AMSC 460 Numerical LinAlg

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1 Gaussian Elimination

We discuss floating point error in the context of Gaussian elimination and build towards pivoting.

1.1 Floating Point Error

Definition 1.1: Machine precision

Given a real number a, in machine computation it is approximated by $\mathrm{fl}(a)$ which has the property

$$\frac{|a - \mathrm{fl}(a)|}{|a|} \leq \mu \tag{1}$$

where μ is the **machine precision**, also called the **machine epsilon**.

Typically the machine precision is of the order $\mu \approx 10^{-16}$.

Corollarly 1.1: Addition of numbers below machine precision has no effect

For any ϵ such that $|\epsilon| < \mu$,

$$\mathrm{fl}(1 + \epsilon) = 1 \tag{2}$$

Corollarly 1.2: μ is the smallest number whose addition has an effect

The machine precision μ is the smallest number such that

$$\mathrm{fl}(1 + \mu) > 1 \tag{3}$$

Corollarly 1.3: Addition to large numbers has no effect

For any ϵ such that $|\epsilon| < \mu$,

$$\mathrm{fl}\left(\frac{1}{\epsilon} \pm 1\right) = \frac{1}{\epsilon} \tag{4}$$

1.2 Gaussian Elimination Example

Consider for example the linear system:

$$\begin{bmatrix} \delta & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \end{bmatrix} \tag{5}$$

where δ is very small, specifically, $\delta < \mu$.

1.2.1 Ideal Solution

First we solve this without floating point error.

For the first step of Gaussian elimination, we have

$$L_1 = \begin{bmatrix} 1 & 0 \\ -\frac{1}{\delta} & 1 \end{bmatrix} \tag{6}$$

This gives us

$$L_1 A = \begin{bmatrix} 1 & 0 \\ -\frac{1}{\delta} & 0 \end{bmatrix} \begin{bmatrix} \delta & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} \delta & 1 \\ 0 & 1 - \frac{1}{\delta} \end{bmatrix} \tag{7}$$

and

$$L_1 b = \begin{bmatrix} 1 \\ 3 - \frac{1}{\delta} \end{bmatrix} \tag{8}$$

Now we compute x:

$$\left(1 - \frac{1}{\delta}\right) x_2 = 3 - \frac{1}{\delta} \tag{9}$$

$$\implies x_2 = \frac{3 - {}^1\!/_\delta}{1 - {}^1\!/_\delta} \tag{10}$$

and

$$\delta x_1 + x_2 = 1 \tag{11}$$

$$\implies x_1 = \frac{1-x_2}{\delta} = \frac{1-\frac{3-1/\delta}{1-1/\delta}}{\delta} = \frac{1-1/\delta-3+1/\delta}{\delta(1-\delta)} = -\frac{2}{\delta-1} \tag{12}$$

Since we are assuming δ is very small ($\delta \ll 1$),

$$x_1 = -\frac{2}{\delta-1} \approx -\frac{2}{-1} = 2 \tag{13}$$

1.2.2 Floating Point Error

Now let us see what floating point error does to the same linear system (equation 5).

In this case we have

$$\mathrm{fl}\left(3-\frac{1}{\delta}\right) = -\frac{1}{\delta} \tag{14}$$

$$\mathrm{fl}\left(1-\frac{1}{\delta}\right) = -\frac{1}{\delta} \tag{15}$$

Thus we have

$$x_2 = \frac{\mathrm{fl}\,(3-1/\delta)}{\mathrm{fl}\,(1-1/\delta)} = \frac{-1/\delta}{-1/\delta} = 1 \tag{16}$$

That is $\mathrm{fl}(x_2) = 1$.

$$x_1 = \frac{1-x_2}{\delta} = \frac{1-1}{\delta} = 0 \tag{17}$$

x_1 and x_2 are completely wrong!

Hence we need pivoting.

