Runge-Kutta Method

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1 Gaussian Quadrature

Quadrature is a process to substitute an integral with a finite sum.

First of all, take a non-negative function $\omega(t)$ acts on an interval (a, b) such that it satisfies

$$0 < \int_a^b \omega(t)dt < \infty \quad , \quad \left| \int_a^b t^i \omega(t)dt \right| < \infty \quad i = 1, 2, 3, ... \tag{1}$$

The ω is called the weight function, and we do the following approximation with it.

$$\int_a^b f(t)\omega(t)dt \approx \sum_{i=1}^{v} b_i f(c_i) \tag{2}$$

where bi values are called *the quadrature weights* and c_i values are called the *the quadrature nodes*. These constants do not depend on the f, but a, b, ω in general. However, the sum (2) still does not consist of a, b. Hence, the boundaries of the integral can be chosen arbitrarily. The can even be $\pm\infty$.

The order of the quadrature is an important point to determine. Of course, it depends on the choice of nodes and weights. However, for all appropriate choices, if the quadrature is exact for any polynomial in $\mathcal{P}(p-1)$, then we have a boundary for the p times **smoothly** differentiable function f as

$$\left| \int_a^b f(t)\omega(t)dt - \sum_{i=1}^{v} b_i f(c_i) \right| \leq c \left| max_{a \leq t \leq b} f^{(p)}(t) \right| \quad , c \geq 0 \tag{3}$$

The above condition is called *the order condition*, and the c value is independent of the f.

Lemma 1.1. *For any given distinct set of nodes $c_1, c_2, c_3, \cdots, c_v$. It is possible to find a unique set of weights $b_1, b_2, \cdots, b_v$ such that the quadrature formula (2) is of order $p \geq v$.*

Proof. By the order condition, for such given nodes, for any arbitrary basis of $\mathcal{P}(v-1)$, the method must be equal to the integral. Lets choose the simplest basis $1, t, t^2, \cdots, t^{v-1}$. Then we should have

$$\sum_{j=1}^{v} b_j c_j^m = \int_a^b t^m \omega(t)dt \quad , m = 0, 1, \cdots, v-1 \tag{4}$$

Now for distinct nodes, we have a v number of equations and v unknowns b_i values. These form a non-singular *Vandermonde Matrix*. Hence, the set of equations has a unique solution, and the order of the method is $p \geq v$ according to the order condition. $\square$

The b_i values can be calculated using *Lagrange Interpolation Polynomials*. Let the basis of the $\mathcal{P}(v-1)$ be the functions $g_m(t)$ interpolation functions as

$$g_m(t) = \sum_{j=1}^{v} \rho_j(t) g_m(c_j) \tag{5}$$

Now take the quadrature where $\int_0^1 g_m(t)\omega(t)dt = \sum_{i=1}^{v} b_j g_m(c_j)$. By the (5), we have

$$\int_0^1 \left[\sum_{j=1}^{v} \rho_j(t) g_m(c_j)\right] \omega(t)dt = \sum_{j=1}^{v} \left[\int_0^1 \rho_j(t)\omega(t)\right] g_m(c_j) \tag{6}$$

Consequently, we have

$$b_j = \int_0^1 \rho_j(t)\omega(t) \tag{7}$$

where the $\rho_j(t)$ is the j^{th} Lagrange Polynomial.

Another important point for a quadrature is to choose the set of nodes c_i. Choosing them as equispaced points of the interval $[a, b]$ seems natural. However, its order is not good as it could be. By making an intelligent choice, we can increase the order to $2v$.

Before making that choice, we need to define an inner product with respect to a weight function $\omega(t)$ as

$$\langle f,\ g\rangle = \int_a^b f(t)g(t)\omega(t)dt \tag{8}$$

where $f, g \in \{f, \quad \int_a^b |f(t)|^2\omega(t)dt < \infty\}$ Under this inner product, we have orthogonal polynomials $p_m = \mathcal{P}(m)$ such that

$$\forall p \in \mathcal{P}(m-1) \quad \langle p_m,\ p\rangle = 0 \tag{9}$$

The p_m is the m^{th} orthogonal polynomial. Of course, orthogonal polynomials are not unique, but the *monic polynomials*, which are the orthogonal polynomials with the highest degree coefficients are 1, are [1].

Another critical notion for this intelligent choice of the nodes is the locations of the roots of orthogonal polynomials.

