Optimal Backward Error & the Dahlquist Test Problem

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Joint work with Yalçin Kaya[2] and Robert H C Moir[1]

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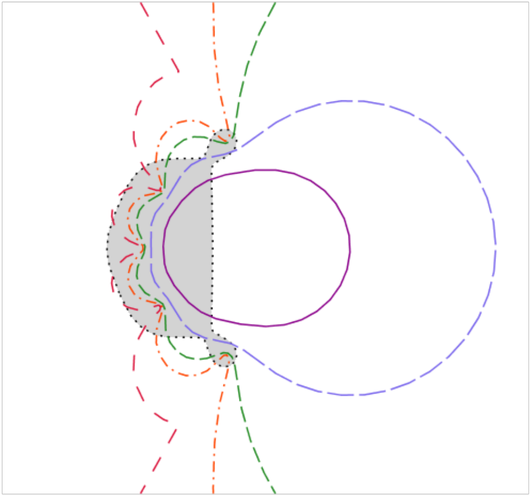


Suppose that you have an initial-value problem (ODE) to solve:

$$\dot{x} = f(t, x), \quad x(t_0) = x_0, \quad t_0 \leq t \leq t_{final}.$$

- Would you bet \$1000 that your numerical solution to *your* initial-value problem was correct?
- What if someone else wrote the solver?
- What if you had an easy way to test the solution before you bet?
- What does "correct" mean anyway?

- Suppose $x_{ref}(t)$ is the "true" reference solution to the IVP $\dot{x} = f(t,x), \quad x(t_0) = x_0$.

We do not know $x_{ref}(t)$ (else why compute?)

- Suppose $z(t)$ is our computed solution, interpolating the *skeleton* (t_k, x_k) which has mesh widths (step sizes) $h_k = t_{k+1} - t_k$.
- The "forward error" is $z(t) - x_{ref}(t)$.
- The "backward error" (residual) is $\Delta = \dot{z}(t) - f(t, z(t))$.

$\Delta(t)$ is computable, and can often be understood or interpreted as a model perturbation: $\dot{z} = f(t, z(t)) + \Delta(t)$.

- The "local error" needs a new concept:

"local reference solution"

the reference solution to $\dot{x} = f(t, x), \quad x(t_k) = x_k$.

- Call these $x_k(t), \quad t_k \leq t \leq t_{k+1}$.
- The "local errors" are $z(t) - x_k(t)$ on $t_k \leq t \leq t_{k+1}$.
- Typically these are largest at t_{k+1}^-.

- Forward error and residual are related by "conditioning" (sensitivity), *e.g.* by

Gröbner-Alexeev nonlinear variation of constants formula

$$z(t) - x_{ref}(t) = \int_{t_0}^{t} G(t, \tau, z, x_{ref})\Delta(\tau)d\tau.$$

- If $\|\Delta(t)\| = O(h^p)$ as $h = mean\ h_k \to 0$ then $\|z - x_{ref}\| = O(h^p)$ also (we say the numerical method has order p).

- J. Wilkinson first popularized backward error in numerical linear algebra.
- He attributed it to Givens, but von Neumann & Goldstine had the notion of "condition number" ("figure of merit").
- Henrici realized the notion was very general.
- Warming & Hyett and then Griffiths & Sanz-Serna looked at "the method of modified equations".
- Zadunaisky invented "defect correction", an iterated improvement scheme using backward error.
- Stetter proved that, asymptotically as $h \to 0$, $\|\Delta\| \sim (\text{local error})/h$.
- Enright, in the 1980s, showed defect (residual) *control* was a viable strategy for RK solvers; Shampine used it for BVP solvers (esp `bvp4c` in MATLAB).
- The book Corless & Fillion uses backward error throughout.

Remark: backward error is not a panacea — there are problems for which small forward error is possible but not backward error.

- Most codes supply interpolants: for graphical output, for event location, for handling delay DE.
- These interpolants should be $O(h^p)$ accurate, but *sometimes aren't*.

Example

In MATLAB, ode45 uses a fifth-order Runge-Kutta Fehlberg formula, but has only a fourth-order interpolant: so $z'(t)$ will only be third-order accurate.
This sometimes overestimates $\Delta(t) := \dot{z}(t) - f(t, z)$.

