Iterative Solvers

Iterative vs. Direct Solvers

- Direct Solver/Method – closed form strategy, e.g. quadratic/Cardano formula, Gaussian Elimination for LU factorization, Cholesky factorization, etc.
- Iterative Solver/Method
  - start with an initial guess c^1
  - use a recursive approach to improve that guess: $c^2, c^3, c^4, \ldots$
  - terminate based on a stopping criterion, e.g. when error is small $\|c^q - c^{exact}\| \leq \epsilon$

- A direct method can be used to obtain an initial guess
- Iterative methods are great for sparse matrices, as they often can ignore 0 entries
  - E.g. by formulating the method via the matrix's action (multiplication) on a vector
- Direct solvers are more commonly used on dense matrices
- Iterative solvers are used for training Neural Networks!

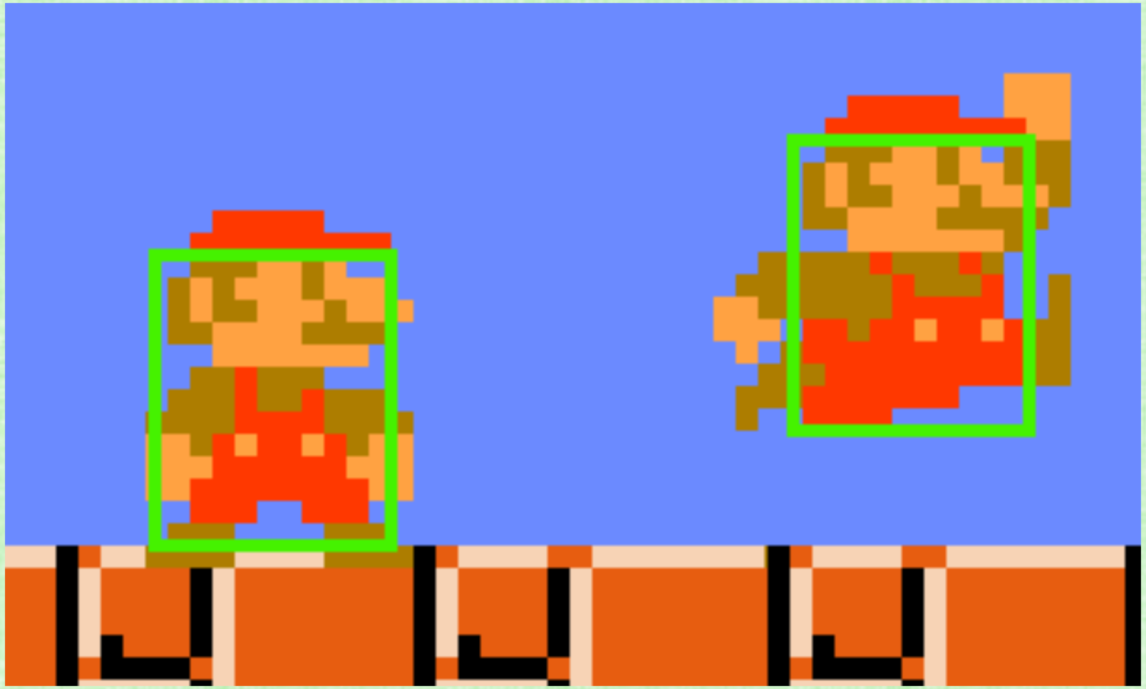
Issues with Direct Methods

- (Recall) Quadratic formula loses precision, and can fail, when $-b \pm \sqrt{b^2 - 4ac}$ has catastrophic cancellation
  - The de-rationalized quadratic formula instead uses $-b \mp \sqrt{b^2 - 4ac}$
  - Using one formula for each root avoids catastrophic cancellation

- Cardano’s formula for the roots of a cubic equation suffers from similar issues, but there is no straightforward fix
- The computed roots too often have unacceptably high error
- To highlight why one might need accurate cubic roots, consider collision detection…

Hit Box

- In order to detect interactions between objects in video games, objects were assigned a hit box
- Anything inside an object's hit box can potentially interact with (i.e. hit) it

