正交多项式

段元兴

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1.1

证明: 当$i=j$时

$$\langle Q_i|Q_j\rangle = \frac{\langle V_i|V_i\rangle}{\alpha_i^2} = 1 = \delta_{ij} \tag{1}$$

当$i>j$时, 假设$\langle Q_{i-1}|Q_j\rangle = 0$成立$(i-1\neq j)$, 现证明$\langle Q_i|Q_j\rangle = 0$:

$$\begin{aligned}\langle Q_i|Q_j\rangle &= \frac{\left\langle xQ_{i-1} - \sum_{k=0}^{i-1}\langle Q_k|xQ_{i-1}\rangle Q_k \middle| Q_j\right\rangle}{\alpha_i\alpha_j} \\ &= \frac{\langle xQ_{i-1}|Q_j\rangle - \sum_{k=0}^{i-1}\langle Q_k|xQ_{i-1}\rangle \langle Q_k|Q_j\rangle}{\alpha_i\alpha_j} \\ &= \frac{\langle xQ_{i-1}|Q_j\rangle - \langle Q_j|xQ_{i-1}\rangle \langle Q_j|Q_j\rangle}{\alpha_i\alpha_j} \\ &= 0\end{aligned} \tag{2}$$

1.2

证明: 对于$i=0,1,\ldots,n-3$:

$$\begin{aligned}\gamma_{i,n-1} &= \langle Q_i|xQ_{n-1}\rangle \\ &= \left\langle \alpha_{i+1}Q_{i+1} + \sum_{k=0}^{i}\langle Q_k|xQ_i\rangle Q_k \middle| Q_{n-1}\right\rangle \\ &= \alpha_{i+1}\langle Q_{i+1}|Q_{n-1}\rangle + \sum_{k=0}^{i}\langle Q_k|xQ_i\rangle \langle Q_k|Q_{n-1}\rangle \\ &= 0\end{aligned} \tag{3}$$

1.3

证明: 由1.2可知:

$$\begin{aligned}\gamma_{n-1,n} &= \alpha\langle Q_n|Q_n\rangle + \sum_{k=0}^{n} -1\langle Q_k|xQ_i\rangle \langle Q_k|Q_n\rangle \\ &= \alpha\end{aligned} \tag{4}$$

2

2.1

由于给出的Legendre多项式递推公式是对已经归一化的, 为减小计算根号的误差, 可以利用未归一化的公式:

$$(2*n+1)xV_n(x) = nV_{n-1}(x) + (n+1)V_{n+1}(x) \tag{5}$$

其中

$$V_n(x) = \sqrt{\frac{2}{2n+1}}P_n(x) \tag{6}$$

且$V_0(x)=1, V_1(x)=x$.

计算结果如下表:

表 1:

	Legendre	Laguerre
2	-0.1976423538	0.1250000000
16	-0.6087144379	0.09265564419
128	-0.2214407353	-0.2278406909
1024	-0.6063038195	0.1340328657

2.2

由Hermite多项式的递推公式知:

$$\alpha_i = \sqrt{\frac{i+1}{2}}, \beta_i = 0, i = 0, 1, \ldots \tag{7}$$

而对于Chebyshev多项式有

$$\alpha_0 = \frac{1}{\sqrt{2}}, \alpha_i = \frac{1}{2}, i = 1, 2, \ldots, \beta_i = 0, i = 0, 1, \ldots \tag{8}$$

写到对称三对角矩阵后即可使用带位移的隐式对称QR求本征值. 以下是计算结果和耗时:

表 2: 求解Hermite多项式和Chebyshev多项式的根耗时(CPU: Ryzen9 3950x, 单线程, 仅含求解特征值的时间, 单位: ms)

规模	Hermite多项式	Chebyshev多项式	Chebyshev多项式根的正确性 (所有根的误差均小于10^{-14})
2	0.002	0.000	是
16	0.011	0.011	是
128	0.515	0.507	是
1024	28.068	28.118	是

