2008 Lecture 7 starts here

Newton-Raphson

- When the derivative of f(x) is known, and when f(x) is well behaved, the celebrated (and ancient) Newton-Raphson method gives the fastest convergence of all ("quadratic", i.e. m = 2, such that $\varepsilon_n = \varepsilon_{n-1}^2$)

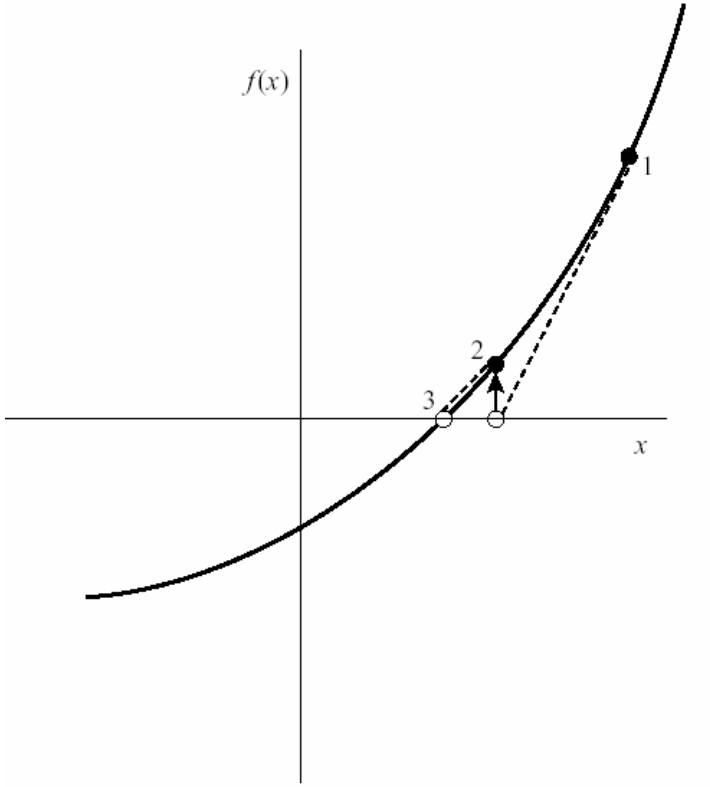
- Relies on the Taylor expansion

  $f(x + \delta) = f(x) + \delta\, f'(x) + \tfrac{1}{2}\, \delta^2\, f''(x) + \ldots..$

  If *ith* iteration, x_i, is close to the root, then for the next iteration, try $x_{i+1} = x_i + \delta$ with $\delta = -f(x_i) / f'(x_i)$

Geometric representation

- Newton-Raphson method: picture from *Recipes*
- Convergence is quadratic, with m=2



Extrapolate the local derivative to find the next estimate of the root

Newton-Raphson

- Convergence is rapid, and the method is very useful for “polishing” a root (i.e. refining an estimate that is nearly correct)

Clearly, a few iterations usually yields an accurate result in the limit of small δ, because terms of order $\frac{1}{2}\,\delta^2\,f''(x)$ or higher are much smaller than $\delta\,f(x)$

$$f(x + \delta) = f(x) + \delta\,f'(x) + \tfrac{1}{2}\,\delta^2\,f''(x) + \ldots..$$

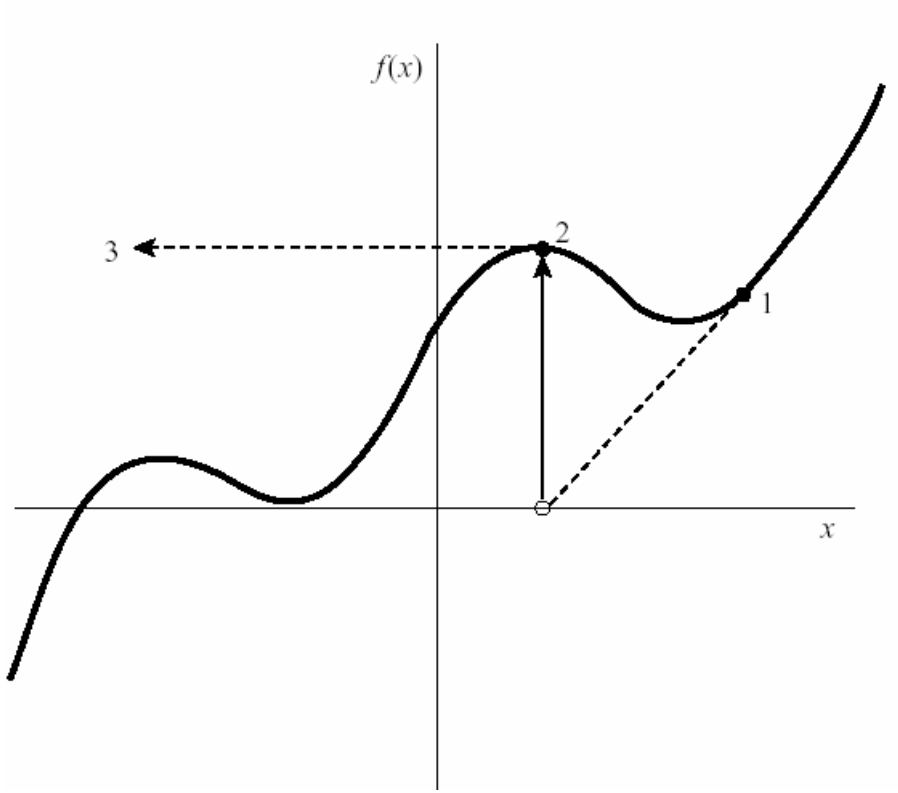
Exception: when $f'(x)$ is very small (or zero)

