10.34: Numerical Methods Applied to Chemical Engineering

Lecture 5:
Eigenvalues and eigenvectors

Permutation

- Reordering through use of permutation matrices:
  - Consider the operation of swapping two rows. This can be done through matrix multiplication.

$$\boldsymbol{P} = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 1 & 0 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{pmatrix}$$

swap row 1 and 2

identity

  - For example:

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x_2 \\ x_1 \\ x_3 \end{pmatrix}$$

Permutation

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$$

swap row 1 and 2

identity

$$
\boldsymbol{PA} = \begin{pmatrix} \boldsymbol{PA}_1^C & \boldsymbol{PA}_2^C & \dots & \boldsymbol{PA}_N^C \end{pmatrix} = \begin{pmatrix} \boldsymbol{A}_2^R \\ \boldsymbol{A}_1^R \\ \boldsymbol{A}_3^R \\ \vdots \\ \boldsymbol{A}_N^R \end{pmatrix}
$$

Permutation

- Reordering through use of permutation matrices:
  - How do I swap columns?

$$\boldsymbol{A}\boldsymbol{P}^T = \left(\boldsymbol{P}\boldsymbol{A}^T\right)^T$$

- Permutation matrices are unitary:

$$\mathbf{P}\mathbf{P}^T = \mathbf{I}$$
$$\mathbf{P}^T = \mathbf{P}^{-1}$$

- Reordering a system of equations:

$$(\boldsymbol{P}_1\boldsymbol{A}\boldsymbol{P}_2^T)(\boldsymbol{P}_2\boldsymbol{x}) = \boldsymbol{P}_1\boldsymbol{b}$$

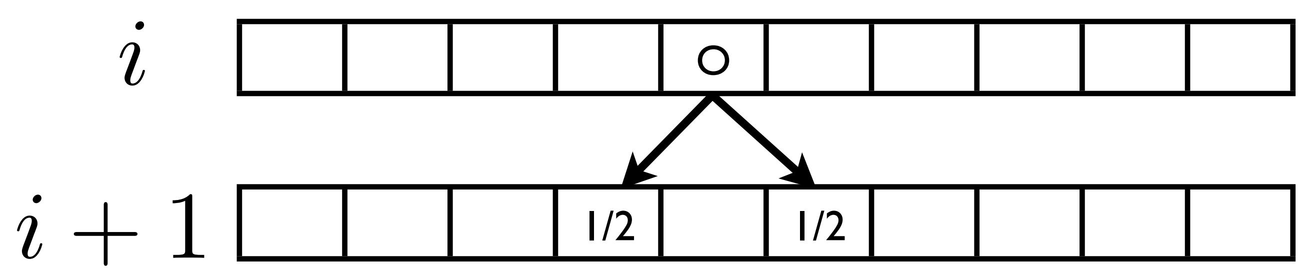
  - Reordering is a form of preconditioning!
  - Reordering can be used for pivoting!

Recap

- Gaussian elimination
- Sparse matrices
- Permutation and reordering

Recap

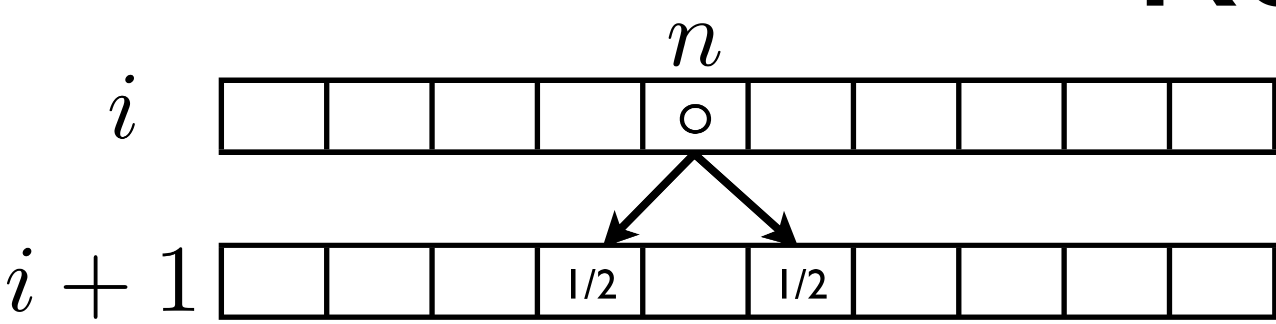
- Example: Plinko:



- Derive a sparse matrix model that maps the probability of the chip location from one level to the next.

$$\mathbf{P}^{i+1} = \mathbf{A}\mathbf{P}^{i}$$

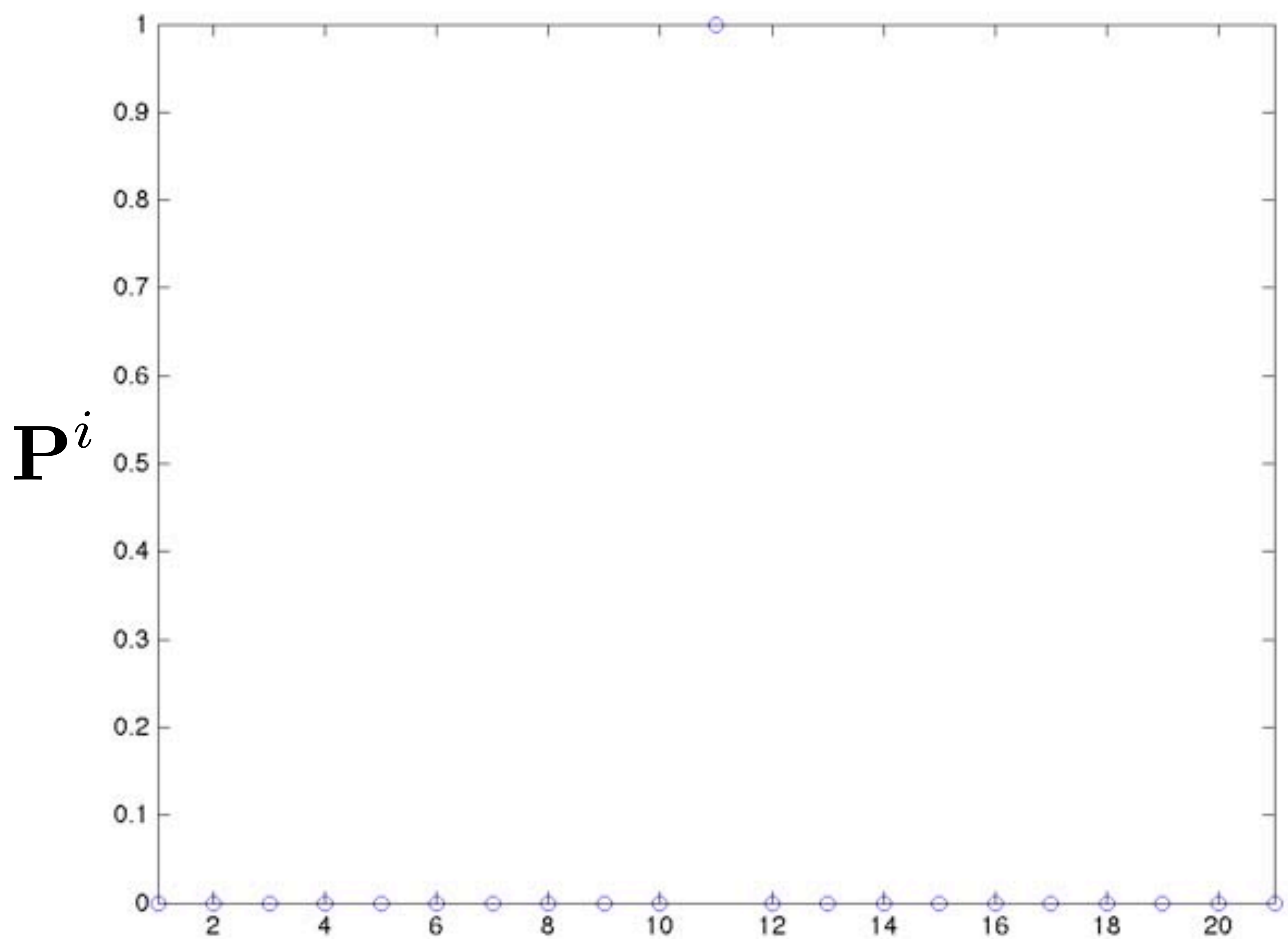
Recap



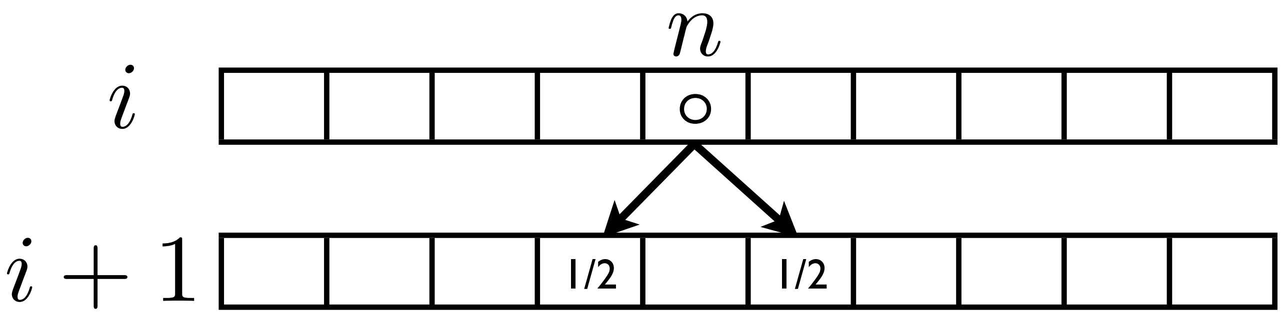
$$P_n^{i+1} = P_{n-1}^i/2 + P_{n+1}^i/2$$

