Statistics and Numerical Method — Problem Set #2 (due 10/21/2019)

1. Eigenvalue problem in hydrodynamics (6pts)

Waves are the basic phenomenon in a wide range of physical systems. Even you understand perfectly how to solve eigensystems, you should never forget the physical meanings behind. In this problem, let us consider waves in hydrodynamics. The basic equations of isothermal hydrodynamics read

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0 \ , \tag{1}$$

$$\frac{d\boldsymbol{v}}{dt} \equiv \frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot (\nabla \boldsymbol{v}) = -a^2 \frac{\nabla \rho}{\rho} \ , \tag{2}$$

where ρ, $\boldsymbol{v}$ are gas density and velocity. The pressure is given by $P = \rho a^2$ with a being a constant.

Now consider a 1D problem along the x direction. Suppose we have a homogenous background with $\rho = \rho_0$ and $\boldsymbol{v} = v_0 \hat{x}$. Linear perturbations on top of this background can be described by linearizing the above equations. Let perturbed quantities be denoted by a subscript '$_1$', which yields

$$\frac{\partial \rho_1}{\partial t} + \rho_0 \frac{\partial v_{x1}}{\partial x} + v_0 \frac{\partial \rho_1}{\partial x} = 0 \ , \quad \frac{\partial v_{x1}}{\partial t} + v_0 \frac{\partial v_{x1}}{\partial x} + \frac{a^2}{\rho_0}\frac{\partial \rho_1}{\partial x} = 0 \ . \tag{3}$$

These equations can be written in matrix form

$$\frac{\partial}{\partial t}\begin{pmatrix} \rho_1 \\ v_{x1} \end{pmatrix} + \begin{pmatrix} v_0 & \rho_0 \\ a^2/\rho_0 & v_0 \end{pmatrix} \frac{\partial}{\partial x}\begin{pmatrix} \rho_1 \\ v_{x1} \end{pmatrix} = 0 \ , \quad \text{or} \quad \frac{\partial}{\partial t}\boldsymbol{W} + A\frac{\partial}{\partial x}\boldsymbol{W} = 0 \ , \tag{4}$$

where $\boldsymbol{W} \equiv (\rho_1, v_{x1})^T$, and A is the constant matrix in the above.

(1). Let $\boldsymbol{W} = \boldsymbol{W}_0 e^{\mathrm{i}(kx - \omega t)}$, where k is given, and we would like to solve for ω (as a function of k), show that the above equation is reduced to an eigenvalue problem on matrix A. (1pt) 转化为求解 $AW_0 = \frac{\omega}{k} W_0$

(2). Compute (analytically) the eigenvalues and eigenvectors of the above, and discuss their physical meanings. (2pts)

$W_0 = \begin{pmatrix} \rho_0/a\, v \\ v \end{pmatrix}, \begin{pmatrix} \rho_0/a\, v \\ -v \end{pmatrix}$

$\omega/k = v_0 + a \ , \ v_0 - a$ 正传播和反传播. Doppler effect.

(3). Real world is in 3D. Even we restrict our problem to 1D, one should not ignore v_y and v_z. This would add two more linearized equations

$W_0 = \begin{pmatrix} \rho_0/a\, v \\ v \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \rho_0/a\, v \\ -v \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ v \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ v \end{pmatrix}$

特征向量仍是 $AW_0 = \frac{\omega}{k} W_0$

$$\frac{\partial v_{y1}}{\partial t} + v_0 \frac{\partial v_{y1}}{\partial x} = 0 \ , \quad \frac{\partial v_{z1}}{\partial t} + v_0 \frac{\partial v_{z1}}{\partial x} = 0 \ . \tag{5}$$

只是 $A = \begin{pmatrix} v_0 & \rho_0 & & \\ a^2/\rho_0 & v_0 & & \\ & & v_0 & \\ & & & v_0 \end{pmatrix}$

仍然可以线性叠加. 波的可叠加性质

Discuss how the eigensystem changes with this addition, and explain their meanings. (2pts)

(4). Solving (magneto-)hydrodynamic equations sometimes requires to solve an eigensystem like this (which contains additional dimensions corresponding to pressure/energy and magnetic fields). What method would you recommend? (1pt)

① 可先做合适的操作, 将其变为实对称的, 例如选 $P = \begin{pmatrix} \rho_0/a & & \\ & 1 & \\ & & 1 \end{pmatrix}$, 则 $P^{-1}AP$ 实对称 然后做 Jacobi 方法 或 Triangular + QR

2. Poisson solver (24 pts)

② 若不能变为实对称, 则可采用 Inverse Power + Shift 或 Hessenberg + QR

We have introduced the Poisson equation in the lecture

$$\nabla^2 \Phi = \rho \ , \tag{6}$$

where we have taken $4\pi G = 1$. In this problem, let us solve the Poisson equation in two dimensions on a uniform, 20×20 rectangular grid whose coordinates span over $([-10, 10], [-10, 10])$. This means the size of each grid cell is 1×1, and the value of that cell is defined at cell centers [e.g., $x_i = -10 + (i - 0.5)$, $y_j = -10 + (j - 0.5)$].