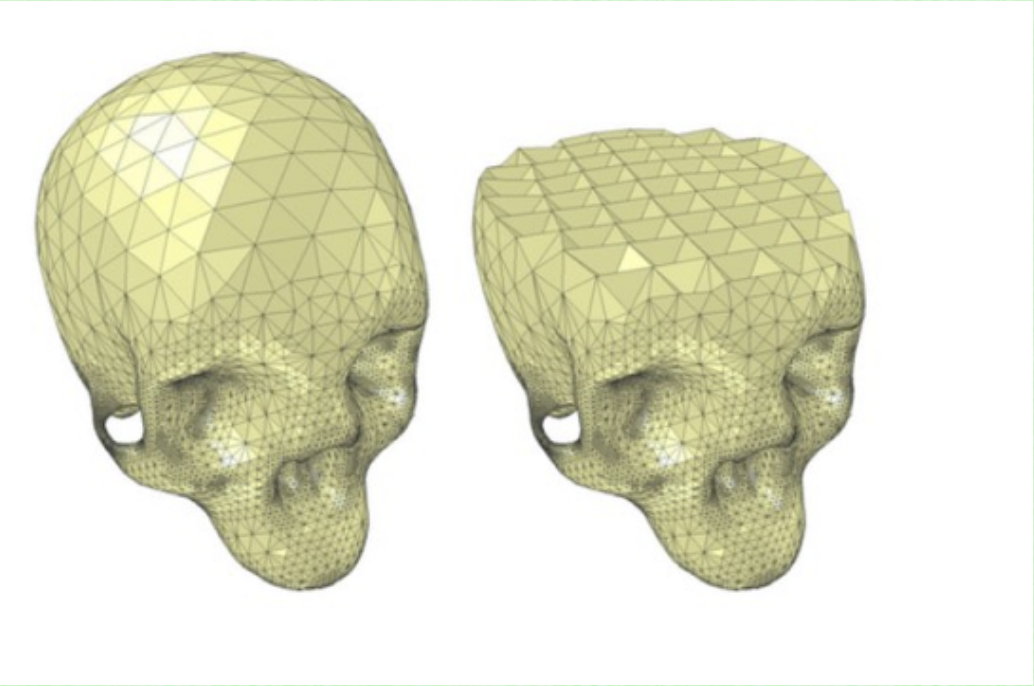


Better Hit Boxes

- These evolved over time to more complicated shapes in both 2D and 3D
  - e.g. spheres, ellipsoids, capsules, etc.
- Anything <u>inside</u> any of an object's hit boxes can potentially interact with it

