Rosenbrock Methods

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We start with a diagonally IRK method

$$k_i^n = hf(y^n + \sum_{j=1}^{i-1} \alpha_{ij} k_j^n + \alpha_{ii} k_i), \quad i = 1, \cdots, s$$

$$y^{n+1} = y^n + \sum_{j=1}^{s} b_j k_j$$

applied to the autonomous differential equation

$$y' = f(y).$$

Linearizing the first formula yields

$$k_i^n = hf(y^n + \sum_{j=1}^{i-1} \alpha_{ij} k_j^n) + hf'(y^n + \sum_{j=1}^{i-1} \alpha_{ij} k_j^n) \alpha_{ii} k_i^n, \quad i = 1, \cdots, s.$$

$$k_i^n = hf(y^n + \sum_{j=1}^{i-1} \alpha_{ij} k_j^n) + hf'(y^n + \sum_{j=1}^{i-1} \alpha_{ij} k_j^n)\alpha_{ii} k_i^n, \quad i = 1, \cdots, s.$$

Replacing the Jacobians with $J = f'(y^n)$ for the computational cost:

$$k_i^n = hf(y^n + \sum_{j=1}^{i-1} \alpha_{ij} k_j^n) + hJ\alpha_{ii} k_i^n, \quad i = 1, \cdots, s.$$

and introducing additional linear combinations of terms to gain further freedom:

$$k_i^n = hf(y^n + \sum_{j=1}^{i-1} \alpha_{ij} k_j^n) + hJ \sum_{j=1}^{i} \gamma_{ij} k_j^n, \quad i = 1, \cdots, s$$

Definition:

An s-stage Rosenbrock method is given by the formulas

$$k_i^n = hf(y^n + \sum_{j=1}^{i-1} \alpha_{ij} k_j^n) + hJ \sum_{j=1}^{i} \gamma_{ij} k_j^n, \quad i = 1, \cdots, s$$

$$y^{n+1} = y^n + \sum_{j=1}^{s} b_j k_j$$

where α_{ij}, γ_{ij}, b_i are the determining coefficients and $J = f'(y^n)$.

Non-autonomous problem:

The equation

$$y' = f(x, y)$$

can be converted to autonomous form by adding $x' = 1$. So the s-stage Rosenbrock method for non-autonomous case could be written as

$$k_i^n = hf(x^n + \alpha_i h, y^n + \sum_{j=1}^{i-1} \alpha_{ij} k_j^n) + \gamma_i h^2 \frac{\partial f}{\partial x}(x^n, y^n) + h \frac{\partial f}{\partial y}(x^n, y^n) \sum_{j=1}^{i} \gamma_{ij} k_j^n$$

$$y^{n+1} = y^n + \sum_{j=1}^{s} b_j k_j$$

where the additional coefficients are given by

$$\alpha_i = \sum_{j=1}^{i-1} \alpha_{ij}, \quad \gamma_i = \sum_{j=1}^{i} \gamma_{ij}.$$

Implicit differential equations:
Suppose the problem is of the form

$$My' = f(x, y)$$

where M is a constant, nonsingular matrix. Then applying an s-stage Rosenbrock method, we can get

$$Mk_i^n = hf(y^n + \sum_{j=1}^{i-1} \alpha_{ij} k_j^n) + hJ \sum_{j=1}^{i} \gamma_{ij} k_j^n, \quad i = 1, \cdots, s$$

$$y^{n+1} = y^n + \sum_{j=1}^{s} b_j k_j.$$

Then the inversion of M is advoided.

Applying the Rosenbrock method to the test equation $y' = \lambda y$, then the numerical solution becomes $y^{n+1} = R(h\lambda)y^n$ with

$$R(z) = 1 + zb^T(I - zB)^{-1}e_n$$

where

$$b^T = (b_1, \cdots, b_s), \quad B = (\alpha_{ij} + \gamma_{ij})_{i,j=1}^{s}.$$

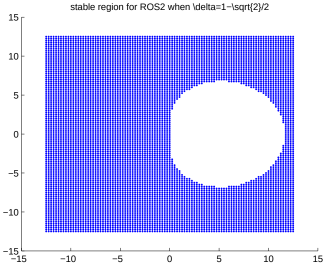
Since B is a lower triangular matrix, the stability function can be investigated similarly as for DIRK methods.

