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Abstract: *We discuss numerical results obtained when computing one-dimensional integral manifolds with Runge-Kutta type methods.*

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Keywords: differential algebraic equations, integral manifolds, Runge-Kutta methods.

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1 Introduction

We shall consider numerical results obtained with the methods analysed in [8]. For a general background we refer to [9].

2 Numerical implementation

The equation to be solved is given in form

$$f(x,\, y,\, y_1,\, y_2,\, \ldots,\, y_q) = 0 \tag{2.1}$$

where $f : \mathbb{R}^m \to \mathbb{R}^k$, $y \in \mathbb{R}^n$ and subscripts denote derivatives; we denote the components of y by upper indices. Here $k \geq n$. Note especially that we allow $k > n$.

There are three subproblems in implementing the algorithm:

1. Given a point $p \in M$, compute the distribution $\mathcal{D}_p$
2. Step size control
3. Orthogonal projection to M.

All of these reduce to fairly standard numerical problems. The implementation was done on Maple V. It would probably be more efficient to produce e.g. Fortran code from the Maple procedures, but this will be considered in a future paper.

2.1 Computing the distribution

As it is seen in [9], the distribution $\mathcal{D}_p$ can be computed as the nullspace of the following $(k + nq) \times (nq + n + 1)$ matrix A:

$$\begin{pmatrix} v & I_{nq} & 0_{nq\times n} \\ & df_p & \end{pmatrix}$$

where $v = -\pi(p)$ where π is the projection picking up components corresponding to $(y_1,\, y_2,\, \ldots, y_q)$. It can be further reduced to computing the nullspace of the $k \times (1 + n)$-matrix:

$$\begin{pmatrix} A_1 - A_2 v & A_3 \end{pmatrix}$$

where $\begin{pmatrix} A_1 & A_2 & A_3 \end{pmatrix}$ is a suitable partition of the jacobian df_p: the sizes of matrices A_j are $k \times 1$, $k \times nq$, $k \times n$, respectively.

When computing numerically the nullspace, we use the singular value decomposition $U\Sigma V^T$ for the matrix above and take the last column of V, which corresponds to the smallest (= zero) singular value. However, often we are able to find an explicit formula for the nullspace.

2.2 Step size control

Here we have used two standard techniques [5]: either take two sequential steps with stepsize h and compare the result with one step with stepsize $2h$, or Fehlberg-like: compare two parallel steps, the other of order p and the other of order $p+1$.

We implemented explicit methods: classical RK4, Fehlberg 4(5) (denote this by RKF45), Dopri 5(4). In case of RK4 the "$2*h$ compared to $2h$" was used.

2.3 Projection

Projection was done by chord Newton iteration. The needed jacobian was evaluated every third step and its $LU-$decomposition is used. Initial point is selected either as

$$\begin{cases} q_{init} = p + hV_p \\ \mu_{init} = 0 \end{cases} \tag{2.2}$$

or yet better as

$$\begin{cases} q_{init} = p + hV_p - (df_p)^t \mu_2 \, h^2 \\ \mu_{init} = \mu_2 \, h^2 = \left(df_p (df_p)^t\right)^{-1} d^2 f_p(V_p,\, V_p) h^2/2 \end{cases} \tag{2.3}$$

The initial point in (2.2) is of order $O(h^2)$ and in (2.3) of order $O(h^3)$. In the numerical examples we use the initial point (2.3). Although it was not extensively studied, this seemed to reduce the number of needed Newton iterations.

Here the h^2-coefficient has an interesting geometrical interpretation:

$$|(df_p)^t \mu_2| = \frac{1}{2} \cdot (\text{normal curvature at } p),$$

see [9]. In the latter case evaluation of $d^2 f$ is needed, which can be considerably slow for large system.

Fortunately this might be overcome by automatic differentiation. But this is a topic of future research and we refer to [2] for more information on this subject.

However, in these moderate size examples we construct $d^2 f$ analytically so only a function evaluation is needed.

Note that $d^2 f$ is used also in the chord Newton.

3 Examples

In this section we study 4 examples. Two of them are hamiltonian and two otherwise interesting. It is well known [7] that in case of hamiltonian systems the symplectic Runge-Kutta methods are superior. However, we have not implemented a symplectic method, mainly because the theory for the symplecticity of the integrator is not directly applicable to our method.

This would require further inspection and will be a topic of future research. At this stage we are interested mainly in the behaviour of 'the most classical' Runge-Kutta integrators in context of our method.