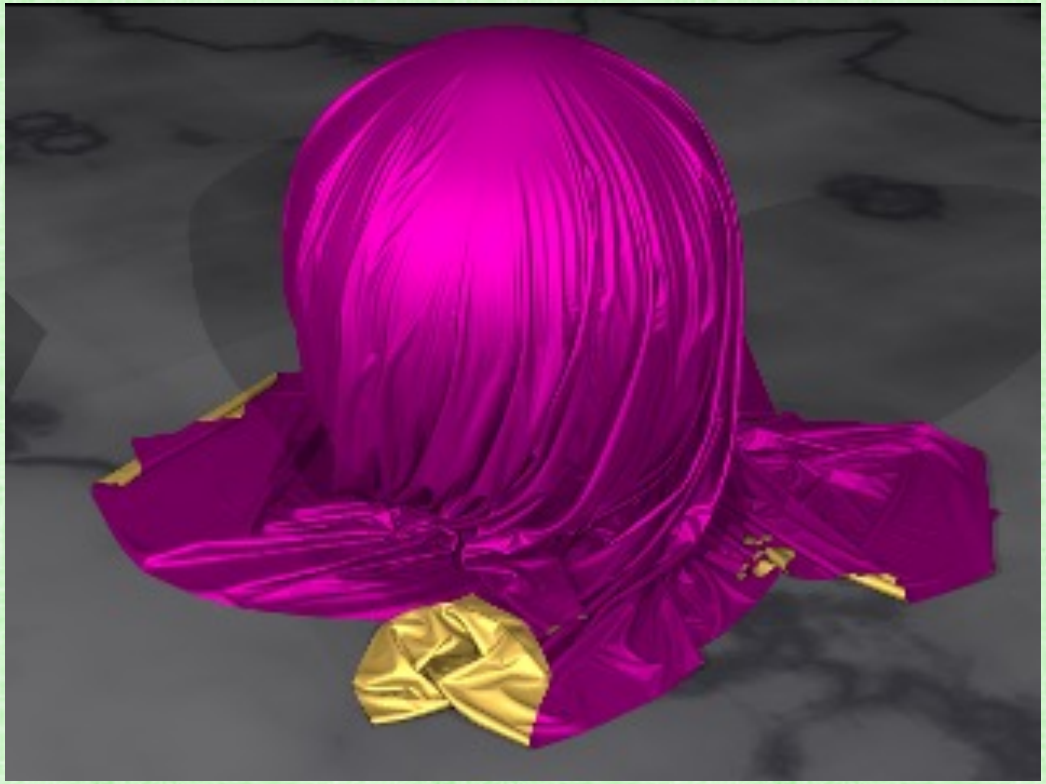
Accurate Collision Detection

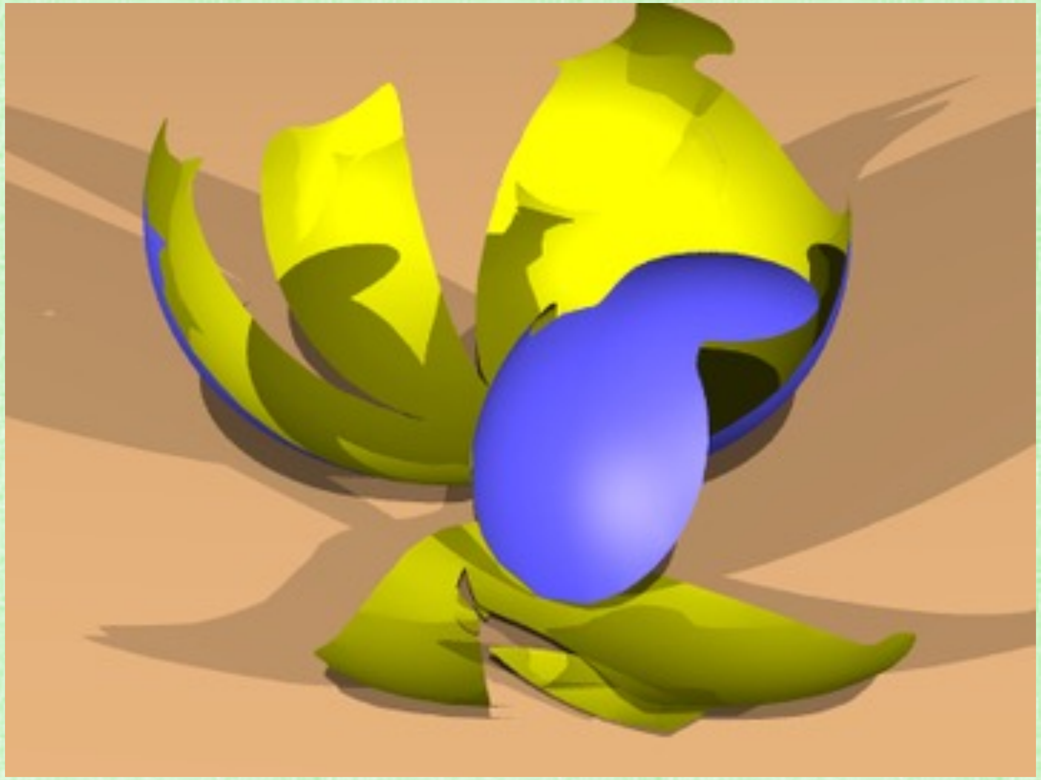
- More complex objects are often modeled by a triangulated surface mesh
- The interior can be filled with tetrahedra, or approximated with other objects
- Anything <u>inside</u> any of an object's interior structures can potentially interact with it



Objects Without Interiors

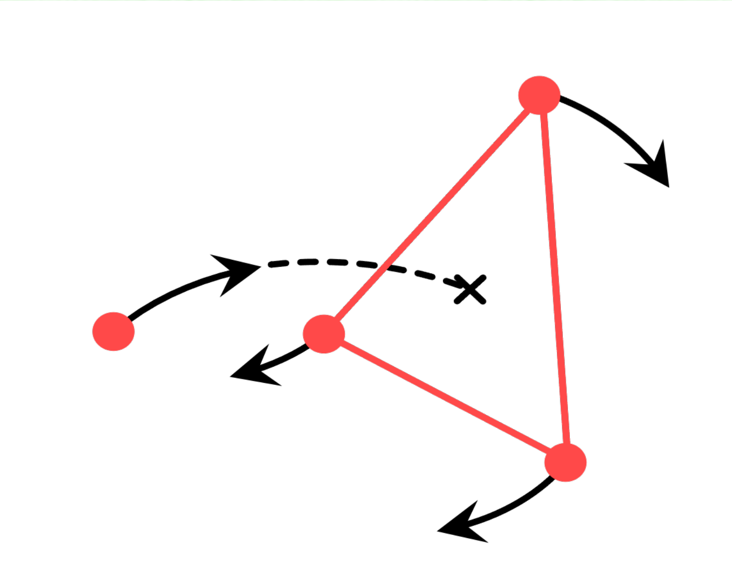
- Very thin objects, such as cloth/shells, do not have an interior region
- One cannot use the same concept of inside to detect potential interactions