1.3 Pivoting

Algorithm 1.1: Pivoting

The process of pivoting is:

1. Find the largest entry in the column below the diagonal, that is the largest of $a_{21}, \ldots, a_{n1}$. Let's say that a_{k1} is the largest entry.
2. Interchange rows 1 and k (so that the largest entry a_{k1} is now in the position $(1, 1)$).
3. Apply the Gaussian elimination strategy.

Interchanging rows can be represented using a **permutation matrix**:

Construction 1.1: Permutation matrix

We represent interchanging row 1 and k using the **permutation matrix**:

$$P_1 = \left[\begin{array}{c|c|c|c} 0 & & 1 & \\ \hline & I_{k-1} & & \\ \hline 1 & & 0 & \\ \hline & & & I_{n-k-1} \end{array}\right] \tag{18}$$

This is just the identity matrix with the 1-st and k-th column swapped.

For the first step of Gaussian elimination, we first compute $P_1 A$, and $P_1 b$. Then we compute L_1 for $P_1 A$. The resulting matrix is then

$$L_1 P_1 A \tag{19}$$

and

$$L_1 P_1 b \tag{20}$$

Next we recursively continue the process of the sub-matrix, finding P_2 and then L_2. The result of the whole Gaussian elimination process is then

$$L_{n-1} P_{n-1} \cdots L_2 P_2 L_1 P_1 A x = L_{n-1} P_{n-1} \cdots L_2 P_2 L_1 P_1 b \tag{21}$$

As before, we call the matrix on the left-hand side U:

Definition 1.2: U

Call

$$U = L_{n-1}P_{n-1}\cdots L_2P_2L_1P_1A \tag{22}$$

Thus

$$A = P_1^{-1}L_1^{-1}\cdots P_{n-1}^{-1}L_{n-1}^{-1}U \tag{23}$$

Note first that each P_i is its own inverse: $P_i = P_i^{-1}$.

Note also that intuitively performing row swaps before each row-reduction is the same as performing all the swaps immediately and then doing row-reduction. That is, it can be shown that

$$P_{n-1}\cdots P_2P_1A = L_{n-1}^{-1}\cdots L_2^{-1}L_1^{-1}U \tag{24}$$

Definition 1.3: LU **decomposition**

Define

$$P = P_{n-1}\cdots P_2P_1 \tag{25}$$

and, as before

$$L = L_{n-1}^{-1}\cdots L_2^{-1}L_1^{-1} \tag{26}$$

Then we have

$$PA = LU \tag{27}$$

That is, the result is the LU decomposition of PA.

We say that $P^{-1}L$ is **psychologically lower triangular**.

2 Error in Gaussian Elimination

2.1 Looking Ahead

Imagine that solving system $Ax = b$ using Gaussian elimination, we compute $\hat{x} \approx x$.

We ask: how big is the error $\frac{\|x-\hat{x}\|}{\|x\|}$?

Claim: The computed $\hat{x}$ is the exact solution to a perturbed problem

$$(A+E)\hat{x} = b \tag{28}$$

Hopefully E is small!

We will first focus up on building up the mathematical machinery necessary to analyze this.

2.2 Norms

For this entire section we are working in $\mathbb{R}^n$.

(Note from me: these defenitions are all generalizable to $\mathbb{C}^n$, but require us to be a little more careful with e.g. complex conjugates).

Definition 2.1: Common Vector Norms

We can define several different notions of a **vector norm** $\|v\|$ for $v \in \mathbb{R}^n$.
The l^2 norm is:

$$\|v\|_2 = \left(\sum_{i=1}^{n} v_i^2\right)^{1/2} \tag{29}$$

The Manhattan norm is:

$$\|v\|_1 = \sum_{i=1}^{n} |v_i| \tag{30}$$

(called the Manhattan norm because it is kind of like "counting blocks in Manhattan" – very silly).

The supremum norm (or uniform norm) is:

$$\|v\|_\infty = \max_{1\leq i\leq n} |v_i| \tag{31}$$

A vector norm induces a matrix norm:

Definition 2.2: Matrix norm

The **matrix norm** of a real-valued matrix A is defined by

$$\|A\| = \max_{v \neq 0} \frac{\|Av\|}{\|v\|} \tag{32}$$

We say that the matrix norm $\|A\|$ is *induced* by the vector norm.

