Composition and Splitting Methods

Book Sections II.4 and II.5

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Seminar on Geometric Numerical Integration

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Outline

Preliminaries

Notation

- autonomous differential equation

$$\dot{y} = f(y)\,, \quad y(t_0) = y_0\,,$$

- its exact flow φ_t, and
- numerical method Φ_h, i.e. $y_1 = \Phi_h(y_0)$.

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- autonomous differential equation

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- numerical method Φ_h, i.e. $y_1 = \Phi_h(y_0)$.

Basic Facts

- $\varphi_h(y) = y + \mathcal{O}(h)$
- p : order of Φ_h
  $e := \Phi_h(y) - \varphi_h(y)$ error

$$e = C(y)h^{p+1} + \mathcal{O}(h^{p+2})$$

Definition of the Adjoint Method

Definition

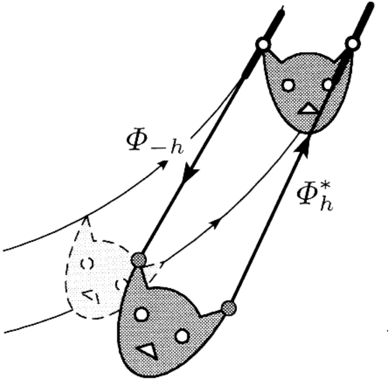
The adjoint of Φ_h is

$$\Phi_h^* := \Phi_{-h}^{-1} .$$

It is defined implicitly by

$$y_1 = \Phi_h^*(y_0) \quad \text{iff} \quad y_0 = \Phi_{-h}(y_1) .$$

Φ_h is symmetric, if $\Phi_h^* = \Phi_h$.



Properties of the Adjoint Method

Remark

- Note that $\varphi_{-t}^{-1} = \varphi_t$, but in general $\Phi_h^* = \Phi_{-h}^{-1} \neq \Phi_h$.
- The adjoint method satisfies $(\Phi_h^*)^* = \Phi_h$ and $(\Phi_h \circ \Psi_h)^* = \Psi_h^* \circ \Phi_h^*$.

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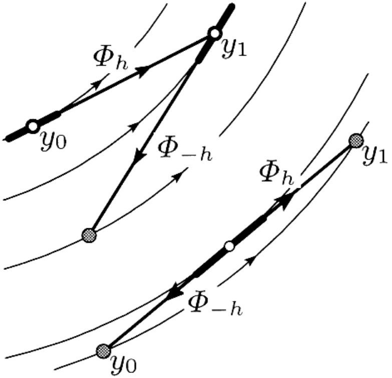
Example

- (explicit Euler)*
  $=$ implicit Euler
- (implicit midpoint)*
  $=$ implicit midpoint



Order of the Adjoint Method

Theorem

1. *If Φ_h has order p and satisfies*

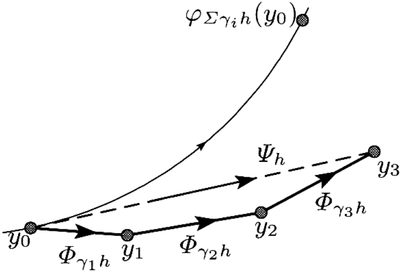
$$\Phi_h(y_0) - \varphi_h(y_0) = C(y_0)h^{p+1} + \mathcal{O}(h^{p+2}),$$

then Φ_h^* also has order p and satisfies

$$\Phi_h^*(y_0) - \varphi_h(y_0) = (-1)^p C(y_0)h^{p+1} + \mathcal{O}(h^{p+2}).$$

2. *In particular, if Φ_h is symmetric, its order is even.*

Definition of Composition Methods



Definition

Let $\Phi_h^1, \ldots, \Phi_h^s$ be one step methods. Composition

$$\Psi_h := \Phi^s_{\gamma_s h} \circ \ldots \circ \Phi^1_{\gamma_1 h},$$

where $\gamma_1, \ldots, \gamma_s \in \mathbb{R}$.