3.1 A simple example

Let us look at a simple system in $J_1(\mathbb{R} \times \mathbb{R})$:

$$y' - 3y - 2x^2 = 0 \tag{3.1}$$

whose explicit solution with initial point $y(0) = 2$ is

$$y(x) = -x^2 - \frac{2}{3}x - \frac{2}{9} + \frac{20}{9}e^{3x}.$$

The motivation for this example is to test the order of the method Dopri5. Note that the theory is so far only up to order 4. We would like to test numerically if the theory could be extended also to higher orders. We compute for $x = 0..0.01$ with constant stepsize $h = 2^{-k}$ where $k \in \{6, 7, \ldots, 13\}$.

The result is encouraging, the order really seems to be 5. In figure 3.1 is shown in log-log scale the errors at $x = 0.002$ and $x = 0.01$. The slopes are 4.836 and 4.952, respectively. At $h = 2^{-13}$ one can see the effect of round-off errors, the computations were done with 30 decimals. Without the points where $h = 2^{-13}$ the slopes would be 5.008 and 5.011, respectively.

It is tempting to conjecture that the main result of [8] can be extended to all orders, i.e. there would be no new order conditions!

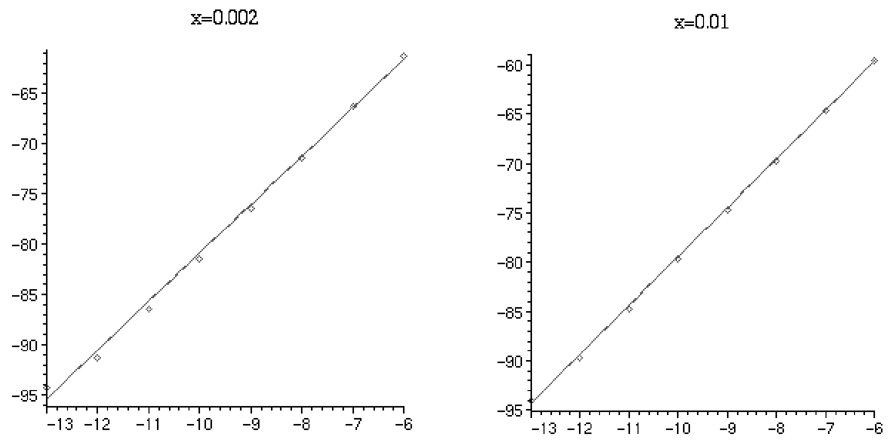

Figure 3.1: Testing the order of dopri5(4).

3.2 Henon-Heiles system

The equations of this famous example from astronomy are:

$$\begin{cases} y^1_2 + y^1 + 2y^1y^2 = 0 \\ y^2_2 + y^2 + (y^1)^2 - (y^2)^2 = 0 \\ \frac{1}{2}\left|y_1\right|^2 + \frac{1}{2}\left|y\right|^2 + (y^1)^2y^2 - \frac{1}{3}(y^2)^3 - a = 0 \end{cases} \tag{3.2}$$

The computation is reduced [9] to:

$$\begin{cases} \frac{1}{2}\left|y_1\right|^2 + \frac{1}{2}\left|y\right|^2 + (y^1)^2y^2 - \frac{1}{3}(y^2)^3 - a = 0 \\ \mathcal{D} = \operatorname{span}(V) \\ V = \left(1, y^1_1, y^2_1, -y^1 - 2y^1y^2, -y^2 - (y^1)^2 + (y^2)^2\right) \end{cases} \tag{3.3}$$

where a is the constant energy. We are interested in quasiperiodic motion, which is achieved by the initial point $(x, y, y_1) = (0, 0.12, 0.12, 0.12, 0.12)$. We take the Poincaré section at the hyperplane $y^1 = 0$ and look at $(y^2,\, y^2_1)$.

We compute 'approximately two rounds' in the Poincaré section, which means taking $x = 0..1100$ and hence about 340 points in the section. The point in the section is chosen by Hermite interpolation between points $p_m\, p_{m+1}$ which are sequential such that $\operatorname{sgn}(y^1)$ changes.

Results: in dopri5 we used the 4^{th} order point as the new starting point for the next step. Although it was not extensively studied, it seemed like using 5^{th} order point required so small tolerance that proceeding along the solution was actually slower than in the 4^{th} order case.

Dopri5 was clearly more efficient than RKF45. Surprisingly, also RK4 was clearly better than RKF45, despite the more elementary step size control. RKF45 required very small stepsize to produce qualitatively correct solution, it was not reasonable to compute even one round. Compared to this Dopri5 and RK4 used quite big steps. Some results of computations are in table 1.

	toler	x=110	x=550	x=1100
Dopri5(4) 4^{th} order pt	$5 \cdot 10^{-5}$	186	920	1837
Dopri5(4) 5^{th} order pt	$1 \cdot 10^{-5}$	242	1201	2404
Dopri5(4) 4^{th} order pt	$5 \cdot 10^{-6}$	268	1373	2722
RK4	$5 \cdot 10^{-4}$	568	2897	5801

Table 1: Some results of Hénon-Heiles (3.3): number of steps.

