

Matrix Decomposition

✓ LU

→ QR

→ Spectral (square matrices)

SVD

Householder Triangularization

Look at G-S again

In G-S, each operation to compute a column of \hat{Q} is an upper triangular matrix multiplication

$$\underline{A} \underbrace{\underline{R}_1 \underline{R}_2 \dots \underline{R}_n}_{\hat{R}^{-1}} = \hat{Q} \Rightarrow \underline{A} = \hat{Q} \hat{R}$$

This is called Triangular Orthogonalization:

R gives Q

Difficulty maintaining orthogonality due to accumulation of round-off errors

Improves by using Modified Gram-Schmidt, rather than Classical Gram-Schmidt, but is still an issue

One can do the reverse : repeated applications of Q give R

$$\underbrace{Q_n Q_{n-1} \dots Q_2 Q_1}_{\hat{Q}^T} A = \hat{R} \Rightarrow A = \hat{Q} \hat{R}$$

where each Q_k is orthogonal

This is called Orthogonal Triangularization

Q gives R

For this, we need to find the Q_k

The main idea is to find a matrix Q_k that zeros out the values below a diagonal while preserving all prior zeros

$$\begin{array}{cccc}
 \begin{bmatrix} x & x & x \\ x & x & x \\ x & x & x \\ x & x & x \end{bmatrix} & \xrightarrow{Q_1} & \begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & x & x \\ 0 & x & x \end{bmatrix} & \xrightarrow{Q_2} & \begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & x \end{bmatrix} & \xrightarrow{Q_3} & \begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & 0 \end{bmatrix} \\
 \underline{A} & & \underline{Q_1 A} & & \underline{Q_2 Q_1 A} & & \underline{Q_3 Q_2 Q_1 A} = \underline{R}
 \end{array}$$

One more requirement: Each \underline{Q}_k must be

unitary $\underline{Q}_k^T \underline{Q}_k = \underline{Q}_k \underline{Q}_k^T = \underline{I}$

Choose the following block matrix

$$\underline{Q}_k = \begin{bmatrix} \underline{I} & \underline{0} \\ \underline{0} & \underline{F} \end{bmatrix}$$

$\underline{I} \in (k-1) \times (k-1)$ identity matrix

$$\underline{F} \in (m-k+1) \times (m-k+1)$$

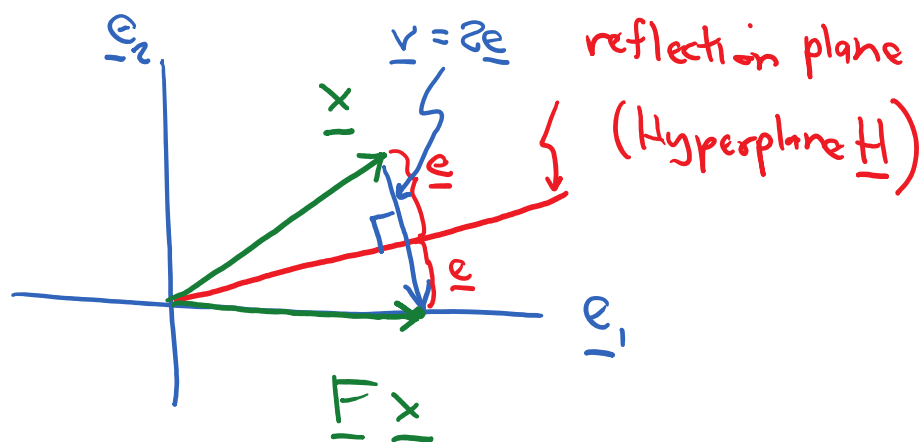
Householder reflector matrix

\underline{F} is a specific type of operation, defined as follows:

$$\underline{x} = \begin{bmatrix} a \\ b \\ c \\ \vdots \end{bmatrix} \quad F \Rightarrow F\underline{x} = \begin{bmatrix} \|\underline{x}\|_2 \\ 0 \\ 0 \\ \vdots \end{bmatrix} = \|\underline{x}\|_2 \underline{e}_1$$

$$\underline{e}_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix}$$

How does this appear in \mathbb{R}^d ?