$$\mathbf{P}^{i+1} = \mathbf{A}\mathbf{P}^i$$

- `A=spdiags(ones(N,2)/2, [-1 1], N, N);`
- `A(1,2)=1; A(N,N-1)=1;`



Recap



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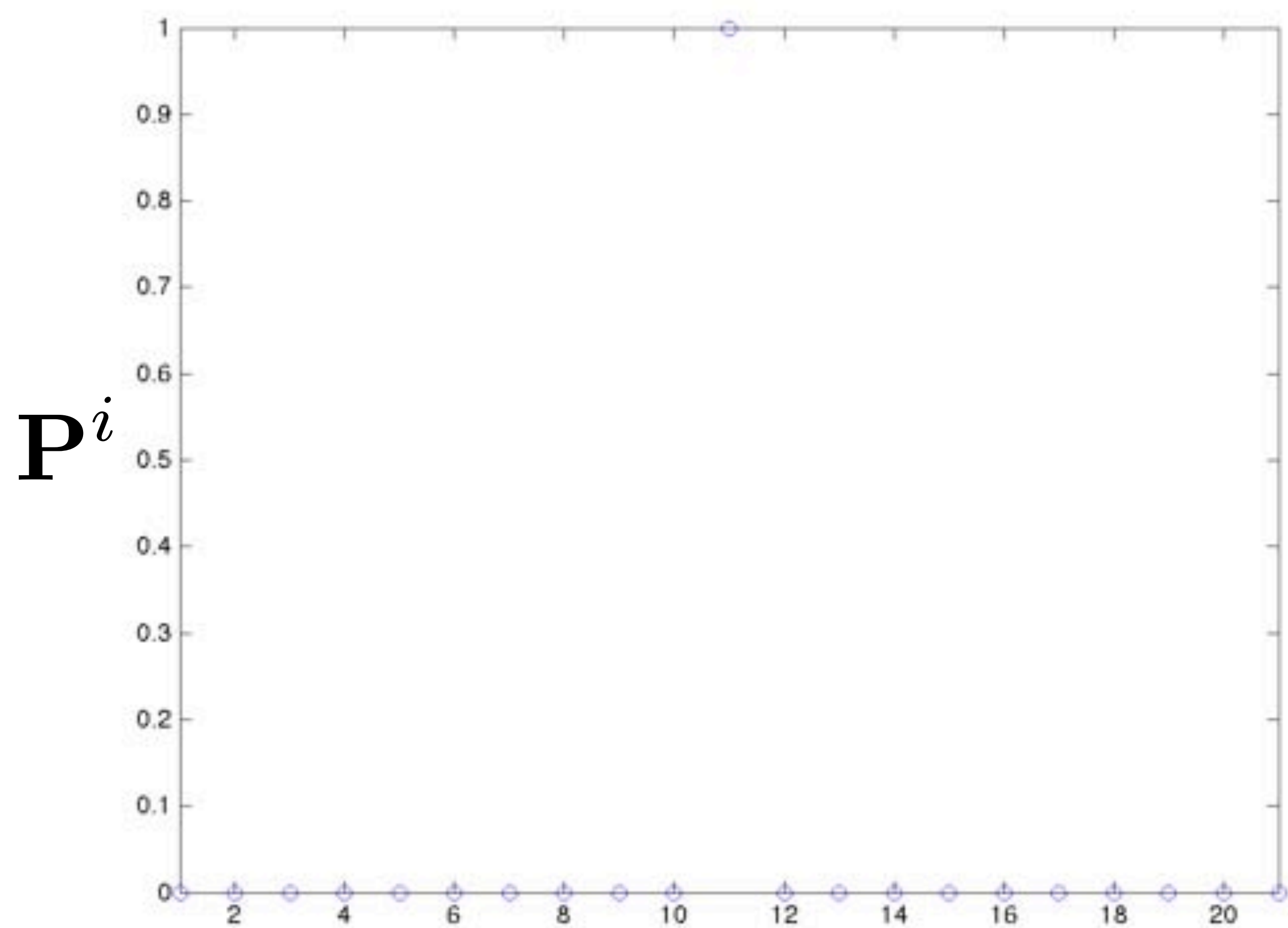
$$\boldsymbol{A} = \left(\qquad \right)$$

Recap

- Notice that after many cycles, the probability distribution becomes "constant." $\mathbf{AAAA\ldots AP}_0$
- In fact there are special distributions such that:

$$(\mathbf{AA})\mathbf{P} = \mathbf{P}$$

- What are examples of those distributions?
- They are called eigenvectors of the matrix: $\mathbf{B} = \mathbf{AA}$



Eigenvalues and Eigenvectors

- The eigenvectors of a matrix are special vectors that are "stretched" on multiplication by the matrix:

$$\mathbf{A}\mathbf{w} = \lambda \mathbf{w}$$

$$\mathbf{A} \in \mathbb{R}^{N \times N} \qquad \mathbf{w} \in \mathbb{C}^{N} \qquad \lambda \in \mathbb{C}$$