Example

1. $\Phi_h^1 = \ldots = \Phi_h^s =: \Phi_h$
2. $\Phi_h^{2k} = \Phi_h$ and $\Phi_h^{2k-1} = \Phi_h^*$

Order Increase

of General Composition Methods

Theorem

Let $\Psi_h := \Phi^s_{\gamma_s h} \circ \ldots \circ \Phi^1_{\gamma_1 h}$ *with* Φ^k_h *of order* p *and*

$$\Phi^k_h(y) - \varphi_h(y) = C_k(y)h^{p+1} + \mathcal{O}(h^{p+2})\,.$$

If

$$\gamma_1 + \ldots + \gamma_s = 1\,,$$

then Ψ_h *has order* $p+1$ *if and only if*

$$\gamma_1^{p+1} C_1(y) + \ldots + \gamma_s^{p+1} C_s(y) = 0\,.$$

Order Increase

of Compositions of a Single Method

Corollary

If $\Psi_h = \Phi_{\gamma_s h} \circ \ldots \circ \Phi_{\gamma_1 h}$, *then the conditions are*

$$\begin{aligned} \gamma_1 + \ldots + \gamma_s &= 1 \\ \gamma_1^{p+1} + \ldots + \gamma_s^{p+1} &= 0\,. \end{aligned}$$

Remark

A solution only exists if p is even.

Order Increase
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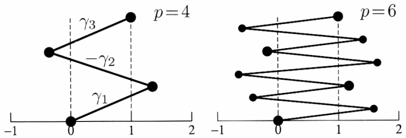
Remark

A solution only exists if p is even.

Example

$s = 3$, Φ_h symmetric, order $p = 2$, $\gamma_1 = \gamma_3$.
Then $\Psi_h = \Phi_{\gamma_3 h} \circ \Phi_{\gamma_2 h} \circ \Phi_{\gamma_1 h}$ is also symmetric, order ≥ 3.
Symmetric $\Rightarrow$ order even $\Rightarrow$ order 4. So repeated application is possible.



Order Increase

of Compositions with the Adjoint Method

Corollary

If

$$\Psi_h = \Phi_{\alpha_s h} \circ \Phi^*_{\beta_s h} \circ \ldots \circ \Phi^*_{\beta_2 h} \circ \Phi_{\alpha_1 h} \circ \Phi^*_{\beta_1 h} \,,$$

then the conditions are

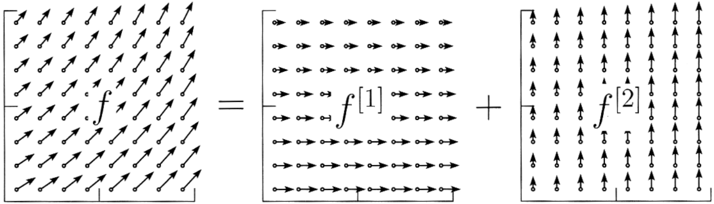
$$\begin{aligned} \beta_1 + \alpha_1 + \ldots + \beta_s + \alpha_s &= 1 \\ (-1)^p \beta_1^{p+1} + \alpha_1^{p+1} + \ldots + (-1)^p \beta_s^{p+1} + \alpha_s^{p+1} &= 0 \,. \end{aligned}$$

Example

$\Psi_h := \Phi_{\frac{h}{2}} \circ \Phi^*_{\frac{h}{2}}$ is symmetric, order $p+1$.