Using finite difference, this system of equations (400 in total!) can be expressed as

非直译的精确 处理，ρ和Φ都 定义在格点的中心；

$$\Phi_{i+1,j} + \Phi_{i-1,j} + \Phi_{i,j+1} + \Phi_{i,j-1} - 4\Phi_{i,j} = \rho_{i,j} \ , \ (i, j = 1, .., 20) \ . \tag{7}$$

In this problem, we take

$$\rho_{i,j} = \exp\left[-0.5(x_i^2 + y_i^2)\right] \ . \tag{8}$$

- 20×20 的格子 ⟺ 400×400 的方程 直接求解使用大矩阵
- 这里的边界条件是不物理的 $\Phi_{20,20}=0$，但 数值上的处理.

Additional boundary conditions must also be prescribed, and we set $\Phi = 0$ at $x, y = \pm 10$. To implement this boundary condition, you will need to include one additional "ghost cell" surrounding your grid, and enforce, e.g., $\Phi_{0,j} = -\Phi_{1,j}$, $\Phi_{N+1,j} = -\Phi_{N,j}$ (and similar in two other boundaries), so that one finds $\Phi = 0$ at the grid boundary after averaging the last grid cell and the ghost cell. Note that this boundary condition must be enforced after every numerical step.

处理 ρ, Φ "定义在格点中心" 与 "边界条件" 的矛盾. 增加 ghost point Φ_{0j}, $\Phi_{i,0}$ 等. $= -\Phi_{1j}$, $-\Phi_{i,1}$

To solve the above equations, we ask you to write your own solver in your favorite programming language using the following iterative methods: a). Jacobi; b). Gauss-Seidel; c). Successive over-relaxation with relaxation factor $\omega = 1.5$; d). Steepest descent; e). Conjugate gradient.

1). How many iterations are required for each of the methods to converge to within $\|R\|_2 < 10^{-6}$? 1076, 539, 173, 1094, 32 Show the converged solution. To better present your results, we further ask you to calculate the residual vector R (i.e. a 20×20 matrix) for up to 100 steps, and plot $\|R\|_2$ as a function of number of iterations. Please attach the original code that should be properly documented. (4 pts for each) 其他的, see the code

2). Further discuss the computation cost per iteration for each method. (4pts) Jacobi, Gauss-Seidel, SOR 复杂度 N^2 $(N=20)$ Steepest descent 和 Conjugate gradient 也是 N^2，但每次算 α_k 和 β_k，所以略大一些（这里是指每次迭代的计算复杂度大致相当）

3. Ionization equilibrium (10 pts)

Level of ionization plays an important role in the dynamics of the diffuse interstellar gas. It strongly affects heating and cooling processes, as well as the level of coupling between gas and magnetic fields. In this problem, we consider a toy model of ionization equilibrium applicable to the dense molecular cloud and protoplanetary disks, first proposed by Oppenheimer & Dalgarno (1974). In this model, there are five species and four reactions, and by assuming equilibrium states, electron abundance $x_e \equiv n_e/n \ll 1$ is found to be determined by

$$P(x_e) = x_e^3 + \frac{\beta}{\alpha} x_M x_e^2 - \frac{\zeta}{\alpha n} x_e - \frac{\zeta \beta}{\alpha \gamma n} x_M = 0 \ . \tag{9}$$

where $\alpha = 3 \times 10^{-6} (T/K)^{-1/2}$ cm^3 s^{-1}, $\gamma = 3 \times 10^{-9}$ cm^3 s^{-1}, $\beta = 3 \times 10^{-11} (T/K)^{-1/2}$ cm^3 s^{-1}, are the reaction rate coefficients for dissociative and radiative recombinations, and charge exchanges, $\zeta = 10^{-17}$ s^{-1} is the ionization rate, and x_M is the abundance "metal" elements (Mg or Fe). This equation can be solved numerically to obtain x_e as a function of n, T and x_M. 利用 $p(x_e) = x_e^3 + a_2 x_e^2 - a_1 x_e - a_0$

$p'(x_e) = 3x_e^2 + 2a_2 x_e - a_1$，导数在 $(0, \infty)$ 仅有一个零点，而 $p(x_e=0) < 0$

1). Show that this equation has only one positive root. Then discuss the (analytic) lower and upper bounds of this root (i.e., bracketing). (2 pts)

root 的范围可由 $p'(x_e)$ 的零点，和 $p(x_e)$ 明显为正的点来取，注意一般 $\alpha > \gamma$ 因为 root $\in \left(\frac{-a_2 + \sqrt{a_2^2 + 3a_1}}{3}, \sqrt{\frac{\zeta}{\alpha n}}\right)$

2). Fix $T = 30$K, $n = 10^5$ cm^{-3}, and $x_M = 10^{-12}$. Write and attach your own code to solve this function numerically using the following methods: a). Bisection; b). Secant method; c). Newton-Raphson method. Discuss how to robustly choose the initial trial value. Show the solution, and plot the relative error ($|x_i - x^*|$) as a function of iteration step i till convergence. (2 pts each)

Newton 找根时，因为 $p(x_e)$ 是下凸的，所以从 root 范围的上界 $\sqrt{\frac{\zeta}{\alpha n}}$ 开始比较好；其他两种方法就用 (1) 的结果. 其他细节见代码

3). Using your favorite method, calculate x_e as a function of n for $n = 10^4$ cm^{-3} to $n = 10^{14}$ cm^{-3}, assuming a). $T = 20$K, $x_M = 10^{-10}$; b). $T = 20$K, $x_M = 10^{-12}$; c). $T = 100$K, $x_M = 10^{-12}$. (2pts)

见代码