- Some years ago RMC proposed finding "optimal" interpolants, that minimized

$$\|\Delta\|_2^2 = \frac{1}{h}\int_{t_n}^{t_{n+1}} \Delta^H(\tau)\Delta(\tau)d\tau.$$

- This leads to the Euler-Lagrange equations

$$\begin{aligned} \dot{z} - f(t,z) &= \Delta \\ \dot{\Delta} + J_f^H\Delta &= 0, \end{aligned}$$

  to be solved as a Boundary-Value problem with $z(t_n) = x_n, \quad z(t_{n+1}) = x_{n+1}.$
- This works, but it's not what we'll talk about today.

- YK suggested we look also at minimizing $\|\Delta\|_\infty$, which leads to optimal control problems: find $u(t)$ such that

$$\dot{z} = f(t, z) + u(t)$$

steers $z(t)$ from $z(t_n) = x_n$ to $z(t_{n+1}) = x_{n+1}$ with minimal $\|u\|_\infty$.
- These turn out to be solvable in some cases using the Pontrjagin maximum principle, and in others by using optimization packages such as `AMPL`.
- We are interested in the *relative* optimality:

$$\dot{z} = f(t, z)(1 + \delta(t)).$$

- We'll just do some "baby" optimal control problems here.

- Suppose $f(t,x)$ is scalar, and separable: $f(x,t) = X(x)T(t)$; so that the equation $\dot{z} = f(t,z)(1+\delta(t))$ is also separable.
- Then,

$$\dot{z} = X(z)T(t)(1+\delta(t)) \Rightarrow \frac{dz}{X(z)} = T(t)dt + T(t)\delta(t)dt.$$

- So,

$$\int_{x_n}^{z(t)} \frac{d\zeta}{X(\zeta)} - \int_{t_n}^{t} T(\tau)d\tau = \int_{t_n}^{t} T(\tau)\delta(\tau)d\tau$$

giving the constraint

$$C = \int_{x_n}^{x_{n+1}} \frac{d\zeta}{X(\zeta)} - \int_{t_n}^{t_n+h} T(\tau)d\tau = \int_{t_n}^{t_n+h} T(\tau)\delta(\tau)d\tau.$$

- C is in principle known.

Optimal Interpolants for Optimal Residual (∞-Norm)

- By the triangle inequality,

$$|C| \leq \int_{t_n}^{t_n+h} |T(\tau)| d\tau \quad \cdot \quad \|\delta(t)\|_\infty .$$

- So no matter what control $\delta(t)$ is chosen,

$$\|\delta\|_\infty \geq \frac{|C|}{\int_{t_n}^{t_n+h} |T(\tau)| d\tau} .$$

- By choosing

$$\delta(\tau) = \overline{\text{signum}(T(\tau))} \cdot \frac{C}{\int_{t_n}^{t_n+h} |T(\tau)| d\tau}$$

(signum$(re^{i\theta}) = e^{i\theta}$) this bound is achieved while satisfying the constraint:

$$\int_{t_n}^{t_n+h} T(\tau)\delta(\tau) d\tau = \int_{t_n}^{t_n+h} T(\tau) \frac{\overline{\text{signum}(T(\tau))} \cdot (C)}{\int_{t_n}^{t_n+h} |T(\tau)| d\tau} d\tau = C.$$

- This explicitly gives us our minimum residual (and the optimal interpolant is $z(t)$).
- Note: more general equations need the full maximum principle.

- We've solved a number of examples this way, including $\dot{x} = x^2$, a non-compact example, and $\dot{x} = -\sqrt{x}$ (Torricelli's law, which is not Lipschitz), and several systems.
- We note that this method of assessment is *independent* of the numerical method used: all we need is $(t_n, x_n), \quad (t_n + h, x_{n+1}),$ and the original equation.
- We have examined several such methods.
- Today we'll look at perhaps the simplest interesting problem:

$$\dot{x} = \lambda x, \qquad x(t_n) = x_n.$$

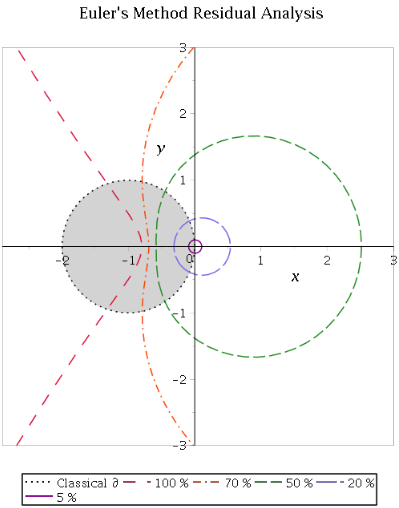
- Without loss of generality we can shift the origin to t_n