Lemma 1.2. *All "m" zeros of an orthogonal polynomial p_m with respect to $\omega(t)$ reside in the interval (a, b) and* ***they are simple****.*

Proof. Because $p_m(t)$ is orthogonal, we have $\langle p_m,\ 1\rangle = 0$. We also have $\omega(t) \geq 0$. Hence, there must be at least one point where the p_m changes sign in the interval.

[1] Proof of this is in the handwritten notes.

Let say there exist a k number of roots residing in the interval. We know that $k \geq 1$. Let bound the k as $m-1 \geq k \geq 1$. Let $x_1, x_2, \cdots, x_k$ be the corresponding roots. Let define a $q(t)$ as

$$q(t) = \prod_{i=1}^{k}(t - x_i) = \sum_{i=1}^{k} q_i x_i$$

Now consider the function $p_m(t)q(t)$. At every point that p_m changes sign, q also changes sign, and they have the same sign. Hence, the $p_m(t)q(t) \geq 0$. Thus, we have

$$\int_a^b p_m(t)q(t)\omega(t)dt \geq 0$$

However, $\langle p_m,\ q\rangle = 0$ due to the orthogonality. Consequently, we have a contradiction, so all of the roots of p_m must be in the interval (a, b) □

Theorem 1.1. *Let $c_1, c_2, \cdots, c_v$ be the roots of the orthogonal polynomial p_v. Let the $b_1, b_2, \cdots, b_v$ be the solution of the Vandermonde System (4). Then*

- *The quadrature method is of order $2v$.*
- *No other quadrature can have higher order.*

Proof. Notice that p_v is an order of v polynomial. We want the quadrature to be the order of $k \geq 2v$. Then, by the order condition, the quadrature should be exact for all polynomials $\hat{p} \in \mathcal{P}(2v-1)$. Note that $\exists q, r \in \mathcal{P}(v-1)$ such that

$$\hat{p} = p_v q + r \quad ; p_v \in \mathcal{P}(v) \backslash \mathcal{P}(v-1)$$

Then consider the quadrature

$$\int_a^n \hat{p}(t)\omega(t)dt = \sum_{i=1}^{v} b_i \hat{p}(c_i)$$

Also

$$\int_a^b \hat{p}(t)\omega(t)dt = \langle p_v, q\rangle + \int_a {}_b r(t)\omega(t)dt$$

$\langle p_v, q\rangle = 0$

$$\Rightarrow \int_a^b \hat{p}(t)\omega(t)dt = \sum_{i=1}^{v} b_i r(c_i)$$

Hence,

$$\sum_{i=1}^{v} b_i \hat{p}(c_i) = \sum_{i=1}^{v} b_i r(c_i) \tag{10}$$

Now, we showed that the order condition is satisfied. Hence, we have the order of the quadrature, $p \geq 2v$

Now, let's assume the order of the quadrature is $p \geq 2v + 1$. This is to say that the quadrature must integrate

$$\bar{p}(t) = \prod_{1}^{v}(t - c_i)^2 \int_a^b \bar{p}(t)\omega(t)dt = \int_a^b \left[\prod_{1}^{v}(t - c_i)^2\right]\omega(t)dt > 0$$

but

$$\sum_{i=1}^{v} b_i \bar{p}(c_i) = \sum_{i=1}^{v} b_i \prod_{1}^{v}(c - c_i)^2 = 0$$

Hence, the $\bar{p}(t)$ cannot hold the order condition.

$$\int_a^b \bar{p}(t)\omega(t)dt \neq \sum_{i=1}^{v} b_i \bar{p}(c_i) \tag{11}$$

Consequently, we have

$$p \geq 2v \;\;\&\;\; p < 2v + 1 \iff p = 2v \tag{12}$$

□

Theorem 1.2. *Let $r \in \mathcal{P}(v)$ obey the orthogonality conditions.*

$$\forall \hat{p} \in \mathcal{P}(m - 1) \quad \langle r, \hat{p}\rangle = 0 \;\;\&\;\; \langle r, t^m\rangle \neq 0$$

, so r is an orthogonal polynomial of degree m. Let $c_1, c_2, \cdots, c_v$ be zeros of the r. Let's choose $b_1, b_2, \cdots, b_v$ consistently (4). Then the quadrature formula is an order of $p = v + m$.

