Strang I.4

$Ax = b$

Example

"row view"

$$\begin{bmatrix} 1 & -2 \\ 2 & 3 \end{bmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1 \\ 9 \end{pmatrix}$$

$$A \quad \vec{x} \quad = \quad \vec{b}$$

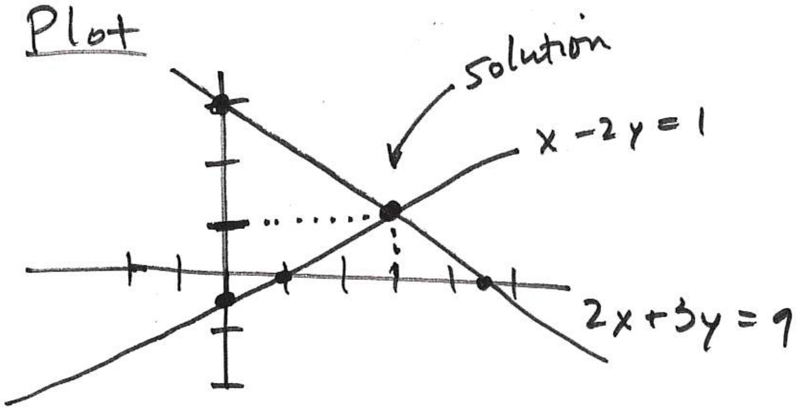
$$\left.\begin{aligned} x - 2y &= 1 \\ 2x + 3y &= 9 \end{aligned}\right\} \text{ two lines in } \mathbb{R}^2$$

$$\vec{x} = \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 3 \\ 1 \end{pmatrix}$$

check:

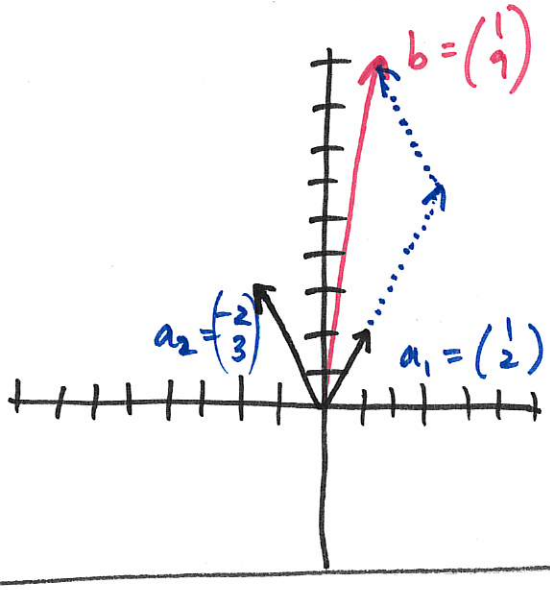
$$\begin{cases} 3 - 2 = 1 \ \checkmark \\ 6 + 3 = 9 \ \checkmark \end{cases}$$

Plot



"column view"

$$b = 3\vec{a}_1 + 1\vec{a}_2$$



"row view" in 3D : 3 planes meet at point

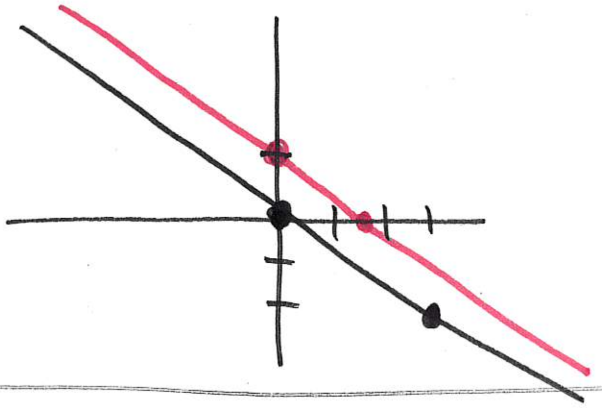
"column view" in 3D : 3 columns combine to give $\vec{b}$.