Newton-Raphson

- Cases where f′(x) is small (i.e. where there is a local extremum) can send the solution shooting off into outer space

  …. unless the method is modified to keep the solution within a known bracket

  (as in routine “RTSAFE”)



Summary of 1-D root finding

- Preferred methods:
  - If f′ is known analytically, “safe Newton-Raphson” is the preferred method
  - If f′ is not known analytically, Brent’s method is the method of choice
    - Could use “safe Newton-Raphson” with the derivative computed numerically, but the latter takes up as much time as is saved by the use of N-R
  - Newton-Raphson is also useful for rapid “polishing” (very close to the solution) and for multidimensional root finding.

Roots of polynomial functions

- General polynomial equation

  $0 = P(x) \equiv \Sigma\, a_k\, x^k$

  has an analytic solution for cases up to and including the quartic

  No general analytic solution for quintics and higher (“the equation that couldn’t be solved”)

Roots of polynomial functions

- General features:

  Polynomial of order N will have N roots, which can be real or complex and may or may not be distinct

  If the a_k are all real, the roots may be real or complex, but any complex roots will occur in pairs of complex conjugates, $a \pm bi$

  Polynomials can be ill-conditioned: a small change in the coefficients can cause a large change in the roots

Roots of polynomial functions

- General features:

  Degenerate roots, or nearly equal roots, present the biggest numerical problems

  Example: $P(x) \equiv (x - c)^2 = 0$

  – Brackets don't exist since P(x) is never negative

  – Derivative $f'(x) = 0$ at the solution $x = c$

  ➔ Newton-Raphson is potentially unstable

Deflation

- Every time a root, x_k, is found, the order of the polynomial can be decreased by one, and the equation becomes

  $0 = P(x) = (x - x_k)\, Q(x)$

  where Q(x) can be obtained by "synthetic division" (see §5.3 in *Recipes*)

- This procedure, known as "deflation", allows the roots to be obtained one-by-one

Laguerre's method for obtaining a single root

- Mathematical background

$$P(x) = (x-x_1)\,(x-x_2)\,\ldots\,(x-x_n)$$

$$\ln|P(x)| = \ln|x-x_1| + \ln|x-x_2| + \ldots. + \ln|x-x_n|$$

$$G \equiv d \ln|P(x)|/dx = (x-x_1)^{-1} + (x-x_2)^{-1} + \ldots + (x-x_n)^{-1}$$

$$H \equiv -\, d \ln|P(x)|/dx^2 = (x-x_1)^{-2} + (x-x_2)^{-2} + \ldots + (x-x_n)^{-2}$$

Laguerre's method for obtaining a single root

- Now make a "drastic set of assumptions"

  We suppose x_1 is located at distance *a* from our current guess, x, and that all the other roots lie at a distance *b*

$$G = (x-x_1)^{-1} + (x-x_2)^{-1} + \ldots + (x-x_n)^{-1} = a^{-1} + (n-1)\, b^{-1}$$

$$H = (x-x_1)^{-2} + (x-x_2)^{-2} + \ldots + (x-x_n)^{-2} = a^{-2} + (n-1)\, b^{-2}$$

We can then eliminate b from the above equations to obtain a quadratic equation for a^{-1} …..