The qualitative performance of RKF45 did not depend on using local extrapolation.

On the left of figure 3.2 is the result with dopri5, tol.= $5 \cdot 10^{-5}$. 1840 points was needed. With bigger tolerances the algorithm rejected considerably more points. By looking at the figure, the result is slightly less 'uniformly distributed' than in the following RK4 case.

On the right of figure 3.2 is the result with RK4, tol.= $5 \cdot 10^{-4}$. 5800 points was needed. It is interesting to compare these two figures: the points in the sections are clearly not at same places, but the shapes of the sections are still the same.

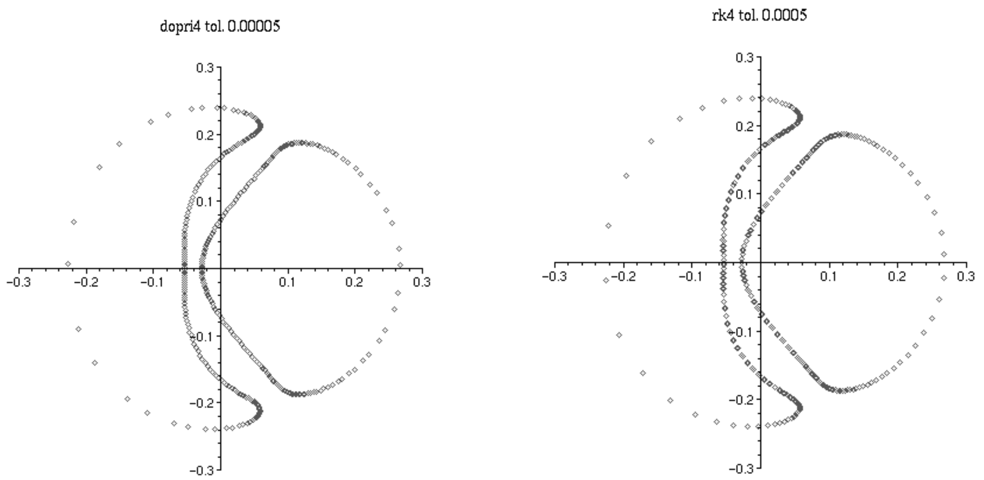

Figure 3.2: Poincaré sections in the (y^2, y^2_1)-plane for the Henon-Heiles system (3.3).

In the light of the RKF45 case, it seems that the traditional step size controlling methods need some revision in the case of our method.

3.3 Stiff pendulum

This is a pendulum with massless, stiff spring and a mass of 1 unit at the end of the spring. The rest length of the spring and the gravitational constant are taken to be 1. The equations are:

$$\begin{cases} y^1_2 + y^1 y^3 = 0 \\ y^2_2 + y^2 y^3 + 1 = 0 \\ \left((y^1)^2 + (y^2)^2\right)\left(\varepsilon^2 y^3 - 1\right)^2 - 1 = 0 \\ \varepsilon^2 y^3_1 + \left(y^1 y^1_1 + y^2 y^2_1\right)\left(\varepsilon^2 y^3 - 1\right)^3 = 0 \\ \left(\varepsilon^2 y^3 - 1\right)\varepsilon^2 y^3_2 - 3\varepsilon^4 (y^3_1)^2 \\ \quad + \left((y^1_1)^2 + (y^2_1)^2 - y^2\right)\left(\varepsilon^2 y^3 - 1\right)^4 - y^3\left(\varepsilon^2 y^3 - 1\right)^2 = 0 \end{cases} \tag{3.4}$$

and the computation in reduced form [9]:

$$\begin{cases} \left((y^1)^2 + (y^2)^2\right)\left(\varepsilon^2 y^3 - 1\right)^2 - 1 = 0 \\ \mathcal{D} = \operatorname{span}(V) \\ V = \left(1, y^1_1, y^2_1, -\left(y^1 y^1_1 + y^2 y^2_1\right)\left(\varepsilon^2 y^3 - 1\right)^3/\varepsilon^2, -y^1 y^3, -y^2 y^3 - 1\right) \end{cases} \tag{3.5}$$

We investigate the cases $\varepsilon \in \{0.1,\, 0.01\}$.