Hyperplane: A plane with a dimension one less than the embedding plane

(in \mathbb{R}^d , H is \mathbb{R}^{d-1} ; in \mathbb{R}^3 , H is \mathbb{R}^2, \dots)

To determine this projection, look at the

"error" vector between $\underline{F}\underline{x}$ and \underline{x} .

Let

$$\underline{v} = \underline{F}\underline{x} - \underline{x} = \|\underline{x}\|_2 \underline{e}_1 - \underline{x}$$



Is defined once \underline{x} is defined

The key is that \underline{v} is perpendicular to the hyperplane H (see diagram above in \mathbb{R}^d)

To develop \underline{F} , project a vector \underline{y} onto

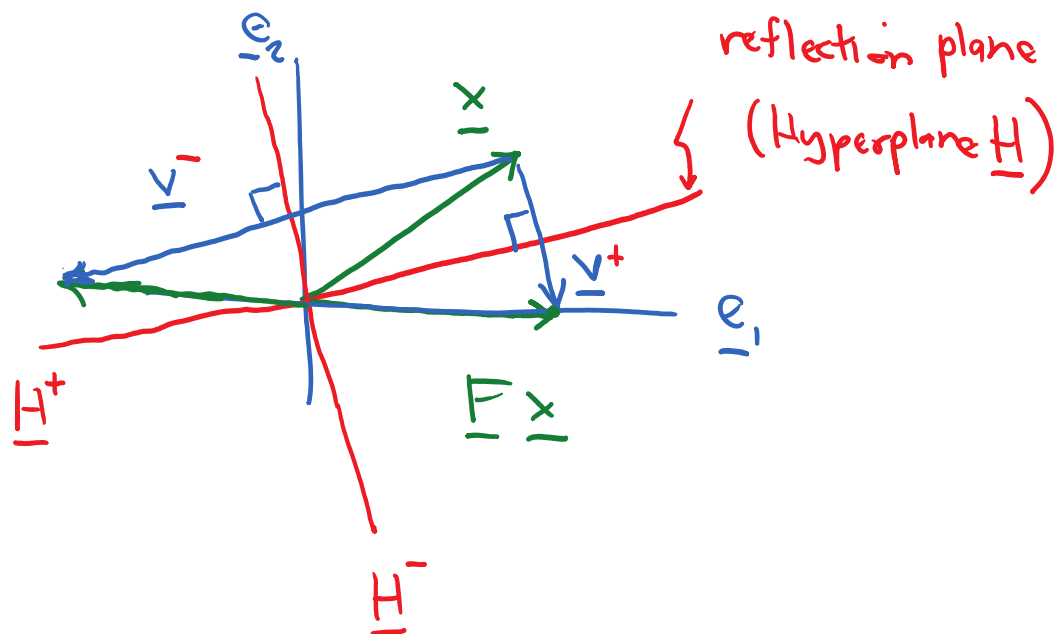
\underline{H} :

$$\underline{P}\underline{y} = \left(\underline{I} - \frac{\underline{v}\underline{v}^T}{\underline{v}^T\underline{v}} \right) \underline{y} = \underline{y} - \underline{v} \left(\frac{\underline{v}^T \underline{y}}{\underline{v}^T \underline{v}} \right)$$

However, we actually need to go twice as far (see diagram above)

$$\underline{F}\underline{y} = \underbrace{\left(\underline{I} - \frac{2\underline{v}\underline{v}^T}{\underline{v}^T\underline{v}} \right)}_{\underline{F}} \underline{y} = \underline{y} - 2\underline{v} \left(\frac{\underline{v}^T \underline{y}}{\underline{v}^T \underline{v}} \right)$$