Laguerre's method for obtaining a single root

We then obtain

$$a = \frac{n}{G \pm \sqrt{(n-1)(nH - G^2)}}$$

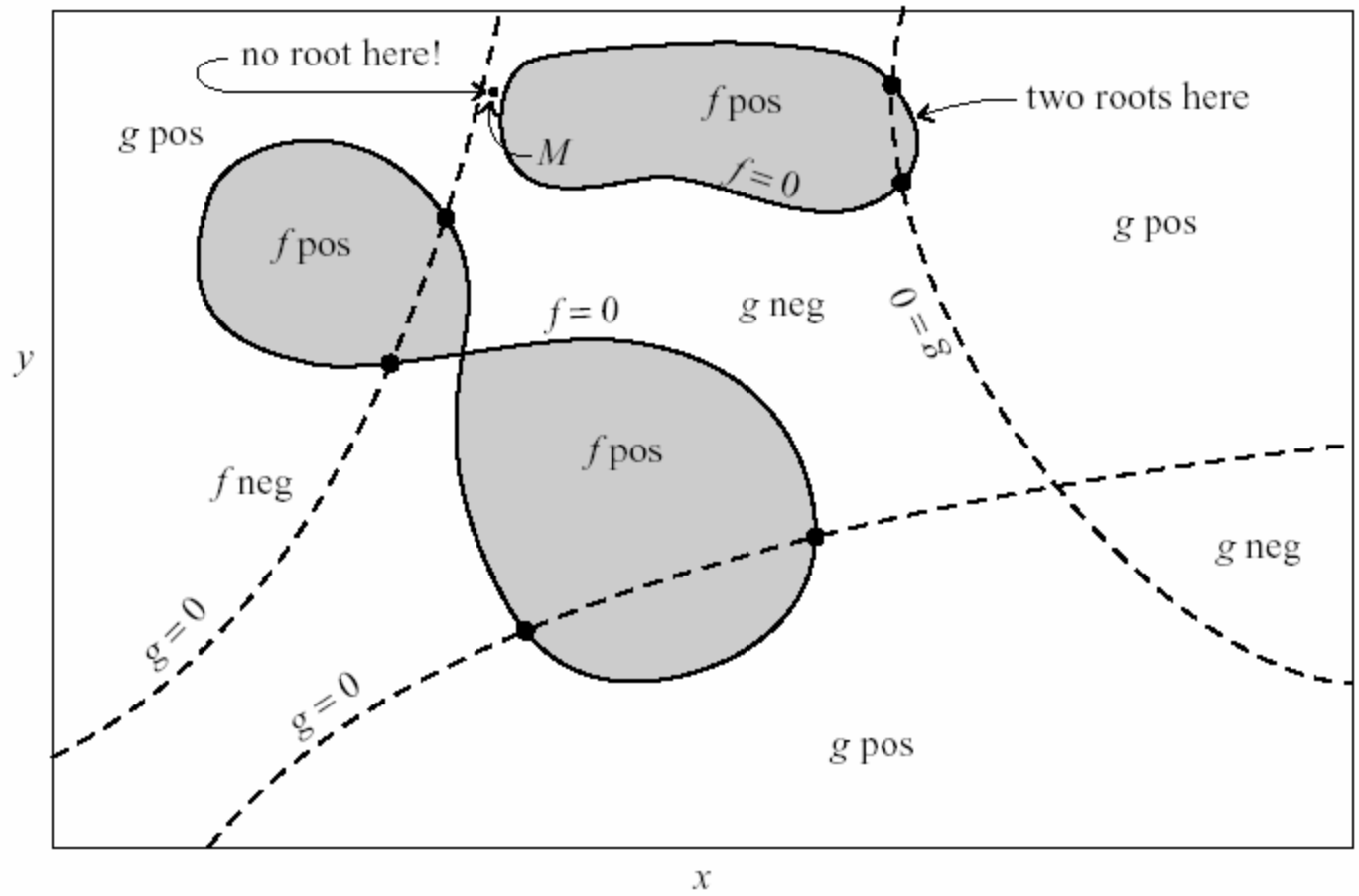
This, of course, is not the exact value of $(x - x_1)$, because of the approximation made in obtaining it, but it is useful for obtaining the next estimate of x_1, which we take as $(x - a)$

Overview

- Find roots one at a time, using Laguerre's method iteratively until *a* is sufficiently small
- After each root is found, reduce the order of the polynomial by deflation.

Multidimensional non-linear systems of equations

- In general, a horrible problem, for reasons shown schematically in *Recipes*, Fig 9.6.1



Multidimensional non-linear systems of equations

- The only general algorithm is Newton-Raphson

Generalization to multidimensional case

$f(x + \delta) = f(x) + \delta\, f'(x) + (1/2)\, \delta^2\, f''(x) + \ldots..$

becomes

$\mathbf{f}(\mathbf{x} + \delta) = \mathbf{f}(\mathbf{x}) + \mathbf{J}(\mathbf{x})\, \delta + O(\delta^2)$

where **J** is the Jacobian matrix, with $J_{ik} = \partial f_i / \partial x_k$

Multidimensional non-linear systems of equations

The next iteration on **x** is therefore

$$\mathbf{x}' = \mathbf{x} + \delta = \mathbf{x} - \mathbf{J}^{-1} f(\mathbf{x})$$

where $\delta = -\mathbf{J}^{-1}\,\mathbf{f}(\mathbf{x})$ is obtained by the solution of the linear set of equations $\mathbf{J}\,\delta = -\mathbf{f}$

