Numerical Methods in Physics

Numerische Methoden in der Physik, 515.421.

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Room: TDK Seminarraum

Time: 8:30-10 a.m.

Exercises: Computer Room, PH EG 004 F

http://itp.tugraz.at/LV/boeri/NUM_METH/index.html
(Lecture slides, Script, Exercises, etc).

Important notice :

This will be the **last lecture** for the course of Numerical Methods in Physics, WS 2013-14. There will be **<u>no lecture</u> <u>on the 21st of January</u>** (next week).

Next week you will have the possibility to present your exercises.

Depending on how many people are left after next week we will add one or two additional dates for the presentation after the end of the semester to present your exercises (12th of March + 11th of February, if needed).

We will post the dates on the web site (and send you an email) when this is decided.

If **after the 12th of March** you haven't presented all four exercises, you will **lose all points** for the exercises and will have to take the class again.

Important notice 2 (exam dates):

Exams for the lecture in numerical methods in Physics will take place in my office PH3.108, starting 22th of January 2013 (Wednesday).

For the **winter semester**, I will offer the following dates:

- 22nd, 23rd, 27th, 28th, 29th, 30th, 31st of January
- 3rd-7th of February.

A list with available dates and slots is pasted outside my offic**e.** You can register writing your name on the list, **up to the 17th of January.**

There will be additional dates in May-June and October 2014 – check the web page of the course!

Important notice 2 (exam topics):

The topics for the exam are the chapters of the script which have been explained in the main lecture. You can study the **German (D)** or **English (E)** version of the script, they are now both available on the web site…

- **D(1) E(1)** Introduction.
- **D(2) E(2)** Numerical Methods for Linear, Inhomogeneous Systems of Equations.
- **D(4) E(3)** Least Squares Approximation.
- **D(5) E(4)** Numerical Solution of Transcendental Equations.
- **D(7) E(5)** Eigenvalues and Eigenvectors of Real Matrices.
- **D(8) E(6)** Numerical Methods for Ordinary Differential Equations: Initial value problems.

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- **D(8) E(6)** Numerical Methods for Ordinary Differential Equations: Initial value problems.

Last week(7/1/2014)

Eigenvalues and Eigenvectors of Real Matrices (part II)

- ***Von Mises Method:*** *iterative method to find the lowest or highest eigenvalue of a matrix.*
- **Jacobi Method** for real matrices: reducing a matrix into a diagonal form by iteration of similarity operations.
- **Jacobi Method**: optimizing convergence speed.
- **Generalized eigenvalue** problem: reduction to a standard eigenvalue problem using **Cholesky's decomposition**.

This week (14/1/2014)

Eigenvalues and Eigenvectors of Real Matrices (Part III)

- Jacobi method and Cholesky decomposition: Summary, derivations and examples.
- Upper Hessenberg form for real matrices.
- Hyman's method: characteristic polynomial of Upper Hessenberg matrices; formulas and examples.

Jacobi Method:

We diagonalise a **symmetric** matrix A using a **sequence of similarity operations** U_t.

$$A^{(1)} = U_0^T A U_0$$

$$A^{(2)} = U_1^T A^{(1)} U_1 = U_1^T U_0^T A U_0 U_1$$

$$\dots$$

$$A^{(t+1)} = U_t^T A^{(t)} U_t = U_t^T U_{t-1}^T \dots U_0^T A U_0 \dots U_{t-1} U_t$$

This series converges to:

$$\lim_{t\to\infty} A^{(t)} = D$$

$$\lim_{t\to\infty} U_0 U_1 \dots U_{t-1} U_t \to U$$

Where U is the matrix of the **eigenvectors** of A.

Jacobi Matrices:

The matrices U_t are **orthogonal rotation matrices** of the form:

$$U_t(i,j,\varphi) = \begin{pmatrix} 1 & 0 & & & \dots & & & & 0 \\ & 1 & & & & & & & \\ & & \dots & & & & & & \\ & & & \cos\varphi & & -\sin\varphi & & & \\ & & & & 1 & & & & \\ & & & \sin\varphi & & \cos\varphi & & & \\ & & & & & & 1 & & \\ & & & & & & & \dots & \\ 0 & & & & \dots & & & 0 & 1 \end{pmatrix} \begin{matrix} \\ \\ \\ i \\ \dots \\ j \\ \\ \\ \\ \end{matrix}$$

$$i \qquad \dots \qquad j$$

i.e. each matrix is specified by two indexes *i* and *j* (rows and columns) and a ***rotation angle*** ϕ.

