Runge Kutta

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1 The Problem

An *instance* of the ODE problem is an ordered triple (f, x_0, y_0) where x_0, y_0 are real numbers, and where $f(x, y)$ is a function of two variables such that $f(x, y)$ is defined in some neighborhood of (x_0, y_0).

A *solution* to the ODE instance (f, x_0, y_0) is a function F such that $F(x_0) = y_0$, and, for x in some neighborhood of x_0, $F(x)$ is defined and $F'(x) = f(x, F(x))$.

1.1 Reduction

We can greatly simplify our proofs if we assume that we start at $(0, 0)$, and that $F'(0) = 0$. We will give a reduction of the general problem to the restricted problem that satisfies these criteria.

It is important to realize that the purpose of this reduction is only to simplify proofs. No simplification of the actual calculations results from the reduction, in fact, it would make the calculations longer.

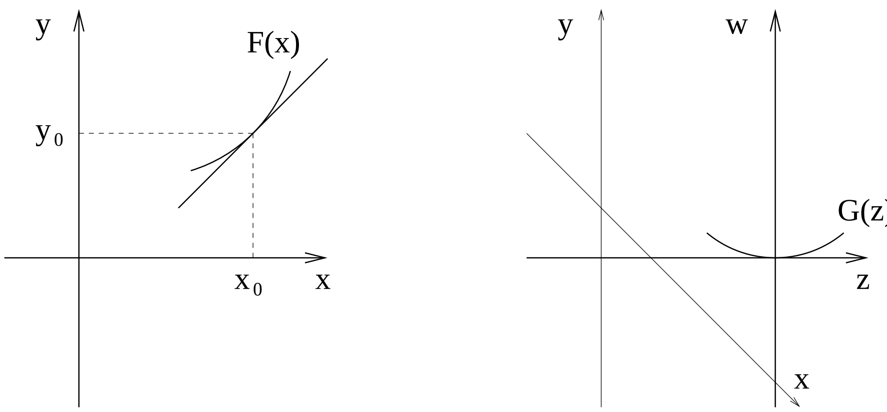

Figure 1

The reduction is essentially an affine transformation of the plane, as indicated in Figure 1

Lemma 1.1 *Any ODE instance* (f, x_0, y_0) *can be reduced to an ODE instance* $(g, 0, 0)$ *such that* $g(0, 0) = 0$.

Proof: Let $m = f(x_0, y_0)$. Let $g(z, w) = f(z + x_0, w + y_0 + mz) - m$, which is defined in a neighborhood of $(0, 0)$. For any function F defined on a neighborhood of x_0, such that $F(x_0) = y_0$, let $G(z) = F(z + x_0) - y_0 - mz$; note that G is defined on a neighborhood of 0, that $G(0) = 0$, and $G'(0) = 0$. We need to prove that F is a solution to (f, x_0, y_0) if and only if G is a solution to $(g, 0, 0)$.

Suppose F is a solution to (f, x_0, y_0). Then

$$\begin{aligned} G'(z) &= F'(z + x_0) - m \\ &= f(z + x_0, F(z + x_0)) - m \\ &= f(z + x_0, G(z) + y_0 + mz) - m \\ &= g(z, G(z)) + m - m = g(z, G(z)) \end{aligned}$$

That is, G is a solution to $(g, 0, 0)$.

Conversely, Suppose G is a solution to $(g, 0, 0)$. Then

$$\begin{aligned} F'(x) &= G'(x - x_0) + m \\ &= g(x - x_0, G(x - x_0)) + m \\ &= f(x - x_0 + x_0, F(x) - y_0 - m(x - x_0) + y_0 + m(x - x_0)) + m - m \\ &= f(x, F(x)) \end{aligned}$$

That is, F is a solution to (f, x_0, y_0). $\square$

2 Runge Kutta Algorithms

A Runge Kutta algorithm for approximating the solution to an ODE takes the following form. We are given a number s (the order of the algorithm) and constants $\alpha_{i,j}$ for $1 \leq i < j \leq d$, β_i for $1 \leq i \leq d$, and γ_j for $1 \leq j \leq d$.

