Eigenvalue problems

- Actually eigenvalue and eigenvector problems
- Sometimes only interested in one of them, e.g. might be interested in just some energies, not the wavefunctions in QM
- Standard analytical approach:

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

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

- Matrix eq $M\bar{x} = 0$ has non-trivial solution $\bar{x}$ iff $\det(M) = 0$
- So look at $\det(A-\lambda I) = 0$ where $\det(A-\lambda I)$ is a polynomial of degree N in λ
  - "characteristic polynomial"

    $$P(\lambda) = \det(A - \lambda I) = (\lambda_1 - \lambda)(\lambda_2 - \lambda)\ldots$$

  - Eigenvalues are the N roots of $P(\lambda)$.
  - The roots (eigenvals) of A is called "the spectrum", denoted as

    $$\lambda(A) = \{\lambda_1, \lambda_2, \ldots, \lambda_N\}$$

    and $\det(A) = \lambda_1\lambda_2 \ldots \lambda_N$ (product of eigenvals)

- Nice analytically, but inefficient to compute $\det(A-\lambda I)$ when N is large
- Here: Jacobi's rotation method: Ch. 7.1 – 7.4

  Other methods discussed in Ch. 7.5 – 7.7

- Basis for Jacobi's method (and other methods): <u>Similarity transf.</u>

  - Transformations with orthogonal matrix S: $S^T = S^{-1}$

    $$S^T S = S S^T = I$$

  - Here we assume A is <u>real</u> and <u>symmetric</u>

  - A is $N \times N$, with N eigenvalues: $\lambda^{(1)}, \lambda^{(2)}, \dots, \lambda^{(N)}$

    (not nec. distinct)

$\Rightarrow$ Then there <u>exists</u> an orthogonal matrix S such that

$$S^T A S = D = \begin{bmatrix} d_{11} & & & 0 \\ & d_{22} & & \\ & & \ddots & \\ 0 & & & d_{NN} \end{bmatrix} \quad \text{diagonal matrix}$$

- Apply S from the left

$$AS = SD$$

- Express S as column vectors: $S = \left[\left(\bar{s}_1\right) \left(\bar{s}_2\right) \left(\bar{s}_3\right) \dots \left(\bar{s}_N\right) \right]$

$$A \times \begin{bmatrix} \bar{s}_1 & \bar{s}_2 & \dots & \bar{s}_N \end{bmatrix} = \begin{bmatrix} \bar{s}_1 & \bar{s}_2 & \dots & \bar{s}_N \end{bmatrix} \begin{bmatrix} d_{11} & & & 0 \\ & d_{22} & & \\ & & \ddots & \\ 0 & & & d_{NN} \end{bmatrix}$$

$$= \begin{bmatrix} d_{11} \bar{s}_1 & d_{22} \bar{s}_2 & \dots & d_{NN} \bar{s}_N \end{bmatrix}$$

- This is a set of N equations

$$A \bar{s}_1 = d_{11} \bar{s}_1$$
$$A \bar{s}_2 = d_{22} \bar{s}_2$$
$$\vdots$$
$$A \bar{s}_N = d_{NN} \bar{s}_N$$

<u>So:</u>

- The elements along the diagonal in D are the <u>eigenvalues</u> of A
- The columnvectors in S are the <u>eigenvectors</u> of A

- Idea behind Jacobi's rotation method:

Find the final S by applying a series of similarity transformations $S_1, S_2, \ldots, S_M$

$$A$$
$$S_1^T A S_1$$
$$S_2^T S_1^T A S_1 S_2$$
$$\vdots$$

until finally we have a diagonal matrix

$$S_M^T \cdots S_1^T A S_1 \cdots S_M = D$$

- Then we know that

$$S = S_1 S_2 S_3 \ldots S_M$$

and we have found the eigenvals. (in D) and eigenvectors (columns in S)

End lecture

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- Note that eigenvals. are preserved at each step:

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

$$\times S_1^T \rightarrow \quad S_1^T(A \underset{S_1 S_1^T}{\wedge} \bar{x}) = S_1^T(\lambda \bar{x})$$

The same eigenvalue

$$\Rightarrow \quad (S_1^T A S_1)(S_1^T \bar{x}) = \lambda (S_1^T \bar{x})$$

New matrix

New ~~vector~~ eigenvector

$$\Rightarrow \quad (S_2^T S_1^T A S_1 S_2)(S_2^T S_1^T \bar{x}) = \lambda (S_2^T S_1^T \bar{x})$$

etc...