Numerical Methods in Physics

Numerische Methoden in der Physik, 515.421.

Instructor: Ass. Prof. Dr. Lilia Boeri
Room: PH 03 090
Tel: +43-316-873 8191
Email Address: l.boeri@tugraz.at

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 (exam):

Exams for the lecture in numerical methods in Physics will take place in my office PH3.108, starting 20th of January 2013.

For the **winter semester**, I will offer dates in the weeks:

- 20th-26th of January
- 27th – 31st of January
- 3rd-9th of February.

A list with available dates and slots **is available today at the end of the lecture and during the exercises,** and then I will paste it outside my office**.** You can register writing your name on the list, **up to 14th of January.**

There will be additional dates in May-June and October 2014.

TOPICS (this year):

- **Chapter 1: Introduction.**
- **Chapter 2: Numerical methods for the solution of linear inhomogeneous systems.**
- Chapter 3: Interpolation of point sets.
- **Chapter 4: Least-Squares Approximation.**
- **Chapter 5: Numerical solution of transcendental equations.**
- Chapter 6: Numerical Integration.
- **Chapter 7: Eigenvalues and Eigenvectors of real matrices.**
- **Chapter 8: Numerical Methods for the solution of ordinary differential equations: initial value problems.**
- Chapter 9: Numerical Methods for the solution of ordinary differential equations: marginal value problems.

Last week(10/12/2013)

Ordinary Differential Equations: Initial Value problems (part II)

- Practical use of Runge-Kutta methods.
- Why do we need an adaptive stepsize?
- Methods for error estimate.
- Implementing a simple Runge-Kutta method with **adaptive stepsize**.

Runge-Kutta Methods:

Runge-Kutta *ansatz* for arbitrary *p* order:

$$\hat{y}_i(x_0 + h) = y_i(x_0) + h\sum_{j=1}^{p} c_j g_j$$

Using Runge-Kutta Methods in Practice:

Calculating a single Runge-Kutta step is of not much help. In practice, if we want to integrate a differential system, we want to perform *several steps one* after the other:

$$\hat{y}_i(x_0 + h) \equiv \hat{y}_{i,1} = y_i(x_0) + h \cdot \sum_{j=1}^{p} c_j g_{i,j}(x_0; y_{1,0}, \ldots, y_{n,0})$$

$$\hat{y}_i(x_0 + 2h) \equiv \hat{y}_{2,1} = \hat{y}_{i,1} + h \cdot \sum_{j=1}^{p} c_j g_{i,j}(x_0 + h; \hat{y}_{1,1}, \ldots, \hat{y}_{n,1})$$

In the first step, the initial values are known exactly, and given by the boundary conditions. For all other steps, the initial values are given by previous R-K moves, and thus known only approximately.

In Runge-Kutta methods, the choice of the stepsize is a crucial ingredient to ensure stability of the algorithm (example, satellite problem).