We will assume that

$$\begin{aligned} \gamma_1 &= 0 \\ \sum_{1 \leq i < j} \alpha_{i,j} &= \gamma_j \\ \sum_{1 \leq i \leq s} \beta_i &= 1 \end{aligned}$$

The algorithm is then

$$
\begin{aligned}
k_1 &= hf(x_n, y_n) \\
k_2 &= hf(x_n + \gamma_1 h, y_n + \alpha_{12} k_1) \\
&\dots \\
k_j &= hf(x_n + \gamma_j h, y_n + \sum_{1 \le i < j} \alpha_{i,j} k_i \\
&\dots \\
y_{n+1} &= \sum_{1 \le i \le s} \beta_i k_i
\end{aligned}
$$

These constants can be arranged in a *Butcher tableau.*

Exercise 2.1

(a) *Write the Butcher tableau for the third order method we discussed in class.*

(b) *Euler's method is actually a Runge Kutta algorithm of order 1. Write the Butcher tableau for this algorithm. (This is so easy it's hard.)*

3 Power Series Approximation

Without loss of generality, $x_i = y_i = 0$. Assume that $F'(x) = f(x, F(x))$ for all x is some neighborhood of x. We also assume that the Taylor series for F converges in some neighborhood of x, and that the Taylor series for f converges in some neighborhood of $(0,0)$. Without loss of generality, $f(0,0) = 0$.

There exist constants a_2, a_3, a_4 such that, for x in some neighborhood of 0:

$$F(x) = a_2 x^2 + a_3 x^3 + a_4 x^4 + O(|x|^5)$$

Also there exist constants $b_{10}, b_{20}, b_{30}, b_{01}, b_{11}$ such that, for (x, y) in some neighborhood of $(0,0)$:

$$f(x,y) = b_{10} x + b_{20} x^2 + b_{30} x^3 + b_{01} y + b_{11} xy + O(|x|^4) + O(|x|^2 |y|) + O(|y|^2)$$

Differentiating with respect to x, we obtain

$$F'(x) = 2a_2 x + 3a_3 x^2 + 4a_4 x^3 + O(|x|^4)$$

$F'(x) = f(x, F(x))$, and we can use the Taylor series for F and f to obtain:

$$
\begin{aligned}
2a_2 &= b_{10} \\
3a_3 &= b_{20} + \tfrac{1}{2} b_{01} b_{10} \\
4a_4 &= b_{30} + \tfrac{1}{2} b_{10} b_{11} + \tfrac{1}{3} b_{01} b_{20} + \tfrac{1}{6} b_{01}^2 b_{10} \\
5a_5 &= \dots \\
\dots
\end{aligned}
$$

That is

$$
\begin{aligned}
a_2 &= \tfrac{1}{2}b_{10} \\
a_3 &= \tfrac{1}{3}b_{20} + \tfrac{1}{6}b_{01}b_{10} \\
a_4 &= \tfrac{1}{4}b_{30} + \tfrac{1}{8}b_{10}b_{11} + \tfrac{1}{12}b_{01}b_{20} + \tfrac{1}{24}b_{01}^2 b_{10} \\
a_5 &= \ldots \\
\ldots
\end{aligned}
$$

4 Second Order Runge Kutta

A Runge Kutta algorithm is characterized by its *Butcher tableau.* There are multiple Runge Kutta algorithm of each order. The Butcher tableaux for the two order 2 methods we have presented in class are

$$
\begin{array}{c|cc}
0 & & \\
\frac{1}{2} & \frac{1}{2} & \\
\hline
 & 0 & 1
\end{array}
\qquad \text{and} \qquad
\begin{array}{c|cc}
0 & & \\
1 & 1 & \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

We will use the second tableau. Our algorithm is then

$$
\begin{aligned}
k_1 &= hf(x_n, y_n) \\
k_2 &= hf(x_n + h, y_n + k_1) \\
x_{n+1} &= x_n + h \\
y_{n+1} &= y_n + \tfrac{1}{2}k_1 + \tfrac{1}{2}k_2
\end{aligned}
$$

Lemma 4.1 *If f is analytic, the error of the above second order Runge Kutta algorithm is $O(h^3)$.*

Proof: Without loss of generality, $n = 0$, $x_0 = 0$, $y_0 = 0$, and $f(0,0) = 0$. Then

$$
\begin{aligned}
f(x,y) &= b_{10}x + O(|x|^2 + |y|) \\
F(x) &= a_2x^2 + O(|x|^3)
\end{aligned}
$$

We need to show that $y_1 = F(x_1) + O(h^3)$, where $x_1 = x_0 + h = h$. We have

$$
\begin{aligned}
k_1 &= 0 \\
k_2 &= hf(h,0) \\
&= b_{10}h^2 + O(h^3) \\
&= 2a_2h^2 + O(h^3) \\
y_1 &= \tfrac{1}{2}k_1 + \tfrac{1}{2}k_2 \\
&= a_2h^2 + O(h^3) \\
&= F(h) + O(h^3)
\end{aligned}
$$

$\square$

5 Third Order Runge Kutta

Exercise 5.1 *Write the Butcher tableau for the third order Runge Kutta method we discussed in class.*

Exercise 5.2 *Prove that the error of that third order method is $O(h^4)$ per step.*