- The amount of stretch λ is called the eigenvalue
- Finding an eigenvector/eigenvalue involves solving:
  - N equations
  - which are nonlinear ($\lambda \mathbf{w}$)
  - for $N+1$ unknowns
- Eigenvectors are not unique:
  - If $\mathbf{w}$ is an eigenvector, so is $c\mathbf{w}$

Eigenvalues

- Finding eigenvalues:

$$\mathbf{A}\mathbf{w} = \lambda\mathbf{w} \Rightarrow (\mathbf{A} - \lambda\mathbf{I})\,\mathbf{w} = 0$$

  - either $\mathbf{w} = 0$
  - or $\mathbf{w} \in \mathcal{N}(\mathbf{A} - \lambda\mathbf{I})$ and $\det(\mathbf{A} - \lambda\mathbf{I}) = 0$

- For the right values of λ, $\mathbf{A} - \lambda\mathbf{I}$ is singular!
  - $\det(\mathbf{A} - \lambda\mathbf{I}) = 0 = p^N(\lambda)$
  - $p^N(\lambda)$ is called the characteristic polynomial.
  - The N roots of $p^N(\lambda)$ are the eigenvalues of
  - $p^N(\lambda) = c(\lambda_1 - \lambda)(\lambda_2 - \lambda)\ldots(\lambda_N - \lambda)$