Let us choose first $\varepsilon = 0.01$ and use the initial point $(0, 0.85, 0, -1765, 0, 0)$, which is not exactly on the manifold but close enough: then $f = 0.00005$. This initial point will quickly be iterated to correct manifold. We compute $x = 0..1.5$.

Dopri5 is, as in previous example, clearly more efficient than RKF45. The latter has trouble keeping the solution qualitatively correct, it suffers from dissipativity (figure 3.3) for all reasonable stepsizes. Some results of computations are in table 2.

	toler	$x = 0.5$	$x = 1.5$
Dopri5(4)	10^{-4}	357	1141
Dopri5(4)	10^{-5}	685	2051
RK4	10^{-2}	643	1931
RK4	10^{-3}	957	2857

Table 2: Stiff pendulum (3.5) $\varepsilon = 0.01$, number of steps.

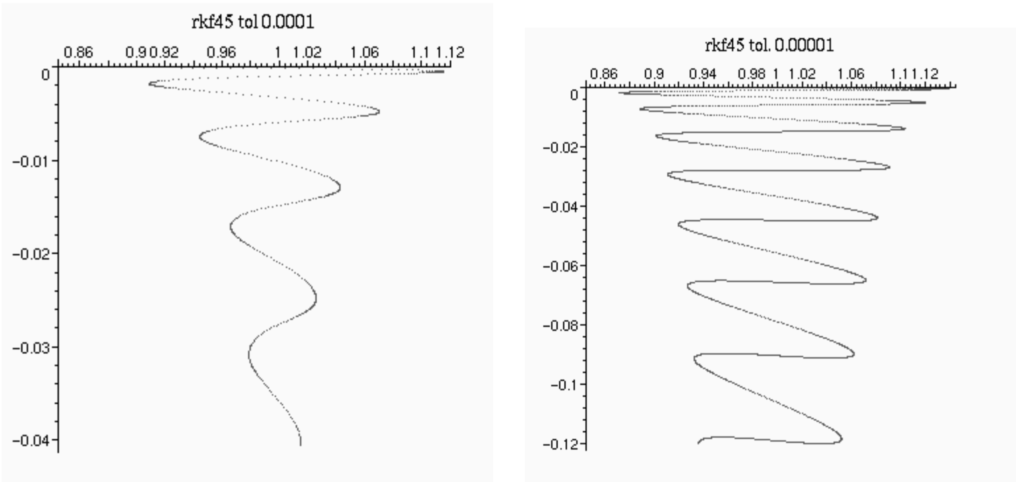

Figure 3.3: Dissipativity of RKF45 in stiff pendulum (3.5), $\varepsilon = 0.01$.

Comparing dopri5 and RK4: on the left of figure 3.4 is the result with dopri5 tol. $= 10^{-4}$, we use the usual 5^{th} order point as the new point on solution. 1141 points was needed. With tolerances bigger than that, dopri5 lost the qualitatively correct behaviour. With tolerances 10^{-6} or smaller, the propagation along the solution was painfully slow.

In RK4 the computed solution has good quality even with 'big' tolerances. Hence in this example RK4 easily beats RKF45. RK4 is also more reliable but slower than dopri5, which hopefully (to be seen in the near future...) is of higher order.

On the right of figure 3.4 is the result with RK4 tol. $= 10^{-2}$, 1931 points was needed. In dopri5 the effect of tolerance is clearly more visible than in RK4 case.

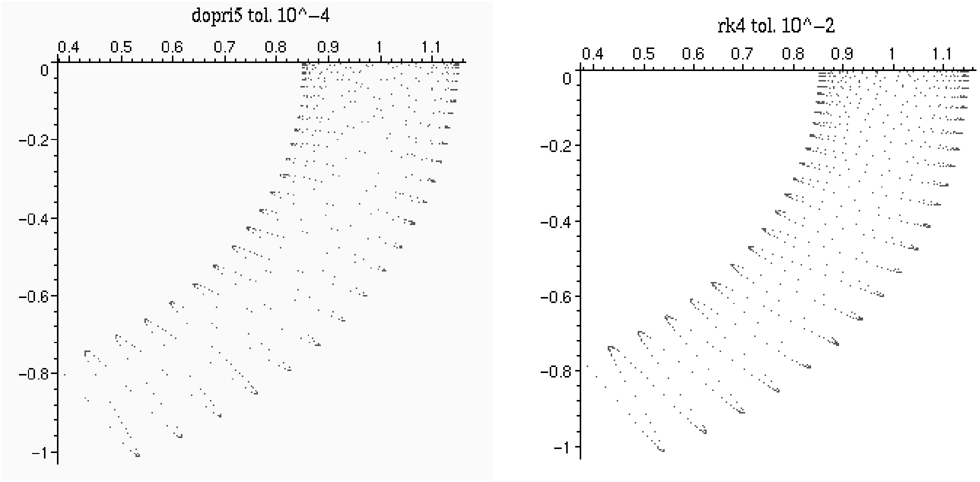

Figure 3.4: Stiff pendulum (3.5) $\varepsilon = 0.01$, $x = 0...1.5$.

