计算物理 HW1 Problem3

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2021 年 10 月 16 日

题目. Hilbert 矩阵 本题中我们将考虑一个著名的、接近奇异的矩阵，称为 Hilbert 矩阵。

解答: (a) 应有 $\frac{\partial D}{\partial c_i} = \int_0^1 2x^{i-1}\left(\sum_{j=1}^{n} c_j x^{j-1} - f(x)\right)dx = 0$

满足 $\sum_{j=1}^{n}(H_n)_{ij}c_j = b_i,\ i,j = 1,\cdots,n$

可得 $(H_n)_{ij} = \frac{2}{i+j-1},\ b_i = \int_0^1 2x^{i-1}f(x)dx$

(b) 已知 $(H_n)_{ij} = (H_n)_{ji} = \frac{2}{i+j-1}$

可得 $\forall c \in \mathbb{R}^{n\times n}, c = \begin{pmatrix} c_1 \\ c_2 \\ \cdots \\ c_n \end{pmatrix}, c^T H_n c = \sum_{i=1}^{n}\sum_{j=1}^{n}\frac{c_i c_j}{i+j-1} = \sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j \int_0^1 x^{i+j-2}dx = \int_0^1\left(\sum_{i=1}^{n} c_i x^{i-1}\right)^2 dx \geq 0$, 仅当 $c = 0$ 时取等号;

综上，H_n 是对称的正定矩阵，根据线性代数知识，有 H_n 的最大主子行列式 $|H_n| > 0$，非奇异得证.

(c) 已知 $c_n = 1!\cdot 2!\cdots(n-1)!$，根据 Stirling's approximation, 当 $n >> 1$ 时, $n! \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$, 可得

$\ln det(H_n) = 4\ln c_n - \ln c_{2n} = 3\sum_{i=1}^{n-1}\ln(i!) - \sum_{i=n}^{2n-1}\ln(i!) \approx 3\sum_{i=1}^{n-1}\left[\left(i+\frac{1}{2}\right)\ln i - i + \frac{\ln 2\pi}{2}\right] - \sum_{i=n}^{2n-1}\left[\left(i+\frac{1}{2}\right)\ln i - i + \frac{\ln 2\pi}{2}\right]$.

但对于 $n<10$ 的情况, 我们可以精确求解得
$\ln det(H_n) = 4\ln c_n - \ln c_{2n} = 3\sum\limits_{i=1}^{n-1}\ln(i!) - \sum\limits_{i=n}^{2n-1}\ln(i!) = 3\sum\limits_{i=1}^{n-1}[(n-i)\ln i] - n\ln(n-1)! - \sum\limits_{i=n}^{2n-1}[(2n-i)\ln i] = \sum\limits_{i=1}^{n-1}[(2n-3i)\ln i] - \sum\limits_{i=n}^{2n-1}[(2n-i)\ln i]$.

所以这里我选择用精确求解的办法而不是 Stirling's approximation, 计算 $n<10$ 的情况代码见文件 1800011105-1-3(c).py

输出结果为:

$det(H_1) = 1$

$det(H_2) = 0.0833333$

$det(H_3) = 0.000462963$

$det(H_4) = 1.65344e^{-07}$

$det(H_5) = 3.7493e^{-12}$

$det(H_6) = 5.3673e^{-18}$

$det(H_7) = 4.8358e^{-25}$

$det(H_8) = 2.73705e^{-33}$

$det(H_9) = 9.72023e^{-43}$

$det(H_{10}) = 2.16418e^{-53}$

(d) 代码见 1800011105-1-3-(d).py

GEM 的输出结果如下

When n=1, the solution x is [0.5]

When n=2, the solution x is [-1.0, 3.0]

When n=3, the solution x is [1.5, -12.0, 15.0]

When n=4, the solution x is [-2.0, 30.0, -90.0, 70.0]

When n=5, the solution x is [2.5, -60.0, 315.0, -560.0, 315.0]

When n=6, the solution x is [-3.0, 105.0, -840.0, 2520.0, -3150.0, 1386.0]

When n=7, the solution x is [3.5, -168.0, 1890.0, -8400.0, 17325.0, -16632.0, 6006.0]

When n=8, the solution x is [-4.0, 252.0, -3780.0, 23100.0, -69300.0, 108108.0, -84084.0, 25740.0]

When n=9, the solution x is [4.5, -360.0, 6929.98, -55439.83, 225224.35, -504502.67, 630628.46, -411839.06, 109394.77]

When n=10, the solution x is [-5.0, 494.93, -11878.5, 120106.35, -630564.86, 1891710.83,

-3363065.89, 3500355.66, -1968960.67, 461857.15]

Cholesky 的输出结果如下

When n=1, the solution x is [0.5]

When n=2, the solution x is [-1.0, 3.0]

When n=3, the solution x is [1.5, -12.0, 15.0]

When n=4, the solution x is [-2.0, 30.0, -90.0, 70.0]

When n=5, the solution x is [2.5, -60.0, 315.0, -560.0, 315.0]

When n=6, the solution x is [-3.0, 105.0, -840.0, 2520.0, -3150.0, 1386.0]

When n=7, the solution x is [3.5, -168.0, 1890.0, -8400.0, 17325.0, -16632.0, 6006.0]

When n=8, the solution x is [-4.0, 252.0, -3780.0, 23100.0, -69300.0, 108108.0, -84084.0, 25740.0]

When n=9, the solution x is [4.5, -360.0, 6929.97, -55439.8, 225224.28, -504502.52, 630628.29, -411838.96, 109394.74]

When n=10, the solution x is [-5.0, 494.94, -11878.72, 120108.41, -630574.89, 1891738.93, -3363112.74, 3500401.56, -1968985.06, 461862.57]

两种方法的结果随 n 增大开始逐渐有差别, 我认为 Cholesky 更精确, 因为它利用了对称性, 节省了一半的运算次数, 这样舍入误差也应该更小, 结果的稳定性更好.