

On Lawson methods and trees

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$$y^{(4)}(0) = (f'''[f, f, f])(y_0) + 3(f''[f'f, f])(y_0)$$

+ $(f'f''[f, f])(y_0) + (f'f'f'f)(y_0)$
 \downarrow

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Outline



- 1. Lawson methods
- 2. Outdoor excursion
- 3. Order and convergence
- 4. Example: Linear problems

Outline



1. Lawson methods

2. Outdoor excursion

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Problem



consider semilinear stiff problem

$$u'(t) = Au(t) + g(u(t)), \qquad u(0) = u_0$$

A matrix of large norm or A differential operator (unbounded) s.t.

$$\left| \mathrm{e}^{t \mathsf{A}} \right| \leq C, \qquad t \geq 0$$

w.l.o.g.
$$C = 1$$
 (for $C > 1$ use $||v||_{\star} = \sup_{t \ge 0} ||e^{tA}v||$)
q "nice"

applications: (discretizations of) pdes

- heat equation, convection diffusion equation, etc
- (nonlinear) Schrödinger equation, Maxwell equations

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Lawson methods, 1967: key idea



$$u'(t) = Au(t) + g(u(t)), \qquad u(0) = u_0$$

transformation of variables

$$w(t) = \mathrm{e}^{-t\mathsf{A}}u(t)$$

differentiation yields (hopefully) nonstiff ode for w

$$\mathbf{w}'(t) = \mathrm{e}^{-t\mathbf{A}}(-\mathbf{A}u + u') = \mathrm{e}^{-t\mathbf{A}}g(u) = \mathrm{e}^{-t\mathbf{A}}g(\mathrm{e}^{t\mathbf{A}}\mathbf{w})$$

Lawson method:

- solve ode for w with explicit Runge–Kutta method
- transform back to original u variables

Lawson methods



s-stage Runge–Kutta method given by a_{ij} , b_i , c_i

$$U_{i} = e^{c_{i}hA}u_{0} + h\sum_{j=1}^{i-1} a_{ij}e^{(c_{i}-c_{j})hA}g(U_{j}), \qquad i = 1, \dots, s$$
$$u_{1} = e^{hA}u_{0} + h\sum_{i=1}^{s} b_{i}e^{(1-c_{i})hA}g(U_{i})$$

example: Lawson-Euler method:

$$u_1 = \mathrm{e}^{hA}u_0 + h\mathrm{e}^{hA}g(u_0)$$

Lawson methods



s-stage Runge–Kutta method given by *a_{ij}*, *b_i*, *c_i*

$$U_{i} = e^{c_{i}hA}u_{0} + h\sum_{j=1}^{i-1} a_{ij}e^{(c_{i}-c_{j})hA}g(U_{j}), \qquad i = 1, \dots, s$$
$$u_{1} = e^{hA}u_{0} + h\sum_{i=1}^{s} b_{i}e^{(1-c_{i})hA}g(U_{i})$$

discussion:

- if c₁ ≤ ... ≤ c_s, then scheme is suited for parabolic and hyperbolic problems (excludes Dopri, etc.)
- otherwise, we need $\|e^{tA}\| \leq 1$ for all $t \in \mathbb{R}$
- requires evaluation or approximation of $e^{hA}v$
- special case of exponential integrator (using only exponentials)

Failure of Lawson methods



consider scalar ivp

$$u'(t) = Au(t) + 1$$
, $u(0) = u_0 = -A^{-1}$, $A < 0$

with solution $u(t) = u(0) = -A^{-1}$

exponential Euler method is exact:

$$u_1 = e^{hA}u_0 + h\varphi_1(hA) = u_0, \qquad \varphi_1(z) = \frac{e^2 - 1}{z}$$

Lawson Euler method

$$u_1 = e^{hA}u_0 + he^{hA} = e^{hA}(-A^{-1} + h)$$

gives reasonable results only in nonstiff case hA
ightarrow 0

convergence analysis: H., Ostermann, 2005

Success of Lawson methods



in

- Kassam, Trefethen, 2005 (integrated factor method):
 KdV, Burgers, Kuramoto-Sivashinsky, Allen-Cahn, periodic b.c.
- Cano, Gonzáles-Pachón, 2014: nonlinear Schrödinger equation, periodic b.c.
- Balac, Fernandez, Mahé, Méhats, Texier-Picar, 2014: generalized nonlinear Schrödinger equation in optics

full order of convergence is observed numerically

aim of this talk:

explain this behavior theoretically:

If the solution is sufficiently regular, then the Lawson method converges with the same order as the underlying Runge–Kutta method.