Note: Householder reflectors are not unique
(see \underline{H}^+ and \underline{H}^- below)



$$\underline{v}^+ = + \|\underline{x}\|_2 \underline{e}_1 - \underline{x}$$

$$\underline{v}^- = - \|\underline{x}\|_2 \underline{e}_1 - \underline{x}$$

Mathematically, choice does not matter

Numerically, choice does matter & we

want large $\|\underline{v}\|$

$$\Rightarrow \text{Set } \underline{v} = -\text{sign}(x_1) \|\underline{x}\|_2 \underline{e}_1 - \underline{x}$$

$$w / \text{sign}(x) = 1 \text{ if } x = 0$$

and x_1 = first component of \underline{x}

After clearing the \ominus :

$$\underline{v} = \text{sign}(x_1) \|\underline{x}\|_2 \underline{e}_1 + \underline{x}$$

Algorithm: Householder \mathbb{Q} R

for $k=1:n$

$$\underline{x} = \underline{A}(k:m, k)$$

$$\underline{v}_k = \text{sign}(x_1) \|\underline{x}\|_2 \underline{e}_1 + \underline{x}$$

$$\underline{v}_k = \underline{v}_k / \|\underline{v}_k\|_2$$

$$\underline{A}(k:m, k:n) = \underline{A}(k:m, k:n)$$

$$-2\underline{v}_k (\underline{v}_k^T \underline{A}(k:m, k:n))$$

end

After these steps, \underline{A} will be upper triangular

Note: Here $\hat{\underline{Q}}$ is never computed

To find $\hat{\underline{Q}}$ do the following, first define the operation of $\hat{\underline{Q}} \underline{x}$

for $k = n:-1:1$

$$\underline{x}(k:m) = \underline{x}(k:m) - \underline{Z} \underline{v}_k (\underline{v}_k^T \underline{x}(k:m))$$

end

To find $\hat{\underline{Q}}$ apply this operation to the identity matrix

$$\underline{Q} \underline{I} = \underline{Q} = [\underline{Q} \underline{e}_1 \quad \underline{Q} \underline{e}_2 \quad \dots]$$

$$\text{with } \underline{e}_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \underline{e}_2 = \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}, \dots$$

QR Factorizations

QR Factorizations

Triangular Orthonormalization ($\hat{R} \rightarrow \hat{Q}$)

* Gram-Schmidt (Classical)

* Gram-Schmidt (Modified)

Orthogonal Triangularization ($\hat{Q} \rightarrow \hat{R}$)

* Householder Reflections

Givens Rotations (easier parallelization)

To motivate, consider the solutions to the following ordinary differential equation (ODE)

$$\frac{dy}{dt} = ay \quad \text{for } a = \text{constant}$$

Independent variable: t

Homogeneous: **Yes**

Dependent variable: $y = y(t)$

Linear: **Yes**

Order: 1

Solution is $y(t) = C e^{at}$

$$\text{Check: } \frac{dy}{dt} = \frac{d}{dt} (C e^{at}) = a C e^{at} = a y(t)$$

What happens if we have a set of two ODEs?

$$\frac{dy_1}{dt} = a y_1, \quad \frac{dy_2}{dt} = b y_2$$

$$\text{Then } y_1(t) = C_1 e^{at}, \quad y_2(t) = C_2 e^{bt}$$

However, if instead we have

✓ uncoupled

$$\frac{dy_1}{dt} = ay_2, \quad \frac{dy_2}{dt} = by_1$$

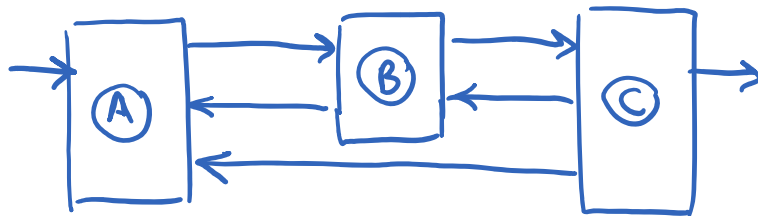
These ODEs are coupled. We need y_1 to solve for y_2 and vice versa

This is quite common in applications!

