10.34, Numerical Methods Applied to Chemical Engineering
Professor William H. Green

Lecture #11: Numerical Calculation of Eigenvalues and Eigenvectors. Singular Value Decomposition (SVD).

Singular Value Decomposition (SVD)

How do you handle poorly conditioned matrices? $\underline{\underline{A}}\cdot\underline{x} = \underline{b}$

What are corresponding eigenvalues for rectangular matrix?

$$\begin{pmatrix} & & \\ & A & \\ & & \end{pmatrix}\begin{pmatrix} \\ \\ \end{pmatrix} \text{ or } \begin{pmatrix} & & \end{pmatrix}\begin{pmatrix} & & \\ & A & \\ & & \end{pmatrix}$$ eigenvalues? eigenvectors?

Lots of equations and not many unknowns ➔ rectangular matrix

$$\left.\begin{array}{ll} \left[\hat{O}f(x) - q(x)\right] = 0 & \int a_n(x)\Re(x)dx = 0 \\ \swarrow & \\ f(x,c) = \sum c_n\phi_n(x) & \end{array}\right\}$$ infinite number of equations, finite number of $\underline{c}_n$

Another scenario:

Determine how plant is operating:

You make more measurements than unknowns.

$\underline{\underline{A}}^T\underline{\underline{A}}$: $$\begin{pmatrix} & A^T & \\ & & \end{pmatrix}\begin{pmatrix} & \\ A & \\ & \end{pmatrix} = \begin{pmatrix} A^TA & \\ & \end{pmatrix}$$ eigenvalues λ: $\sigma_i = \sqrt{\lambda_i}$ ← "singular values of $\underline{\underline{A}}$"

small square matrix

$$\underline{\underline{A}} = \underline{\underline{U}}\begin{pmatrix} \sigma_1 & 0 & 0 & 0 & 0 \\ 0 & \sigma_2 & 0 & 0 & 0 \\ 0 & 0 & \sigma_3 & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & \sigma_n \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}\cdot\underline{\underline{V}}^T \qquad \underline{\underline{U}}^T = \underline{\underline{U}}^{-1} \qquad \underline{\underline{V}}^T = \underline{\underline{V}}^{-1}$$

in the Beers notes
this is called $\underline{\underline{W}}$ square matrix

$\underline{\underline{A}} = \underline{\underline{U}}\cdot\underline{\underline{\Sigma}}\cdot\underline{\underline{V}}^T$ ← Singular value decomposition

big square matrix | rectangular matrix mostly zeros

MATLAB read help for more information about `svd`

```
[U,S,V] = svd(A)
```

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$||\underline{\underline{A}}||_2 = \max(\{\sigma_i\})$

$\mathrm{cond}(\underline{\underline{A}}) = \sigma_{max}/\sigma_{min}$

Pseudo Inverse

$$\underline{\underline{A}}^+ = \underline{\underline{V}}\cdot\begin{pmatrix} \sigma_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sigma_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sigma_3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sigma_n & 0 & 0 \end{pmatrix}\underline{\underline{U}}^T \quad \underline{x} = \underline{\underline{A}}^+\underline{b} \qquad \underline{\underline{A}}\cdot\underline{x} \approx \underline{b}$$

For a poorly conditioned matrix, one of σ_i is close to zero; better to just replace $1/\sigma_n$ (when $\sigma_n \approx 0$) with 0. This gives you a more stable *approximate inverse*.

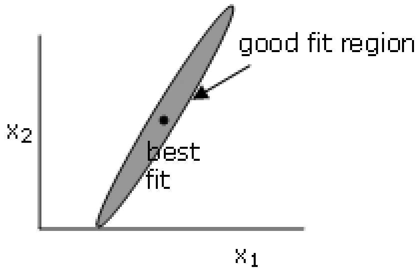

Figure 1. Least squares.

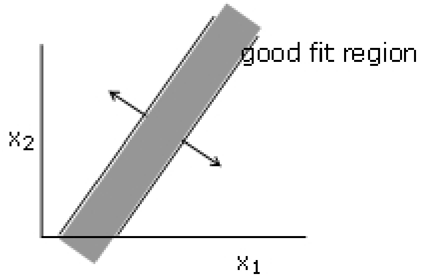

Figure 2. SVD ignores the other direction.