Ex $\quad$ A singular

$$A = \begin{pmatrix} 2 & 3 \\ 4 & 6 \end{pmatrix}$$

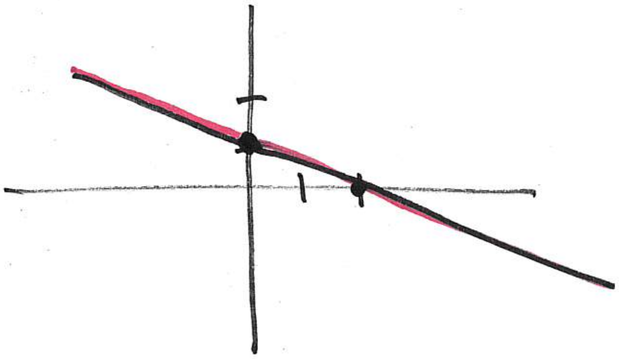
row view

$2x + 3y = 0$
$2x + 3y = 3$



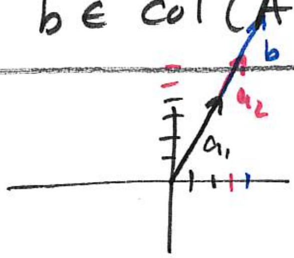
$$\begin{pmatrix} 2 & 3 \\ 4 & 6 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 4 \\ 8 \end{pmatrix}$$

solutions : $\begin{pmatrix} \alpha \\ \frac{1}{3}(4-2\alpha) \end{pmatrix}$



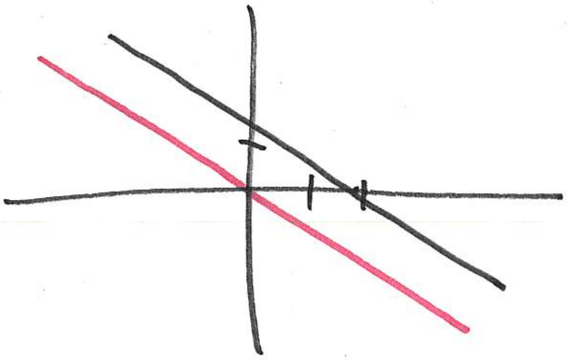
$\boxed{\text{case: } b \in col(A)}$

col view :



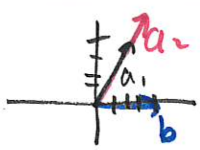
$$\begin{pmatrix} 2 & 3 \\ 4 & 6 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 4 \\ 0 \end{pmatrix}$$

no solutions



$\boxed{\text{case: } b \notin col(A)}$

col view:



$Ax = b$

A $n \times n$ matrix

b $n \times 1$ column vector

A **nonsingular** if any one of

1. has an inverse $AA^{-1} = A^{-1}A = I$

2. $\det(A) \neq 0$

3. $\text{rank}(A) = n$ "full rank"

4. if $\vec{z} \neq \vec{0}$, $A\vec{z} \neq \vec{0}$ (no nontrivial null space)

Existence and Uniqueness

A nonsingular $\Rightarrow$ $Ax = b$ has the unique solution $x = A^{-1}b$

A singular $\Rightarrow$ # of solutions depends on b

- if $b \in$ column space (A) $\Rightarrow$ infinitely many solutions

- if $b \notin$ column space (A) $\Rightarrow$ no solution

Solving $Ax = b$

transform to system that is easier to solve.

