Class 9. Root Finding in Multi-D, and Numerical Differentiation

Nonlinear Systems of Equations

- Consider the system \( f(x, y) = 0, \ g(x, y) = 0 \). Plot zero contours of \( f \) and \( g \):

* No information about \( f \) in \( g \), and *vice versa*.
  - In general, no good method for finding roots.

- If you are near root, best bet is NR.
  
  E.g., For \( \mathbf{F}(x) = 0 \), choose \( x_{i+1} = x_i + \delta \), where \( \mathbf{F}'(x)\delta = -\mathbf{F}(x) \).
  
  - This is a matrix equation: \( \mathbf{F}'(x) \) is a matrix with elements \( \partial F_i/\partial x_j \). The matrix is called the Jacobian.

- Written out (2-D example):
  
  \[
  \frac{\partial f}{\partial x} \delta_x + \frac{\partial f}{\partial y} \delta_y = -f(x, y),
  \]
  
  \[
  \frac{\partial g}{\partial x} \delta_x + \frac{\partial g}{\partial y} \delta_y = -g(x, y).
  \]

- Given initial guess, must evaluate matrix elements and RHS, solve system for \( \delta \), and compute next iteration \( x_{i+1} \). Then repeat (must solve \( 2 \times 2 \) linear system each time).

- Essentially the non-linear system has been linearized to make it easier to work with.

- *NRiC* §9.7 discusses a global convergence strategy that combines multi-D NR with “backtracking” to improve chances of finding solutions.

**Example: Interstellar Chemistry**

- ISM is multiphase plasma consisting of electrons, ions, atoms, and molecules.

- Originally, the ISM was thought to be too hostile for molecules.
But in 1968-69, radio observations discovered absorption/emission lines of NH$_3$, H$_2$CO, H$_2$O, ...

Lots of organic molecules, e.g., CH$_3$CH$_2$OH (ethanol), etc.

In some places, all atoms have been incorporated into molecules.

E.g., molecular clouds: dense, cold clouds of gas composed primarily of molecules.

\( T \sim 30 \text{ K}, \ n \sim 10^6 \text{ cm}^{-3}, \ M \sim 10^{5-6} M_\odot, \ R \sim 10-100 \text{ pc.} \)

How do we predict what the abundances of different molecules should be, given \( n \) and \( T \)?

Need to solve a chemical reaction network.

Consider reaction between two species A and B:

\[ A + B \rightarrow AB \text{ (reaction rate} = n_A n_B R_{AB}). \]

Reverse also possible:

\[ AB \rightarrow A + B \text{ (reaction rate} = n_{AB} R'_{AB}). \]

In equilibrium:

\[ n_A n_B R_{AB} = n_{AB} R'_{AB}; \]
\[ n_A + n_{AB} = n_A^0; \]
\[ n_B + n_{AB} = n_B^0. \]

where \( n_A^0 \) and \( n_B^0 \) are normalizations so that A and B are conserved.

Substitute normalization equations into reaction equation to get quadratic in \( n_{AB} \), easily solved.

However, many more possible reactions:

\[ AC + B \leftrightarrow AB + C \text{ (exchange reaction);} \]
\[ ABC \leftrightarrow AB + C \text{ (dissociation reaction).} \]

Wind up with large nonlinear system describing all forward/reverse reactions, involving known reaction rates \( R \), plus normalizations. Must solve given fixed \( n^0 \) and \( T \).
Numerical Derivatives

• For NR and function minimization, often need derivatives of functions. It’s always better to use an analytical derivative if it’s available.

• If you’re stuck, could try:

\[ f'(x) \approx \frac{f(x + h) - f(x)}{h}, \]

where \(|h|\) is small.

• However, this is very susceptible to RE. Better:

\[ f'(x) \approx \frac{f(x + h) - f(x - h)}{2h}. \]

(This version cancels the second-derivative term in the Taylor series expansion of \(f(x + h) - f(x - h)\), leaving just the third- and higher-order terms.)

• Read *NRiC* §5.7 before trying this!