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Classical order of RK methods



reminder: how to prove error estimates for RK methods consider autonomous ivp

$$y' = f(y), \qquad y(0) = y_0,$$

with *f* sufficiently smooth

Taylor's theorem

$$y(h) = \sum_{k=0}^{p} y^{(k)}(0) \frac{h^{k}}{k!} + O(h^{p+1}), \qquad h \to 0$$

higher derivatives of y obtained by repeated differentiation of the ode





Taylor expansion of exact solution



 τ_2

order *q*(*τ*) = number of nodes of *τ* elementary differential *D*(*τ*) defined recursively by

$$D(\bullet)(y) = f(y),$$

•
$$D(\tau)(y) = f^{(k)}(y) \Big[D(\tau_1)(y), \dots, D(\tau_k)(y) \Big]$$
 for $\tau = \frac{\tau_1}{\tau_1} \frac{\tau_2}{\tau_1} \frac{\tau_k}{\tau_k}$

Theorem (Butcher, 1963; Hairer, Wanner, 1974; ...) The solution of y' = f(y), $y(0) = y_0$ satisfies

$$y^{(k)}(0) = \sum_{\substack{\tau \in \mathcal{T} \\ \varrho(\tau) = k}} \alpha(\tau) D(\tau)(y_0), \qquad k = 1, 2, 3, \dots$$

for certain coefficients $\alpha(\tau)$, which are independent of the ode.

Taylor expansion of numerical solution



for y' = f(y)

$$y_1 = y_0 + h \sum_{i=1}^{s} b_i f(Y_i), \qquad Y_i = y_0 + h \sum_{j=1}^{s} a_{ij} f(Y_j)$$

Theorem (Hairer, Wanner, 1974, ...)

The numerical solution $y_1 \approx y(h)$ satisfies

$$y_1^{(k)}(\mathbf{0}) = \sum_{\substack{\tau \in \mathcal{T} \\ \varrho(\tau) = k}} \phi(\tau) \alpha(\tau) D(\tau)(y_0), \qquad k = 1, 2, 3, \dots$$

with the same coefficients $\alpha(\tau)$ as for the exact solution.

conclusion: RK method is of order p if $\phi(\tau) = 1$ for all τ with $\varrho(\tau) \leq p$

RK methods vs Lawson methods



Runge–Kutta method for y' = f(y), $y(0) = y_0$

$$y_1 = y_0 + h \sum_{i=1}^{s} b_i f(Y_i),$$

 $Y_i = y_0 + h \sum_{j=1}^{i-1} a_{ij} f(Y_j)$

exact solution

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$$y(h) = y_0 + \int_0^h f(y(\sigma)) d\sigma$$

Lawson method for u' = Au + g(u), $u(0) = u_0$ $u_1 = e^{hA}u_0 + h\sum_{i=1}^{s} b_i e^{(1-c_i)hA}g(U_i)$, $U_i = e^{c_ihA}u_0 + h\sum_{j=1}^{i-1} a_{ij}e^{(c_i-c_j)hA}g(U_j)$

exact solution

$$u(h) = e^{hA}u_0 + \int_0^h e^{(h-\sigma)A}g(u(\sigma))d\sigma$$

Iterated v.o.c. formula



notation:

$$g_{\eta} = g(e^{\eta hA}u_{0}), \qquad g_{\eta}^{(k)} = g^{(k)}(e^{\eta hA}u_{0}), \qquad k \ge 1$$
$$u(h) = e^{hA}u_{0} + h \int_{0}^{1} e^{(1-\sigma)hA}g(u(\sigma h))d\sigma$$
$$= e^{hA}u_{0} + h \int_{0}^{1} e^{(1-\sigma)hA}g(e^{\sigma hA}u_{0} + h \int_{0}^{\sigma} e^{(\sigma-\eta)hA}g(u(\eta h))d\eta)d\sigma$$
$$= e^{hA}u_{0} + h \int_{0}^{1} e^{(1-\sigma)hA}g_{\sigma}d\sigma$$
$$+ h^{2} \int_{0}^{1} e^{(1-\sigma)hA}g'_{\sigma} \int_{0}^{\sigma} e^{(\sigma-\eta)hA}g_{\eta}d\eta d\sigma$$
$$+ \mathcal{O}(h^{3})$$