This definition makes some intutive sense: Our intuition for vector norm is a measure of the length of a vector. Recall that matrices are linear transformations–i.e. they transform vectors. It thus makes sense to define the matrix norm as a measure of how much a matrix stretches vectors. Our definition of matrix norm is the maximum amount by which the matrix A stretches a given vector.

Theorem 2.1: Common Matrix Norms

For the vector norms defined above we have the following matrix norms:

$$\|A\|_2 = \text{max singular value of } A = \left(\text{max eigenvalue of } A^T A\right)^{1/2} \tag{33}$$

Note that this is hard to compute.

$$\|A\|_1 = \max_j \sum_i |a_{ij}| \tag{34}$$

That is, $\|A\|_1$ is the maximum column sum (sum over rows).

$$\|A\|_\infty = \max_i \sum_j |a_{ij}| \tag{35}$$

2.3 Error in Gaussian Elimination

Considered the perturbed system given by equation 28.

Theorem 2.2: Error in Perturbed System

We claim that

$$\|E\| \leq \mu\rho(n)\|A\| \tag{36}$$

where $\rho(n)$ is typically of order 1 (and μ is the machine precision).

That is, the relative error for the preturbed system,

$$\frac{\|E\|}{\|A\|} \tag{37}$$

behaves like the machine precision μ.

Note that this is true only when pivoting is done (otherwise a small entry may completely mess the result up)!

Now we analyze the error in our perturbed system:

We know that

$$(A + E)\hat{x} = b \tag{38}$$

$$\implies b - A\hat{x} = E\hat{x} \tag{39}$$

$$\implies \|b - A\hat{x}\| = \|E\hat{x}\| \tag{40}$$

$$\leq \|E\|\|\hat{x}\| \tag{41}$$

by definition of the matrix norm (since $\|E\| = \max_y \|Ey\|/\|y\|$).

Note that

$$x - \hat{x} = A^{-1}(b - A\hat{x}) \tag{42}$$

since $Ax = b \implies x = A^{-1}b$.

And since $b - A\hat{x} = E\hat{x}$, equation 42 becomes

$$x - \hat{x} = A^{-1}E\hat{x} \tag{43}$$

Thus we have

$$\|x - \hat{x}\| = \|A^{-1}E\hat{x}\| \tag{44}$$

$$\leq \|A^{-1}\|\|E\hat{x}\| \tag{45}$$

$$\leq \|A^{-1}\|\|E\|\|\hat{x}\| \tag{46}$$

Thus

$$\frac{\|x-\hat{x}\|}{\|\hat{x}\|} \leq \frac{\|A^{-1}\|\|E\|\|\hat{x}\|}{\|\hat{x}\|} \leq \|A^{1}\|\mu\rho(n)\|A\| \tag{47}$$

by theorem 2.2.

That is,

Theorem 2.3: Almost Error Bound

We have

$$\frac{\|x-\hat{x}\|}{\|\hat{x}\|} \leq \|A^{-1}\|\|A\|\mu\rho(n) \tag{48}$$

The left-hand side is almost the relative error.
The right hand side shows us that it is essentially bounded by the machine precision.

Definition 2.3: Condition Number

Often $\|A^{-1}\|\|A\|$ is called the **condition number** of A, denoted

$$K(A) = \|A^{-1}\|\|A\| \tag{49}$$

Theorem 2.4: True Error Bound

We can show (stated here without proof)

$$\frac{\|x-\hat{x}\|}{\|x\|} \leq \frac{K(A)\rho(n)\mu}{1-K(A)\rho(n)\mu} \tag{50}$$

Note: Gaussian elimination is not truly stable! We can make it fail with so-called "pathological matrices." However these matrices do not seem to arise in natural situations.

3 Singular Value Decomposition

Construction 3.1: Singular Value Decomposition

Statement: Any matrix A can be factored as $A = U\Sigma V^T$.