Triangular System

$$\begin{pmatrix} x & x & x & x \\ & x & x & x \\ & & x & x \\ & & & x \end{pmatrix} \begin{pmatrix} x \\ x \\ x \\ x \end{pmatrix} = \begin{pmatrix} x \\ x \\ x \\ x \end{pmatrix}$$

Q. How would you solve this?

Preconditioning

A, M nonsingular (e.g. $M = D$, diagonal scaling)

$$MAz = Mb$$

$$z = (MA)^{-1} Mb = A^{-1}M^{-1}Mb = A^{-1}b = x \checkmark$$

Permutation Matrix

row permutation (identity with rows permuted)

$$PAx = Pb$$

column permutation (identity with columns permuted)

$$APz = b \quad \Rightarrow \quad z = P^{-1}x$$

$$AP(P^{-1}x) = b \qquad x = Pz$$

The Factorization $A = LU$

3×3 example $\quad A = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 5 & 7 \\ 2 & 7 & 8 \end{pmatrix}$

$$LU = \begin{pmatrix} x & 0 & 0 \\ x & x & 0 \\ x & x & x \end{pmatrix} \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \end{pmatrix}$$

$$= \begin{pmatrix} x \\ x \\ x \end{pmatrix} (x \ x \ x) + \begin{pmatrix} 0 \\ x \\ x \end{pmatrix} (0 \ x \ x) + \begin{pmatrix} 0 \\ 0 \\ x \end{pmatrix} (0 \ 0 \ x)$$

$$= l_1 u_1^* + l_2 u_2^* + l_3 u_3^*$$

$$= \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & x & x \\ 0 & x & x \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & x \end{pmatrix}$$

At each stage $k = 1, \dots, n$, only the vectors l_k, u_k^* will contribute to k^{th} row and k^{th} col of remaining matrix.

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 5 & 7 \\ 2 & 7 & 8 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix} (1 \ 2 \ 3) + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 3 & 2 \end{pmatrix}$$

$$= \begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix} (1 \ 2 \ 3) + \begin{pmatrix} 0 \\ 1 \\ 3 \end{pmatrix} (0 \ 1 \ 1) + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$= \underbrace{\begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix}}_{l_1} \underbrace{(1 \ 2 \ 3)}_{u_1^*} + \underbrace{\begin{pmatrix} 0 \\ 1 \\ 3 \end{pmatrix}}_{l_2} \underbrace{(0 \ 1 \ 1)}_{u_2^*} + \underbrace{\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}}_{l_3} \underbrace{(0 \ 0 \ -1)}_{u_3^*}$$

Therefore

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 5 & 7 \\ 2 & 7 & 8 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 2 & 3 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 & 3 \\ 0 & 1 & 1 \\ 0 & 0 & -1 \end{pmatrix}$$

$$A \quad = \quad L \qquad U$$

Instability of Gaussian Elimination (w/o pivoting)

Example

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$$

full rank
$\kappa_2 = (3+\sqrt{5})/2 \approx 2.618$

but G.E. fails right away!

$$A = \begin{bmatrix} 10^{-20} & 1 \\ 1 & 1 \end{bmatrix}$$

factors $\quad L = \begin{bmatrix} 1 & 0 \\ 10^{20} & 1 \end{bmatrix}, \quad U = \begin{bmatrix} 10^{-20} & 1 \\ 0 & 1-10^{+20} \end{bmatrix}$

assume after rounding $\quad \tilde{L} = \begin{bmatrix} 1 & 0 \\ 10^{20} & 1 \end{bmatrix}, \quad \tilde{U} = \begin{bmatrix} 10^{-20} & 1 \\ 0 & -10^{20} \end{bmatrix}$

$$\tilde{A} = \tilde{L}\tilde{U} = \begin{bmatrix} 10^{-20} & 1 \\ 1 & 0 \end{bmatrix}$$

not close to A! (large backward error

e.g. $\quad Ax = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Rightarrow x \cong \begin{pmatrix} -1 \\ 1 \end{pmatrix}$

$\tilde{A}\tilde{x} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Rightarrow \tilde{x} \approx \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

large error in solve.

Gaussian Elimination (as presented so far) is not stable!