Let us choose then $\varepsilon = 0.1$ and the initial point $p_0 = (0,\ .85,\ 0,\ -17.65,\ 0,\ 0)$. This, as in the previous case, is not exactly on the manifold but close enough: $f(p_0) = 0.00005$. This initial point will quickly be iterated to correct manifold.

We compute $x = 0..20$. The results are quite similar to previous case; RK4 beats RKF45 and dopri5 is clearly superior to both of these. RKF45 is dissipative for all reasonable stepsizes.

Some results of computations are in table 3. The column $x = 3.7$ corresponds to the 'one swing' case mentioned below. In figure 3.5 is the result by

	toler	$x = 3.7$	$x = 20$
Dopri5(4)	10^{-4}	136	751
Dopri5(4)	10^{-5}	260	1444
RK4	10^{-2}	223	1259
RK4	10^{-3}	371	2082

Table 3: Stiff pendulum (3.5) $\varepsilon = 0.1$, number of steps.

dopri5 with tolerance 10^{-4}, on the left only one swing to show the 'speed' of numerical solution, on the right the qualitative behaviour over longer time interval.

3.4 Four bar system

This is a classical example in multibody dynamics. The links are rigid and of negligible mass. Joints are frictionless and joints 0 and 3 are fixed. There

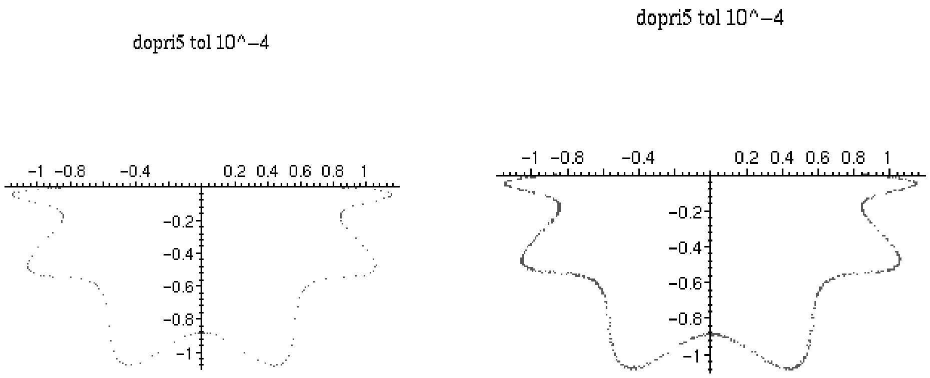

Figure 3.5: Stiff pendulum (3.5), $\varepsilon = 0.1$.

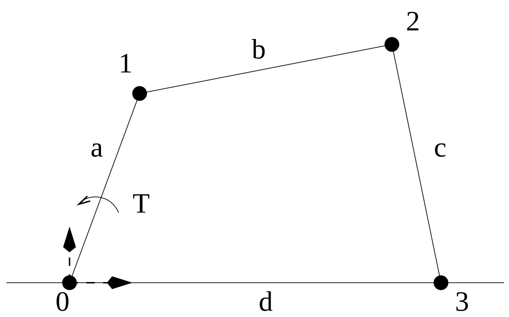

Figure 3.6: Four-bar linkage.

are point masses m_1, m_2 at joints 1 and 2, respectively. The effecting forces are gravity and a constant torque T acting on the origin.

The equations of motion, where (y^1, y^2), (y^3, y^4) are coordinates for joints 1 and 2 respectively, are in descriptor form:

$$\begin{cases} B(x, y, y_1)y_2 + f(x, y, y_1) + (dg)^t\lambda = 0 \\ g(y) = 0 \end{cases} \tag{3.6}$$

with

$$B = \operatorname{diag}(m_1, m_1, m_2, m_2), \qquad \gamma = \text{gravitation constant},$$

$$f = \begin{pmatrix} y^2\, T/a^2 \\ -y^1\, T/a^2 + m_1\gamma \\ 0 \\ m_2\gamma \end{pmatrix}, \quad g = \frac{1}{2}\begin{pmatrix} (y^1)^2 + (y^2)^2 - a^2 \\ (y^3 - y^1)^2 + (y^4 - y^2)^2 - b^2 \\ (d - y^3)^2 + (y^4)^2 - c^2 \end{pmatrix} \tag{3.7}$$