Eigenvalues

- Examples:

  - $\mathbf{A} = \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{pmatrix}$

$$\mathbf{A} - \lambda\mathbf{I} = \begin{pmatrix} -2-\lambda & 0 & 0 \\ 0 & 1-\lambda & 0 \\ 0 & 0 & 3-\lambda \end{pmatrix}$$

$$\det(\mathbf{A} - \lambda\mathbf{I}) = (-2-\lambda)(1-\lambda)(3-\lambda) = 0$$

$$\lambda = -2, 1, 3$$

    - The elements of a diagonal matrix are eigenvalues

  - $\mathbf{A} = \begin{pmatrix} -2 & 1 \\ 1 & -2 \end{pmatrix}$

Eigenvalues

- Examples:
  - The elements of a diagonal matrix are eigenvalues:

$$0 = \det \begin{pmatrix} A_{11}-\lambda & 0 & \dots & 0 \\ 0 & A_{22}-\lambda & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & A_{NN}-\lambda \end{pmatrix}$$
$$= (A_{11}-\lambda)(A_{22}-\lambda)\dots(A_{NN}-\lambda).$$

  - The diagonal elements of a triangular matrix are eigenvalues too:

$$0 = \det \begin{pmatrix} A_{11}-\lambda & A_{12} & \dots & A_{1N} \\ 0 & A_{22}-\lambda & \dots & A_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & A_{NN}-\lambda \end{pmatrix}$$
$$= (A_{11}-\lambda)(A_{22}-\lambda)\dots(A_{NN}-\lambda).$$

Eigenvalues

- Properties of eigenvalues: $\mathbf{A} \in \mathbb{R}^{N \times N}$
  - Inferred from the properties of polynomial equations!
  - $p^N(\lambda)$ is a polynomial of degree N and has no more than N roots. $\mathbf{A}$ has up to N distinct eigenvalues.
  - The eigenvalues, like the factors of a polynomial need not be distinct. Multiple roots are possible, e.g.

    $$p^N(\lambda) = c(\lambda - \lambda_1)^2(\lambda - \lambda_2)\ldots(\lambda - \lambda_{N-1})$$

  - Eigenvalues may be real or complex. Complex eigenvalues appear in conjugate pairs: λ, $\bar{\lambda}$
  - $\det(\mathbf{A}) = \lambda_1 \lambda_2 \ldots \lambda_N$
  - $\mathrm{tr}(\mathbf{A}) = \lambda_1 + \lambda_2 + \ldots + \lambda_N$

Eigenvalues

- Example:
  - A series of chemical reactions: $\mathrm{A} \xrightarrow{k_1} \mathrm{B} \underset{k_3}{\overset{k_2}{\longleftrightarrow}} \mathrm{C} \underset{k_5}{\overset{k_4}{\longleftrightarrow}} \mathrm{D}.$
  - Conservation equation:

$$\frac{d}{dt}\begin{pmatrix} [A] \\ [B] \\ [C] \\ [D] \end{pmatrix} = \begin{pmatrix} -k_1 & 0 & 0 & 0 \\ k_1 & -k_2 & k_3 & 0 \\ 0 & k_2 & -k_3 - k_4 & k_5 \\ 0 & 0 & k_4 & -k_5 \end{pmatrix}\begin{pmatrix} [A] \\ [B] \\ [C] \\ [D] \end{pmatrix}.$$

  - Find the characteristic polynomial of the rate matrix:

$$0 = \det\begin{pmatrix} -k_1 - \lambda & 0 & 0 & 0 \\ k_1 & -k_2 - \lambda & k_3 & 0 \\ 0 & k_2 & -k_3 - k_4 - \lambda & k_5 \\ 0 & 0 & k_4 & -k_5 - \lambda \end{pmatrix}$$

$$\det(\mathbf{A}) = \sum_{j=1}^{N} (-1)^{i+j} A_{ij} M_{ij}(\mathbf{A})$$

  - What are the eigenvalues of the rate matrix?
  - What are they physically?