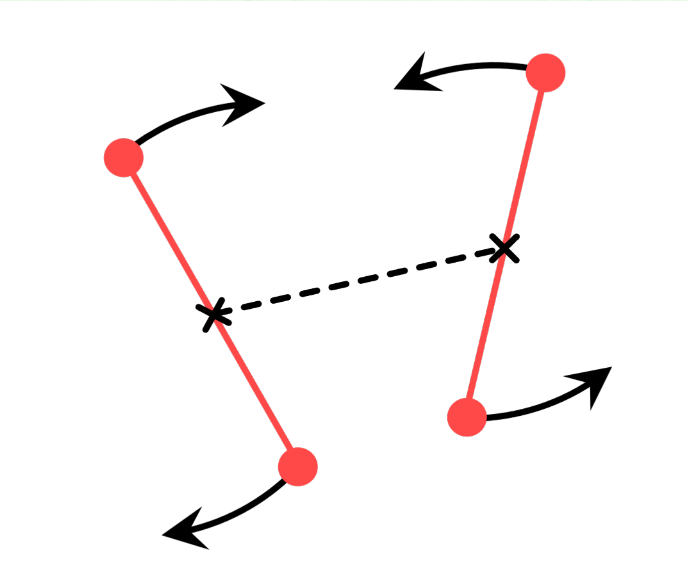




Continuous Collision Detection (CCD)

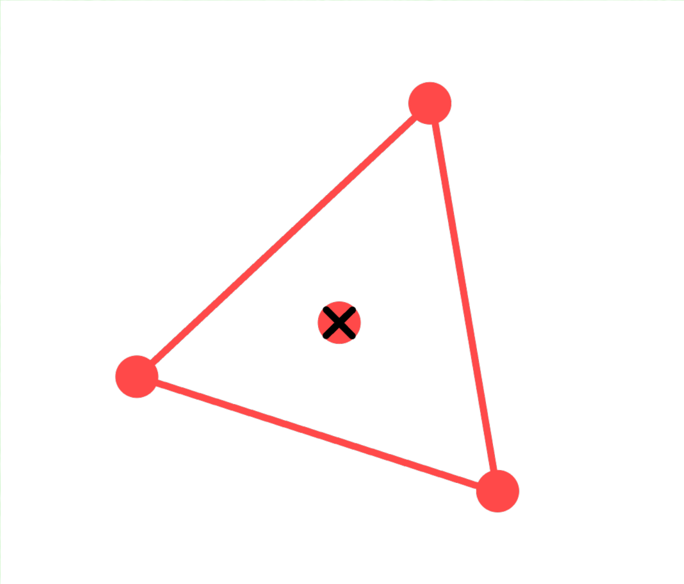
- Model the time varying trajectories of surface triangle vertices to see if/when they collide with each other
- Doesn't depend on the existence of an interior region
- There are two cases to consider: (1) Point-Face, (2) Edge-Edge

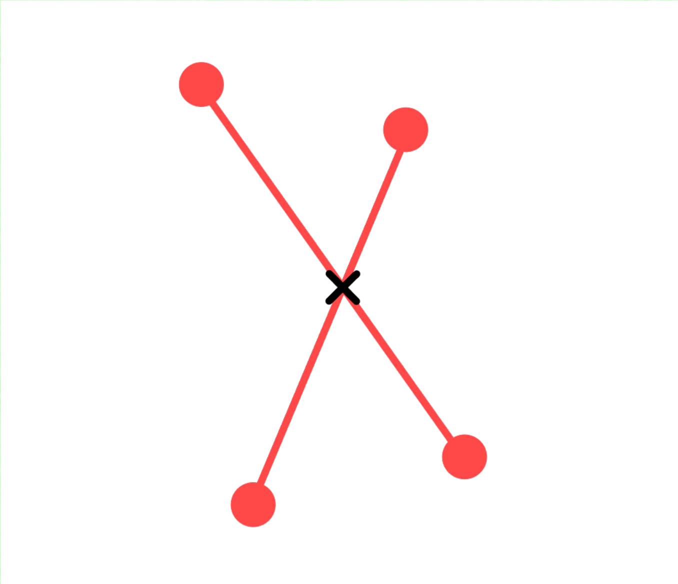




Continuous Collision Detection (CCD)