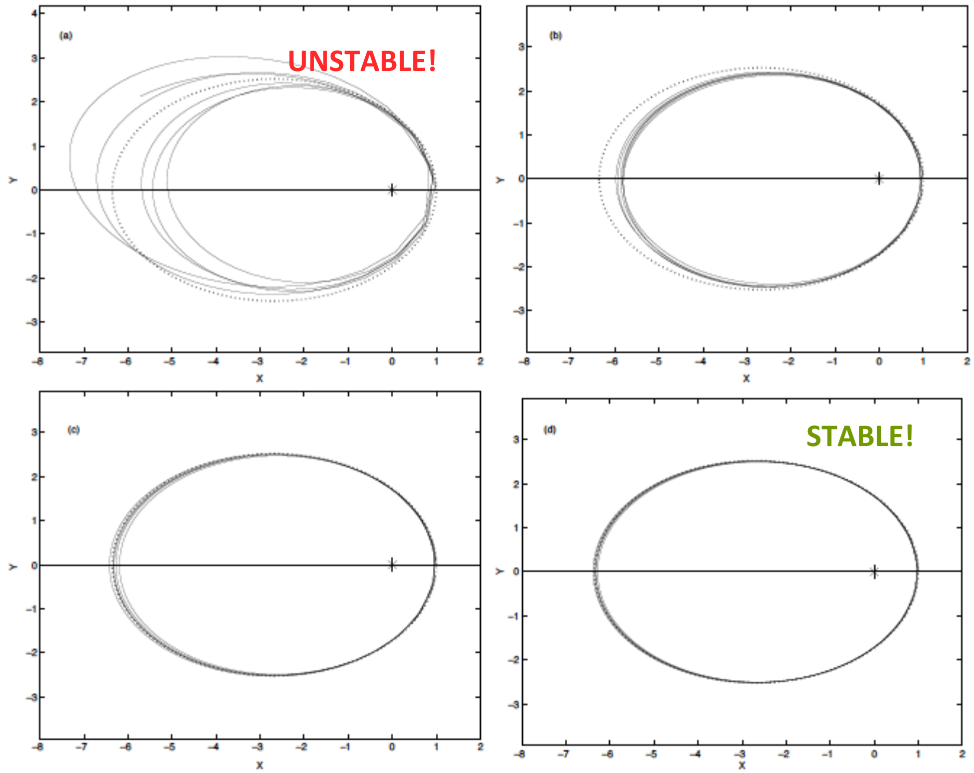


Figure 5.5: Stability test for RUNGETEST. The constant stepsizes have been chosen as follows: (a) $h = 1/50$, (b) $h = 1/60$, (c) $h = 1/70$, (d) $h = 1/80$ of the revolution period. The star indicates the centre of the earth, and the dotted line the exact analytical trajectory of the satellite.

How to estimate the error of a Runge-Kutta step

(and choose the optimal step size):

$$E_V(h) = y_i(x_0 + h) - \hat{y}_i(x_0 + h)$$

A good estimate of $E_V(h)$ is given in practice between the value of y obtained with a single R-K step of size h, and two steps of size h/2:

$$E_V(h) \approx \hat{y}(x_0 + h) - \hat{y}(x_0 + 2\frac{h}{2})$$

This can be used in practice to implement a simple algorithm for **stepsize adaptation** in Runge-Kutta methods. To implement this method in practice, one chooses h and calculates $E_V(h)$ with a standard R-K routine and:

- If $E_V(h)$ is ≤ ε, the R-K move **is accepted** with h.
- If $E_V(h)$ > ε, the R-K move **is refused**, h is reduced, and EV(h) is evaluated again.

Effect of the stepsize adaptation:

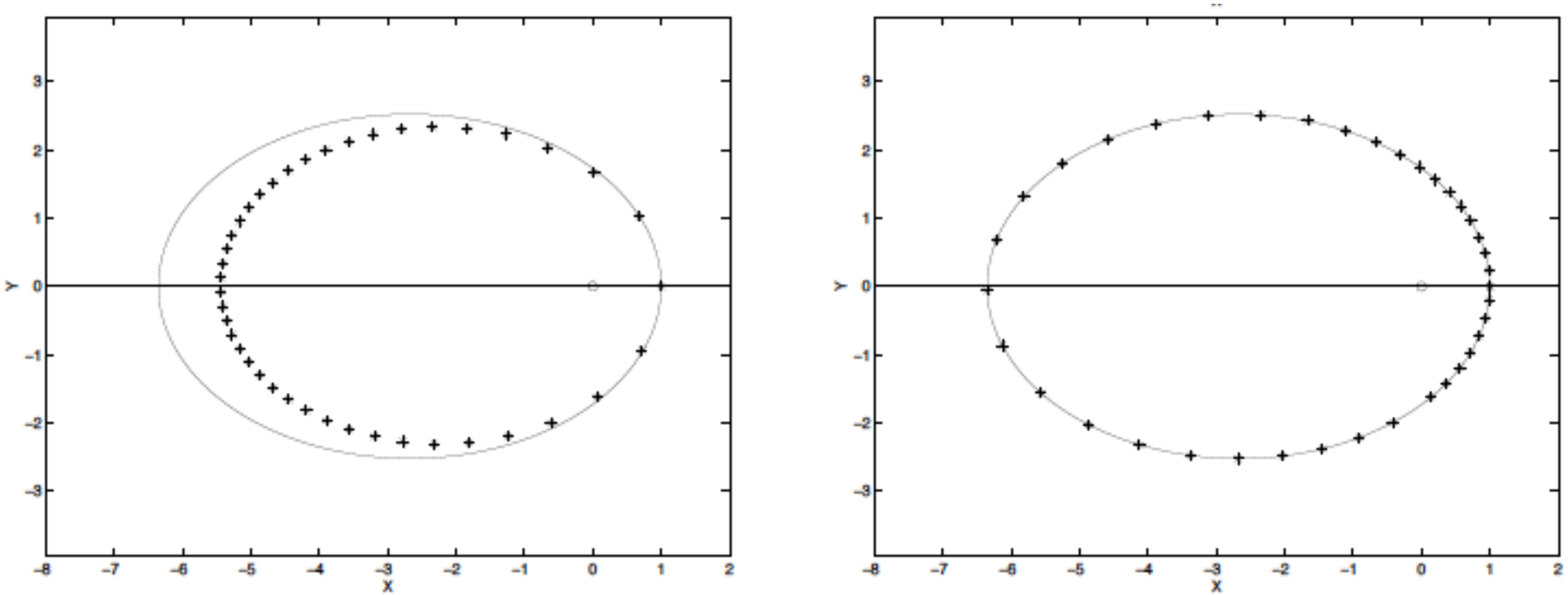


Figure 5.6: Efficiency of the stepsize adaptation in the 'satellite problem'. Comparison of the exact elliptical trajectory (full line) with the numerical values (stars). Above: Runge-Kutta *without* stepsize adaptation; Below: Runge-Kutta *with* stepsize adaptation.

This week (17/12/2013)

Eigenvalues and Eigenvectors of Real Matrices

- Generalized and regular eigenvalue problem: definition.
- Matrices with special forms: symmetric, hermitian, orthogonal, normal.
- Diagonalization of a matrix.
- Von-Mises Method: largest and smallest eigenvalue.
- Von-Mises Method: a simple example (analytical)

Eigenvalues and Eigenvectors of Real Matrices:

We will consider ***homogeneous linear problems*** for which:

$$A \cdot \mathbf{x} = \mathbf{0}$$

There are two possible sub-cases:

1) det(A)≠0 -> the system admits only the *trivial* solution **x=0**!

2) det(A)≠0 -> the system admits *also non-trivial solutions* **x**!

An important case which is often encountered in practice is that of linear systems which depend on a set of external parameters λ_i; in that case the homogeneous system reads:

$$A(\lambda_i) \cdot \mathbf{x} = \mathbf{0}, \quad A(\lambda_i) = \left[a_{ij}(\lambda)\right]$$

Depending on the values of the λ_i's both situations 1) and 2) can be realized.

We are interested in non-trivial solutions, which occur for those values of the λ_i*'s* for which A is *singular*.

$$\det(A(\lambda_i)) = 0$$

The λ_i*'s* and the corresponding $\mathbf{x}_i$ (solutions) are called the **eigenvalues** and **eigenvectors** of A – and the problem of finding them is called a ***generalized eigenvalue problem***.

Regular eigenvalue problems are a sub-class of generalized eigenvalue problems, in which the dependence of the matrix A on λ has a simple form:

$$A(\lambda) = A_0 - \lambda I, \qquad I \text{ is the identity matrix}$$

This means that:

$$(A_0 - \lambda I)\mathbf{x} = \mathbf{0}, \quad \text{i.e.} \quad \mathrm{A}_0\mathbf{x} = \lambda\mathbf{x}$$

The problem has non-trivial solutions if:

$$\det(A_0 - \lambda I) = 0$$

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***.

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

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

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 $\mathbf{x}_i$.

Special forms of matrices:

- A ***real*** matrix is called ***symmetric*** if:

$$A = A^T$$

- A ***complex*** matrix is called ***Hermitian*** if:

$$A = A^+$$

The eigenvalues of symmetric and Hermitian matrices are all real.

- A ***real*** matrix is called ***orthogonal*** if:

$$AA^T = I$$

- A ***complex*** matrix is called ***unitary*** if:

$$AA^+ = I$$

A real or complex matrix is called **normal**, if it **commutes** with its transpose or Hermitian conjugate.

$$AA^T = A^T A \qquad \text{or} \qquad AA^+ = A^+ A$$

Diagonalization:

A matrix A is diagonalizable if one can find a matrix U such that:

$$U^{-1}AU = D$$

Where D is a *diagonal matrix*, i.e. a matrix which has non-zero elements only along its diagonal. A and D are related by a similarity operation, i.e. an operation which does not change the spectrum (eigenvalues) of the matrix.