$$\dot{x} = \lambda x, \quad x(0) = x_n \quad \text{on } 0 \leq t \leq h.$$

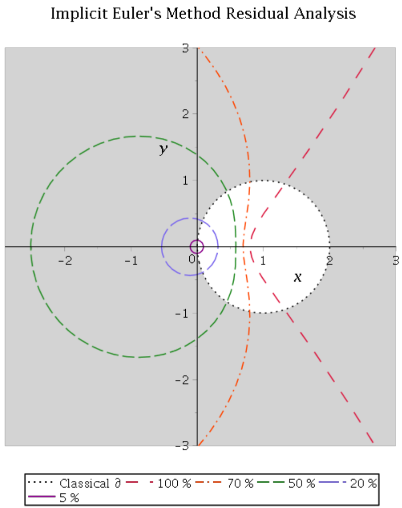
- This is the Dahlquist test problem.
- For $\mathrm{Re}(\lambda) \ll 0$ it is the simplest example of a “stiff” problem.
- It arises also on linearization of nonlinear problems and doing eigenvalue analysis.
- It's more important to numerical analysis than one might think.

- Considering the parameter $\mu = \lambda h$ and the function $R(\mu)$, which is the approximation of the exponential function provided by a given numerical method (the exponential being the solution to the reference problem), we obtain a classical measure of the stability of the numerical method.
- For $|R(\mu)| < 1$, the numerical solution of the Dahlquist test problem is uniformly bounded in $n \geq 0$.
- This determines the classical stability region in the complex plane of the given numerical method.
- These regions give rise to a variety of "familiar diagrams" for familiar numerical methods.

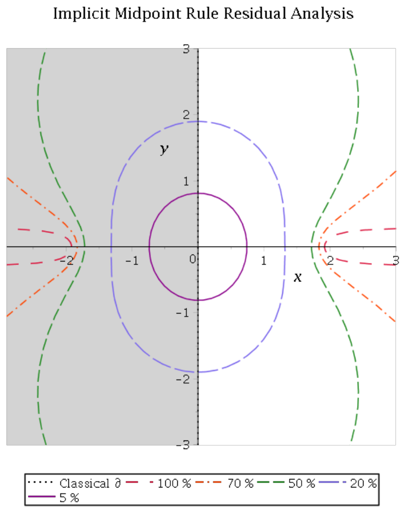
Classical Stability: Euler Method



Classical Stability: Implicit Euler Method

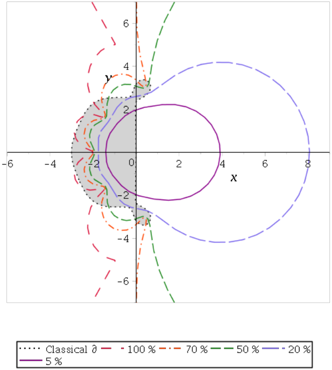


Classical Stability: Implicit Midpoint Rule (Or Any Exactly A-Stable Method)

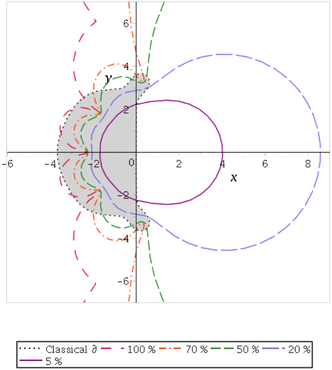


Classical Stability: RKF45

Fourth Order Part RKF45 Method Residual Analysis

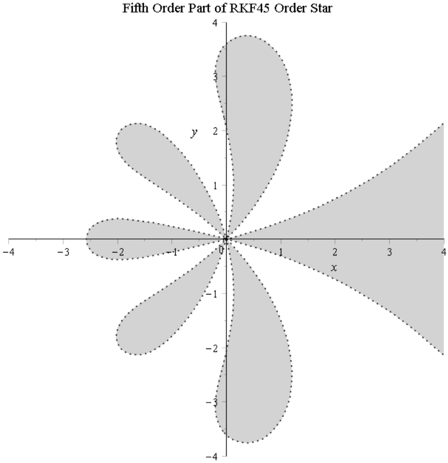


Fifth Order Part RKF45 Method Residual Analysis



RKF45 Order Star

- By considering not $|R(\mu)| < 1$ but the relative forward error $|R(\mu)e^{-\mu}|$ we are led to the theory of "order stars", which considers the regions $A_+ : |R(\mu)e^{-\mu}| > 1, A_0 : |R(\mu)e^{-\mu}| = 1, A_- : |R(\mu)e^{-\mu}| < 1.$