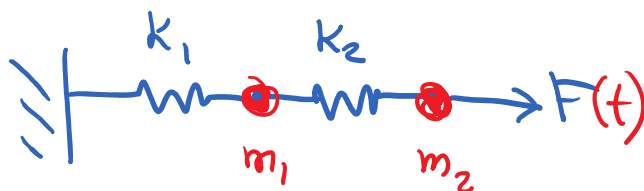
① Chemical reactions



② Flow between tanks



③ Series of springs



Generalize into the following for two dependent variables $y_1(t)$ & $y_2(t)$

$$\frac{dy_1}{dt} = a_{11}y_1 + a_{12}y_2$$

with constants

$$\frac{dy_2}{dt} = a_{21}y_1 + a_{22}y_2$$

$a_{11}, a_{12}, a_{21}, a_{22}$

Let

$$\underline{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}, \quad \underline{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

$$\Rightarrow \frac{d\underline{y}}{dt} = \begin{bmatrix} \frac{dy_1}{dt} \\ \frac{dy_2}{dt} \end{bmatrix} \Rightarrow \frac{d\underline{y}}{dt} = \underline{A} \underline{y}$$

Assume a solution

$$y_1 = x_1 e^{\lambda t}, \quad y_2 = x_2 e^{\lambda t}$$

$$\frac{dy_1}{dt} = \lambda x_1 e^{\lambda t}, \quad \frac{dy_2}{dt} = \lambda x_2 e^{\lambda t}$$

$$\frac{d\underline{y}}{dt} = \underline{A} \underline{y}$$

$$\begin{bmatrix} \cancel{\lambda x_1 e^{\lambda t}} \\ \cancel{\lambda x_2 e^{\lambda t}} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} \cancel{x_1 e^{\lambda t}} \\ \cancel{x_2 e^{\lambda t}} \end{bmatrix}$$

$$\begin{bmatrix} \lambda x_2 e^{\lambda t} \end{bmatrix} = \begin{bmatrix} a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} x_2 e^{\lambda t} \end{bmatrix}$$

$$\underline{A} \underline{x} = \lambda \underline{x} \quad \text{Eigensystem of } \underline{A}$$

$$\underline{A} \underline{x} - \lambda \underline{x} = \underline{0}$$

$$(\underline{A} - \lambda \underline{I}) \underline{x} = \underline{0}$$

λ : Eigenvalue

\underline{x} : Eigenvector

Frequently appears in applications

$$\underline{A} \underline{x} = \lambda \underline{x} \quad \text{Eigensystem of } \underline{A}$$

λ : Eigenvalue

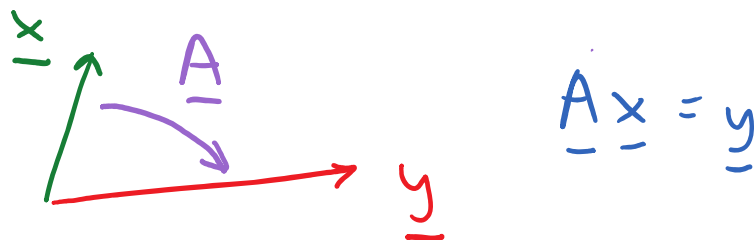
\underline{x} : Eigenvector

Eigensystems appear in many data science applications,
e.g. networks & graphs, Markov chains, physical &
social science systems

$$\underline{A} \underline{x} - \lambda \underline{x} = \underline{0}$$

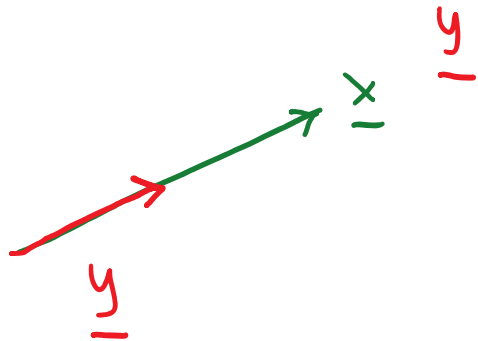
$$(\underline{A} - \lambda \underline{I}) \underline{x} = \underline{0}$$

What, in general, does a matrix do?



