Even more amazing result

- $x_0 = Pb$ is the smallest solution to $Ax = b$ (i.e. the one that minimizes the length $|x_0|$)
- Consider another solution, $(x_0 + x')$, where $x'$, of course, must lie in the nullspace of $A$
- But, $x_0 = VQUTb$ must be orthogonal to the nullspace:
  - $x_0$ is a linear combination of those columns of $V$ for which $w_k$ is non-zero (since $Q_{kk} = 0$ when $w_k = 0$)
  - $x'$ is a linear combination of those columns of $V$ for which $w_k$ is zero
- Hence $|x_0 + x'|$ is always larger than $|x_0|$
  $\Rightarrow x_0 = Pb$ is the shortest vector that satisfies $Ax = b$
Least squares solution when $b$ lies outside the range of $A$

- This is related to the case of the $M \times N$ matrix considered in Lecture 1 (for the case $M > N$)

The solution that comes closest to satisfying $A \mathbf{x} = b$ (i.e. which minimizes $| A \mathbf{x} - b |$) is again $\mathbf{x} = P b$
Nearly singular matrices

- Even if $A$ is non-singular, numerical problems can arise as a result of roundoff error when solving $Ax = b$, particularly when the matrix $A$ is “nearly” singular.
- Here, none of singular values is actually zero, but some are very small relative to others.
- Define condition number = largest $w_i$/smallest $w_i$.
  When the condition number is very large, LU decomposition fails.
Nearly singular matrices

- SVD can often help here. We obtain the SVD of the nearly singular matrix, then zero out the small $w_i$ values, then find the least squares solution to $A \mathbf{x} = \mathbf{b}$ (i.e. write $\mathbf{x} = \mathbf{P} \mathbf{b}$)

- The error caused by replacing the smallest $w_i$ values with zero is often not as bad as the roundoff errors that result when the condition number is very large $\Rightarrow$ it sometimes pays to deliberately make a nearly singular matrix singular and then use SVD rather than LU decomposition
Numerical integration
(Numerical recipes, Chapter 4)

• Analytical differentiation is easy, but analytical integration is “hard”: more of an art than a science
  – Led to the development of numerical techniques, even back in the 18th Century
  – Even simple classical methods are still useful
Numerical integration

- Numerical integration is always equivalent to the solution of a differential equation:
  \[ y = \int f(x) \, dx \quad \text{then} \quad \frac{dy}{dx} = f(x) \]

There are several modern algorithms for solving differential equations (that are particularly useful when \( f(x) \) is not smooth)

These involve adaptive step size and will be discussed later
Basic integration techniques

• These harken back the Riemann definition of the integral

\[ \int_a^b f(x) \, dx = \lim_{N \to \infty} \sum_{i=1}^{N} \Delta x_i \, f(x_i) \]

• First consider methods that use a constant step size (\(\Delta x_i = h\) for all \(i\))
Trapezoidal rule

• Break integral into N – 1 equally spaced intervals

\[ I = h \left( \frac{1}{2} f_1 + f_2 + f_3 + \ldots + f_{N-1} + \frac{1}{2} f_N \right) \]

\[ + h^2 \left( \frac{f_1' - f_N'}{12} \right) + \ldots \]

with stepsize \( h = \frac{x_b - x_a}{(N - 1)} \)

• Error is proportional to \( h^2 \propto \frac{1}{N^2} \)
  – Need to cover regions where \( f'' \) is large with high density of points
Simpson’s rule

• Slightly better performer for fairly smooth functions

• Again, break integral into \( N - 1 \) equally spaced intervals, but now use

\[
I = h \left( f_1 + 4f_2 + 2f_3 + 4f_4 + 2f_5 + \ldots + 2f_{N-2} + 4f_{N-1} + f_N \right)/3
+ h^4 \frac{(f_1'' - f_N'')}{180} + \ldots
\]

with \( N \) odd

• Now error is proportional to \( f'''/N^4 \)
Geometric interpretation

- Black – integrand; red – trapezoid; blue – Simpson’s
Control of truncation errors

• The choice of N must reflect the obvious tradeoff between
  accuracy (\( \propto 1/N^2 \) or \( 1/N^4 \)) and computational expense (\( \propto N \))

• We keep increasing N until the answer stops changing (or changes only by an acceptably small amount)
Romberg integration

- We can even plot $I$ vs $h$

- If the resultant function is smooth (good polynomial fit), we can extrapolate to $h = 0$
Complications

• Integrable singularity at the lower limit
  – Suppose the integrand has a singularity at $x = a$ (lower limit of integration), which diverges as $(x - a)^{-\gamma}$ with $0 \leq \gamma < 1$
  – Then use the change of variable $t = (x - a)^{1-\gamma}$, which yields

\[
\int_{a}^{b} f(x) dx = \frac{1}{1-\gamma} \int_{0}^{(b-a)^{1-\gamma}} t^{\gamma/(1-\gamma)} f(t^{1/(1-\gamma)} + a) dt
\]
Complications