Lubich, Jahnke, 2000; Thalhammer, 2008; Lubich, 2008



notation:

$$g_{\eta} = g(\mathrm{e}^{\eta h A} u_0), \qquad g_{\eta}^{(k)} = g^{(k)}(\mathrm{e}^{\eta h A} u_0), \qquad k \geq 1$$

$$\begin{split} u(h) &= \mathrm{e}^{hA} u_0 + h \int_0^1 \mathrm{e}^{(1-\sigma)hA} g_{\sigma} \mathrm{d}\sigma \\ &+ h^2 \int_0^1 \mathrm{e}^{(1-\sigma)hA} g_{\sigma}' \int_0^{\sigma} \mathrm{e}^{(\sigma-\eta)hA} g_{\eta} \mathrm{d}\eta \mathrm{d}\sigma \\ &+ h^3 \int_0^1 \mathrm{e}^{(1-\sigma)hA} g_{\sigma}' \int_0^{\sigma} \mathrm{e}^{(\sigma-\eta)hA} g_{\eta}' \int_0^{\eta} \mathrm{e}^{(\eta-\xi)hA} g_{\xi} \mathrm{d}\xi \mathrm{d}\eta \mathrm{d}\sigma \\ &+ \frac{1}{2} h^3 \int_0^1 \mathrm{e}^{(1-\sigma)hA} g_{\sigma}'' \Big[\int_0^{\sigma} \mathrm{e}^{(\sigma-\eta)hA} g_{\eta} \mathrm{d}\eta, \int_0^{\sigma} \mathrm{e}^{(\sigma-\xi)hA} g_{\xi} \mathrm{d}\xi \Big] \mathrm{d}\sigma \\ &+ \mathcal{O}(h^4) \end{split}$$



notation:

$$g_{\eta} = g(\mathrm{e}^{\eta h A} u_0), \qquad g_{\eta}^{(k)} = g^{(k)}(\mathrm{e}^{\eta h A} u_0), \qquad k \geq 1$$

$$\begin{split} u(h) &= \mathrm{e}^{hA} u_0 + h \int_0^1 \mathrm{e}^{(1-\sigma)hA} g_\sigma \, \mathrm{d}\sigma \quad \bullet \\ &+ h^2 \int_0^1 \mathrm{e}^{(1-\sigma)hA} g_\sigma' \int_0^\sigma \mathrm{e}^{(\sigma-\eta)hA} g_\eta \, \mathrm{d}\eta \, \mathrm{d}\sigma \\ &+ h^3 \int_0^1 \mathrm{e}^{(1-\sigma)hA} g_\sigma' \int_0^\sigma \mathrm{e}^{(\sigma-\eta)hA} g_\eta' \int_0^\eta \mathrm{e}^{(\eta-\xi)hA} g_{\xi} \, \mathrm{d}\xi \, \mathrm{d}\eta \, \mathrm{d}\sigma \\ &+ \frac{1}{2} h^3 \int_0^1 \mathrm{e}^{(1-\sigma)hA} g_\sigma'' \Big[\int_0^\sigma \mathrm{e}^{(\sigma-\eta)hA} g_\eta \, \mathrm{d}\eta, \int_0^\sigma \mathrm{e}^{(\sigma-\xi)hA} g_{\xi} \, \mathrm{d}\xi \Big] \, \mathrm{d}\sigma \\ &+ \mathcal{O}(h^4) \end{split}$$



notation:

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notation:

$$g_{\eta} = g(\mathrm{e}^{\eta h A} u_0), \qquad g_{\eta}^{(k)} = g^{(k)}(\mathrm{e}^{\eta h A} u_0), \qquad k \geq 1$$