- But we want the relative backward error:
- For $f(x) = \lambda x$, we get $\frac{dz}{z} = \lambda dt + \delta(t)dt$, so

$$\int_{x_n}^{x_{n+1}} \frac{dz}{z} - \lambda \int_{t_n}^{t_n+h} d\tau = \lambda \int_{t_n}^{t_n+h} \delta(\tau)d\tau,$$

or

$$\left|\ln_k\left(\frac{x_{n+1}}{x_n}\right) - \lambda h\right| = \left|\lambda \int_{t_n}^{t_n+h} \delta(\tau)d\tau\right| \leq |\lambda h| \, \|\delta\|_\infty.$$

- So, $\|\delta\|_\infty \geq \left|\frac{1}{\mu}\ln_k(R(\mu)) - 1\right|$, and equality is obtained if

$$\delta(\mu) = \frac{1}{\mu}\ln_k(R(\mu)) - 1.$$

- N.B. $\ln_k a := \ln a + 2\pi ik$

- Indeed this is the exact solution to the *same kind* of problem

$$x_n = R(\mu)^n x_0 = e^{\frac{\ln_k R(\mu)}{h} nh} x_0 .$$

- So,

$$\Lambda = \frac{\ln_k R(\mu)}{h} = \lambda \frac{\ln_k R(\mu)}{\mu}, \quad \dot{y} = \Lambda y!$$

$$y_{n+1} = R(\mu)y_n \qquad \text{e.g. } R(\mu) = 1+\mu \quad \text{Euler}$$
$$\text{or } R(\mu) = (1-\mu)^{-1} \quad \text{Implicit Euler}$$

Then $y_n = R^n(\mu)y_0$ by induction

$$= \mathrm{e}^{n \ln R(\mu)} y_0 \qquad = \mathrm{e}^{n(\ln R(\mu)+2\pi i k)} y_0$$
$$= \mathrm{e}^{n \ln_k R(\mu)} y_0 \qquad = \mathrm{e}^{nh\mu \frac{\ln_k R(\mu)}{\mu}} y_0$$
$$= \mathrm{e}^{\lambda t_n \cdot (1+\delta)} y_0 \quad \text{if } 1+\delta = \frac{\ln_k R(\mu)}{\mu}$$

$\therefore$ interpolant $z(t) = \mathrm{e}^{\lambda(1+\delta)t} y_0$ satisfies

$$\dot{z}(t) = \lambda(1+\delta)z(0) = y_0 \,.$$

Define:

$$K_R(\mu) = \mathrm{round}\left(\frac{\mathrm{Im}(\mu - \ln R(\mu))}{2\pi}\right)$$

(a kind of unwinding number, cf $K(z) = \frac{z - \ln e^z}{2\pi i} = \lceil \frac{\mathrm{Im}(z) - \pi}{2\pi} \rceil$)

Theorem:

$$K_R(\mu) = \arg_k \min |\delta|$$

Proof:

$$\begin{aligned}
\arg_k \min |\delta| &= \frac{\arg_k \min |\ln_k(R\mu)) - \mu|}{\mu} \\
&= \arg_k \min \left| \ln_k(\rho e^{i\theta}) - (\sigma + i\tau) \right| \\
&= \arg_k \min |\ln \rho - \sigma + i(\theta + 2\pi i k - \tau)|
\end{aligned}$$

k cannot affect the real part, and minimizes the imaginary part exactly when k is the nearest integer to $\frac{\tau-\theta}{2\pi}$. QED.

N.B. there may be more than one such k but they give the same δ .

- This will give us a *quantitative* assessment of the quality of the method $x_{n+1} = R(\mu)x_n$.