• Integrable singularity at the upper limit
  – Suppose the integrand has a singularity at $x = b$
    (lower limit of integration), which diverges as $(b - x)^{-\gamma}$
    with $0 \leq \gamma < 1$
  – Then use the change of variable $t = (b - x)^{1-\gamma}$, which yields

\[
\int_{a}^{b} f(x) \, dx = \frac{1}{1-\gamma} \int_{0}^{(b-a)^{1-\gamma}} t^{\gamma/(1-\gamma)} f(b - t^{1/(1-\gamma)}) \, dt
\]
Complications

• Integrable singularity in the middle of the range at \( x = c \), where \( a < c < b \)

Simply write

\[
\int_{a}^{b} f(x)\,dx = \int_{a}^{c} f(x)\,dx + \int_{c}^{b} f(x)\,dx
\]

and use both formulae
Complications

• Bottom line: hard to devise a general numerical integrator
  – We always evaluate the function at a finite number of points, so we rarely detect an integrable singularity
  – Need to identify integrable singularities by analytical methods
Complications

• Upper or lower limit of ±∞
  – Use change of variables to map ∞ to a finite number (e.g. zero)
  e.g. for
    \[ I = \int_{1}^{\infty} \frac{1}{x^2} g(x) \, dx \]

  use \( x = 1/t \) \( \Rightarrow \) \( dx = - \frac{dt}{t^2} = - x^2 \, dt \)

  to obtain \[ I = \int_{0}^{1} g(1/t) \, dt \]
Irregular step sizes
(see Numerical Recipes, §4.5, for details)

• So far, we have only used methods that compute the integral as

\[ I = \sum w_i f(x_i) \]

where \( w_i \) are the weights
(e.g. \( \frac{1}{2}, 1, 1, 1, \ldots, 1, \frac{1}{2} \) for the trapezoid rule)
and the \( x_i \) are evenly-spaced

• For smooth functions, better accuracy can be achieved if we permit the \( x_i \) to be unevenly spaced

• For the right choices of \( w_i \) and \( x_i \), we can arrange for the sum to be exact for \( f(x) \) equal to any polynomial of degree \( 2N - 1 \) or less! (Gaussian quadrature)
Multidimensional integrals
(see *Numerical Recipes*, §4.6)

- So far, we’ve only considered 1-D integrals.
- Methods for multidimensional integrals:
  1) for highly symmetric cases, can sometimes be rewritten as 1-D integral

  Example: when integrating a spherically-symmetric 3-D function of \(x, y, \text{ and } z\), we can use

\[
\int \int \int f(x,y,z) \, dx \, dy \, dz = \int f(r) \, 4\pi \, r^2dr
\]
Multidimensional integrals

2) Can write as N nested 1-D integrals
\[ \int d^\alpha x \, f(x) = \int dx_1 \int dx_2 \ldots \int dx_\alpha \, f(x_1, x_2, \ldots, x_\alpha) \]

But..

- we need to know about function pathologies
- the boundary has to be simple (which it often isn’t)
- we need \( N^\alpha \) evaluations of the function
Multidimensional integrals

If the function is smooth, but the boundary is complex, then Monte Carlo methods can work quite well

→ Use multiple function evaluations at random locations within the boundary

Next topic: random number generation
Monte Carlo Integration

- Basic idea:

\[ \int f(x) \, dV = \bar{f} \, V \]

where \( \bar{f} \) is the average value of \( f \) within the volume \( V \)
Monte Carlo Integration

- How do we estimate $\bar{f}$?

- Throw down points at random within the volume, and compute the average of $f$ evaluated for those points

- If the boundary is complex, choose a hypercube that encloses it and discard points that lie outside the boundary
Monte Carlo Integration

If there are N points within the boundary:

Best estimate of $f$ is $\bar{f} \equiv (1/N) \sum f(x_i)$

Standard error on that estimate is $\sqrt{(\langle f^2 \rangle - \langle f \rangle^2)/N}$
Monte Carlo Integration

• So, Monte Carlo integration yields an estimate of the integral

\[ I = \frac{V}{N} \sum f(x_i) \]

with a typical error

\[ \delta I = V \sqrt{\langle f^2 \rangle - \langle f \rangle^2} / N \]

Unfortunately, the \( N^{-\frac{1}{2}} \) dependence is not very favorable
Monte Carlo Integration

• The fractional error $\delta I/I$ is of order
  $\sqrt{(\langle f^2 \rangle / \langle f \rangle^2 - 1)/N}$

The quantity $(\langle f^2 \rangle / \langle f \rangle^2 - 1)$ can be large if $f(x)$ is strongly peaked

For example, if $f$ is very high in a small fraction of the volume, we are oversampling (i.e. wasting points) on regions where $f$ is small.
Monte Carlo Integration

• Accuracy is improved if we can find a change of variables $dV' = g(x) \, dV$ such that $g(x)$ has a strong dependence similar to that of $f(x)$

• Then $\int f(x) \, dV = \int [f(x)/g(x)] \, dV'$

| Strongly peaked | Not strongly peaked |