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notation:

$$g_{\eta} = g(\mathrm{e}^{\eta h A} u_0), \qquad g_{\eta}^{(k)} = g^{(k)}(\mathrm{e}^{\eta h A} u_0), \qquad k \geq 1$$

$$\begin{split} u(h) &= \mathrm{e}^{hA} u_0 + h \int_0^1 \mathrm{e}^{(1-\sigma)hA} g_{\sigma} \mathrm{d}\sigma & \bullet \\ &+ h^2 \int_0^1 \mathrm{e}^{(1-\sigma)hA} g_{\sigma}' \int_0^\sigma \mathrm{e}^{(\sigma-\eta)hA} g_{\eta} \mathrm{d}\eta \mathrm{d}\sigma \\ & \to h^3 \int_0^1 \mathrm{e}^{(1-\sigma)hA} g_{\sigma}' \int_0^\sigma \mathrm{e}^{(\sigma-\eta)hA} g_{\eta}' \int_0^\eta \mathrm{e}^{(\eta-\xi)hA} g_{\xi} \mathrm{d}\xi \mathrm{d}\eta \mathrm{d}\sigma \\ & \bullet + \frac{1}{2} h^3 \int_0^1 \mathrm{e}^{(1-\sigma)hA} g_{\sigma}'' \Big[\int_0^\sigma \mathrm{e}^{(\sigma-\eta)hA} g_{\eta} \mathrm{d}\eta, \int_0^\sigma \mathrm{e}^{(\sigma-\xi)hA} g_{\xi} \mathrm{d}\xi \Big] \mathrm{d}\sigma \\ & + \mathcal{O}(h^4) \end{split}$$

Elementary integrals



Definition

For $\tau \in \mathcal{T}$ and $0 \leq \zeta \leq 1$ we define $G_{\zeta}(\tau)$ recursively as:

•
$$G_{\zeta}(\bullet)(v) = \int_0^{\zeta} e^{(\zeta - \sigma)hA} g(e^{\sigma hA}v) d\sigma$$

for
$$\tau = \tau_1^{\tau_2} \cdots \tau_k$$
 set

$$G_{\zeta}(\tau)(\mathbf{v}) = \int_{0}^{\zeta} e^{(\zeta-\sigma)h\mathbf{A}} g^{(k)} (e^{\sigma h\mathbf{A}} \mathbf{v}) [G_{\sigma}(\tau_{1})(\mathbf{v}), \dots, G_{\sigma}(\tau_{k})(\mathbf{v})] d\sigma.$$

• $G(\tau) = G_1(\tau)$; $F(\tau)$ denotes integrand of $G(\tau)$.

 $G(\tau)$ is $\varrho(\tau)$ -fold multivariate integral, $F(\tau)$ is function of $\varrho(\tau)$ variables.

Expansion of exact solution



Theorem

The solution of u' = Au + g(u), $u(0) = u_0$ satisfies

$$u(h) = e^{hA}u_0 + \sum_{\tau \in \mathcal{T}} h^{\varrho(\tau)}\gamma(\tau)G(\tau)(u_0)$$

with certain coefficients $\gamma(\tau)$ which are independent of the differential equation.

Proof. Isomorphism $\tau \simeq D(\tau) \simeq G(\tau)$

Expansion of numerical solution



$$\begin{aligned} u_{1} &= e^{hA}u_{0} + h\sum_{i=1}^{s} b_{i}e^{(1-c_{i})hA}g_{c_{i}} \\ &+ h^{2}\sum_{i=1}^{s} b_{i}e^{(1-c_{i})hA}g_{c_{i}}'\sum_{j=1}^{i-1} a_{ij}e^{(c_{i}-c_{j})hA}g_{c_{j}} \\ &+ h^{3}\sum_{i=1}^{s} b_{i}e^{(1-c_{i})hA}g_{c_{i}}'\sum_{j=1}^{i-1} a_{ij}e^{(c_{i}-c_{j})hA}g_{c_{j}}'\sum_{k=1}^{j-1} a_{jk}e^{(c_{j}-c_{k})hA}g_{c_{k}} \\ &+ \frac{1}{2}h^{3}\sum_{i=1}^{s} b_{i}e^{(1-c_{i})hA}g_{c_{i}}'\left[\sum_{j=1}^{i-1} a_{jj}e^{(c_{i}-c_{j})hA}g_{c_{j}}, \sum_{k=1}^{i-1} a_{ik}e^{(c_{i}-c_{k})hA}g_{c_{k}}\right] \\ &+ \mathcal{O}(h^{4}) \end{aligned}$$