Example: Euler Method

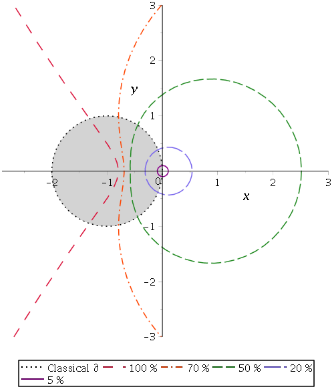
$$x_{n+1} = x_n + h\lambda x_n = (1 + h\lambda)x_n = (1 + \mu)x_n.$$

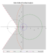
- Now, $R(\mu) \approx e^{\mu}$ so $\delta = \frac{\ln_k R(\mu)}{\mu} - 1 \approx 0$, but the *size* of δ tells us the relative backward error
- Note: In general $|\delta| = O(h^p)$ as $h \to 0$, so this is a nonlinear pseudospectral problem (plot contours of $|\delta|$ in the complex μ plane).

- If $|\delta| > 1$ then the problem we've solved is more than 100% different to the problem we wanted to solve.
- The curve $|\delta| = 1$ gives a qualitative upper limit: μ outside that region means the solution (decaying or not) is pretty lousy (probably worthless).
- If $|\delta| < 0.05$ then we've solved a problem within 5% of the one we wanted to (analogous to the 95% confidence limit!)
- If $|\delta| < \varepsilon$ (user's tolerance) then the solver has done its job [you win your bet!]

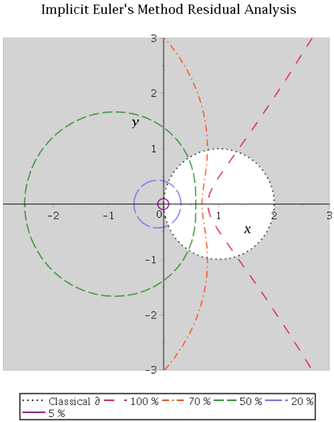
Euler Method

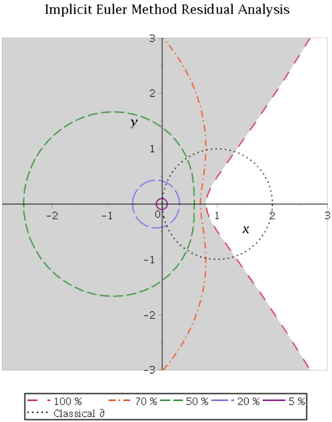
Euler's Method Residual Analysis



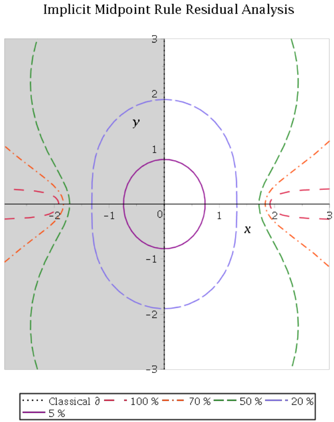


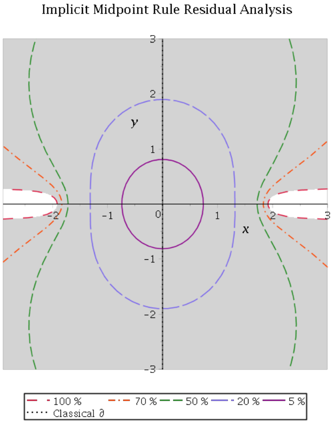
Implicit Euler Method





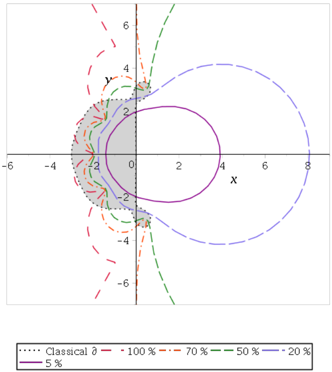
Implicit Midpoint Rule



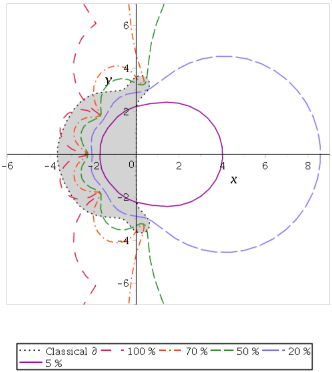


RKF45

Fourth Order Part RKF45 Method Residual Analysis



Fifth Order Part RKF45 Method Residual Analysis



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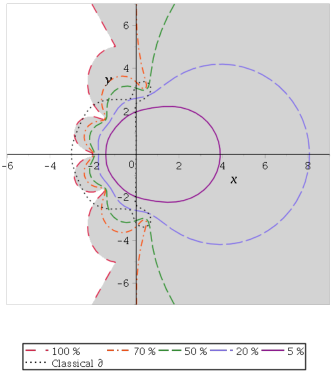