Add pivoting to stabilize.

permute rows so that next pivot is element w/ largest magnitude in column

$$\begin{pmatrix} 10^{-20} & 1 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 10^{20} \end{pmatrix} \begin{pmatrix} 10^{-20} & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1-10^{20} \end{pmatrix}$$

$$\approx \begin{pmatrix} 1 \\ 10^{20} \end{pmatrix} \begin{pmatrix} 10^{-20} & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & -10^{20} \end{pmatrix}$$

approximation due to <u>finite precision</u>

$$= \begin{pmatrix} 1 \\ 10^{20} \end{pmatrix} \begin{pmatrix} 10^{-20} & 1 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & -10^{20} \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 \\ 10^{20} & 1 \end{pmatrix} \begin{pmatrix} 10^{-20} & 1 \\ 0 & -10^{20} \end{pmatrix}$$

<u>check</u>

$$= \begin{pmatrix} 10^{-20} & 1 \\ 1 & 0 \end{pmatrix} \not\approx \begin{pmatrix} 10^{-20} & 1 \\ 1 & 1 \end{pmatrix}$$

<u>bad</u>

Row pivoting

$$A = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 3 & 7 \\ 2 & 4 & 8 \end{pmatrix}$$

$$\begin{pmatrix} 1 \\ ? \\ ? \end{pmatrix} \begin{pmatrix} 0 & 1 & 1 \end{pmatrix}$$ can't use 0 as a pivot!

Let's choose the largest element in col 1 (that's in row 3).

$$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 3 & 7 \\ 2 & 4 & 8 \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{1}{2} \\ 1 \end{pmatrix} \begin{pmatrix} 2 & 4 & 8 \end{pmatrix} + \begin{pmatrix} 0 & 1 & 1 \\ 0 & 1 & 3 \\ 0 & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 \\ \frac{1}{2} \\ 1 \end{pmatrix} \begin{pmatrix} 2 & 4 & 8 \end{pmatrix} + \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 \\ \frac{1}{2} \\ 1 \end{pmatrix} \begin{pmatrix} 2 & 4 & 8 \end{pmatrix} + \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 1 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 2 \end{pmatrix}$$

$$= \underbrace{\begin{pmatrix} 0 & 1 & 0 \\ \frac{1}{2} & 1 & 1 \\ 1 & 0 & 0 \end{pmatrix}}_{\text{\underline{not} lower triangular}} \underbrace{\begin{pmatrix} 2 & 4 & 8 \\ 0 & 1 & 1 \\ 0 & 0 & 2 \end{pmatrix}}_{\text{upper triangular ✓}}$$

How to fix this?

pivot order was 3, 1, 2

if we want it to be 1, 2, 3, we need to permute the rows of A

$$PA = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 3 & 7 \\ 2 & 4 & 8 \end{pmatrix} = \begin{pmatrix} 2 & 4 & 8 \\ 0 & 1 & 1 \\ 1 & 3 & 7 \end{pmatrix}$$

Then

$$PA = \begin{pmatrix} 2 & 4 & 8 \\ 0 & 1 & 1 \\ 1 & 3 & 7 \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \frac{1}{2} & 1 & 1 \end{pmatrix}}_{\text{lower triangular } \checkmark} \underbrace{\begin{pmatrix} 2 & 4 & 8 \\ 0 & 1 & 1 \\ 0 & 0 & 2 \end{pmatrix}}_{\text{upper triangular } \checkmark}$$

Every invertible $n \times n$ matrix has $PA = LU$, P permutation

To solve $Ax = b$,

1. find $PA = LU$, then
2. $PA = LUx = Pb$
3. Solve $Ly = Pb$ by forward substitution
4. Solve $Ux = y$ by backward substitution