If $A \in \mathbb{R}^{m\times m}$, then U is an orthogonal matrix of order n, V is an orthogonal matrix of order n, and

$$\Sigma = \begin{pmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ 0 & & & \sigma_n \end{pmatrix} \tag{51}$$

where $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$.

σ_i are called **singular values**.

3.1 Orthogonal Matrices and Given's Rotation

Definition 3.1: Orthogonal Matrices

A square matrix X is orthogonal if

$$X^T X = XX^T = I \tag{52}$$

That is, the columns/rows of X are orthonormal.

Note on orthogonality: the (i, j) entry of $X^T X$ is the inner product of the i-th row of X^T (i.e. the i-th column of X) and the j-th column of X. If all columns are orthonormal, the inner product is 0 for $i \neq j$ (orthogonality) and 1 for $i = j$ (normalization).

An important example of an orthogonal matrix in $2D$ is

$$Q = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \tag{53}$$

We check that this matrix is indeed orthogonal:

$$Q^TQ = \begin{bmatrix} \cos^2\theta + \sin^2\theta & -\cos\theta\sin\theta + \cos\theta\sin\theta \\ -\sin\theta\cos\theta + \sin\theta\cos\theta & (-\sin\theta)^2 + \cos^2\theta \end{bmatrix} \tag{54}$$

$$= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{55}$$

Thus Q is orthogonal.

Let's further analyze Q.

Take any vector v such that $\|v\|_2 = 1$, and consider $w = Qv$.

$$\|w\|_2^2 = \langle Qv, Qv\rangle \tag{56}$$

$$= (Qv)^TQv \tag{57}$$

$$= v^TQ^TQv \tag{58}$$

$$= v^Tv \tag{59}$$

$$= \langle v, v\rangle \tag{60}$$

$$= \|v\|_2^2 = 1 \tag{61}$$

where $\langle\cdot,\cdot\rangle$ is the inner product (in this case the conventional dot product/Euclidean inner product).

Thus Q preserves the norm of a vector.

(Note: the professor has alternated a bit between $\langle\cdot,\cdot\rangle$ and $(\cdot,\cdot)$ notation for inner products in the past. In this section he used the latter notation, but I used the former since I think it is somewhat more common).

Let ϕ be the angle between v and w for any v.

$$\cos\phi = \frac{\langle v, w\rangle}{\|v\|\|w\|} \tag{62}$$

$$= \frac{\big\langle (v_1, v_2), Q(v_1, v_2)\big\rangle}{\|v\|\|Qv\|} \tag{63}$$

Without writing out all the tedious trig calculations, we note that

$$\big\langle (v_1, v_2), Q(v_1, v_2)\big\rangle = \big\langle (v_1, v_2), (v_1\cos\theta - v_2\sin\theta, v_1\sin\theta + v_2\cos\theta)\big\rangle \tag{64}$$

$$= \cos\theta\|v\|^2 \tag{65}$$

Thus

$$\cos\phi = \frac{\cos\theta\|v\|^2}{\|v\|\|Qv\|} \tag{66}$$

$$= \frac{\cos\theta\|v\|^2}{\|v\|^2} \tag{67}$$

$$= \cos\theta \tag{68}$$

Thus

$$\theta = \phi \tag{69}$$

So Q rotates v by an angle of θ.

Theorem 3.1: Given's Rotation

The matrix

$$\begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \tag{70}$$

represents counter-clock-wise rotation by θ in $\mathbb{R}^2$.

3.2 Intro to Singular Value Decomposition

The goal of singular value decomposition (SVD) is:

Given matrix $A \in \mathbb{R}^{n\times m}$ (or $\mathcal{M}_{n\times m}(\mathbb{R})$ in more familiar notation), factor

$$A = U\Sigma V^T \tag{71}$$

where U, V are orthogonal matrices (columns are orthonormal), U of order n, V of order m, and Σ diagonal.

Let's say without loss of generality $n \geq m$

Then

$$\Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_m \\ & & 0 & \end{bmatrix} \tag{72}$$

(i.e. diagonal matrix for the first m rows, and all zeros below that).