Examples of L-stable Rosenbrock methods:

$\gamma = 2.928932188134e-01$	
$\alpha_{21} = 1.000000000000e+00$	$\gamma_{21} = -5.857864376269e-01$
$b_1 = 5.000000000000e-01$	$b_2 = 5.000000000000e-01$

Table: ROS2

A-stability and L-stability



And you can also do the time step control with embeded methods [6]:

$\gamma = 4.358665215084e-01$	
$\alpha_{21} = 6.666666666666e-01$	$\gamma_{21} = 3.635068368900e-01$
$\alpha_{31} = 6.666666666666e-01$	$\gamma_{31} = -8.996866791992e-01$
$\alpha_{32} = 6.666666666666e-01$	$\gamma_{32} = -1.537997822626e-01$
$b_1 = 2.500000000000e-01$	$\hat{b}_1 = 7.467047032740e-01$
$b_2 = 2.500000000000e-01$	$\hat{b}_2 = 1.144064078371e-01$
$b_3 = 5.000000000000e-01$	$\hat{b}_3 = 1.388888888888e-01$

Table: ROS3w (with a strongly A-stable 2rd order method embeded)

s-stage Rosenbrock method:

$$k_i^n = hf(y^n + \sum_{j=1}^{i-1} \alpha_{ij} k_j^n) + hJ \sum_{j=1}^{i} \gamma_{ij} k_j^n, \quad i = 1, \cdots, s$$

$$y^{n+1} = y^n + \sum_{j=1}^{s} b_j k_j.$$

Theorem 7.4 [5]:
A Rosenbrock method with $J = f'(y_0)$ is of order p iff

$$\sum_j b_j \Phi_j(t) = \frac{1}{\gamma(t)}, \quad \forall t \in T(p).$$

Therefore, we can apply the Rooted trees method to derive the order conditions just as what we do for Runge-Kutta methods.

The only difference is that at singly-branched vertices of the corresponding trees α_{jk} is replaced by $\alpha_{jk} + \gamma_{jk}$. The conditions up to order 4 are showed as in Table 3.

order	RHS($=1/\gamma(t)$)	$\Phi_j(t)$
1	1	1
2	$\frac{1}{2}$	$\sum_k(\alpha_{jk} + \gamma_{jk})$
3	$\frac{1}{3}$	$\sum_{k,l} \alpha_{jk}\alpha_{jl}$
3	$\frac{1}{6}$	$\sum_{k,l}(\alpha_{jk} + \gamma_{jk})(\alpha_{kl} + \gamma_{kl})$
4	$\frac{1}{4}$	$\sum_{k,l,m} \alpha_{jk}\alpha_{jl}\alpha_{jm}$
4	$\frac{1}{8}$	$\sum_{k,l,m} \alpha_{jk}(\alpha_{kl} + \gamma_{kl})\alpha_{jm}$
4	$\frac{1}{12}$	$\sum_{k,l,m}(\alpha_{jk} + \gamma_{jk})\alpha_{kl}\alpha_{km}$
4	$\frac{1}{24}$	$\sum_{k,l,m}(\alpha_{jk} + \gamma_{jk})(\alpha_{kl} + \gamma_{kl})(\alpha_{lm} + \gamma_{lm})$

Table: order conditions for original Rosenbrock

s-stage Rosenbrock method:

$$k_i^n = hf(y^n + \sum_{j=1}^{i-1} \alpha_{ij} k_j^n) + hJ \sum_{j=1}^{i} \gamma_{ij} k_j^n, \quad i = 1, \cdots, s$$

$$y^{n+1} = y^n + \sum_{j=1}^{s} b_j k_j.$$

When $\gamma_{ii} = \gamma$ for all i, we only need to do the LU decomposition once. Then the order conditions can be derived similarly as IRK methods, except that these diagonal γ appear only for singly-branched vertices.

The conditions up to order 4 are showed as in Table 4.

order	RHS	$\Phi_j(t)$
1	1	1
2	$\frac{1}{2} - \gamma$	$\sum_k'(\alpha_{jk} + \gamma_{jk})$
3	$\frac{1}{3}$	$\sum_{k,l}' \alpha_{jk}\alpha_{jl}$
3	$\frac{1}{6} - \gamma + \gamma^2$	$\sum_{k,l}'(\alpha_{jk} + \gamma_{jk})(\alpha_{kl} + \gamma_{kl})$
4	$\frac{1}{4}$	$\sum_{k,l,m}' \alpha_{jk}\alpha_{jl}\alpha_{jm}$
4	$\frac{1}{8} - \frac{\gamma}{3}$	$\sum_{k,l,m}' \alpha_{jk}(\alpha_{kl} + \gamma_{kl})\alpha_{jm}$
4	$\frac{1}{12} - \frac{\gamma}{3}$	$\sum_{k,l,m}'(\alpha_{jk} + \gamma_{jk})\alpha_{kl}\alpha_{km}$
4	$\frac{1}{24} - \frac{\gamma}{2} + \frac{3\gamma^2}{2} - \gamma^3$	$\sum_{k,l,m}'(\alpha_{jk} + \gamma_{jk})(\alpha_{kl} + \gamma_{kl})(\alpha_{lm} + \gamma_{lm})$