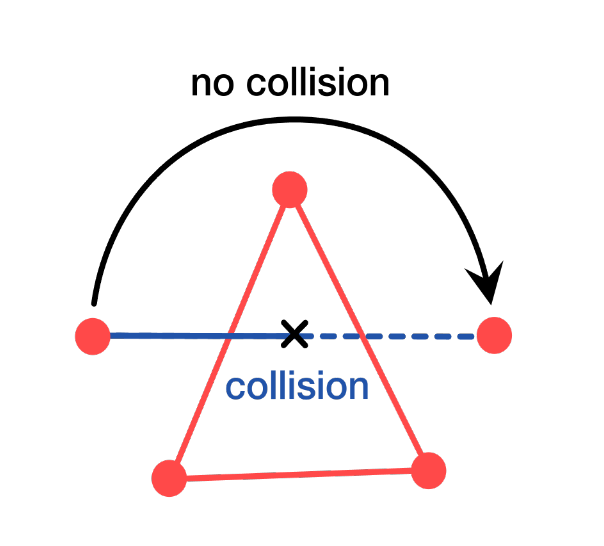
- In both cases, the 4 relevant points need to become <u>coplanar</u> in order to (potentially) collide
- Once deemed coplanar, a second check determines whether: the lone point is inside the triangle (for Point-Face) or the two edges intersect (for Edge-Edge)

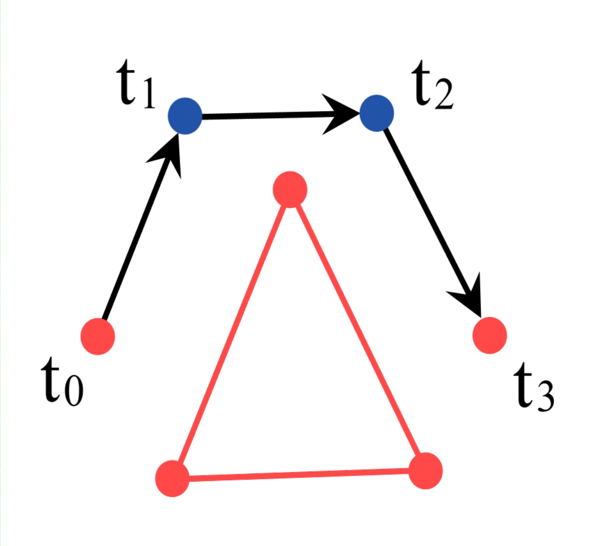




Continuous Collision Detection (CCD)

- Consider time t_o to time t_f and assume that the points have constant velocities during that time interval: $V_i(t_o)$ for $\mathrm{i} = 1, 2, 3, 4$
- The time evolving positions are: $X_i(t) = X_i(t_o) + V_i(t_o)(t - t_o)$ for $t \in [t_o, t_f]$
- Although their paths are (generally) curved, considering piecewise linear increments is sufficient for preventing self-intersecting states





Continuous Collision Detection (CCD)

- Coplanarity occurs when $X_4(t) - X_1(t), X_3(t) - X_1(t)$, and $X_2(t) - X_1(t)$ are not a basis for R^3, which can be checked by making them the columns of a 3x3 matrix and setting the determinant to zero (obtaining a cubic equation in t)
- Find the first root of this cubic equation in the interval $\left[t_o, t_f\right]$
- Cubic equation solvers are so error prone that collisions are (very) often missed, and the cloth/shell ends up in a spurious self-intersecting state

- A very carefully devised/implemented <u>iterative solver</u> for <u>cubic equations</u> was able to detect all collisions:
  - It requires <u>double precision</u> (and fails too often in single precision)
  - See Bridson et al. “Robust Treatment of Collisions, Contact, and Friction for Cloth Animation” (2002)