Moreover, we impose the restriction that

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_m \geq 0 \tag{73}$$

It is interesting to note that Galois theory says that we cannot get an exact closed-form solution of Σ, but we can get away with numerical computation because we don't care if the error in Σ is below the machine precision.

3.3 Householder Reflection

Now we construct an orthogonal matrix that will be useful to us

Construction 3.2: Orthonormal matrix

Given $u \in \mathbb{R}^n$, consider

$$Q = I - \frac{2}{u^T u} u u^T \tag{74}$$

The matrix Q is called the **Householder reflection** (it will become apparent why in the end of this sub-section).

3.3.1 Proof that Q is Orthogonal

$$Q^T Q = (I - \frac{2}{u^T u} u u^T)^T (I - \frac{2}{u^T u} u u^T) = (I - \frac{2}{u^T u} u u^T)(I - \frac{2}{u^T u} u u^T) \tag{75}$$

here we have distributed the transpose, noting that $I^T = I$ and $(uu^T)^T = (u^T)^T u^T = uu^T$.

We continue to distribute this equation

$$Q^TQ = (I - \frac{2}{u^Tu}uu^T)(I - \frac{2}{u^Tu}uu^T) \tag{76}$$
$$= I - \frac{4}{u^Tu}uu^T + \frac{4}{u^Tuu^Tu}uu^Tuu^T \tag{77}$$
$$= I - \frac{4}{u^Tu}uu^T + \frac{4}{(u^Tu)(u^Tu)}u(u^Tu)u^T \tag{78}$$
$$= I - \frac{4}{u^Tu}uu^T + \frac{4}{u^Tu}uu^T \tag{79}$$
$$= I \tag{80}$$

Thus Q is orthogonal.

3.3.2 Geometric Interpretation of Q

There is a very nice geometric interpretation of Q for $n = 3$.

Suppose $u \in \mathbb{R}^3$ and $u_2, u_3 \in \mathbb{R}^3$ span the plane orthogonal to u.

Since u is orthogonal to u_2 and u_3, it is linearly independent, meaning that all three of them span $\mathbb{R}^3$ and thus form a basis.

Any vector $x \in \mathbb{R}^3$ can be written in this basis

$$x = cu + c_2u_2 + c_3u_3 \tag{81}$$

Now consider

$$Q = I - \frac{2}{u^Tu}uu^T \tag{82}$$

$$Qx = x - \frac{2}{u^Tu}uu^Tx \tag{83}$$

We can expand u^Tx into

$$u^Tx = u^T(cu + c_2u_2 + c_3u_3) \tag{84}$$

Since u is orthogonal to u_2, u_3, the inner product $u^Tu_2 = u^Tu_3 = 0$, so only the cu term in equation 84 is non-zero:

$$u^Tx = cu^Tu \tag{85}$$

Therefore

$$Qx = (cu + c_2u_2 + c_3u_3) - \frac{2}{u^Tu}u(cu^Tu) \tag{86}$$
$$= (cu + c_2u_2 + c_3u_3) - 2cu \tag{87}$$
$$= -cu + c_2u_2 + c_3u_3 \tag{88}$$

We've inverted the orthogonal component–that is Q reflected x through the plane orthogonal to u (spanned by u_2, u_3). This is called the **Householder reflection**.

3.4 Singular Value Decomposition

In a previous lecture we defined the matrix norm:

Definition 3.2: Matrix norm

A norm of matrix A is induced by the l^2 norm. We define the norm of matrix A as follows:

$$\|A\|_2 = \max_{v \neq 0} \frac{\|Av\|_2}{\|v\|_2} \tag{89}$$

We also state (for now without proof) that the norm of an orthogonal matrix U is 1:

$$\|U\|_2 = 1 \tag{90}$$

and that given orthogonal matrix U,

$$\|UX\|_2 = \|X\|_2 \; \forall X \tag{91}$$

We will show that $\|A\|_2 = \sigma_1$. To do so, we will try to bound $\|A\|_2$ on both sides.