Matrix \underline{A} transforms vector \underline{x}
into \underline{y}

Now, consider $\underline{A} \underline{x} = \lambda \underline{x}$



\underline{x} is a special set of vectors of \underline{A}
such that applying \underline{A} to \underline{x} does
nothing but scale \underline{x}

Consider

$$\underline{A} = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}, \quad \underline{x} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\underline{A} \underline{x} = \begin{bmatrix} 3 \\ 3 \end{bmatrix} = 3 \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$\updownarrow \quad \updownarrow$
 $\lambda \quad \underline{x}$

Eigenvalue $\lambda = 3$

$\square \quad \cdot \quad \square 17$

$$\text{Eigenvector } \underline{x} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Let $\underline{A} \in M_{n \times n}$ (Eigensystems such as these
only valid for square matrices)

Given \underline{A} , find $\lambda + \underline{x}$

$$\underline{A}\underline{x} = \lambda \underline{x}$$

$$\underline{A}\underline{x} - \lambda \underline{x} = \underline{0}$$

$$(\underline{A} - \lambda \underline{I})\underline{x} = \underline{0}$$

Here \underline{x} must be in the nullspace

of $\underline{A} - \lambda \underline{I}$

We do not want the trivial solution. Thus,

$\Rightarrow \underline{A} - \lambda \underline{I}$ can not be of full rank

$\Rightarrow (\underline{A} - \lambda \underline{I})^{-1}$ does not exist

$$\Rightarrow \det(\underline{A} - \lambda \underline{I}) = 0$$

unknown eigenvalue

$\det(\underline{A} - \lambda \underline{I}) \Rightarrow$ Characteristic polynomial
of matrix A (in terms of λ)

Eigensystem Procedure:

Given $\underline{A} \in M_{n \times n}$

① Solve for all λ 's such that

$$\det(\underline{A} - \lambda \underline{I}) = 0$$

(Find roots of characteristic
polynomial)

② For each λ_i , find the corresponding
 \underline{x}_i , such that

$$\underline{A} \underline{x}_i = \lambda_i \underline{x}_i$$

$$\text{or} \\ (\underline{A} - \lambda \underline{I}) \underline{x} = \underline{0}$$

Example: Let $\underline{A} = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$

$$\begin{aligned} \underline{A} - \lambda \underline{I} &= \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\ &= \begin{bmatrix} 1-\lambda & 2 \\ 2 & 1-\lambda \end{bmatrix} \end{aligned}$$

$$\det(\underline{A} - \lambda \underline{I}) = (1-\lambda)^2 - 4 = 0$$

Characteristic
equation

$$(1-\lambda)^2 = 4, \quad 1-\lambda = \pm 2$$

↓

$$\left. \begin{array}{l} \lambda_1 = -1 \\ \lambda_2 = 3 \end{array} \right\} \text{Eigenvalues} \\ \text{of } \underline{A}$$

For $\lambda_1 = -1$

$$\text{Solve } (\underline{A} - \lambda_1 \underline{I}) \underline{x}_1 = \underline{0}$$

$$\begin{bmatrix} 1 - (-1) & 2 \\ 2 & 1 - (-1) \end{bmatrix} \underline{x}_1 = \underline{0}$$

$$\begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix} \begin{bmatrix} x_{11} \\ x_{12} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Note: Rows are
linearly dependent,
 $\det(\underline{A} - \lambda_1 \underline{I}) = 0$