Example with pivoting

$$A = \begin{pmatrix} 1 & 2 & 2 \\ 4 & 4 & 2 \\ 4 & 6 & 4 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 2 & 2 \\ 4 & 4 & 2 \\ 4 & 6 & 4 \end{pmatrix} = \begin{pmatrix} \frac{1}{4} \\ 1 \\ 1 \end{pmatrix} \begin{pmatrix} 4 & 4 & 2 \end{pmatrix} + \begin{pmatrix} 0 & 1 & \frac{3}{2} \\ 0 & 0 & 0 \\ 0 & 2 & 2 \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{4} \\ 1 \\ 1 \end{pmatrix} \begin{pmatrix} 4 & 4 & 2 \end{pmatrix} + \begin{pmatrix} \frac{1}{2} \\ 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 2 & 2 \end{pmatrix} + \begin{pmatrix} 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{4} \\ 1 \\ 1 \end{pmatrix} \begin{pmatrix} 4 & 4 & 2 \end{pmatrix} + \begin{pmatrix} \frac{1}{2} \\ 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 2 & 2 \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & \frac{1}{2} \end{pmatrix}$$

permutation 2, 3, 1

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 2 & 2 \\ 4 & 4 & 2 \\ 4 & 6 & 4 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ \frac{1}{4} & \frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} 4 & 4 & 2 \\ 0 & 2 & 2 \\ 0 & 0 & \frac{1}{2} \end{pmatrix}$$

$$P \quad A = L \quad U$$

Example w/o pivoting (for comparison)

$$A = \begin{pmatrix} 1 & 2 & 2 \\ 4 & 4 & 2 \\ 4 & 6 & 4 \end{pmatrix}$$

$$= \begin{pmatrix} 1 \\ 4 \\ 4 \end{pmatrix} \begin{pmatrix} 1 & 2 & 2 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & -4 & -6 \\ 0 & -2 & -4 \end{pmatrix}$$

$$= \begin{pmatrix} 1 \\ 4 \\ 4 \end{pmatrix} \begin{pmatrix} 1 & 2 & 2 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ \frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 & -4 & -6 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 \\ 4 \\ 4 \end{pmatrix} \begin{pmatrix} 1 & 2 & 2 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ \frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 & -4 & -6 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & -1 \end{pmatrix}$$

$$= \underbrace{\begin{pmatrix} 1 & 0 & 0 \\ 4 & 1 & 0 \\ 4 & \frac{1}{2} & 1 \end{pmatrix}}_{L} \underbrace{\begin{pmatrix} 1 & 2 & 2 \\ 0 & -4 & -6 \\ 0 & 0 & -1 \end{pmatrix}}_{U}$$

LU operation counts

$$\begin{pmatrix} l_{11} & & & \\ l_{21} & l_{22} & & \\ \vdots & & \ddots & \\ l_{n1} & \cdots & & l_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

Forward Substitution

for $j = 1, \ldots, n$

  $x_j = b_j / l_{jj}$ [solve for x_j]

  for $i = j+1, \ldots, n$ [subtract $x_j \vec{l}_j$ from rhs]

    $b_i \leftarrow b_i - x_j l_{ij}$

  end

end

Operation count:

$$= \sum_{j=1}^{n} \left(1 + \sum_{i=j+1}^{n} 2 \right)$$

$$= n + \sum_{j=1}^{n} 2(n-(j+\cancel{1})+\cancel{1}) = n + \sum_{j=1}^{n} 2(n-j)$$

$$\left(k = n-j \Rightarrow (j=1 \Rightarrow k=n-1), \ (j=n \Rightarrow k=0)\right)$$

$$= n + \sum_{k=0}^{n-1} 2k = n + 2\sum_{k=1}^{n-1} k$$

$$= n + \cancel{2}\frac{(n-1)n}{\cancel{2}} = \cancel{n} + n^2 - \cancel{n} = n^2$$

LU factorization

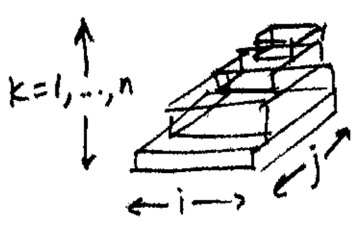
```
for k = 1, ..., n
    if a_kk == 0 stop
    for i = k+1, ..., n
        l_ik = a_ik / a_kk
    end
    for i = k+1, ..., n
        for j = k+1, ..., n
            a_ij ← a_ij - l_ik a_kj
        end
    end
end
```

operation count

$$= \sum_{k=1}^{n} \left(\sum_{i=k+1}^{n} 1 + \sum_{i=k+1}^{n} \sum_{j=k+1}^{n} 2 \right) = \left\langle \sum_{i=1}^{n} i^2 = \frac{n(n+1)(2n+1)}{6} \right\rangle$$

$$= \frac{n(n-1)(2n-1)}{3} + \frac{n(n-1)}{2}$$

or geometric estimate :