Residual and Solution Error

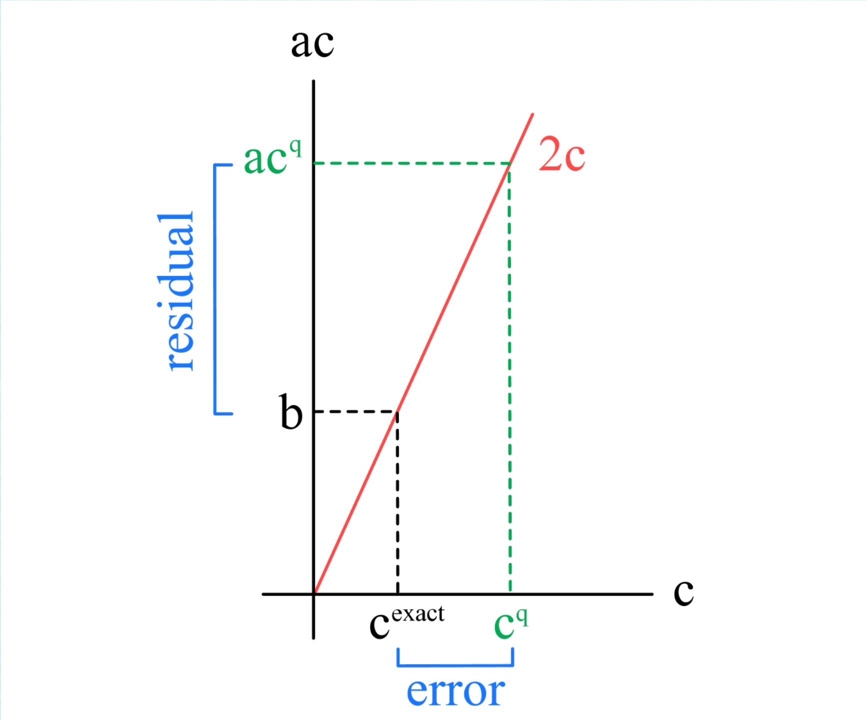
- When solving $Ac = b$, a current guess c^q has residual $r^q = b - Ac^q$
- The residual measures the errors in the equations, not the error in the solution
- The error in the solution $e^q = c^q - c^{exact}$ relates to the residual via:

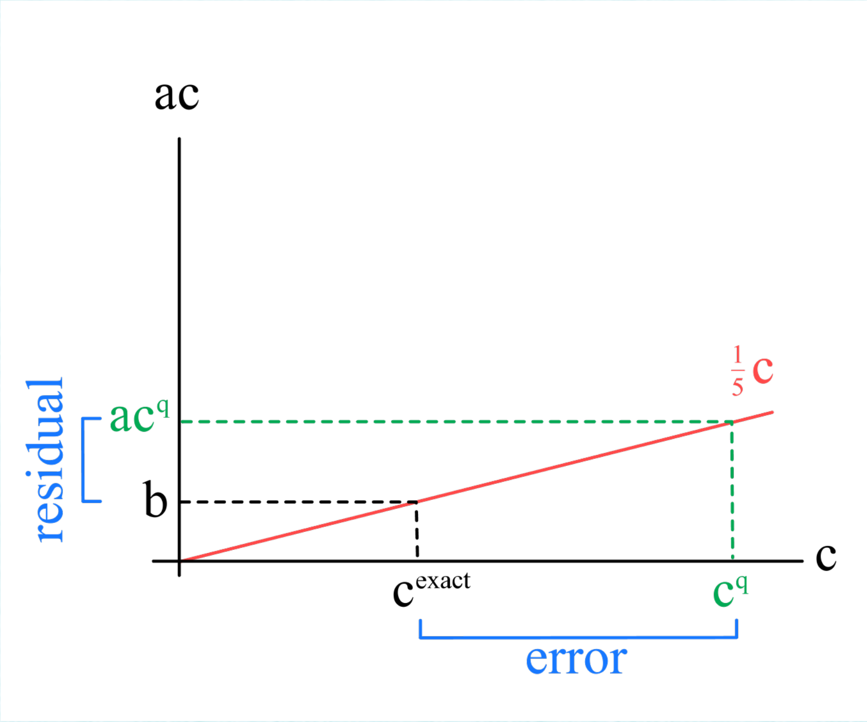
$$r^q = b - Ac^q = Ac^{exact} - Ac^q = A(c^{exact} - c^q) = -Ae^q$$

- That is, the residual is the solution error transformed into the space that b lives in (the range of A)

1D example

- Consider a simple size $1x1$ matrix, i.e. $[a]c = b$ with exact solution $c = \frac{b}{a}$
- Since $r^q = -ae^q$, smaller a values lead to deceivingly small residuals even when the error is large