- The eigenvalues of A are the non-zero elements of D:

$$\lambda_i = d_{ii}$$

- The columns of U are the eigenvectors of the matrix A.

$$u_{ij} = x_j^i$$

A matrix is diagonalizable if its eigenvectors form a *linearly independent system*.

Proof:

$$U^{-1} A U = D$$

$$U U^{-1} \cdot A \cdot U = U D$$

$$A \cdot U = U \cdot D$$

$$U = \begin{pmatrix} u_{11} & \cdots & u_{1n} \\ u_{21} & & \vdots \\ \vdots & & \\ u_{n1} & & u_{nn} \end{pmatrix} = \begin{pmatrix} \underline{u}_1 & \underline{u}_2 & \underline{u}_n \end{pmatrix}$$

$$\underline{u}_1 = \begin{pmatrix} u_{11} \\ u_{21} \\ \vdots \\ u_{n1} \end{pmatrix} \cdots \quad \underline{u}_n = \begin{pmatrix} u_{1n} \\ \vdots \\ u_{nn} \end{pmatrix}$$

$$(U D)_{ij} = \sum_{\ell} u_{i\ell} d_{\ell j} = u_{ij} d_{jj} = \lambda_j u_{ij}$$

$$\Rightarrow (U D) = \begin{pmatrix} \lambda_1 \underline{u}_1 & \lambda_2 \underline{u}_2 & \cdots & \lambda_n \underline{u}_n \end{pmatrix}$$

$$A \cdot U = \tilde{\lambda} U$$

$$A(\underline{u}_1, \ldots, \underline{u}_n) = (\lambda_1 \underline{u}_1, \ldots, \lambda_n \underline{u}_n)$$

i.e. $\underline{u}_i$ are eigenvectors of A.

Properties of normal matrices:

Normal matrices are diagonalizable. Their eigenvectors are ***orthonormal***:

$$\mathbf{x}_i \cdot \mathbf{x}_j^* = \delta_{ij}$$

And therefore the transformation matrices U are ***orthogonal*** and ***unitary***:

$$UU^T = I \qquad \text{and} \qquad UU^+ = I$$

Von Mises's method

The method of von Mises is a very robust iterative method for the calculation of the eigenvalue of a matrix which has the largest absolute value, and the corresponding eigenvector. With a simple modification, it can also return the eigenvalue with the smallest absolute value (and the corresponding eigenvector).

Hypotheses: A is diagonalizable and one of its eigenvalues is dominant.

$$|\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_n|$$

Von-Mises Iteration: Starting from an arbitrary vector $\mathbf{v}^{(0)}$ and applying t-times the matrix A one obtains a sequence of vectors:

$$\mathbf{v}^{(t)} = (A)^t \mathbf{v}^{(0)}$$

For large *t*'s the ratio between the components of two subsequent vectors converge to the largest eigenvalue, and $\mathbf{v}^{(t)}$ converges to the corresponding eigenvector:

$$\frac{v_l^{(t+1)}}{v_l^{(t)}} = \lambda_1 \qquad \text{and} \qquad \lim_{t\to\infty} \mathbf{v}^{(t)} = \mathbf{x}_1$$

I want to prove that the method of von Mises converges to the largest eigenvalue and the corresponding eigenvector: (P) VM2

$\underline{v}^{(0)} = \sum_{i=1}^{m} \alpha_i \underline{x}_i$, $\underline{x}_i$ are the eigenvectors of A.

$$A \cdot \underline{v}^{(0)} = \underline{v}^{(1)} = \sum_{i=1}^{m} \alpha_i \lambda_i \underline{x}_i$$

$$\underline{v}^{(2)} = A \cdot \underline{v}^{(1)} = \sum_{i=1}^{m} \alpha_i \cdot \lambda_i^2 \cdot \underline{x}_i$$

...