2.3

证明: 由对应不同特征值的特征向量的正交性和零点得:

$$\begin{aligned} f_j(x_i) &= \sum_{k=0}^{n-1} Q_k(x_i)Q_k(x_j) \\ &= \begin{cases} 0, & i \neq j \\ \sum_{k=0}^{n-1} Q_k(x_i)Q_k(x_i) = \frac{1}{\omega_i^2}, & i = j \end{cases}. \end{aligned} \tag{9}$$

即证明其是在高斯节点上的插值多项式. 现证明对于任何不超过$2n-1$次的多项式$f(x)$均有

$$\int_a^b f(x)\rho(x)dx = \int_a^b \sum_{k=0}^{n-1} f(x_k)g_k(x)\rho(x)dx = \sum_{k=0}^{n-1} f(x_k)A_k. \tag{10}$$

其中

$$A_k = \int_a^b g_k(x)\rho(x)dx, \tag{11}$$

而

$$g_k(x) = \omega_k^2 f_k(x) \tag{12}$$

为归一化后的基函数. 设$\Omega_n(x) = \prod_{k=0}^{n-1}(x - x_i)$, 通过多项式除法得到:

$$f(x) = \Omega_n(x)q(x) + r(x). \tag{13}$$

其中$q(x), r(x)$均为不超过$n-1$次的多项式. 从而

$$\int_a^b f(x)dx = \int_a^b \Omega_n(x)\rho(x)q(x)dx + \int_a^b r(x)\rho(x)dx \tag{14}$$

由于对于不超过$n-1$次的多项式, 其插值得到的积分式精确的, 所以对$r(x)$的积分是精确的. 而由于$\Omega_n(x)$与$Q_n(x)$的次数和零点一致, 所以仅差一个常数系数, 又任意小于等于$n-1$次的多项式可以用$\{Q_0(x), Q_1(x), \ldots, Q_{n-1}(x)\}$展开, 故

$$\int_a^b \Omega_n(x)\rho(x)q(x)dx = 0 \tag{15}$$

得证.

现求其系数: 从上面的证明可以看出权值

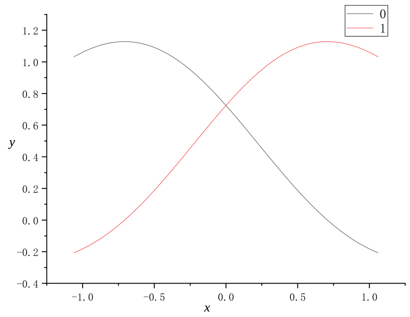
$$\begin{aligned} A_j &= \int_a^b g_j(x)\rho(x)dx \\ &= \sum_{i=0}^{n-1}\int_a^b \omega_j^2 Q_i(x_j)Q_i(x)\rho(x)dx \\ &= \sum_{i=0}^{n-1}\omega_j^2 \langle Q_0|Q_0\rangle = \omega_j^2. \end{aligned} \tag{16}$$

下表是求出不同规模的A_j的耗时 (1024阶Hermite多项式在计算时超出了double的范围):

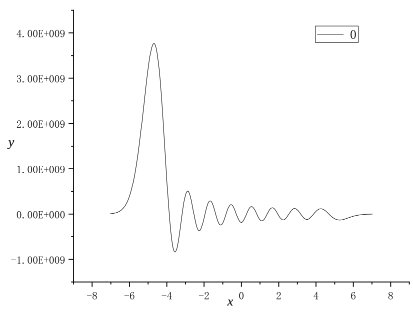
表 3: 求基函数权重A_j的耗时(CPU: Ryzen9 3950x, 单线程, 单位: ms)

耗时	Hermite多项式	Chebyshev多项式
2	0.005	0.000
16	0.022	0.003
128	10.263	1.196
1024	-	736.279