3.4.1 Upper Bound

For any $v \in R^n$,

$$\frac{\|Av\|_2}{\|v\|_2} = \frac{\|U\Sigma V^Tv\|_2}{\|v\|_2} = \frac{\|\Sigma V^Tv\|_2}{\|v\|_2} \tag{92}$$

since U is orthogonal.

Let $w = V^T v$.

Since V is orthogonal,

$$Vw = VV^T v = Iv = v \tag{93}$$

Plugging this into equation 92,

$$\frac{\|\Sigma w\|_2}{\|Vw\|_2} = \frac{\|\Sigma w\|_2}{\|w\|_2} \tag{94}$$

since V is orthogonal.

Now we expand this using the fact that Σ is diagonal (of the form given in equation 72) and the defenition of the l^2 norm:

$$\frac{\|\Sigma w\|_2}{\|w\|_2} = \frac{\left[(\sigma_1 w_1)^2 + (\sigma_2 w_2)^2 + \cdots + (\sigma_n w_n)^2\right]^{1/2}}{(w_1^2 + w_2^2 + \cdots + w_n^2)^{1/2}} \tag{95}$$

Since $\sigma_1 \geq \sigma_2 \geq \cdots \sigma_n \geq 0$ (equation 73), the numerator of expression 95 is bounded by:

$$\left[(\sigma_1 w_1)^2 + (\sigma_2 w_2)^2 + \cdots + (\sigma_n w_n)^2\right]^{1/2} \tag{96}$$

$$\leq (\sigma_1^2 w_1^2 + \sigma_1^2 w_2^2 + \cdots + \sigma_1^2 w_n^2)^{1/2} \tag{97}$$

$$= \sigma_1 (w_1^2 + \cdots + w_n^2)^{1/2} \tag{98}$$

Thus, the entire expression 95 is bounded by:

$$\frac{\left[(\sigma_1 w_1)^2 + (\sigma_2 w_2)^2 + \cdots + (\sigma_n w_n)^2\right]^{1/2}}{(w_1^2 + w_2^2 + \cdots + w_n^2)^{1/2}} \leq \sigma_1 \tag{99}$$

In other words,

$$\|A\|_2 \leq \sigma_1 \tag{100}$$

3.4.2 Lower Bound

Since norm is defined as the maximum, to show the lower bound we only need to find one v such that $\frac{\|Av\|_2}{\|v\|_2} = \sigma_1$.

Take

$$v = V \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{101}$$

that is,

$$w = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{102}$$

in $v = Vw$.

For this v and w,

$$\frac{\|Av\|_2}{\|v\|_2} = \frac{\|\Sigma w\|_2}{\|w\|_2} = \frac{\left\| \begin{matrix} \sigma_1 \\ 0 \\ \vdots \\ 0 \end{matrix} \right\|_2}{1} = \sigma_1 \tag{103}$$

Thus

$$\max_v \frac{\|Av\|_2}{\|v\|_2} \geq \sigma_1 \tag{104}$$

Theorem 3.2: l^2 norm of A is its first singular value

This gives us the result

$$\|A\|_2 = \sigma_1 \tag{105}$$

This result will be important for computing the SVD.

3.5 Computing SVD

This is where all of the previous constructions come together.

Let $n \times m$ matrix

$$A = \begin{bmatrix} a_1 & a_2 & \cdots & a_m \end{bmatrix} \tag{106}$$

We claim that there exists a matrix $Q_1 = I - 2\frac{uu^T}{u^T u}$ such that

$$Q_1 A = \left(\begin{array}{c|c} * & \mathbf{b_1^T} \\ \hline 0 & \\ \vdots & * \\ 0 & \end{array}\right) \tag{107}$$

This is (allegedly) proved in a HW exercise.

Similarly, we claim that there exists P_1 such that

$$P_1 b_1 = \begin{pmatrix} * \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{108}$$

an $m-1$ length vector.