↓ rref

$$\left[\begin{array}{cc|c} 1 & 1 & 0 \\ 0 & 0 & 0 \end{array} \right] \rightarrow \underline{x}_1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

Eigenvector associated with $\lambda_1 = -1$

$$\text{Let } \lambda_2 = 3$$

$$\begin{bmatrix} 1 - \lambda_2 & 2 \\ 2 & 1 - \lambda_2 \end{bmatrix} \underline{x}_2 = \underline{0}$$

$$\left[\begin{array}{cc|c} -2 & 2 & 0 \\ 2 & -2 & 0 \end{array} \right] \xRightarrow{\text{rref}} \left[\begin{array}{ccc|c} 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right]$$

$$\therefore \underline{x}_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad \text{Eigenvector associated with } \lambda_2 = 3$$

Summary for $\underline{A} = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$

Two eigenvalues & eigenvectors

$$\lambda_1 = -1, \quad \underline{x}_1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$\lambda_2 = 3, \quad \underline{x}_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Note: Eigenvectors can be multiplied by any non-zero constant & remain eigenvectors

Check:

$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \end{bmatrix} = (-1) \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$\underline{A} \quad \underline{x}_1 = \lambda_1 \quad \underline{x}_1 \quad \checkmark$$

$$\underline{A} \underline{x}_1 = \lambda_1 \underline{x}_1 \quad \checkmark$$

$$\begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \end{bmatrix} = (3) \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\underline{A} \underline{x}_2 = \lambda_2 \underline{x}_2 \quad \checkmark$$

Summary:

λ is an eigenvalue of square matrix \underline{A}
with eigenvector \underline{x} iff

$$\underline{A} \underline{x} = \lambda \underline{x}$$

To determine λ , we need

$$(\underline{A} - \lambda \underline{I}) \underline{x} = \underline{0}$$

For non-trivial solutions

$$\det(\underline{A} - \lambda \underline{I}) = |\underline{A} - \lambda \underline{I}| = 0$$

characteristic polynomial of \underline{A}

Find roots λ of characteristic polynomial

Example 2: Let $\underline{A} = \begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix}$

$$|\underline{A} - \lambda \underline{I}| = \begin{vmatrix} 1-\lambda & 2 \\ 2 & 3-\lambda \end{vmatrix} = (1-\lambda)(3-\lambda) - 4 = 0$$

$$\lambda^2 - 4\lambda - 1 = 0 \Rightarrow \lambda = \frac{-b \pm (b^2 - 4ac)^{1/2}}{2a}$$

$$\lambda = \frac{4 \pm (16 + 4)^{1/2}}{2} = 2 \pm \sqrt{5}$$

To find eigenvector, use λ for each root

1) $\lambda = 2 + \sqrt{5}$

$$\begin{bmatrix} 1 - (2 + \sqrt{5}) & 2 \\ 2 & 3 - (2 + \sqrt{5}) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

↙

$\det(\underline{A} - \lambda \underline{I}) = 0 \rightarrow$ rows must be linearly dependent

singular, rank < 2

$$(-1 - \sqrt{5})x_1 + 2x_2 = 0 \rightarrow \underline{x} = \begin{bmatrix} 1 \\ \frac{1 + \sqrt{5}}{2} \end{bmatrix}$$

2) $\lambda = 2 - \sqrt{5}$

$$\begin{bmatrix} 1 & 1 \end{bmatrix}$$

✓ 1 ✓ ✓

Similar procedure, $\underline{x} = \begin{bmatrix} 1 \\ \frac{1-\sqrt{5}}{2} \end{bmatrix}$

Summary:

$$\lambda_1 = 2 + \sqrt{5}, \quad \underline{x}_1 = \begin{bmatrix} 1 \\ \frac{1+\sqrt{5}}{2} \end{bmatrix}$$

$$\lambda_2 = 2 - \sqrt{5}, \quad \underline{x}_2 = \begin{bmatrix} 1 \\ \frac{1-\sqrt{5}}{2} \end{bmatrix}$$