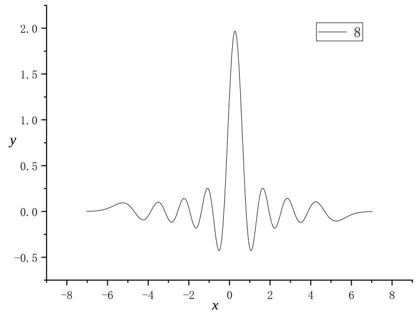
对于$N = 2, 16, 128$, 分别做出$j = 0, \frac{N}{2}$的各种图像:



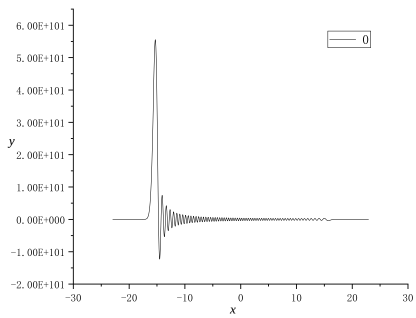
(a) Hermite(2), $j = 0, 1$



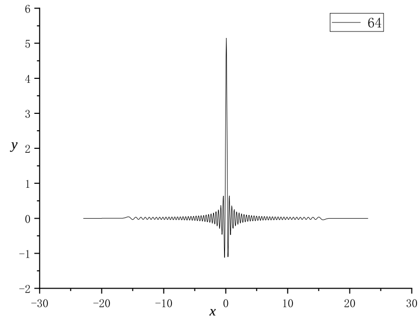
(b) Hermite(16), $j = 0$



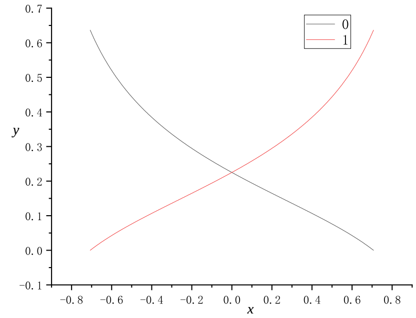
(c) Hermite(16), $j = 8$



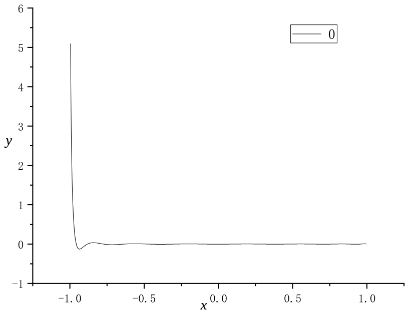
(d) Hermite(128), $j = 0$



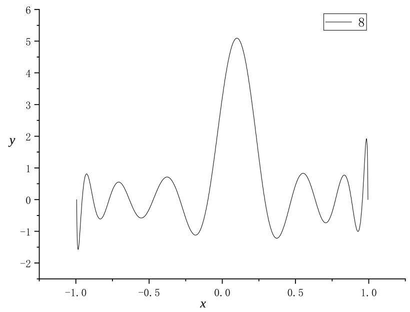
(e) Hermite(128), $j = 64$



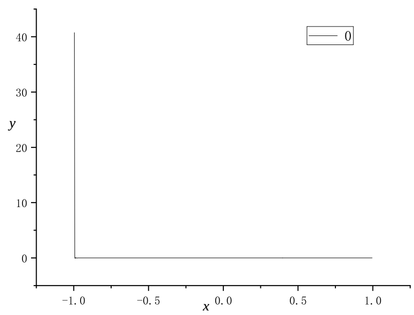
(f) Chebyshev(2), $j = 0, 1$



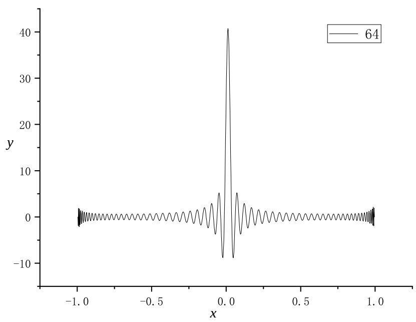
(g) Chebyshev(16), $j = 0$



(h) Chebyshev(16), $j = 0, 8$



(i) Chebyshev(128), $j = 0$



(j) Chebyshev(128), $j = 64$