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Expansion of numerical solution



$$u_{1} = e^{hA}u_{0} + h\sum_{i=1}^{s} b_{i}e^{(1-c_{i})hA}g_{c_{i}} \quad \bullet$$

$$+ h^{2}\sum_{i=1}^{s} b_{i}e^{(1-c_{i})hA}g'_{c_{i}}\sum_{j=1}^{i-1} a_{jj}e^{(c_{i}-c_{j})hA}g_{c_{j}}$$

$$+ h^{3}\sum_{i=1}^{s} b_{i}e^{(1-c_{i})hA}g'_{c_{i}}\sum_{j=1}^{i-1} a_{jj}e^{(c_{i}-c_{j})hA}g'_{c_{j}}\sum_{k=1}^{i-1} a_{jk}e^{(c_{j}-c_{k})hA}g_{c_{k}}$$

$$+ \frac{1}{2}h^{3}\sum_{i=1}^{s} b_{i}e^{(1-c_{i})hA}g''_{c_{i}}\left[\sum_{j=1}^{i-1} a_{jj}e^{(c_{i}-c_{j})hA}g_{c_{j}}, \sum_{k=1}^{i-1} a_{ik}e^{(c_{i}-c_{k})hA}g_{c_{k}}\right]$$

$$+ \mathcal{O}(h^{4})$$

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Elementary quadrature formulas



Definition

For $\tau \in \mathcal{T}$ we define $\widehat{\mathbf{G}}(\tau)$ recursively as:

$$\widehat{G}(\bullet)(v) = \sum_{i=1}^{s} b_i e^{(1-c_i)hA} g_{c_i}, \qquad \widehat{G}_i(\bullet)(v) = \sum_{j=1}^{i-1} a_{ij} e^{(c_i-c_j)hA} g_{c_j}$$

$$\widehat{G}(\bullet)(v) = \sum_{j=1}^{i-1} a_{jj} e^{(c_j-c_j)hA} g_{c_j}$$

$$\widehat{G}(\bullet)(v) = \sum_{j=1}^{i-1} a_{jj} e^{(c_j-c_j)hA} g_{c_j}$$

$$\widehat{G}(\tau)(\mathbf{v}) = \sum_{i=1}^{s} b_{i} e^{(1-c_{i})hA} g_{c_{i}}^{(k)} [\widehat{G}_{i}(\tau_{1})(\mathbf{v}), \dots, \widehat{G}_{i}(\tau_{k})(\mathbf{v})]$$

$$\widehat{G}_{i}(\tau)(\mathbf{v}) = \sum_{j=1}^{i-1} a_{ij} e^{(c_{i}-c_{j})hA} g_{c_{j}}^{(k)} [\widehat{G}_{j}(\tau_{1})(\mathbf{v}), \dots, \widehat{G}_{j}(\tau_{k})(\mathbf{v})]$$

Expansion of numerical solution



Theorem

The Lawson approximation satisfies

$$u_{1} = e^{hA}u_{0} + \sum_{\tau \in \mathcal{T}} h^{\varrho(\tau)}\gamma(\tau)\widehat{G}(\tau)(u_{0})$$

with the same coefficients $\gamma(\tau)$ as for the exact solution.