In addition to these, the energy of the system is constant and expressed by

$$energy = \frac{1}{2}\left(m_1((y_1^1)^2 + (y_1^2)^2) + m_2((y_1^3)^2 + (y_1^4)^2)\right) + (m_1 y^2 + m_2 y^4)\gamma \tag{3.8}$$

The constraints are holonomic, hence we can use in computations the reduced form introduced in [9]:

$$\begin{cases} g(y) = 0 \\ dg\, y_1 = 0 \\ \mathcal{D} = \operatorname{span}(V) \\ V = \left(1, y_1, y_2\right) \\ \begin{pmatrix} B & (dg)^t \\ dg & 0 \end{pmatrix}\begin{pmatrix} y_2 \\ \lambda \end{pmatrix} + \begin{pmatrix} f \\ d^2g\,(y_1, y_1) \end{pmatrix} = 0 \end{cases} . \tag{3.9}$$

We shall consider the motion of joint 2 with different choices of a, b, c, d. Also, we will see the same phenomenon as in the multibody example of [9]: augmenting the system by constant energy condition changes the qualitative behaviour of the solution quite radically.

Choose $(a, b, c, d) = (1,\ 2,\ 1.5,\ 2)$ and $T = 0.8$, $m_1 = 0.2$, $m_2 = 0.1$. We look at component y^4. The initial point is $(0,\ 0.5,\ ..., 0, 0, 0, 0)$ In figure 3.7 is the result with the energy equation augmented (solid line) and without it (dashed line). The change of energy in the latter case is shown in figure 3.8. In the constant energy case the result is beautifully oscillatory, as one might heuristically expect, since the effecting forces (gravitation and torque T) are constants. In the non-constant energy case the result is likewise oscillatory but the period of the oscillation is clearly shorter than in the 'correct' case of constant energy. Also, in down position the behaviour is quite different: it makes only a small 'cup' there.

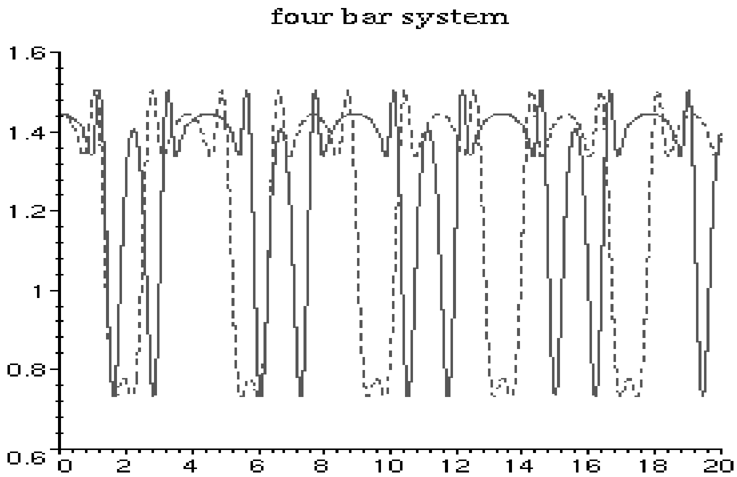

Figure 3.7: Results of 4bar system (3.7) without (dashed line) and with (solid line) (3.8), $T = 0.8$.

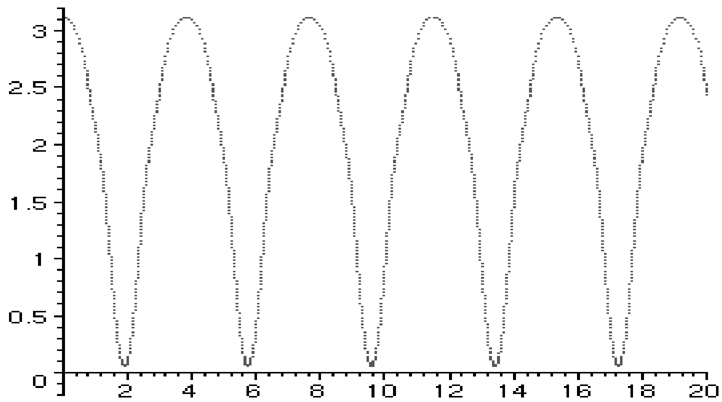

Figure 3.8: Evolution of energy of 4bar system (3.7), $T = 0.8$.

The case where $a + b = c + d$ is interesting, since it produces singularities: then the linkage is capable of reaching position where all the bars are collinear. In that case, the rank of dg is not maximal and the equations of motion become singular. This is called *constraint singularity.* The physical interpretation for the singularity is that there is a bifurcation: the system can move either both joints 1 and 2 down (or up) or another joint moves upwards while the other one moves downwards.