Matrix Elements of the Transformation:

The matrix elements of the transformation $U^T AU$ at time *t* read:

$$a_{ii}^{(t)} = a_{ii}^{(t-1)} \cos^2\varphi + 2a_{ij}^{(t-1)} \cos\varphi \sin\varphi + a_{jj}^{(t-1)} \sin^2\varphi$$

$$a_{jj}^{(t)} = a_{jj}^{(t-1)} \cos^2\varphi - 2a_{ij}^{(t-1)} \cos\varphi \sin\varphi + a_{ii}^{(t-1)} \sin^2\varphi$$

$$a_{ij}^{(t)} = a_{ij}^{(t-1)} (\cos^2\varphi - \sin^2\varphi) + (a_{jj}^{(t-1)} - a_{ii}^{(t-1)}) \cos\varphi \sin\varphi$$

And the series is convergent if the size of the off-diagonal matrix elements decreases with t, *i.e.*

$$S(t) < S(t-1)$$

with

$$S(t) = 2\sum_{m=1}^{n-1} \sum_{m'=m+1}^{n} \left(a_{mm'}^{(t)} \right)^2$$

Cholesky Decomposition:

The Cholesky Decomposition of a symmetric real matrix is the decomposition of the original matrix A into the product of a lower triangular matrix with its transpose. It is similar to the LU decomposition (for general Hermitian matrices), but twice as efficient.

$$A = LL^T$$

$$l_{jj} = \sqrt{a_{jj} - \sum_{t=1}^{j-1} l_{jt}^2}$$

$$l_{ij} = \frac{a_{ij} - \sum_{t=1}^{j-1} l_{it} l_{jt}}{l_{jj}}, \quad i = j+1, \ldots, n$$

The Cholesky Decomposition greatly simplifies the solution of generalised eigenvalue problems:

$$(A - \lambda S)\mathbf{x} = 0$$

Where S is a symmetric matrix (structure matrix).

We have in fact:

$$(A-\lambda S)\mathbf{x} = (A-\lambda LL^T)\mathbf{x} = 0$$

$$(A\left(L^T\right)^{-1} - \lambda L)(L^T\mathbf{x}) = 0$$

$$(L^{-1}A(L^T)^{-1} - \lambda I)(L^T\mathbf{x}) = 0$$

$$(C-\lambda I)\mathbf{y} = 0$$

$$\mathbf{y} = L^T\mathbf{x}$$

Once we have the Cholesky decomposition of S, we construct an auxiliary Cholesky matrix C, solve the regular eigenvalue problem for it, and apply the transpose Cholesky matrix to the solution (**y**) to obtain the solution of the original problem (**x**).

Exercise: Cholesky decomposition of a 3x3 matrix:

CHOLESKY DECOMPOSITION

(4)

$$A = \begin{pmatrix} 4 & 12 & -16 \\ 12 & 37 & -43 \\ -16 & -43 & 98 \end{pmatrix}$$

$$l_{11} = \sqrt{a_{11}} = 2$$

$$l_{i1} = \frac{a_{i1}}{l_{11}} \Rightarrow l_{21} = \frac{12}{2} = 6 \quad ; \quad l_{31} = \frac{-16}{2} = -8$$

$$l_{22} = \sqrt{a_{22} - l_{21}^2} = \sqrt{37 - 36} = 1$$

$$\underset{ij}{l_{32}} = \frac{\underset{ij}{a_{32}} - \sum_{t=1}^{j-1} l_{it} l_{jt}}{\underset{jj}{l_{22}}} = \frac{a_{32} - l_{31} l_{21}}{l_{22} = 1} = \frac{-43 + 6 \cdot 8}{1} = 5$$

$$l_{33} = \sqrt{a_{33} - l_{31}^2 - l_{32}^2} = \sqrt{98 - 64 - 25} = 3$$

$$L = \begin{pmatrix} 2 & \emptyset & \emptyset \\ 6 & 1 & \emptyset \\ -8 & 5 & 3 \end{pmatrix}$$