Proof. Isomorphism $\tau \simeq D(\tau) \simeq G(\tau) \simeq \widehat{G}(\tau)$

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Example: methods of order one



$$u_{1} = e^{hA}u_{0} + h\sum_{i=1}^{s} b_{i}e^{(1-c_{i})hA}g(e^{c_{i}hA}u_{0}) + \mathcal{O}(h^{2})$$

$$u(h) = e^{hA}u_0 + h \int_0^1 e^{(1-\sigma)hA}g(e^{\sigma hA}u_0)d\sigma + \mathcal{O}(h^2) \qquad \bullet$$

hence $u_1 - u(h) = \mathcal{O}(h^2)$ if

$$\widehat{G}(\bullet)(u_0) - G(\bullet)(u_0) = \mathcal{O}(h)$$

well known:

$$\widehat{G}(\bullet)(u_0) - G(\bullet)(u_0) = h \int_0^1 \kappa_p(\sigma) F'(\bullet)(\sigma) \mathrm{d}\sigma$$

order only depends on bounds on $F'(\bullet)$

Convergence



Theorem

A Lawson method is of order p if

$$\widehat{G}(\tau)(u_0) - G(\tau)(u_0) = \mathcal{O}(h^{p+1-\varrho(\tau)}), \quad \text{for all } \tau \in \mathcal{T}, \quad \varrho(\tau) \le p$$

Proof. Follows directly from expansion of exact and numerical solution.

Theorem

lf

$$F(\tau) \in C^{p+1-\varrho(\tau)}$$
 for all $\tau \in \mathcal{T}$, $\varrho(\tau) \leq p$

and if the underlying the Runge–Kutta method is of order p, then the Lawson method is of order p.

Main result



Theorem

lf

- $F(\tau) \in C^{p+1-\varrho(\tau)}$ for all $\tau \in \mathcal{T}$ with $\varrho(\tau) \leq p$ and
- underlying Runge–Kutta method is of order p
- $0 < h \le h_0$

then the Lawson method converges with order p, i.e.

$$\|u(t_n)-u_n\|\leq Ch^p, \qquad t_n=nh\leq T,$$

where C and h_0 are independent of n, h, and A.

Sketch of proof



- expand $F(\tau)(\sigma_1, \dots, \sigma_{\varrho(\tau)})$ into a Taylor polynomial of degree $p + 1 \varrho(\tau)$
- underlying RK method is of order k, hence multivariate quadrature formula is exact for all polynomials of degree p + 1 ρ(τ)
- stability
- Lady Windermere's fan

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Linear problems



$$u' = Au + Bu$$
, $u(0) = u_0$, *B* bounded

integrands of elementary integrals

$$F(\bullet)(\mathbf{v})(\sigma) = e^{(1-\sigma)hA}Be^{\sigma hA}\mathbf{v}$$

$$F(\checkmark)(\mathbf{v})(\sigma) = e^{(1-\sigma_1)hA}Be^{(\sigma_1-\sigma_2)hA}Be^{\sigma_2hA}\mathbf{v}$$

$$F(\checkmark)(\mathbf{v})(\sigma) = e^{(1-\sigma_1)hA}Be^{(\sigma_1-\sigma_2)hA}Be^{(\sigma_2-\sigma_3)hA}Be^{\sigma_3hA}\mathbf{v}$$

• order one: $F(\bullet) \in C^1$

$$F'(\bullet)(v) = e^{(1-\sigma)hA}[B, A]e^{\sigma hA}v, \qquad [B, A] = BA - AB$$

 same regularity condition as for splitting methods (Jahnke, Lubich, 2000; Thalhammer, 2008; Lubich, 2008)

Linear problems – order two



• order two:
$$F(\tau) \in C^{3-\varrho(\tau)}, \, \varrho(\tau) \leq 2$$

$$F''(\bullet)(\mathbf{v})(\sigma) = e^{(1-\sigma)hA}[A, [A, B]]e^{\sigma hA}\mathbf{v}$$

$$F'(\checkmark)(\mathbf{v})(\sigma) = \left[e^{(1-\sigma_1)hA}[B, A]e^{(\sigma_1-\sigma_2)hA}Be^{\sigma_2hA}\mathbf{v}, e^{(1-\sigma_1)hA}Be^{(\sigma_1-\sigma_2)hA}[B, A]e^{\sigma_2hA}\mathbf{v}\right]$$

Summary



- Lawson methods for u' = Au + g(u)
- expansion of exact and numerical solution based on iterated v.o.c. formula
- interprete Lawson methods as multivariate quadrature formulas
- convergence result showing exactly the required regularity assumptions
- for linear problems: same assumptions as for splitting methods
- for semilinear problems: additional terms, not just commutators
- generalization to nonlinear v.o.c. formula possible