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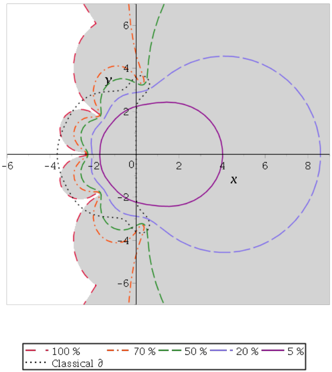
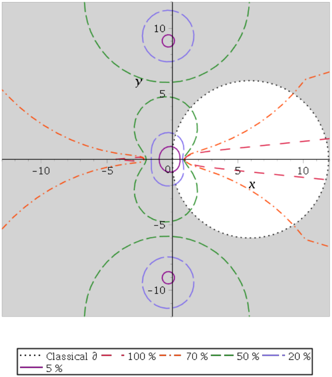
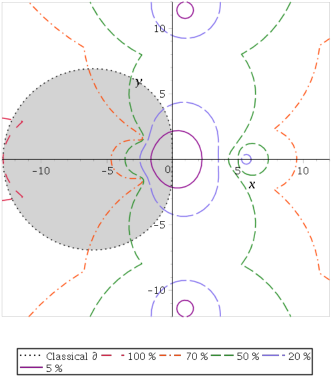