A few examples:

Matrix:

6.000	4.000	4.000	1.000
4.000	6.000	1.000	4.000
4.000	1.000	6.000	4.000
1.000	4.000	4.000	6.000

exact solution:

Eigenvalue:	Eigenvector:			
15	0.5	0.5	0.5	0.5
-1	0.5	-0.5	-0.5	0.5
5	-0.5	0.5	-0.5	0.5
5	-0.5	-0.5	0.5	0.5

Jacobi Solution:

Eigenvalue:	Eigenvector:			
15.000000	0.500000	0.500000	0.500000	0.500000
-1.000000	-0.500000	0.500000	0.500000	-0.500000
5.000000	0.226248	-0.669934	0.669934	-0.226248
5.000000	-0.669934	-0.226248	0.226248	0.669934

***Jacobi**, eigenvectors are not unique!*

Cholesky decomposition:

```
Numerical Solution of the extended eigenvalue problem:

       [A - lambda . B] x  =  0

Matrix A (symmetrical)
 5.0000    4.0000    1.0000    1.0000
 4.0000    5.0000    1.0000    1.0000
 1.0000    1.0000    4.0000    2.0000
 1.0000    1.0000    2.0000    4.0000

Matrix B (symmetrical and definite positive):
 5.0000    7.0000    6.0000    5.0000
 7.0000   10.0000    8.0000    7.0000
 6.0000    8.0000   10.0000    9.0000
 5.0000    7.0000    9.0000   10.0000

The program CHOLESKY extracts from the original matrices
A and B through the Cholesky-decomposition of B:

              B = L . L^T

the matrix

C = L^(-1) . A . (L^(-1))^T
```

```
The lower triangular matrix L is:

   2.2361     0.0000     0.0000     0.0000
   3.1305     0.4472     0.0000     0.0000
   2.6833    -0.8944     1.4142     0.0000
   2.2361    -0.0000     2.1213     0.7071

This marix C is symmetrical and has the same
eigenvalues as the original extended eigenvalue problem:

   1.0000    -3.0000    -3.4785     7.9057
  -3.0000    18.0000    16.4438   -41.1096
  -3.4785    16.4438    18.0000   -43.0000
   7.9057   -41.1096   -43.0000   110.0000

At this point, using the Jacobi prorgram it is possible to determine
the 4 eigenvalues of the matrix C.

These are: 0.2623  2.3078  1.1530  143.2769
```

Other Methods (general):

For general (non-symmetric) matrices the eigenvalues and eigenvectors are found with a two-step procedure:

1) Reduction into an Upper Hessenberg form (Hausholder method)

2) Diagonalization of the Upper Hessenberg matrix through QR or QL methods.

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

Upper Hessenberg form (upper): all elements below the first sub-diagonal are zero.

Hyman's Method:

Hyman's method permits to calculate the real eigenvalues of a matrix in Upper Hessenberg form without explicit ***diagonalization***. In fact, Hyman showed that the characteristic polynomial of an upper Hessenberg matrix is given by:

$$P_n(\lambda) = (-1)^{n+1} \cdot a_{21} a_{32} \ldots a_{nn-1} \cdot H(\lambda)$$

with

$$(A - \lambda I) \cdot \begin{pmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ x_{n-1} \\ 1 \end{pmatrix} = H(\lambda) \begin{pmatrix} 1 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{pmatrix}$$

$$x_i = \frac{1}{a_{i+1,i}} \left[\lambda x_{i+1} - \sum_{l=0}^{n-i-1} a_{i+1,n-l} x_{n-l} \right], \qquad i = n-1, n-2, \ldots, 2, 1.$$

Definition:

The **characteristic polynomial** of a matrix A is obtained solving the equation:

$$\det(A_0 - \lambda I) = 0 \equiv P_n(\lambda) = \lambda^n + \sum_i^n p_i \lambda^{n-i}$$

The order *n* of the polynomial is the same as the order *n* of the matrix. The *n* roots are either real, or form complex-conjugate pairs. Some of these roots can be ***degenerate***.