Table: order conditions for simplified Rosenbrock 1

s-stage Rosenbrock method:

$$k_i^n = hf(y^n + \sum_{j=1}^{i-1} \alpha_{ij} k_j^n) + hJ \sum_{j=1}^{i} \gamma_{ij} k_j^n, \quad i = 1, \cdots, s$$

$$y^{n+1} = y^n + \sum_{j=1}^{s} b_j k_j.$$

In Rosenbrock, the Jacobian matrix $J = \frac{\partial f}{\partial y}$ must be evaluated at every step, which can make the computations costly. So people searched for Rosenbrock methods which assure classical order for all approximations A of $\frac{\partial f}{\partial y}$, and this kind of methods are called **Methods with Inexact Jacobian** or W-Methods for short.

The order conditions up to order 3 are showed as in Table 5.

order	RHS	$\Phi_j(t)$
1	1	1
2	$\frac{1}{2}$	$\sum_k \alpha_{jk}$
2	0	$\sum_k \gamma_{jk}$
3	$\frac{1}{3}$	$\sum_{k,l} \alpha_{jk}\alpha_{jl}$
3	$\frac{1}{6}$	$\sum_{k,l} \alpha_{jk}\alpha_{kl}$
3	0	$\sum_{k,l} \alpha_{jk}\gamma_{kl}$
3	0	$\sum_{k,l} \gamma_{jk}\alpha_{kl}$
3	0	$\sum_{k,l} \gamma_{jk}\gamma_{kl}$

Table: order conditions for W-Rosenbrock

Here we compare ROS2 and Crank-Nicolson method for a Burger's equation with the following form

$$u_t + (\frac{u^2}{2})_x = \epsilon u_{xx} + g(u, x, t)$$

where

$$g(u, x, t) = (\cos(x+t) - \cos^2(x+t) + \sin(x+t))u + \cos(x+t)u^2$$

with the initial condition

$$u(x, 0) = e^{\sin(x)}.$$

The accurate solution is computted by setting $\Delta t = 0.0001$. Here we discretize u in space with 1000 points. The computing region is $[-\pi, \pi]$, with end time $T = 1.0$.

When $\epsilon = 1.0$, the L-2 errors are listed in table 6 and the time cost are listed in table 7.

Table: L-2 error at $T = 1.0$, $\Delta x = 2\pi/999$, $\Delta t = T/N$

N	10	20	40	80	160
ROS2	1.357e-03	2.951e-04	6.574e-05	1.279e-05	4.413e-06
CN	7.354e-04	1.806e-04	4.203e-05	8.590e-06	5.221e-06

Table: time cost (seconds) at $T = 1.0$, $\Delta x = 2\pi/999$, $\Delta t = T/N$

N	10	20	40	80	160
ROS2	7	13	28	55	106
CN	30	48	85	148	245

To sum up, Rosenbrock methods have the following advantages

- Do not need iterations for each step.
- Can be made L-stable, suitable for stiff problems.
- Easily derived order conditions with rooted trees.

and disadvantages

- Problems at dealing with boundary conditions for interior stages.

- H.H. Rosenbrock, Some general implicit processes for the numerical solution of differential equations, Comput. J. , 5, 329330, 1963.
- J.G. Verwer, An analysis of Rosenbrock methods for nonlinear stiff initial value problems, SIAM J. Numer. Anal. 19, 155-170, 1982.
- J.G. Verwer, Instructive experiments with some Runge-Kutta-Rosenbrock methods, Comp. and Math. with Appls. 7, 217-229, 1982.
- J.G. Verwer, S. Scholz, J.G. Blom and M. Louter-Nool, A class of Runge-Kutta-Rosenbrock methods for stiff differential equations, ZAMM 63, 13-20, 1983.

- E. Hairer and G. Wanner, Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Equations, Springer Series in Computational Mathematics 14, Springer Verlag, 2nd edition, 1996.
- J.Rang and L.Angermann, New Rosenbrock W-Methods of Order 3 for Partial Differentail Algebraic Equations of Index 1, BIT Numerical Mathematics 45, 761-787, 2005.