SDIRK 2-Stage 3rd Order

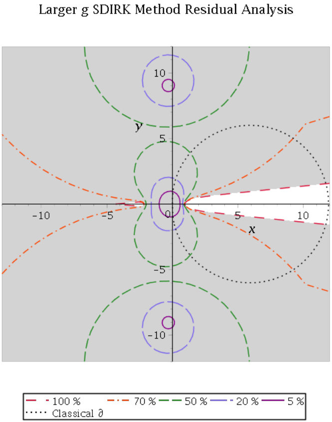
Larger g SDIRK Method Residual Analysis

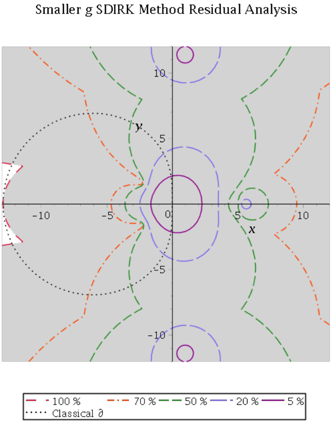


Smaller g SDIRK Method Residual Analysis

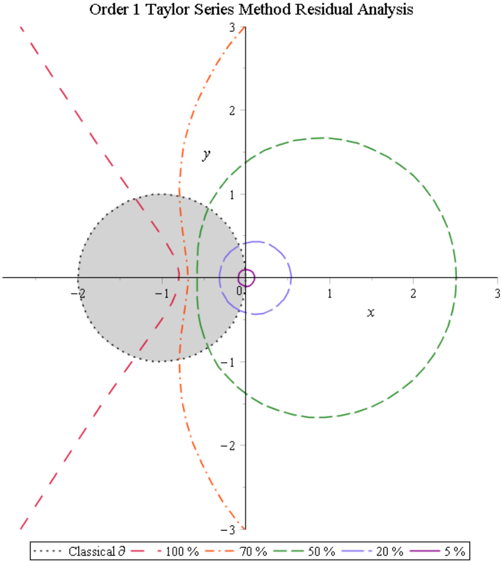


SDIRK 2-Stage 3rd Order





High Order Talyor Series Methods



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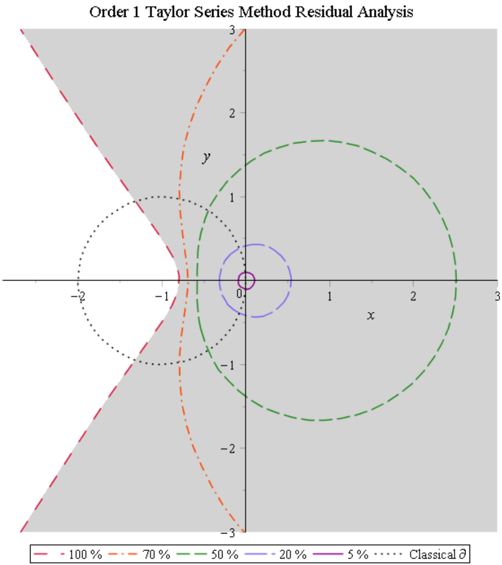
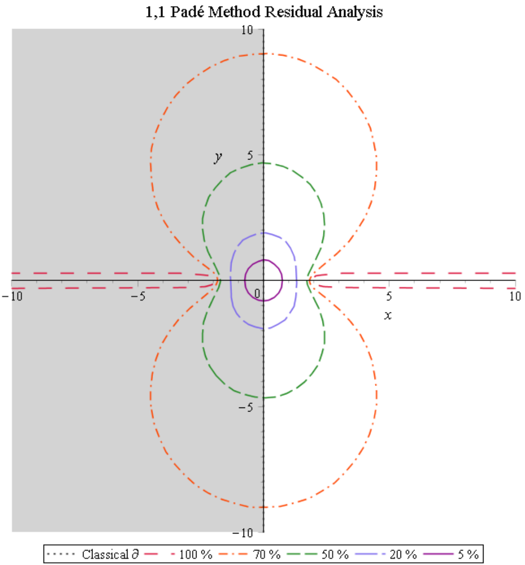
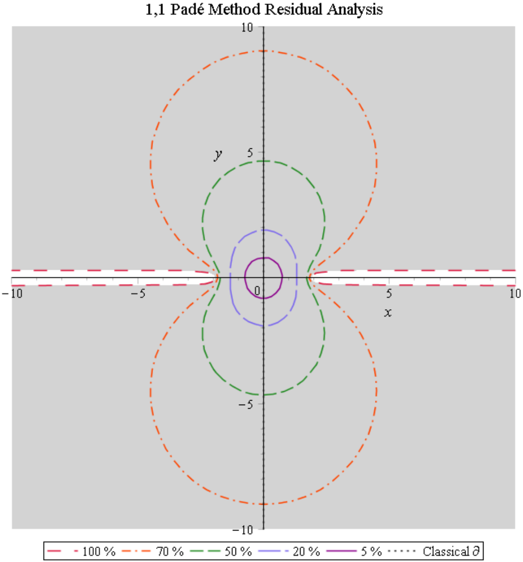


High Order Diagonal Padé Methods



High Order Diagonal Padé Methods



Future work on this project will include:

- look at more methods, more pictures, more systems
- try to test the "preference change" predictions
- look at symplectic methods
- prove some things about the pictures

Calvo, MP, Murua, A, & Sanz-Serna, JM. 1994. Modified equations for ODEs. *Contemporary Mathematics*, **172**, 63–63.

Corless, Robert M. 1994. Error backward. *Contemporary Mathematics*, **172**, 31–31.

Enright, Wayne H. 1989. A new error-control for initial value solvers. *Applied Mathematics and Computation*, **31**, 288–301.

Enright, Wayne H, & Hayes, Wayne B. 2007. Robust and reliable defect control for Runge-Kutta methods. *ACM Transactions on Mathematical Software (TOMS)*, **33**(1), 1.

Grcar, Joseph F. 2011. John von Neumann's analysis of Gaussian elimination and the origins of modern Numerical Analysis. *SIAM review*, **53**(4), 607–682.

Griffiths, DF, & Sanz-Serna, JM. 1986. On the scope of the method of modified equations. *SIAM Journal on Scientific and Statistical Computing*, **7**(3), 994–1008.

Henrici, Peter. 1964. *Elements of numerical analysis*. Wiley.

Turing, Alan M. 1948. Rounding-off errors in matrix processes. *The Quarterly Journal of Mechanics and Applied Mathematics*, **1**(1), 287–308.

Von Neumann, John, & Goldstine, Herman H. 1947. Numerical inverting of matrices of high order. *Bulletin of the American Mathematical Society*, **53**(11), 1021–1099.

Warming, RF, & Hyett, BJ. 1974. The modified equation approach to the stability and accuracy analysis of finite-difference methods. *Journal of computational physics*, **14**(2), 159–179.

Wilkinson, James Hardy. 1963. *Rounding errors in algebraic processes*. Prentice-Hall Series in Automatic Computaton. Prentice-Hall.

Thank You!

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