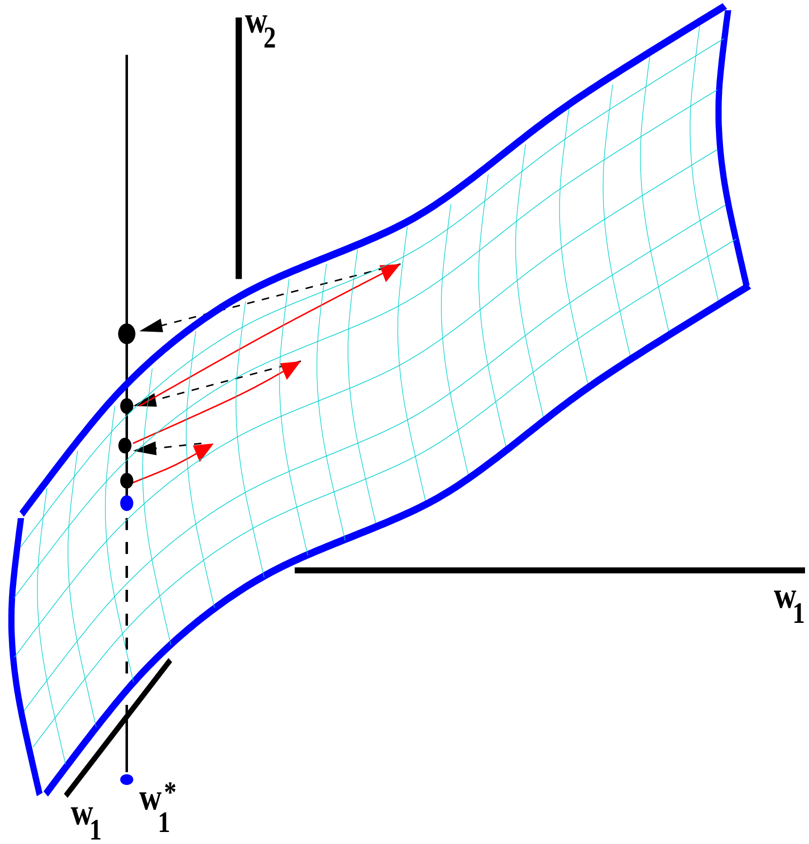

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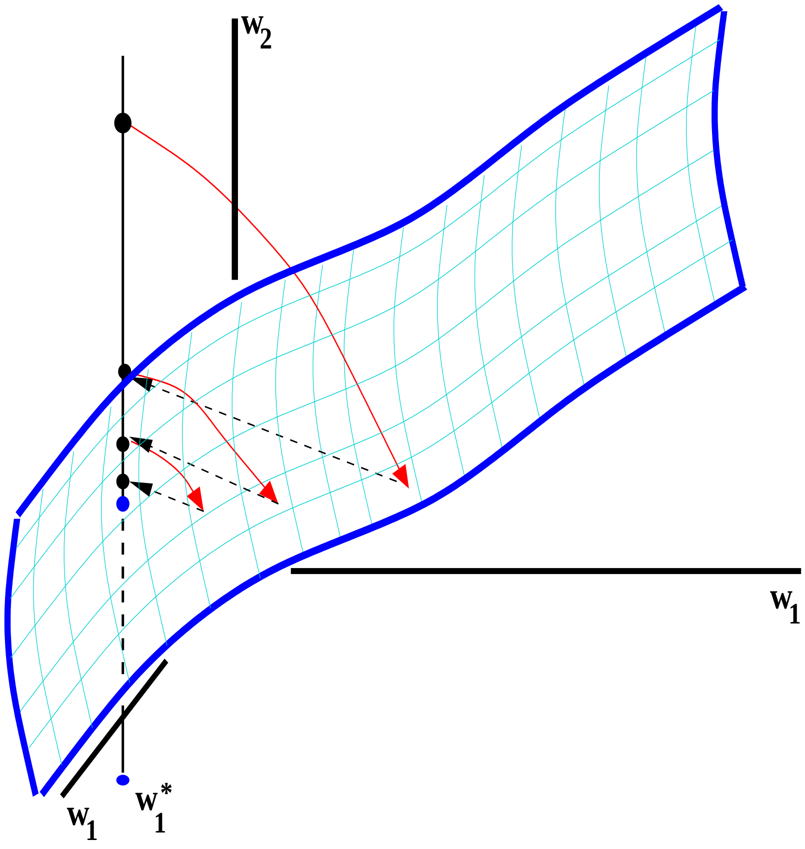

The relative orientation of the slow manifold
and the fast fibers affects algorithm convergence

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Summary

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

vertical fibration		non-vertical fibration	
$m = 0$	$m \geq 1$	$m = 0$	$m \geq 1$
$\mathbb{R} \longrightarrow$ stable	$\mathbb{R} \longrightarrow$ stable	$\mathbb{R} \longrightarrow$ unstable	$\mathbb{R} \longrightarrow$ unstable
$\mathbb{C} \longrightarrow$ stable	$\mathbb{C} \longrightarrow$ unstable	$\mathbb{C} \longrightarrow$ unstable	$\mathbb{C} \longrightarrow$ unstable

- stabilization possible
  - Krylov subspace methods
  - implicit functional iteration
  - more intelligent resetting $w_1 = w_1^*$