(which we know how to do! ☺)

As in 1-D, this only works with a smooth function or a good first guess

Newton-Raphson with a modified step size

- Can improve the robustness of multidimensional N-R by considering the quantity:

  $Q \equiv \frac{1}{2} | \mathbf{f} |^2 = \frac{1}{2} \Sigma f_i f_i$

  which tends to zero at the root

  Any good step should make Q smaller

Newton-Raphson with a modified step size

- Consider now the gradient of Q

$$\partial Q/\partial x_j = \partial(\tfrac{1}{2}\,|\mathbf{f}|^2)/\partial x_j = \Sigma\, f_i\, \partial f_i/\partial x_j$$

$$\rightarrow \quad \nabla Q = \mathbf{f}^T\, \mathbf{J}$$

Our step $\delta = -\mathbf{J}^{-1}\,\mathbf{f}$ is in the *right direction* to reduce Q, because

$$\nabla Q \,.\, \delta = -\,\mathbf{f}^T\,(\mathbf{J}\,\mathbf{J}^{-1})\,\mathbf{f} = -\,2Q < 0$$

Newton-Raphson with a modified step size

So if adding δ to $\mathbf{x}$ doesn't decrease Q, a sufficiently small step in *the same direction* must

Strategy: if the solution starts to overshoot – as indicated by monitoring of $Q \equiv \frac{1}{2} |\mathbf{f}|^2$ – use a smaller step $\lambda\delta$ in the same direction (where λ is a positive scalar < 1)

See *Recipes* §9.7 for the details of how to choose λ

This is implemented in the function NEWT, which will successfully find a root for almost any reasonable initial guess.

Example application: interstellar chemistry

- More than one hundred different molecules have been detected in the interstellar gas

- They are formed and destroyed by a complex network of reactions involving bimolecular reactions and unimolecular processes such as photodissociation

Example application: interstellar chemistry

- Consider the reaction A + B → C + D:

  This destroys A and B (and creates C and D) at a rate k_r n(A)n(B) per unit volume, where n(X) is the density of species X (number per unit volume) and k_r is the rate coefficient (units: $cm^3\ s^{-1}$) for the reaction in question

- Molecule A might also be destroyed by photodissociation, A + hν → E + F

  This destroys A (and creates E and F) at a rate ζ_p n(A) per unit volume, where n(X) is the density of species X (number per unit volume) and ζ_p is the photodissociation rate (units: s^{-1}) for this process

Rate equations for interstellar chemistry

- The density of the *i*th molecule therefore obeys the rate equation:

Processes that create *i*th molecule

Reactions that destroy *i*th molecule

$$\partial n_i / \partial t = \sum_j \sum_k k_{ijk}\, n_j\, n_k + \sum_k \zeta_{ik}\, n_k - n_i \sum_m \sum_k k_{mik}\, n_k - n_i \sum_m \zeta_{mi}$$

Sum of rate coefficients for all reactions of j and k that produce i

Total rate at which k undergoes unimolecular processes to produce i

Equilibrium solution

- In equilibrium, the molecular densities will obey **f**(**n**) = **0**

  where n_i is the density of molecule number *i* , and $f_i \equiv \partial n_i / \partial t$ is a quadratic function of the n_i

  A multidimensional root-finding problem!

  …and one for which the Jacobian is easily computed (quadratic function)

$$\partial f_i / \partial n_k = \sum_j k_{ijk}\, n_j + \zeta_{ik} - n_i \sum_m k_{mik} \qquad (i \neq k)$$

$$\partial f_i / \partial n_i = -\sum_m k_{mik}\, n_k - \sum_m \zeta_{mi} \qquad \text{(diagonal elements)}$$

  Newton's method generally works well

Complication

- The equilbrium equations, as written, are singular, since they don't uniquely specify the total density of molecules

  We need to apply some constraints of the form

$$\sum n_i N_{ic} = n(E_c)$$

N_{ic} = number of atoms of element C contained in molecule i

$n(E_c)$ = (fixed) density of C nuclei

Non-equilibrium solution

- In astrochemistry, the timescale for reaching equilibrium can sometimes be long compared to the ages of molecular clouds

  Therefore, it is also interesting to integrate the equations

$$\partial n_i / \partial t = \sum_j \sum_k k_{ijk}\, n_j\, n_k + \sum_k \zeta_{ik}\, n_k - n_i \sum_m \sum_k k_{mik}\, n_k - n_i \sum_m \zeta_{mi}$$

  (a coupled set of ODE's, to be considered later)

  In the limit of large t, this tends to the equilibrium solution

  ➔ an alternative method even if we are uninterested in the time evolution