$$\underline{v}^{(t)} = A \cdot v^{(t-1)} = \sum_{i=1}^{m} \alpha_i \cdot \lambda_i^t \cdot \underline{x}_i$$

if $|\lambda_1| >> \lambda_j$, $(\lambda_i^t)^{-1} (\lambda_j)^t \to \emptyset$

$$\Rightarrow \underline{v}^{(t)} \to \alpha_{imax} \cdot (\lambda_{imax})^t \cdot \underline{x}_{imax} \propto \underline{x}_{imax}$$

$$\underline{v}_\ell^{(t)} = \alpha_{imax} \cdot (\lambda_{imax})^t \cdot \underline{x}_{imax}^{(\ell)}$$

$$\frac{v_\ell^{(t+1)}}{v_\ell^{(t)}} \to \frac{\alpha_{imax} \cdot (\lambda_{imax})^{t+1} \cdot x_{imax}^{(\ell)}}{\alpha_{imax} \cdot (\lambda_{imax})^t \cdot x_{imax}^{(\ell)}} \to \lambda_{imax} \quad \text{c.v.d.}$$

In practice, it is not convenient to use the von-Mises iteration for a single component, which might become equal to zero, but it is convenient to average over all components which are non-zero, *i.e.*:

$$\frac{1}{n'}\sum_{\mu}\frac{\mathrm{v}_{\mu}^{(t+1)}}{\mathrm{v}_{\mu}^{(t)}}=\lambda_1 \qquad \text{with} \qquad \left|v_{\mu}^{(t)}\right|\geq\varepsilon$$

Smallest Eigenvalue:

The inverse matrix of A, A^{-1}, has the same eigenvectors. The eigenvalues are:

$$A^{-1}\cdot\mathbf{x}_i=\frac{1}{\lambda_i}\cdot\mathbf{x}_i$$

Therefore the smallest eigenvalue and eigenvector of A can be found applying the von Mises method to the inverse of A.

$$\mathbf{v}^{(t)}=(A^{-1})^t\,\mathbf{v}^{(0)} \qquad \text{and} \qquad \lim_{t\to\infty}\frac{v_l^{(t)}}{v_l^{(t+1)}}=\lambda_{\min}$$

A simple example:

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

Useful formulas:

For a 2x2 matrix:

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \qquad A^{-1} = \frac{1}{\det(A)} \begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{pmatrix}$$

$$\det(A) = a_{11}a_{22} - a_{12}a_{21}$$

Von-Mises iteration:

$$\mathbf{v}^{(t)} = (A)^t \, \mathbf{v}^{(0)} \qquad \frac{v_l^{(t+1)}}{v_l^{(t)}} = \lambda_1 \qquad \text{and} \qquad \lim_{t \to \infty} \mathbf{v}^{(t)} = \mathbf{x}_1$$

A simple example:

$$A = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} \qquad \mathbf{x}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and} \quad \mathbf{x}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$\lambda_1 = 3, \qquad \lambda_2 = -1$$

Useful formulas:

For a 2x2 matrix:

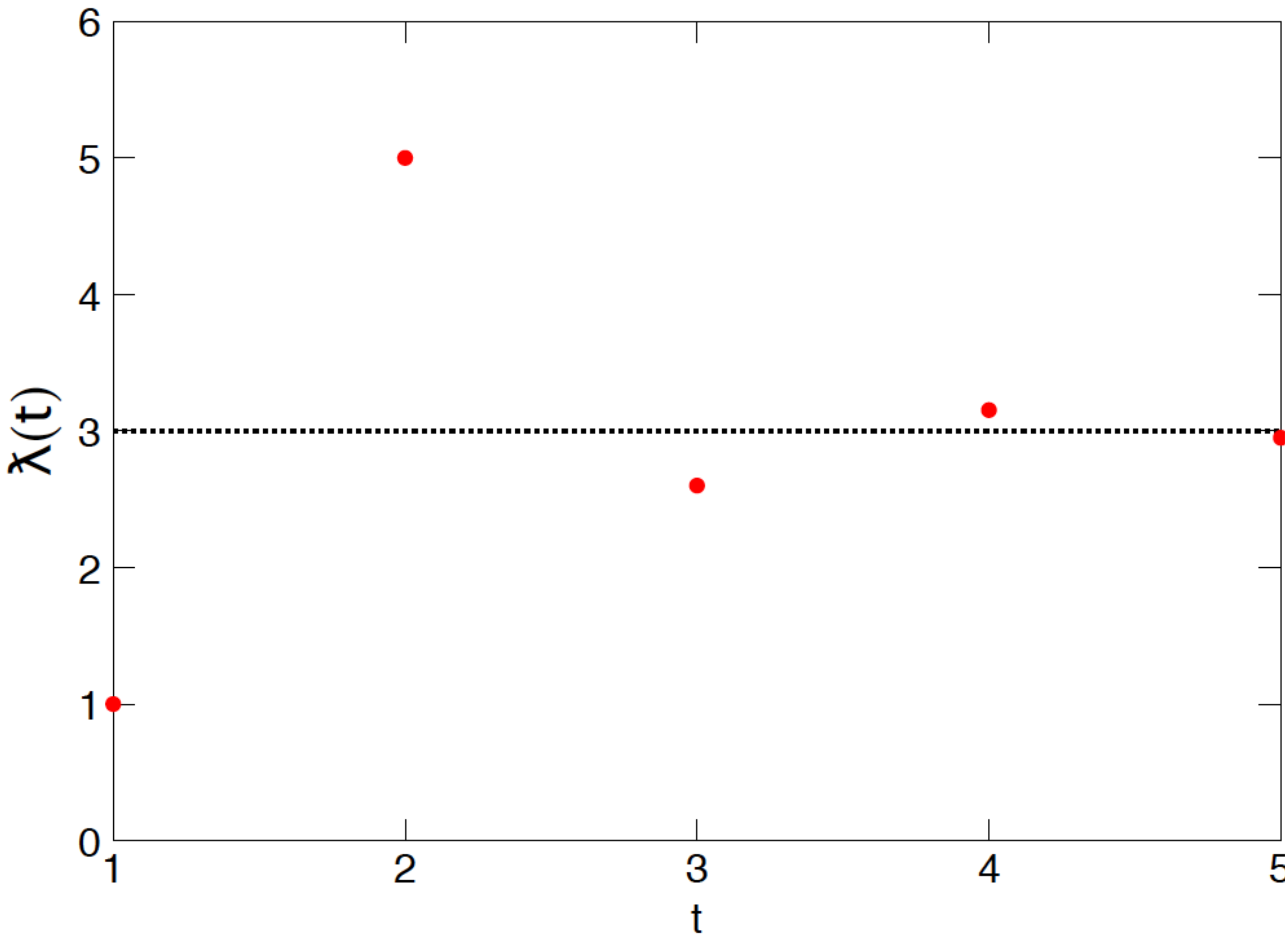
$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \qquad A^{-1} = \frac{1}{\det(A)}\begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{pmatrix}$$