- Φ_h explicit Euler $\Rightarrow$ Ψ_h implicit midpoint
- Φ_h implicit Euler $\Rightarrow$ Ψ_h trapezoidal rule

Idea: Split the Vector Field



Idea

- Split the vector field f into
$$\dot{y} = f(y) = f^{[1]}(y) + f^{[2]}(y) + \ldots + f^{[N]}(y)$$
- Calculate exact flow $\varphi_t^{[i]}$ of $\dot{y} = f^{[i]}$ explicitly
- Use "composition" of $\varphi_h^{[i]}$ to solve $\dot{y} = f(y)$, e.g.
$$\Psi_h = \varphi_{a_s h}^{[1]} \circ \varphi_{b_s h}^{[2]} \circ \ldots \circ \varphi_{a_1 h}^{[1]} \circ \varphi_{b_1 h}^{[2]}$$

Motivation

Example

$\dot{y} = (a+b)y$, then $\varphi_t^a(y_0) = e^{at}y_0$ and $\varphi_t^b(y_0) = e^{bt}y_0$, so

$$(\varphi_t^a \circ \varphi_t^b)(y_0) = e^{at}e^{bt}y_0 = e^{(a+b)t}y_0 = \varphi_t(y_0)$$

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Lie-Trotter Formula

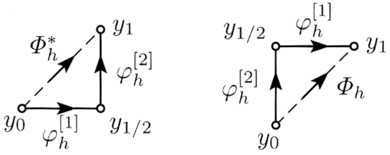
$\dot{y} = (A+B)y \quad$ for $A, B \in \mathbb{C}^{N\times N}$.

$$\varphi_t^A(y_0) = e^{At}y_0 \quad \text{and} \quad \varphi_t^B(y_0) = e^{Bt}y_0$$

Lie Trotter formula $\qquad \lim_{n\to\infty} \left(e^{A\frac{t}{n}}e^{B\frac{t}{n}}\right)^n = e^{(A+B)t}$

so $\qquad \left(\varphi_{\frac{t}{n}}^A \circ \varphi_{\frac{t}{n}}^B\right)^n (y_0) \to \varphi_t(y_0)$

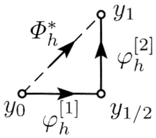
Examples of Splittings

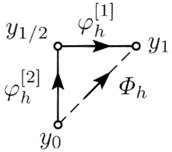


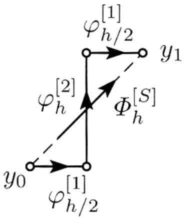
Example (Lie-Trotter Splitting)

$$\Phi_h = \varphi_h^{[1]} \circ \varphi_h^{[2]}$$
$$\Phi_h^* = \varphi_h^{[2]} \circ \varphi_h^{[1]}$$

Examples of Splittings







Example (Lie-Trotter Splitting)

$$\begin{aligned} \Phi_h &= \varphi_h^{[1]} \circ \varphi_h^{[2]} \\ \Phi_h^* &= \varphi_h^{[2]} \circ \varphi_h^{[1]} \end{aligned}$$

Example (Strang Splitting)

$$\Phi_h = \varphi_{\frac{h}{2}}^{[1]} \circ \varphi_h^{[2]} \circ \varphi_{\frac{h}{2}}^{[1]} = \Phi_h^*$$

Application to Separable Hamiltonian Systems

Example

- Separable Hamiltonian $H(p,q) = T(p) + U(q)$

$$\begin{pmatrix} \dot{p} \\ \dot{q} \end{pmatrix} = \begin{pmatrix} -H_q \\ H_p \end{pmatrix} = \begin{pmatrix} 0 \\ T_p \end{pmatrix} + \begin{pmatrix} -U_q \\ 0 \end{pmatrix}$$

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- Exact flows

$$\varphi_t^T \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} = \begin{pmatrix} p_0 \\ q_0 + t\, T_p(p_0) \end{pmatrix}, \quad \varphi_t^U \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} = \begin{pmatrix} p_0 - t\, U_q(q_0) \\ q_0 \end{pmatrix}$$

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- Lie-Trotter splitting $\Phi_h = \varphi_h^T \circ \varphi_h^U$

$$\begin{aligned} p_{n+1} &= p_n - h \cdot U_q(\qquad q_n) \\ q_{n+1} &= q_n + h \cdot T_p(p_{n+1} \qquad) \end{aligned}$$