Properties of Eigensystems:

- ① Eigenvalues of \underline{A}^2 are the square of the eigenvalues of \underline{A} , but eigenvectors are exactly the same

Assume $\underline{A}\underline{x} = \lambda\underline{x}$ is known

Then,

$$\underline{A}^2 \underline{x} = \underline{A}(\underline{A}\underline{x}) = \underline{A}(\lambda\underline{x}) = \lambda \underline{A}\underline{x}$$

$$= \lambda (\lambda \underline{x}) = \lambda^2 \underline{x} \Rightarrow \underline{A}^2 \underline{x} = \lambda^2 \underline{x}$$

Higher powers:

$$\underline{A}^3 \underline{x} = \underline{A} (\underline{A}^2 \underline{x}) = \underline{A} (\lambda^2 \underline{x}) = \lambda^2 \underline{A} \underline{x} = \lambda^3 \underline{x}$$

$$\Rightarrow \underline{A}^3 \underline{x} = \lambda^3 \underline{x}$$

In general, eigenvalues of \underline{A}^n are λ^n of

$$\underline{A} \underline{x} = \lambda \underline{x}$$

Recall Markov Chains:

\underline{M} is transition matrix

Columns of \underline{M} sum to one; all entries > 0

\underline{P}_n probability of states after step n

$$\underline{P}_n = \underline{M} \underline{P}_{n-1}$$

$$\underline{P}_n = \underline{M} (\underline{M} \underline{P}_{n-2})$$

...

$$\underline{P}_n = \underline{M}^n \underline{P}_0$$

↙
may need to raise M to a large
power; find eigensystem of M

② Row reduction does not preserve eigenvalues

Row reduction involves the scaling + addition
of the matrix rows

Example: $\underline{A} = \begin{bmatrix} 4 & -1 & 0 \\ 0 & 1 & 0 \\ 2 & -3 & 6 \end{bmatrix}$

$$\begin{vmatrix} 4-\lambda & -1 & 0 \\ 0 & 1-\lambda & 0 \\ 2 & -3 & 6-\lambda \end{vmatrix} = (4-\lambda)(1-\lambda)(6-\lambda) = 0$$

$$\therefore \lambda = 4, 1, 6$$

Flip rows 1 \leftrightarrow 3

$$\underline{B} = \begin{bmatrix} 2 & -3 & 6 \\ 0 & 1 & 0 \\ 4 & -1 & 0 \end{bmatrix}$$

$$\begin{vmatrix} 2-\lambda & -3 & 6 \\ \dots & \dots & \dots \end{vmatrix}$$

$$\begin{vmatrix} 2-\lambda & -3 & 6 \\ 0 & 1-\lambda & 0 \\ 4 & -1 & -\lambda \end{vmatrix} = (2-\lambda)(1-\lambda)(-\lambda) - 4(1-\lambda)6$$

$$= -(2-3\lambda+\lambda^2)\lambda - 24(1-\lambda)$$

$$= -\lambda^3 + 3\lambda^2 - 2\lambda + 24\lambda - 24$$

$$= -[\lambda^3 - 3\lambda^2 - 22\lambda + 24]$$

$$= -(\lambda-1)(\lambda+4)(\lambda-6)$$

$$\therefore \lambda = 1, \underline{-4}, 6$$

$$\therefore \lambda \text{ of } \underline{B} \neq \lambda \text{ of } \underline{A}$$

③ The product of the eigenvalues of A equals $\det(\underline{A})$ and the sum of the eigenvalues equals $\text{tr}(\underline{A})$, where

$$\text{tr}(\underline{A}) = \text{trace of } \underline{A} = \text{sum of the diagonal}$$

Aside: ERO of swapping rows. What happens to $\det(\underline{A})$ after swap?