Eigenvalues

- Example:
  - A series of chemical reactions: $\mathrm{A} \xrightarrow{k_1} \mathrm{B} \underset{k_3}{\overset{k_2}{\longleftrightarrow}} \mathrm{C} \underset{k_5}{\overset{k_4}{\longleftrightarrow}} \mathrm{D}.$
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$$= \lambda(\lambda + k_1)\left[\lambda^2 + (k_2 + k_3 + k_4 + k_4)\,\lambda + k_2k_4 + k_2k_5 + k_3k_5\right]$$

  - What are the eigenvalues of the rate matrix?
  - What are they physically?

Eigenvectors

- Finding eigenvectors:
  - Given an eigenvalue: λ_i , what is the corresponding eigenvector: $\mathbf{w}_i$?
  - The eigenvector belongs to the null space of $\mathbf{A} - \lambda_i \mathbf{I}$
  - The eigenvector is not unique: $\mathbf{A}(c\mathbf{w}_i) = \lambda_i(c\mathbf{w}_i)$
  - One option: do Gaussian elimination on $[\mathbf{A} - \lambda_i \mathbf{I}|\mathbf{0}]$
    - At some point the eliminated matrix will look like:

$$\left(\begin{array}{cccc|ccc} U_{11} & U_{12} & \dots & U_{1r} & U_{1(r+1)} & \dots & U_{1M} \\ 0 & U_{22} & \dots & U_{2r} & U_{2(r+1)} & \dots & U_{2M} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & U_{rr} & U_{r(r+1)} & \dots & U_{rM} \\ \hline 0 & 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & \underline{0} & \underline{\dots} & \underline{0} \end{array}\right)$$

    - These $r - N$ components of $\mathbf{w}_i$ are arbitrary
    - # of all zero rows = multiplicity of eigenvalue

Eigenvectors

- Examples:

  - Find the eigenvectors of: $\mathbf{A} = \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{pmatrix}$

$$\lambda_1 = -2, \; \lambda_2 = 1, \; \lambda_3 = 3$$

$$[\mathbf{A} + 2\mathbf{I}|\mathbf{0}] = \left[\begin{array}{ccc|c} 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 5 & 0 \end{array} \right]$$

$$\mathbf{w}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \mathbf{A} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} -2 \\ 0 \\ 0 \end{pmatrix}$$

  - What are the others?

Eigenvectors

- Example:
  - A series of chemical reactions: $\mathrm{A} \xrightarrow{k_1} \mathrm{B} \underset{k_3}{\overset{k_2}{\longleftrightarrow}} \mathrm{C} \underset{k_5}{\overset{k_4}{\longleftrightarrow}} \mathrm{D}.$
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  - Find the eigenvector of the rate matrix with eigenvalue 0:

$$\left[\begin{array}{cccc|c} -k_1 & 0 & 0 & 0 & 0 \\ k_1 & -k_2 & k_3 & 0 & 0 \\ 0 & k_2 & -k_3 - k_4 & k_5 & 0 \\ 0 & 0 & k_4 & -k_5 & 0 \end{array}\right]$$

  - What does this eigenvector represent?

Eigenvectors

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    - What does this eigenvector represent?

Eigenvectors

- Example:
  - Find the eigenvalues and linearly ind. eigenvectors:

$$\mathbf{A} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

  - Find the eigenvalues and linearly ind. eigenvectors:

$$\mathbf{A} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

Eigenvectors

- Example:
  - Find the eigenvalues and linearly ind. eigenvectors:

$$\mathbf{A} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \qquad \begin{array}{c} p(\lambda) = \lambda^2 \\ \lambda = 0, 0 \end{array} \qquad \mathbf{w} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

algebraic multiplicity = 2 geometric multiplicity = 2

  - Find the eigenvalues and linearly ind. eigenvectors:

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geometric multiplicity = 1

algebraic multiplicity = 2

Eigenvectors

- Example:
  - Find the eigenvalues and linearly ind. eigenvectors:

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Eigenvectors

- Properties of eigenvectors:
  - If an eigenvalue is distinct (algebraic multiplicity 1):
    - $\dim \mathcal{N}(\mathbf{A} - \lambda_i \mathbf{I}) = 1$
      - There is only one corresponding eigenvector
  - If an eigenvalue has algebraic multiplicity M:
    - $1 \leq \dim \mathcal{N}(\mathbf{A} - \lambda_i \mathbf{I}) \leq M$
    - There could be as many as M linearly independent eigenvectors.
  - Geometric multiplicity is the number of linear independent eigenvectors for an eigenvalue: $\dim \mathcal{N}(\mathbf{A} - \lambda_i \mathbf{I})$
  - When geometric and algebraic multiplicity are the same, the matrix is said to have a "complete set" of eigenvectors.

Eigendecomposition

- For a matrix with a complete set of eigenvectors one can write:

$$\mathbf{A}\mathbf{W} = \mathbf{W}\mathbf{\Lambda}$$

  - where $\mathbf{W} = (\mathbf{w}_1 \ \mathbf{w}_2 \ \dots \ \mathbf{w}_N)$
  - and

$$\mathbf{\Lambda} = \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_N \end{pmatrix}$$

  - equivalently: $\mathbf{\Lambda} = \mathbf{W}^{-1}\mathbf{A}\mathbf{W}$
    - the matrix can be diagonalized
  - equivalently: $\mathbf{A} = \mathbf{W}\mathbf{\Lambda}\mathbf{W}^{-1}$
    - the matrix can be easily reconstructed

Eigendecomposition

- Solving systems of equations is easy when a complete set of eigenvectors and eigenvalues are known:

$$\mathbf{A}\mathbf{x} = \mathbf{b} \Rightarrow \mathbf{W}\mathbf{\Lambda}\mathbf{W}^{-1}\mathbf{x} = \mathbf{b}$$

  - step 1: $\mathbf{\Lambda}(\mathbf{W}^{-1}\mathbf{x}) = \mathbf{W}^{-1}\mathbf{b} \Rightarrow \mathbf{\Lambda}\mathbf{y} = \mathbf{c}$
  - step 2: $\mathbf{y} = \mathbf{\Lambda}^{-1}\mathbf{c} \Rightarrow \mathbf{W}^{-1}\mathbf{x}\mathbf{\Lambda}^{-1}\mathbf{W}^{-1}\mathbf{b}$
  - step 3: $\mathbf{x} = \mathbf{W}\mathbf{\Lambda}^{-1}\mathbf{W}^{-1}\mathbf{b}$

  - But how is $\mathbf{W}^{-1}$ computed?
    - $(\mathbf{W}^{-1})^T$ are the eigenvectors of $\mathbf{A}^T$
    - If $\mathbf{A} = \mathbf{A}^T$ and $\|\mathbf{w}_i\|_2 = 1$, then $\mathbf{W}^{-1} = \mathbf{W}^T$
      - Eigenvalue matrix is unitary: $\mathbf{W}\mathbf{W}^T = \mathbf{I}$
      - Eigenvectors are orthogonal: $\mathbf{w}_i \cdot \mathbf{w}_j = \delta_{ij}$

Eigendecomposition

- Useful when analyzing linear systems of ordinary differential equations:

$$\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}$$

  - substitute: $\mathbf{A} = \mathbf{W}\mathbf{\Lambda}\mathbf{W}^{-1}$
  - let: $\mathbf{y}(t) = \mathbf{W}^{-1}\mathbf{x}(t)$
  - then: $\dot{\mathbf{y}}(t) = \mathbf{\Lambda}\mathbf{y}(t)$ or $\dot{y}_i(t) = \lambda_i y_i(t)$
    - The system of ODEs is decoupled and easy to solve!
- What if there is not a complete set of eigenvectors?
  - Matrix cannot be diagonalized.
  - Components cannot be decoupled.
  - Jordan Normal Form: $\mathbf{A} = \mathbf{M}\mathbf{J}\mathbf{M}^{-1}$
    - $\mathbf{J}$ is almost diagonal