$$\det(A) = a_{11}a_{22} - a_{12}a_{21}$$

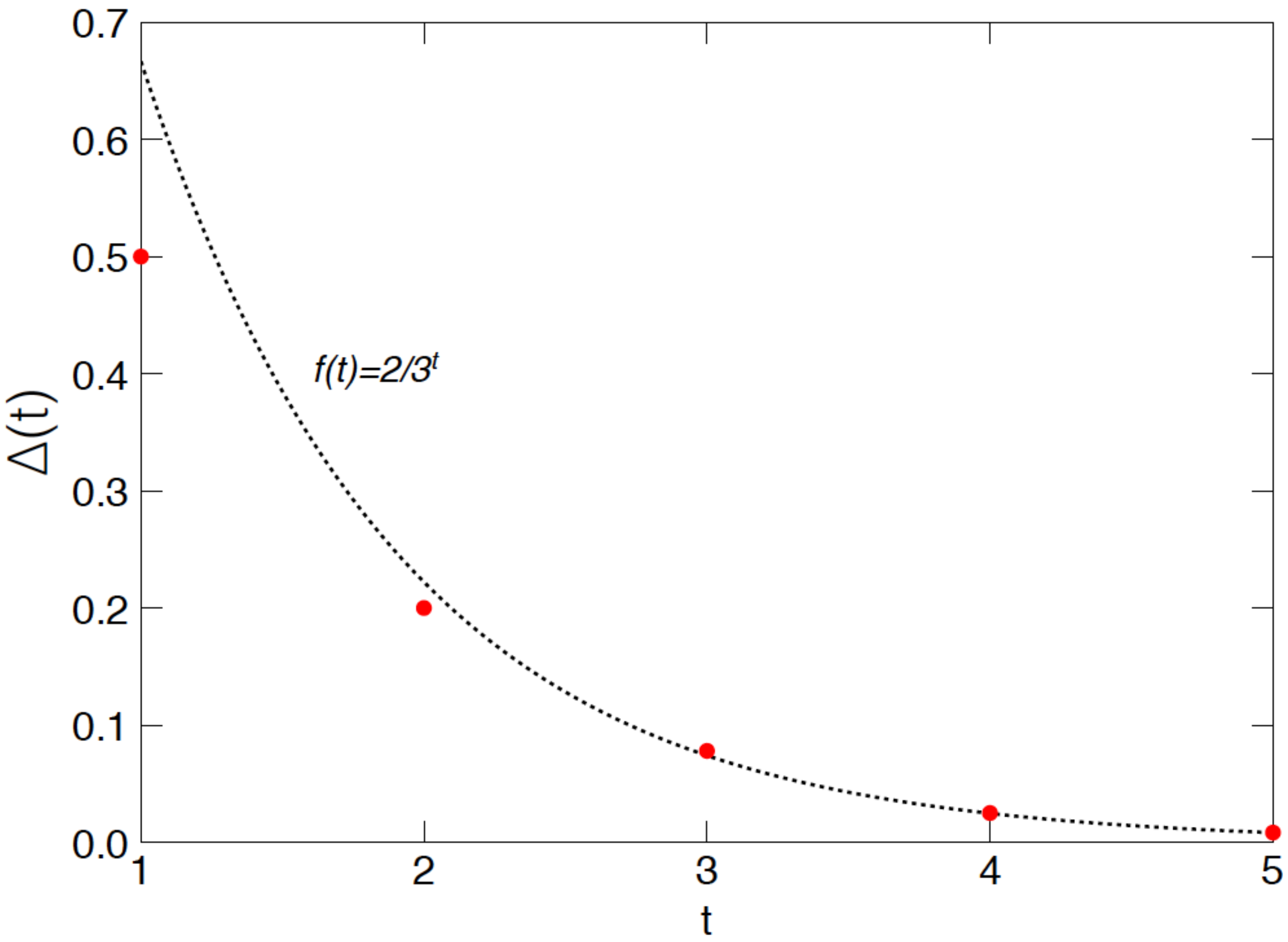
Von-Mises iteration:

$$\mathbf{v}^{(t)} = (A)^t\,\mathbf{v}^{(0)} \qquad \frac{v_l^{(t+1)}}{v_l^{(t)}} = \lambda_1 \qquad \text{and} \qquad \lim_{t\to\infty}\mathbf{v}^{(t)} = \mathbf{x}_1$$

Von-Mises iteration: Eigenvalue



Von-Mises iteration: Error on the eigenvector



① vh

$A = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}$ $\det A = 1 - 4 = -3$

<u>Eigenvalues:</u>

$(1-\lambda)^2 - 4 = \lambda^2 - 2\lambda + 1 - 4 = \lambda^2 - 2\lambda - 3 \stackrel{!}{=} 0$

$\lambda_{1,2} = 1 \pm \sqrt{1+3} = 1 \pm 2 \begin{cases} 3 = \lambda_1 \\ -1 = \lambda_2 \end{cases}$

Eigenvectors:

$\boxed{\lambda_1:}$ $\begin{pmatrix} -2 & 2 \\ 2 & -2 \end{pmatrix} \underline{x} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ $\underline{x} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \underline{x}(3)$

$\boxed{\lambda_2:}$ $\begin{pmatrix} 2 & 2 \\ 2 & 2 \end{pmatrix} \underline{x} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ $\underline{x} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = x(-1)$

Von Mises iteration should return $\lambda_1 = 3$ and $\underline{x}_1 = x(3)$ ②

$\underline{v}^{(0)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$(A)^t \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \underline{v}^{(t)}$$

$$\underline{v}^{(1)} = \begin{pmatrix} 1 \\ 2 \end{pmatrix} \qquad \underline{v}^{(2)} = \begin{pmatrix} 5 \\ 4 \end{pmatrix} \qquad \underline{v}^{(3)} = \begin{pmatrix} 13 \\ 14 \end{pmatrix} \qquad \underline{v}^{(4)} = \begin{pmatrix} 41 \\ 40 \end{pmatrix}$$

$$v^{(5)} = \begin{pmatrix} 121 \\ 122 \end{pmatrix} \quad \cdots \quad \to \quad \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$\Delta = \dfrac{|\Delta \underline{v}^{(t)}|}{|\underline{v}^{(t)}|}$ = Approximate estimate of the accuracy of the v-M method after t steps:

$\Delta^{(1)} = \frac{1}{2} \simeq 50\%$. $\Delta^{(2)} = \frac{1}{5} \simeq 20\%$; $\Delta^{(3)} = \frac{1}{13} \simeq 8\%$; $\Delta^{(4)} = \frac{1}{40} \simeq 2.5\%$

$\Delta^{(5)} \propto \frac{1}{120} \sim 0.83\%$

$$\boxed{\Delta^{(t)} \propto \frac{\alpha}{3^t} \simeq \frac{2}{3^t}}$$

$\lambda^{(1)} = 1$; $\lambda^{(2)} = 5$; $\lambda^{(3)} = \frac{13}{5} \simeq 2.6$; $\lambda^{(4)} = \frac{41}{13} \simeq 3.153\ldots$; $\lambda^{(5)} = \frac{121}{41} = 2.95$

Inverse of A:

$$\frac{1}{\det A} \cdot \begin{pmatrix} 1 & -2 \\ -2 & 1 \end{pmatrix} = -\frac{1}{3} \begin{pmatrix} 1 & -2 \\ -2 & 1 \end{pmatrix}$$

③

Eigenvalues:

$$\left(-\frac{1}{3} - \lambda\right)^2 - \frac{4}{9} = \frac{1}{9} + \frac{2}{3}\lambda + \lambda^2 - \frac{4}{9} = \emptyset$$

$$\lambda^2 + \frac{2}{3}\lambda - \frac{1}{3} = \emptyset$$

$$\lambda = -\frac{1}{3} \pm \frac{1}{3}\sqrt{1+3} = -\frac{1}{3} \pm \frac{2}{3} \quad \begin{cases} \frac{1}{3} & \lambda_1 \\ -1 & \lambda_2 \end{cases}$$

Eigenvectors:

$$\underline{x}(-1) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\underline{x}\left(\frac{1}{3}\right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

With the v-M iteration I can find the eigenvalue λ_2, since $|\lambda_2| > |\lambda_1|$. (9) VM

$\lambda_2 = -1$

$$(A^{-1})^t \underline{v}_0$$

$$\left(-\frac{1}{3}\right)^t \cdot \begin{pmatrix} 1 & -2 \\ -2 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\underline{v}^{(t)} \to \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\underline{v}^{(1)} = -\frac{1}{3} \begin{pmatrix} 1 \\ -2 \end{pmatrix}$$

$$\underline{v}^{(2)} = \frac{1}{9} \begin{pmatrix} 5 \\ -4 \end{pmatrix}$$

$$\underline{v}^{(3)} = -\frac{1}{27} \begin{pmatrix} 13 \\ -14 \end{pmatrix}$$

$$\underline{v}^{(4)} = \frac{1}{81} \begin{pmatrix} 41 \\ -40 \end{pmatrix}$$

$$\underline{v}^{(5)} = -\frac{1}{243} \begin{pmatrix} 121 \\ -122 \end{pmatrix} \quad \ldots$$

$\lambda^{(t)} =$

$$\lambda^{(1)} = -\frac{1}{3}$$

$$\lambda^{(2)} = -\frac{1}{3} \cdot 5 = -\frac{5}{3}$$

$$\lambda^{(3)} = -\frac{9}{27} \cdot \frac{13}{5} = -\frac{13}{5} \cdot \frac{1}{3}$$

$$\lambda^{(4)} = -\frac{1}{3} \quad \frac{41}{13} \quad \ldots$$

$$\lambda^{(5)} = -\frac{1}{3} \quad \frac{121}{41} \quad \ldots$$

$$\lambda^{(t)} \to (-1)$$

This week (17/12/2013)

Eigenvalues and Eigenvectors of Real Matrices

- Generalized and regular eigenvalue problem: definition.
- Matrices with special forms: symmetric, hermitian, orthogonal, normal.
- Diagonalization of a matrix.
- Von-Mises Method: largest and smallest eigenvalue.
- Von-Mises Method: a simple example (analytical)