Root Finding in Multi-D, and Numerical Differentiation

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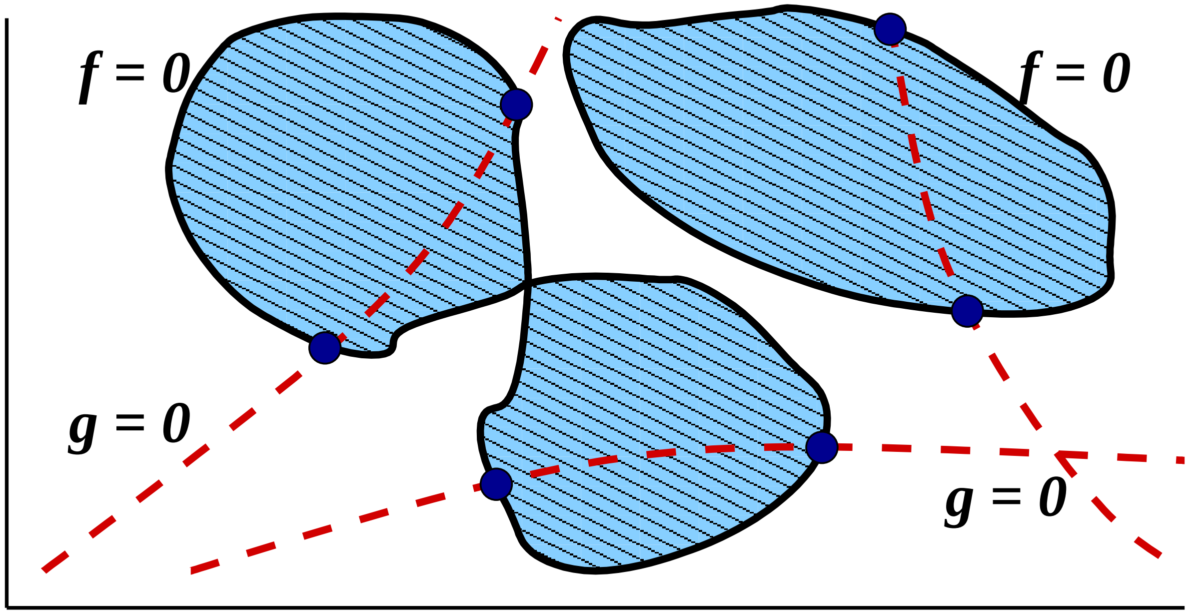
Nonlinear Systems of Equations

- 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 $\mathbf{F}(\mathbf{x}) = \mathbf{0}$, choose $\mathbf{x}_{i+1} = \mathbf{x}_i + \boldsymbol{\delta}$, where $\mathbf{F}'(\mathbf{x})\boldsymbol{\delta} = -\mathbf{F}(\mathbf{x})$.
  - This is a matrix equation: $\mathbf{F}'(\mathbf{x})$ is a matrix with elements $\partial F_i/\partial x_j$. The matrix is called the Jacobian.
- Written out (2-D example):

$$
\begin{aligned}
\frac{\partial f}{\partial x}\delta_x + \frac{\partial f}{\partial y}\delta_y &= -f(x, y), \\
\frac{\partial g}{\partial x}\delta_x + \frac{\partial g}{\partial y}\delta_y &= -g(x, y).
\end{aligned}
$$

- Given initial guess, must evaluate matrix elements and RHS, solve system for $\boldsymbol{\delta}$, and compute next iteration $\mathbf{x}_{i+1}$. Then repeat (must solve 2×2 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_2CO, H_2O, ...
- Lots of organic molecules, e.g., CH_3CH_2OH (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.

  ($T \sim 30$ K, $n \sim 10^6$ cm^{-3}, $M \sim 10^{5\text{–}6} M_\odot$, $R \sim 10$–100 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 $\longrightarrow$ AB (reaction rate = $n_{\rm A} n_{\rm B} R_{\rm AB}$).
- Reverse also possible:

  AB $\longrightarrow$ A + B (reaction rate = $n_{\rm AB} R'_{\rm AB}$).
- In equilibrium:

$$\begin{aligned} n_{\rm A} n_{\rm B} R_{\rm AB} &= n_{\rm AB} R'_{\rm AB}; \\ n_{\rm A} + n_{\rm AB} &= n^0_{\rm A}; \\ n_{\rm B} + n_{\rm AB} &= n^0_{\rm B}. \end{aligned}$$

  where $n^0_{\rm A}$ and $n^0_{\rm B}$ are normalizations so that A and B are conserved.
- Substitute normalization equations into reaction equation to get quadratic in $n_{\rm AB}$, easily solved.

- However, many more possible reactions:

$$\text{AC + B} \longleftrightarrow \text{AB + C} \quad \text{(exchange reaction);}$$

$$\text{ABC} \longleftrightarrow \text{AB + C} \quad \text{(dissociation reaction).}$$

- 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:

$$f'(x) \simeq \frac{f(x+h) - f(x)}{h},$$

where $|h|$ is small.

- However, this is <u>very</u> susceptible to RE. Better:

$$f'(x) \simeq \frac{f(x+h) - f(x-h)}{2h}.$$

  (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!