From these two observations we get

$$Q_1 A P_1^T = \left(\begin{array}{c|cccc} * & * & 0 & \cdots & 0 \\ \hline 0 & & & & \\ \vdots & & & A_1 & \\ 0 & & & & \end{array}\right) \tag{109}$$

Next we repeat these constructions for A_1 and get

$$Q_2 Q_1 A P_1^T P_2^T = \left(\begin{array}{cc|cccc} * & * & 0 & 0 & \cdots & 0 \\ 0 & * & * & 0 & \cdots & 0 \\ \hline 0 & 0 & & & & \\ \vdots & \vdots & & & A_2 & \\ 0 & 0 & & & & \end{array}\right) \tag{110}$$

If we keep doing this $m-1$ times, we get

$$Q_{m-1}\cdots Q_2 Q_1 A P_1^T P_2^T \cdots P_{m-1}^T \begin{bmatrix} * & * & & & \\ & * & * & & \\ & & * & \ddots & \\ & & & \ddots & * \\ & & & & * \\ & & 0 & & \end{bmatrix} \tag{111}$$

Call this matrix Γ.

Equivalently (by orthonormality):

$$A = Q_1^T Q_2^T \cdots Q_{m-1}^T \Gamma P_{m-1} \cdots P_2 P_1 \tag{112}$$

This is step 1 of construction of the SVD.

An outline of step 2:

Let Γ be the bidiagonal matrix we get after step 1

$$\Gamma = \begin{bmatrix} * & * & 0 \\ 0 & * & * \\ 0 & 0 & * \end{bmatrix} \tag{113}$$

Multiply by Given's rotation

$$\begin{bmatrix} * & * & 0 \\ 0 & * & * \\ 0 & 0 & * \end{bmatrix} \begin{bmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} * & 0 & 0 \\ + & * & * \\ 0 & 0 & * \end{bmatrix} \tag{114}$$

Then compute

$$\begin{bmatrix} \hat{c} & -\hat{s} & 0 \\ \hat{s} & \hat{c} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} * & 0 & 0 \\ + & * & * \\ 0 & 0 & * \end{bmatrix} = \begin{bmatrix} * & * & 0 \\ 0 & * & * \\ 0 & 0 & * \end{bmatrix} \tag{115}$$

Repeta this for row pair.

Overall superdiagonal goes to 0 over many iterations.

4 Principal Component Analysis

Suppose we have p variables

$$X_1, X_2, \ldots, X_p \tag{116}$$

and n sample values of each of them, say

$$x_{i1}, x_{i2}, \ldots, x_{in} \tag{117}$$

for variable X_i.

The data can be represented as a matrix:

$$X = \begin{array}{c@{}l} \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{12} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{p1} & x_{p2} & \cdots & x_{pn} \end{bmatrix} & \begin{array}{l} \text{Var } 1 \\ \text{Var } 2 \\ \\ \text{Var } p \end{array} \end{array} \tag{118}$$

Compute the sample mean for each variable

$$\mu_i = \frac{1}{n} \sum_{j=1}^{n} x_{ij} \tag{119}$$

Compute matrix A with mean substracted fromeach random variable (the **mean zero matrix**).

Compute the sample covariance matrix

$$C(X_i, X_i') = \frac{1}{n-1} \sum_{k=1}^{n} (X_{ik} - \mu_i)^2 = \sigma_{x_i}^2 \tag{120}$$

Correlation between variables (covariance normalized by standard deviation):

$$\frac{C(X_i, X_i')}{\sigma_{x_i} \sigma_{x_i'}} \tag{121}$$

Next compute the SVD of A:

$$A = U \Sigma V^T = U_1 \Sigma_1 V^T \tag{122}$$

where U_1 and Σ_1 have the zeros truncated out.

This gives us

$$A^T V = U_1 \Sigma_1 \tag{123}$$

The columns of U_1 are called the **principal components** of A.

U_1 is associated with largest singular values and etc. (it is the change of coordinate matrix into the principal component system).

Largest principal component $\implies$ variable highly correlated.