$$\det(A_0 - \lambda I) = 0 \equiv P_n(\lambda) = \lambda^n + \sum_i^n p_i \lambda^{n-i}$$

$$P_n(\lambda) = 0 \text{ for } \lambda : \lambda_1, \lambda_2, \ldots, \lambda_k = \lambda_{k+1} = \ldots = \lambda_{k+q} = \ldots = \lambda_n$$

The λ_i*'s* are the eigenvalues of the matrix A. The vectors $\mathbf{x}_i$ associated to them are the eigenvectors. ***Solving the eigenvalue problem*** means determining the λ_i*'s* and $\mathbf{x}_i$.

Derivation of the Hyman's formula:

(H).

HYMAN'S METHOD [Proof]

We have an upper Hessenberger matrix of this form:

$$A = \begin{pmatrix} a_{11} & \cdots & a_{n1} \\ & & \vdots \\ a_{n1} & \cdots & a_{nn} \end{pmatrix} \xrightarrow{\text{UHF}} \begin{pmatrix} a_{11} & \cdots & & & \\ \vdots & & & & \\ \emptyset & \cdots \emptyset & a_{n-1\,n-2} & a_{n-1\,n-1} & a_{n-1\,n} \\ \emptyset & & \cdots \emptyset & a_{n\,n-1} & a_{nn} \end{pmatrix}$$

Hyman's EQUATIONS read:

$$(\hat{A} - \lambda \hat{I}) \cdot \begin{pmatrix} x_1 \\ \vdots \\ x_{n-1} \\ 1 \end{pmatrix} = H(\lambda) \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

- To derive the equations for the x_i coefficients we write the equations row-by-row starting from the bottom $(i=n)$; we obtain:

$i=n$

$$a_{n\,n-1}\, x_{n-1} + (a_{nn} - \lambda)\, x_n = \emptyset \qquad x_n = 1$$

$$x_{n-1} = \frac{1}{a_{n\,n-1}} \left[\lambda x_n - a_{nn} \right]$$

$i = n-1$ (H)[2]

$$a_{n-1,n-2}\, x_{n-2} + (a_{n-1\,n-1} - \lambda)\, x_{n-1} + a_{n-1\,n}\, x_n = \phi$$

$$x_{n-2} = \frac{1}{a_{n-1\,n-2}} \left[\lambda x_{n-1} - a_{n-1\,n-1}\, x_{n-1} - a_{n-1\,n}\, x_n \right]$$

As a general rule we can write for the i^{th} row:

$$x_i = \frac{1}{a_{i+1,i}} \left[\lambda x_{i+1} - \sum_{\ell=0}^{m-i-1} a_{i+1,n-\ell}\, x_{n-\ell} \right]$$

For the function $H(\lambda)$ we obtain (first equation, $i=1$):

$$H(\lambda) = \left(\sum_{i=1}^{m} a_{1i}\, x_i - \lambda x_1 \right)$$

; this is a n^{th} degree polynomial, with n zeroes.

The zeroes can be found, for example, with the bissection method.

Simple example: Hyman's formula for a 2x2 matrix.

$a_{11} = 1 \qquad a_{12} = 2 \qquad a_{21} = 1 \qquad a_{22} = 1$

$x_2 = 1$

$$x_1 = \frac{1}{a_{21}}\left[\lambda x_2 - a_{22} x_2\right] = \frac{1}{1}\left[\lambda - 1\right] = (\lambda - 1)$$

$x_2 = 1$

$x_1 = (\lambda - 1)$

$$H(\lambda) = a_{11} x_1 + a_{12} x_2 - \lambda x_1 = x_1 + 2 x_2 - \lambda x_1 = (\lambda - 1) + 2 - \lambda(\lambda - 1) =$$

$$= (\lambda - 1) + 2 - \lambda^2 + \lambda = \left\{-\lambda^2 + 2\lambda + 1\right\} \iff \lambda^2 - 2\lambda - 1$$

$$\boxed{\lambda_{\pm} = 1 \pm \sqrt{1 + 1} = 1 \pm \sqrt{2}}$$

c.v.d.

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