$\frac{1}{3} bh$

$$\sim \frac{2}{3} n^3$$

Operation Count

$$\sum_{k=1}^{n-1}\left[\left(\sum_{i=k+1}^{n} 1\right) + \sum_{j=k+1}^{n}\sum_{i=k+1}^{n} 2\right]$$

$$= \sum_{k=1}^{n-1}\left[n-(k+1)+1 + 2\sum_{j=k+1}^{n} n-(k+1)+1\right]$$

$$= \sum_{k=1}^{n-1}\left[n-k + 2\sum_{j=k+1}^{n} n-k\right]$$

$$= \sum_{k=1}^{n-1}\left[n-k + 2(n-k)\left(n-(k+1)+1\right)\right]$$

$$= \sum_{k=1}^{n-1}\left[(n-k) + 2(n-k)(n-k)\right]$$

$$= \sum_{k=1}^{n-1}(n-k)\left[2(n-k)+1\right]$$

$$m = n-k$$

$$k=1 \Rightarrow m = n-1$$

$$k = n-1 \Rightarrow m = n-n+1 = 1$$

$$= \sum_{m=1}^{n-1} m\left[2m+1\right]$$

$$S_n = \sum_{i=1}^{n} i^2 = \frac{n(n+1)(2n+1)}{6}$$

$$= \sum_{m=1}^{n-1}\left(2m^2+m\right)$$

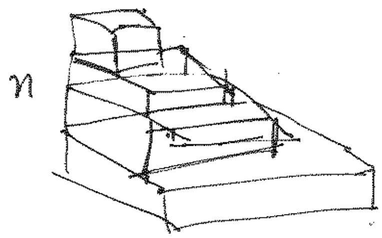
$$= 2\,\frac{(n-1)(n)(2n-2+1)}{6} + \frac{(n-1)n}{2}$$

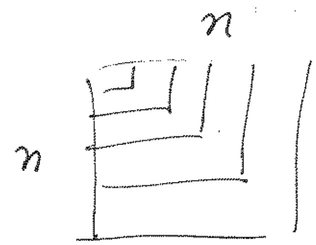
dominant term

$$= \frac{n(n-1)(2n-1)}{3} + \frac{n(n-1)}{2} \sim \frac{2}{3}n^3$$

How to estimate operation count geometrically

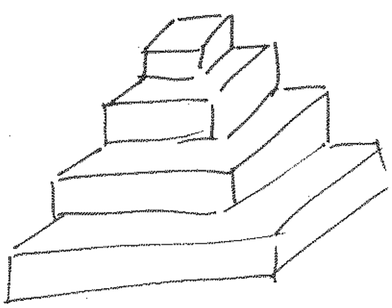
- dominate by operation in inner most loop
  2 flops

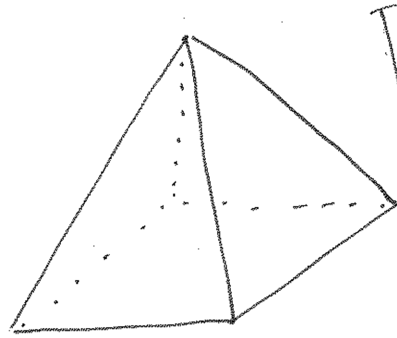




$$V = \frac{1}{3} bh = \frac{1}{3} n^3$$

$$\text{ops} \sim \frac{2}{3} n^3$$





pyramid with
Volume = $\frac{1}{3}bh$