However, if we are modelling a real mechanical device, we might expect that our system has some (non-modelled) supportive structures that eliminate the possibility of a bifurcation. In this case, we have to modify the equations to remove the singularity also from the equations. See also [1, 6] for other approaches to this problem.

The technique for resolving this problem is *ideal decomposition.* We need some definitions and results (which we state without proofs) from algebraic geometry [3]:

Definition 3.1 *Denote by* $\mathbb{C}[y_1, \ldots, y_n]$ *the ring of polynomials in* $y_1, \ldots, y_n$. *A subset* $\mathcal{I} \subset \mathbb{C}[y_1, \ldots, y_n]$ *is an* ***ideal*** *if it satisfies*

(i) $0 \in \mathcal{I}$.

(ii) If $f, g \in \mathcal{I}$, *then* $f + g \in \mathcal{I}$.

(iii) If $f \in \mathcal{I}$ *and* $h \in \mathbb{C}[y_1, \ldots, y_n]$, *then* $hf \in \mathcal{I}$.

Definition 3.2 *Let* $f_1, \ldots, f_s \in \mathbb{C}[y_1, \ldots, y_n]$. *Then we set*

$$\langle f_1, \ldots, f_s \rangle = \{\sum_{i=1}^{s} h_i f_i : h_1, \ldots, h_s \in \mathbb{C}[y_1, \ldots, y_n]\}.$$

We call $\langle f_1, \ldots, f_s \rangle$ *the* ***ideal generated by*** $f_1, \ldots, f_s$.

We skip the proof of the fact that $\langle f_1, \ldots, f_s \rangle$ really is an ideal.

Definition 3.3 *An ideal* $\mathcal{I}$ *is* ***radical*** *if* $f^m \in \mathcal{I}$ *for any integer* $m \geq 1$ *implies that* $f \in \mathcal{I}$.

An ideal $\mathcal{I}$ *is* ***prime*** *if whenever* $f, g \in \mathbb{C}[y_1, \ldots, y_n]$ *and* $fg \in \mathcal{I}$, *then either* $f \in \mathcal{I}$ *or* $g \in \mathcal{I}$.

Definition 3.4 *Let* $\mathcal{I}$ *be an ideal. The* ***radical*** *of* $\mathcal{I}$, *denoted by* $\sqrt{\mathcal{I}}$, *is the set*

$$\{f \in \mathbb{C}[y_1, \ldots, y_n] : f^m \in \mathcal{I} \text{ for some integer } m \geq 1\}.$$

Lemma 3.1 *If* $\mathcal{I}$ *is an ideal, then* $\sqrt{\mathcal{I}}$ *is an ideal. Furthermore,* $\sqrt{\mathcal{I}}$ *is a radical ideal.*

Finally, a strong theorem from algebraic geometry:

Lemma 3.2 *Every radical ideal $\mathcal{I}$ in $\mathbb{C}[y_1, \ldots, y_n]$ can be written uniquely as a finite intersection of prime ideals,*

$$\mathcal{I} = \mathcal{I}_1 \cap \cdots \cap \mathcal{I}_r,$$

where $\mathcal{I}_i \not\subset \mathcal{I}_j$ for $i \neq j$.

An essential thing is that this decomposition can be computed algorithmically through the use of the generators of the ideal.

To demonstrate, suppose $(a, b, c, d) = (1, 2, 1, 2)$. Our g is a polynomial, hence it generates an ideal $\mathcal{I} \in \mathbb{C}[y^1, y^2, y^3, y^4]$ which then generates a *radical* ideal $\sqrt{\mathcal{I}}$. This decomposes to intersection of prime ideals:

$$\sqrt{\mathcal{I}} = \mathcal{I}_1 \cap \mathcal{I}_2$$

where $\mathcal{I}_i$ is the prime ideal generated by g_i,

$$g_1 := \begin{cases} (y^3)^2 + (y^4)^2 - 4y^3 + 3 \\ y^2 - y^4 \\ y^1 - y^3 + 2 \end{cases}$$

$$g_2 := \begin{cases} (y^3)^2 + (y^4)^2 - 4y^3 + 3 \\ 4y^2y^3 - 3y^2 + 3y^4 \\ 4y^2y^4 + 3y^1 - 3y^3 + 6 \end{cases} .$$

In computing these we found Singular [4] very helpful. Using these equations actually removes the singularity! For example, if we have the parallelogram case where both joints 1 and 2 move at the same height, we use g_1 in place of g. The situation $y^2 = y^4 = 0$ is no longer a singularity, g_1 is of maximal rank everywhere. Of course, in this simple case we can eliminate y^3 and y^4, a geometric fact which is also clearly visible in g_1.