6 Fourth Order Runge Kutta

We will use the standard RK4 method:

$$\begin{aligned}
k_1 &= hf(x_n, y_n) \\
k_2 &= hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_1) \\
k_3 &= hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_2) \\
k_4 &= hf(x_n + h, y_n + k_3) \\
x_{n+1} &= x_n + h \\
y_{n+1} &= y_n + \tfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)
\end{aligned}$$

whose Butcher tableau is

$$\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2} & & & \\
\frac{1}{2} & 0 & \frac{1}{2} & & \\
1 & 0 & 0 & 1 & \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}$$

Lemma 6.1 *If f is analytic, the error of the above fourth order Runge Kutta algorithm is $O(h^5)$.*

Proof: Without loss of generality, $n = 0$, $x_0 = 0$, $y_0 = 0$, and $f(0,0) = 0$. Then

$$\begin{aligned}
f(x,y) &= b_{10}x + b_{20}x^2 + b_{30}x^3 + b_{01}y + b_{11}xy + O(|x|^4 + |x|^2|y| + |y|^2) \\
F(x) &= a_2x^2 + a_3x^3 + a_4x^4 + O(|x|^5)
\end{aligned}$$

We need to show that $y_1 = F(x_1) + O(h^5)$, where $x_1 = x_0 + h = h$. We have

$$
\begin{aligned}
F(h) &= a_2h^2 + a_3h^3 + a_4h^4 + O(h^5) \\
&= \tfrac{1}{2}b_{10}h^2 + \tfrac{1}{3}b_{20}h^3 + \tfrac{1}{6}b_{01}b_{10}h^3 + \tfrac{1}{4}b_{30}h^4 + \tfrac{1}{8}b_{11}b_{10}h^4 + \tfrac{1}{12}b_{01}b_{20}h^4 + \tfrac{1}{24}b_{01}^2b_{10}h^4 + O(h^5)
\end{aligned}
$$

and

$$
\begin{aligned}
k_1 &= 0 \\
k_2 &= hf(\tfrac{1}{2}h, \tfrac{1}{2}k_1) \\
&= hf(\tfrac{1}{2}h, 0) \\
&= \tfrac{1}{2}b_{10}h^2 + \tfrac{1}{4}b_{20}h^3 + \tfrac{1}{8}b_{30}h^4 + O(h^5) \\
k_3 &= hf(\tfrac{1}{2}h, \tfrac{1}{2}k_2) \\
&= \tfrac{1}{2}b_{10}h^2 + \tfrac{1}{4}b_{20}h^3 + \tfrac{1}{8}b_{30}h^4 + \tfrac{1}{4}b_{01}b_{20}h^4 + \tfrac{1}{8}b_{11}b_{10}h^4 + O(h^5) \\
k_4 &= hf(h, k_3) \\
&= b_{10}h^2 + b_{20}h^3 + b_{30}h^4 + \tfrac{1}{2}b_{01}b_{10}h^3 + \tfrac{1}{4}b_{01}b_{20}h^4 + \tfrac{1}{4}b_{01}^2b_{10}h^4 + \tfrac{1}{2}b_{11}b_{10}h^4 + O(h^5) \\
y_1 &= \tfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \\
&= \tfrac{1}{6}\big(3b_{10}h^2 + 2b_{20}h^3 + \tfrac{3}{2}b_{30}h^4 + b_{01}b_{10}h^3 + \tfrac{1}{2}b_{01}b_{20}h^4 + \tfrac{1}{4}b_{01}^2b_{10}h^4 + \tfrac{3}{4}b_{11}b_{10}h^4\big) + O(h^5) \\
&= F(h) + O(h^5)
\end{aligned}
$$

□

7 "Big Oh" for Functions which Converge to Zero

The precise mathematical definition of $O(n^2)$, or, for that matter, $O(f(n))$ where f is any positive increasing function, can be found in any computer science textbook. But what about decreasing functions?

Exercise 7.1 *What is the precise mathematical definition of $O(\frac{1}{n})$, or for that matter, $O(f(n))$, where $f(n) \to 0$ as $n \to \infty$? Is the same as for increasing functions?*

Exercise 7.2 *What is the precise mathematical definition of $O(h^2)$, or, for that matter, $O(f(h))$, where $f(h) \to 0$ as $h \to 0$? You clearly cannot use the same definition as before.*

Exercise 7.3 *We say that Newton's method is* quadratically convergent. *Does this mean that the error is $O(n^2)$, where n is the number of iterations? Can you express the true meaning of quadratic convergence in "big Oh" terms?*

8 Vector Functions

Why can't $F(x)$ be a vector of n variables? Answer, it can. For example, a ballistic problem involving launching a rocket needs variables for its position and variables for its velocity. If the acceleration increases as the fuel is used up, the ODE is also time dependent, as opposed to problems involving passive falling bodies.

The standard RK4 method has error $O(h^5)$ even for vector examples.