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Homework

$$V(\phi)=\sum_{0}^{N} y_n\cos(n\phi)$$

$$\begin{array}{c|c} \phi_i & V_i \\ \hline 0 & 0 \\ \vdots & 2.1 \\ \vdots & 0.5 \\ \vdots & 8.6 \\ \frac{5\pi}{3} & \vdots \end{array}$$

$$\overset{\phi_i}{\begin{pmatrix} \cos(0\cdot 0) & \cos(1\cdot 0) & \\ \cos(0\cdot \pi/3) & \cos(1\cdot \pi/3) & \cos(2\cdot \pi/3) \\ & & \\ & & \\ & & \end{pmatrix}} \overset{y_i}{\begin{pmatrix} y_0 \\ \vdots \\ \vdots \\ \vdots \\ y_5 \end{pmatrix}}$$

setup_interV.m

$$\phi_i \cdot y_i \Rightarrow \overset{v_i}{\begin{pmatrix} 0 \\ 2.1 \\ 0.5 \\ \vdots \end{pmatrix}}$$

set tolerances in MatLAB and use: *interpolateV.m*

SVD – answers are not as sensitive to numerical noise
condA = $8.988\cdot10^{15}$ ← HIGH

$$\underline{\underline{A}}^T \underline{V}_\varphi = \underline{\underline{V}}\cdot \begin{pmatrix} 1/\sigma_1 & 0 & 0 & 0 & 0 \\ 0 & 1/\sigma_2 & 0 & 0 & 0 \\ 0 & 0 & 1/\sigma_3 & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & \ddots \end{pmatrix} \underline{\underline{U}}^T \underline{V}_\varphi$$

From MatLAB; singular values, $\underline{\underline{S}}$:

$$\begin{pmatrix} 2.495 & & & & & \\ & 2.495 & & & & \\ & & 2.495 & & & \\ & & & 2.495 & & \\ & & & & 0 & \\ & & & & & 0 \end{pmatrix}$$

Very poorly conditioned matrix means that there is a lot of flexibility in the unknown variables.

```
y = y + ((U(i,i)'*Vphi)./S(j,j)).*V(i,j);
```

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$$\underset{\text{rectangle}}{\begin{pmatrix} & & \\ & A & \\ & & \\ & & \end{pmatrix}} = \underset{\substack{\text{same long}\\ \text{dimension as A}}}{\begin{pmatrix} & & \\ & U & \\ & \text{square} & \\ & & \end{pmatrix}} \begin{pmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \\ 0 & 0 & 0 \end{pmatrix} \underset{\substack{\text{square; same as}\\ \text{short dimension of A}}}{\begin{pmatrix} & & \\ & V^T & \\ & & \end{pmatrix}}$$

$$\underline{\underline{A}} \cdot \underline{\underline{V}} = \underline{\underline{U}} \cdot \underline{\underline{\Sigma}} \cdot \underline{\underline{V}}^T \underline{\underline{V}}$$

$$\underline{\underline{A}} \cdot \underline{\underline{V}} = \underline{\underline{V}} \cdot \underline{\underline{\Lambda}} \qquad \underline{\underline{A}}^T \underline{\underline{A}} \cdot \underline{\underline{V}} = \underline{\underline{V}} \cdot \overbrace{\underline{\underline{\Sigma}}^T \cancel{\underline{\underline{U}}^T \underline{\underline{U}}} \cdot \underline{\underline{\Sigma}}}^{\underline{\underline{\Lambda}}}$$

$$\underline{\underline{A}}\,\underline{\underline{A}}^T \underline{\underline{U}} = \underline{\underline{U}}\,\underline{\underline{\tilde{\Lambda}}}$$

Deconvolution of experimental data

SVD is very good for this.

$\underline{\underline{S}}(\lambda,t) = \Sigma c_i f_i(t) g_i(\lambda)$

See homework for an example.

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