Let's look more closely at g_2. First, condition $y^2 = y^4$ (parallelogram-like motion) yields easily $y^2 = y^4 = 0$. Hence the parallelogram motion is possible only with g_1, not with g_2.

Second, the middle equation of g_2 gives

$$y^4 = y^2(1 - \frac{4}{3}y^3)$$

where the multiplier of y^2 is negative by the first equation of g_2, which is

$$0 = (y^3 - 2)^2 + (y^4)^2 - 1$$

and yields $1 \leq y^3 \leq 3$.

That is, when nonzero, y^2 and y^4 have different signs. Hence g_2 corresponds to situations where the joints 1 and 2 are at different sides of the d-bar, as expected.

Third, the rank of g_2 is maximal everywhere and hence the singularity is vaporized! Let us take an example using g_2 in place of g: the initial

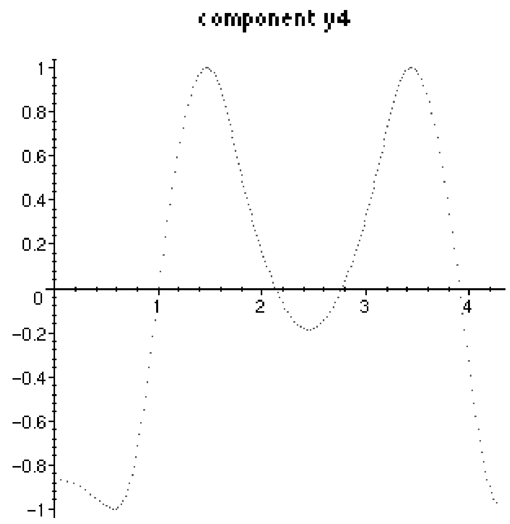

Figure 3.9: The component y^4 of the 'singular' 4bar linkage.

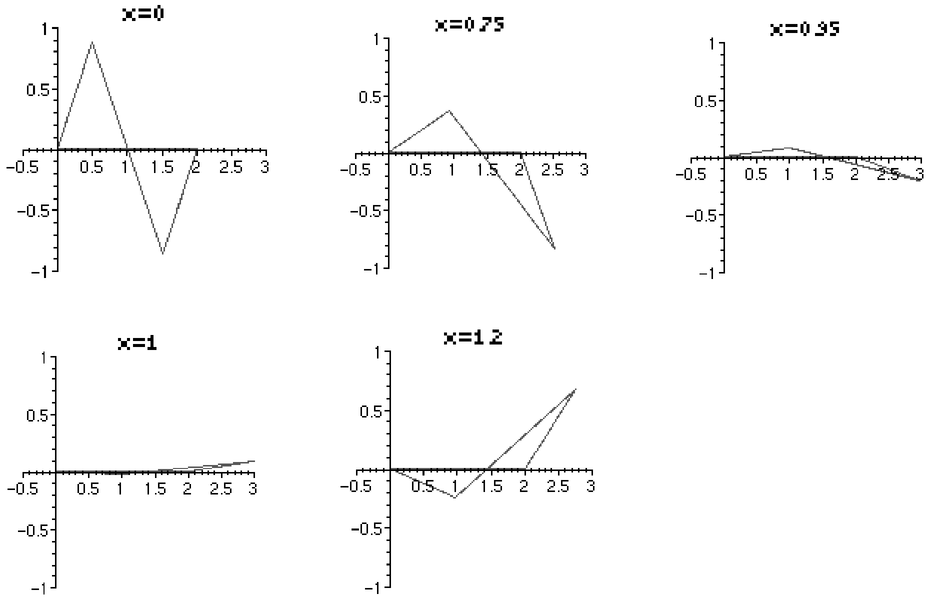

Figure 3.10: Some configurations of the 'singular' 4bar linkage.

point is $(0, 0.5, \sqrt{3}/2, 1.5, -\sqrt{3}/2, 0, 0, 0, 0)$ and T, m_1, m_2 as above. The component y^4 is in figure 3.9 and some of the configurations of the linkage are in figure 3.10. There is no problem passing through points $y^4 = 0$ which would be singularities when using the original g.

Remark. If we had used the Lagrange 2^{nd} kind of equations (i.e. using a minimal set of coordinates, e.g. an angle between bars a and d) for representing the equations of motion, we would have less equations but they would still include an algebraic constraint. Moreover, this constraint would be of non-polynomial type and the ideal decomposition could not be applied.

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