2 Runge-Kutta Method

Now we will start with the identity

$$y(t_{n+1}) = y(t_n) + \int_{t_n}^{t_{n+1}} f(t, y(t))dt \tag{13}$$

let $t \to t_n + ht$

$$y(t_{n+1}) = y(t_n) + h\int_0^1 f(t_n + ht, y(t_n + ht))dt \tag{14}$$

Then, to obtain the Runge-Kutta method, we will use the quadrature method to approximate the integral.

$$y_{n+1} = y_n + h\sum_{i=1}^{v} b_j f(t_n + hc_j, y(t_n + hc_j)) \quad , n = 0, 1, 2, \cdots \tag{15}$$

The main problem with that method is that we don't know the $y(t)$ values on the nodes $\{t_n + c_1 h, t_n + c_2 h, \cdots, t_n + c_v h, \}$. To solve that, we will also approximate these values defining a new quantity,ϵ, such that $y(t_n + hc_j) = \epsilon_j$ as the following

$$\epsilon_1 = y_n \epsilon_2 = y_n + ha_{21} f(t_n, \epsilon_1) \epsilon_3 = y_n + ha_{31} f(t_n, \epsilon_1) + ha_{32} f(t_n + hc_2, \epsilon_2)$$

$$\vdots$$

$$\epsilon_v = y_n + \sum_{1}^{v-1} ha_{vi} f(tn + hc_i, \epsilon_i) \tag{16}$$

The a_{ij} values create a matrix A called *Runge-Kutta Matrix*. Also, we write the weights b_i and nodes c_i as vectors and call them *Runge-Kutta Weights* and *Runge-Kutta Nodes* respectively.

3 Calculation oF R.K. Matrix

One way to calculate an R.K matrix is simply using Tylor expansion. For example, let's calculate it for $v = 2$ case.

Let $\epsilon_1 = y_n$, $c_1 = 0$

$$\epsilon_2 = y_n + ha_{21} f(t_n, y_n) \tag{17}$$

$$\Rightarrow f(t_n + hc_2, \epsilon_2) = f(t_n + hc_2, y_n + ha_{21} f(t_n, y_n))$$

Then, Taylor expansion of the function around the point (t_n, y_n) gives

$$f(t_n + hc_2, \epsilon_2) = f(t_n, y_n) + c_2 h \partial_t f(t_n, y_n) + ha_{21} \partial_y f(t_n, y_n) \dot{y} + \mathcal{O}(h^2) \tag{18}$$

Then the (16) becomes

$$y_{n+1} = y_n + \left[b_1 f(t_n, y_n) + b_2 \left[f(t_n, y_n) + h \left(c_2 \partial_t f(t_n, y_n) + a_{21} \partial_y f(t_n, y_n) \dot{y} + \mathcal{O}(h^2)\right)\right]\right] \tag{19}$$

After some simplifications, we got

$$y_{n+1} = y_n + (b_1 + b_2) f(t_n, y_n) + b_2 h^2 (c_2 \partial_t f(t_n, y_n) + a_{21} \partial_y f(t_n, y_n) f(t_n, y_n)) + \mathcal{O}(h^3) \tag{20}$$

Now let $\tilde{y}(t)$ with the condition $\tilde{y}(t_n) = y_n$ be the exact solution of the ODE. Then again the Taylor expansion gives

$$\tilde{y}(t_{n+1}) = y_n + hf(t_n, y_n) + \frac{1}{2} h^2 (\partial_t f(t_n, y_n) + \partial_y f(t_n, y_n) f(t_n, y_n)) + \mathcal{O}(h^3) \tag{21}$$

Finally, we have the following result by simply comparing the (21) and (20)

$$b_1 + b_2 = 1 \quad , b_2 c_2 = \frac{1}{2} \quad , b_2 a_{21} = \frac{1}{2} \tag{22}$$

$$\Rightarrow a_{21} = c_2 \tag{23}$$

All of the solutions of the above equations give a Runge-Kutta scheme. Hence, obviously, for a given v, we don't have a unique scheme generally. Also, there are many ways to calculate these schemes rather than using Taylor expansion. Before mentioning the other methods, the followings are popular schemes for the $v = 2$ case. **PUT THE FIGURES FOR SCHEMES**