Diagonalizing the Residual/Error Equation

- ”All matrices are diagonal matrices”
- And, diagonal matrices represent decoupled 1D scalar problems

- Using the SVD, $r^q = -Ae^q$ becomes $(U^T r^q) = -\Sigma(V^T e^q)$ which is a decoupled set of diagonal equations
- Each decoupled equation has the form $\hat{r}_k^q = -\sigma_k \hat{e}_k^q$ (seen on the previous slide)
- Small σ_k lead to deceivingly small residuals even when the error is large

- A small residual indicates a small error for larger singular values, but not for smaller singular values

Line Search

- Choose a search direction s^q and move some distance α^q in that direction to update the current guess to the next guess: $c^{q+1} = c^q + \alpha^q s^q$
  - There are various strategies for choosing α^q, including the notion of safe sets that clamp its maximum magnitude
  - Subtract c^{exact} from both sides of this recursion to get $e^{q+1} = e^q + \alpha^q s^q$
  - Multiply through by $-A$ to get $r^{q+1} = r^q - \alpha^q A s^q$
- Optimally, one would follow s^q until all the error in that direction was eliminated
  - That is, until the remaining error is orthogonal to s^q, i.e. $e^{q+1} \cdot s^q = 0$
  - However, the error is unknown (otherwise, the solution would be known)
- Instead, follow s^q until the residual is orthogonal to s^q, i.e. $r^{q+1} \cdot s^q = 0$
  - Plugging in the recursion for r^{q+1} gives $\alpha^q = \frac{s^q \cdot r^q}{s^q \cdot A s^q}$

Steepest Descent

- Steepest Descent chooses the steepest downhill direction as the search direction
  - That turns out to be the residual, i.e. choose $s^q = r^q$
- Iterate: $r^q = b - Ac^q$, $\alpha^q = \frac{r^q \cdot r^q}{r^q \cdot Ar^q}$, $c^{q+1} = c^q + \alpha^q r^q$, until r^q is considered small enough
- Note: can replace $r^q = b - Ac^q$ with $r^q = r^{q-1} - \alpha^{q-1} Ar^{q-1}$
  - Since Ar^{q-1} had already been computed to find α^{q-1}, this eliminates one of the (possibly expensive) multiplications by A
- Drawback: Steepest Descent repeatedly searches in overlapping (non-orthogonal) directions, especially for higher condition number matrices (more on this later)

Conjugate Gradients (CG)

- A very efficient and robust method for SPD systems
- Converges (theoretically) in at most n-steps for an nxn matrix
  - Theoretically, only need one step for each distinct eigenvalue
  - Almost converged when taking one step for each eigenvalue cluster
  - Thus, preconditioning makes a big difference (assuming it clusters eigenvalues)
- Motivation: choosing **orthogonal** search directions precludes repeatedly searching in overlapping directions (in contrast to Steepest Descent)
  - But, it is difficult to implement this orthogonality
- Instead: choose **A-orthogonal** search directions
  - Instead of $< s^q, s^{\hat{q}} > = 0$, choose $< s^q, s^{\hat{q}} >_A = 0$ for $q \neq \hat{q}$

Error Analysis for CG

- In the A-orthogonal basis of search directions, the initial error is $e^1 = \sum_{\hat{q}=1}^{n} \beta^{\hat{q}} s^{\hat{q}}$; so, $< s^q, e^1 >_A = \beta^q < s^q, s^q >_A$
- Error recursion gives $e^q = e^1 + \sum_{\hat{q}=1}^{q-1} \alpha^{\hat{q}} s^{\hat{q}}$; so, $< s^q, e^q >_A = < s^q, e^1 >_A$
- Progressing until $r^{q+1} \cdot s^q = 0$ gives $\alpha^q = \frac{s^q \cdot r^q}{s^q \cdot A s^q} = -\frac{<s^q, e^q>_A}{<s^q, s^q>_A} = -\beta^q$
- Thus, $e^1 = \sum_{\hat{q}=1}^{n} (-\alpha^{\hat{q}}) s^{\hat{q}}$ and $e^q = \sum_{\hat{q}=q}^{n} \left(-\alpha^{\hat{q}}\right) s^{\hat{q}}$
  - This proves that the error is indeed cancelled out in n steps, i.e. $e^{q+1} = 0$

- Aside: If $\tilde{q} < q$, then $s^{\tilde{q}} \cdot r^q = -< s^{\tilde{q}}, e^q >_A = 0$; so, the residual is orthogonal to all previous search directions (not just the previous one)