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- Lie-Trotter splitting $\Phi_h = \varphi_h^T \circ \varphi_h^U \rightsquigarrow$ symplectic Euler

$$\begin{aligned} p_{n+1} &= p_n - h \cdot U_q(p_{n+1}, q_n) \\ q_{n+1} &= q_n + h \cdot T_p(p_{n+1}, q_n) \end{aligned}$$

Construction as a Composition Method

Lemma

$\Phi_h^{[i]}$ *consistent method for* $\dot{y} = f^{[i]}(y)$.

$$\Phi_h := \Phi_h^{[1]} \circ \Phi_h^{[2]} \circ \ldots \circ \Phi_h^{[N]},$$

then Φ_h *has order* 1 *for* $\dot{y} = f(y) = f^{[1]}(y) + f^{[2]}(y) + \ldots + f^{[N]}(y)$.

Construction as a Composition Method

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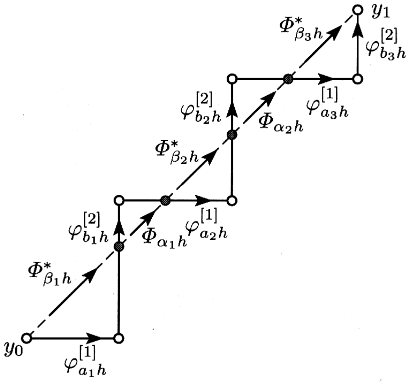
Idea

Compose Φ_h, Φ_h^* to construct method Ψ_h of higher order.

In the case $N = 2$: $\Phi_h = \Phi_h^{[1]} \circ \Phi_h^{[2]}$, $\Phi_h^* = \Phi_h^{[2]*} \circ \Phi_h^{[1]*}$ and

$$\begin{aligned}\Psi_h &= \Phi_{\alpha_s h} \circ \Phi^*_{\beta_s h} \circ \ldots \circ \Phi^*_{\beta_2 h} \circ \Phi_{\alpha_1 h} \circ \Phi^*_{\beta_1 h} \\ &= \Phi^{[1]}_{\alpha_s h} \circ \Phi^{[2]}_{\alpha_s h} \circ \Phi^{[2]*}_{\beta_s h} \circ \Phi^{[1]*}_{\beta_s h} \circ \ldots \circ \Phi^{[2]}_{\alpha_1 h} \circ \Phi^{[2]*}_{\beta_1 h} \circ \Phi^{[1]*}_{\beta_1 h}\end{aligned}$$

Calculate Exact Flows Explicitly



Remark

If $\Phi_h^{[i]} = \varphi_h^{[i]}\ \forall i$, then $\Phi_h^{[i]*} = \varphi_h^{[i]}$ and

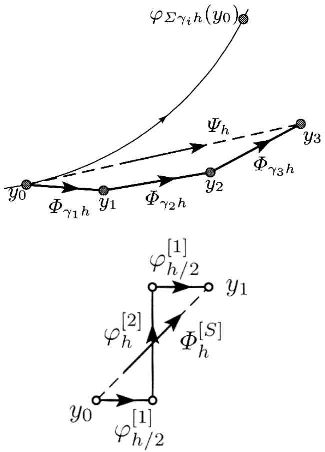
$$\Psi_h = \varphi^{[1]}_{\alpha_s h} \circ \varphi^{[2]}_{(\alpha_s+\beta_s)h} \circ \ldots \circ \varphi^{[1]}_{\beta_1 h}.$$

Remark

For $N = 2$, Ψ_h can be thought of as

- a composition of Φ_h, Φ_h^*
- a “composition” of $\varphi_h^{[i]}$

Summary



1. Composition methods
   - construct methods of high order
   - preserve properties (e.g. symmetry)
2. Splitting methods
   - construct methods for specific problems
   - calculate exact flows of parts of the vector field explicitly