Taylor expansion for $v = 3$ case gives the following equations

$$b_1 + b_2 + b_3 = 1 \quad , c_2 b_2 + c_3 b_3 = \frac{1}{2} \quad , b_2 c_2^2 + b_3 c_3^2 = \frac{1}{3} \quad , b_3 a_{32} c_2 = \frac{1}{6} \tag{24}$$

One can get the following schemes from these equations.**Schemes**

4 Implicit Runge-Kutta Method

The approximation values ϵ_j has the following general form

$$\epsilon_j = y_n + h \sum_{i=1}^{v} a_{ji} f(t_n + hc_i, \epsilon_i) \tag{25}$$

This approximation gives the general form of the Implicit Runge-Kutta Methods

$$y_{n+1} = y_n + h \sum_{i=1}^{v} b_j f(t_n + hc_i, \epsilon_i) \tag{26}$$

An important difference between the explicit and Implicit R.K methods is that the R.K matrix A is lower triangular for the explicit schemes. On the other hand, it is just an arbitrary matrix for implicit schemes.

An advantage of the I.R.K method is that it has superior stability properties. Also, for all $v \geq 1$, there exists an I.R.K method with order $2v$ as a natural extension of the above theorem, **Theorem 1.2**. An example of the I.R.K scheme is the following $v = 2$ with order 3.**Example Scheme** Then we have,

$$\epsilon_1 = y_n + \frac{hf(t_n, \epsilon_1)}{4} - \frac{hf(t_n + \frac{2h}{3}, \epsilon_2)}{4} \tag{27}$$

$$\epsilon_2 = y_n + \frac{hf(t_n, \epsilon_1)}{4} + \frac{5hf(t_n + \frac{2}{3}h, \epsilon_2)}{12} \tag{28}$$

Thus, the corresponding method[2] is

$$y_{n+1} = y_n + \frac{hf(t_n, \epsilon_1)}{4} + \frac{3hf(t_n + \frac{2h}{3}, \epsilon_2)}{4} \tag{29}$$

[2]Check the handwritten notes for the error analysis and order calculation.

5 Collocation & IRK Method

Suppose we know the values (t_j, v_j) up to (t_n, y_n). We want to advance the integration to the value (t_{n+1}, y_{n+1}). To achieve this, we choose v distinct collocation parameters $c_1, c_2, \cdots, c_v \in [0, 1]$. The choice of the range is not essential, but it [0,1] is preferable. Then seek a polynomial $u \in \mathcal{P}(v)$ as

$$u(t_n) = y_n \tag{30}$$

$$\dot{u}(t_n + hc_j) = f(t_n + hc_j, u(t_n + hc_j)) \quad j = 1, 2, \cdots, v \tag{31}$$

This is to say that the polynomial u satisfies the ODE exactly at v distinct points and obeys the initial condition. A collocation method is basically a method for finding such a u. Finally, we set

$$y(t_{n+1}) = u(t_{n+1}) \tag{32}$$

Note that this is nothing but an IRK method.

Lemma 5.1. *Let*

$$q(t) = \prod_{1}^{v}(t - c_j) \quad , q_l(t) = \prod_{j=1, j\neq l}^{v} \frac{(t - c_j)}{c_l - c_j}$$

Then the collocation method is identical to the IRK, and the matrix A and the weight vector b are calculated as

$$a_{ji} = \int_0^{c_j} \frac{q_i(t)}{q_i(c_i)} dt \tag{33}$$

$$b_j = \int_0^{c_j} \frac{q_j(t)}{q_j(c_j)} dt \tag{34}$$

where $j, i = 1, 2, \cdots, v$

Proof. The proof is in the handwritten notes for now. □

With a given node vector c, one can obtain many R.K schemes, but only one of them originated from a collocation. However, it is much easy to calculate the matrix A and the weight b rather than doing cumbersome expansions. Also, for the collocation schemes there is a very important theorem.

Theorem 5.1. *Suppose that $\int_0^1 q(t)t^i dt = 0$ w/ $i = 0, 1, 2, \cdots, m-1$ for some $m \in 0, 1, 2, \cdots, v$. If one chooses the node C as the root of the $q(t)$. Then the collocation method has the order $m + v$.*

Theorem 5.2. *If the nodes C are chosen as the roots of an orthogonal polynomial $p_v \in \mathcal{P}(v)$ with respect to the weight function $\omega(t) = 1$ and $0 \leq t \leq 1$. Then the order of the corresponding collocation method is exactly $2v$.*