Gram-Schmidt

- Orthogonalizes a set of vectors
- For each new vector, subtract its (weighted) dot product overlap with all prior vectors, making it orthogonal to them
- A-orthogonal Gram-Schmidt simply uses an A-weighted dot/inner product
- Given vector $\bar{S}^q$, subtract out the A-overlap with s^1 to s^{q-1} so that the resulting vector s^q has $< s^q, s^{\hat{q}} >_A = 0$ for $\hat{q} \in \{1,2,\cdots,q-1\}$
- That is, $s^q = \bar{S}^q - \sum_{\hat{q}=1}^{q-1} \frac{<\bar{S}^q, s^{\hat{q}}>_A}{<s^{\hat{q}}, s^{\hat{q}}>_A} s^{\hat{q}}$ where the two non-normalized $s^{\hat{q}}$ both require division by their norm (and $< s^{\hat{q}}, s^{\hat{q}} >_A = \left\| s^{\hat{q}} \right\|_A^2$)
- Proof: $< s^q, s^{\tilde{q}} >_A = < \bar{S}^q, s^{\tilde{q}} >_A - \frac{<\bar{S}^q, s^{\tilde{q}}>_A}{<s^{\tilde{q}}, s^{\tilde{q}}>_A} < s^{\tilde{q}}, s^{\tilde{q}} >_A = 0$

Gram-Schmidt for CG

- Choose candidate search directions $\bar{S}^q = r^q$, and make A-orthogonal via Gram-Schmidt
- That is, $s^q = r^q - \sum_{\hat{q}=1}^{q-1} \frac{<r^q, s^{\hat{q}}>_A}{<s^{\hat{q}}, s^{\hat{q}}>_A} s^{\hat{q}}$
- Dot product with $r^{\tilde{q}}$ to get: $s^q \cdot r^{\tilde{q}} = r^q \cdot r^{\tilde{q}} - \sum_{\hat{q}=1}^{q-1} \frac{<r^q, s^{\hat{q}}>_A}{<s^{\hat{q}}, s^{\hat{q}}>_A} s^{\hat{q}} \cdot r^{\tilde{q}}$
  - If $\tilde{q} > q$, then $0 = r^q \cdot r^{\tilde{q}} + 0$ implies that all the residuals are orthogonal
  - If $\tilde{q} = q$, then $s^q \cdot r^q = r^q \cdot r^q + 0$ implies $\alpha^q = \frac{r^q \cdot r^q}{<s^q, s^q>_A}$
- Dot product $r^q = r^{q-1} - \alpha^{q-1} A s^{q-1}$ with $r^{\tilde{q}}$ to get
  - $r^{\tilde{q}} \cdot r^q = r^{\tilde{q}} \cdot r^{q-1} - \alpha^{q-1} < r^{\tilde{q}}, s^{q-1} >_A$
  - If $\tilde{q} > q$, then $0 = 0 - \alpha^{q-1} < r^{\tilde{q}}, s^{q-1} >_A$ implies that only the last term in the sum is nonzero
  - If $\tilde{q} = q$, then $r^q \cdot r^q = 0 - \alpha^{q-1} < r^q, s^{q-1} >_A$ for the last term in the sum
- Finally, $s^q = r^q + \frac{r^q \cdot r^q}{\alpha^{q-1} <s^{q-1}, s^{q-1}>_A} s^{q-1} = r^q + \frac{r^q \cdot r^q}{r^{q-1} \cdot r^{q-1}} s^{q-1}$

Conjugate Gradients Method

- Start with: $s^1 = r^1 = b - Ac^1$
- Iterate:
  - $\alpha^q = \frac{r^q \cdot r^q}{<s^q, s^q>_A}$
  - $c^{q+1} = c^q + \alpha^q s^q$ and $r^{q+1} = r^q - \alpha^q A s^q$ (both as usual for line search)
  - $s^{q+1} = r^{q+1} + \frac{r^{q+1} \cdot r^{q+1}}{r^q \cdot r^q} s^q$

- Note: Gram-Schmidt drifts, making search directions less A-orthogonal over time; thus, occasionally throw out all search directions and start over with $s^1 = r^1 = b - Ac^1$

Non-Symmetric and/or Indefinite

- GMRES, MINRES, BiCGSTAB, etc…
- Generally speaking, iterative methods for non-symmetric and/or indefinite matrices are less stable, more error prone, and slower than CG on an SPD matrix