Introduction to GNU Octave

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1 Basics

1.1 What is Octave?

Octave is an interactive programming language specifically suited for vectorizable numerical calculations. It provides a high level interface to many standard libraries of numerical mathematics, e.g. LAPACK or BLAS.

The syntax of Octave resembles that of Matlab. An Octave program usually runs unmodified on Matlab. Matlab, being commercial software, has a larger function set, and so the reverse does not always work, especially when the program makes use of specialized add-on toolboxes for Matlab.

1.2 Help!

- `help` lists the names of all built-in functions and internal variables.
- `help name` further explains the variable or function “name”.

Example:

```
octave:1> help eig
```
1.3 Input conventions

- All commands can be typed in at the prompt or read from a script.
- Scripts are plain text files with file suffix `.m`. They are imported by calling the file name without the suffix and behave as if their content was typed in line by line.
- `;` separates several commands within a line. A command terminated by `;` does not display its result on-screen.
- `,` separates two commands without suppressing on-screen output.
- `...` at the end of the line denotes that an expression continues into the next line.
- Comments are preceded by `%`.
- Octave is case sensitive.

1.4 Variables and standard operations

- `varname = expression` assigns the result of `expression` to `varname`.
- Octave has all the usual mathematical functions `+`, `-`, `*`, `/`, `^`, `sin`, `cos`, `exp`, `acos`, `abs`, etc.
- The operators of elementary logic are:
  - `<` smaller
  - `<=` smaller or equal
  - `&` and
  - `>` greater
  - `>=` greater or equal
  - `|` or
  - `==` equal
  - `~=` not equal
  - `~` not

When debugging user-defined objects, the following commands are useful:

- `whos` shows all user-defined variables and functions (see Section 3.1).
- `clear name` clears `name` from memory; if no name is given, all variables and functions will be cleared.
- `type name` displays information about the variable or function `name` on the screen.

Examples:

```
octave:1> x12 = 1/8, long_name = 'A String'
x12 = 0.12500
long_name = A String
octave:2> sqrt(-1)-i
ans = 0
octave:3> x = sqrt(2); sin(x)/x
ans = 0.69846
```

And here is a script `doless`, saved in a file named `doless.m`: 
one = 1;
two = 2;
three = one + two;

Calling the script:

octave:1> doless
octave:2> whos
*** local user variables:
prot type rows cols name
==== ==== ==== ==== ====
wd real scalar 1 1 three
wd real scalar 1 1 one
wd real scalar 1 1 two

2 Vector and matrix operations

Matrices and vectors are the most important building blocks for programming in Octave.

2.1 Vectors

- Row vector: $v = (1, 2, 3)$:
  \[ v = [1 \, 2 \, 3] \]
- Column vector: $v = (1, 2, 3)^T$:
  \[ v = [1; \, 2; \, 3] \]
- Automatic generation of vectors with constant increment:
  \[ \text{Start}[:\text{Increment}]:\text{End} \]

Examples:

\begin{verbatim}
octave:1> x = 3:6
x =
3 4 5 6
octave:2> y = 0:.15:.7
y =
0.00000 0.15000 0.30000 0.45000 0.60000
octave:3> z = pi:-pi/4:0
z =
3.14159 2.35619 1.57080 0.78540 0.00000
\end{verbatim}

2.2 Matrices

A matrix $A = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$ is generated as follows.

\begin{verbatim}
octave:1> A = [1 2; 3 4]
A =
1 2
3 4
\end{verbatim}
Matrices can be assembled from submatrices:

\[
\text{octave:2}\ b = [5; 6];
\text{octave:3}\ M = [A \ b]
\]

\[
M = \\
1 & 2 & 5 \\
3 & 4 & 6 
\]

There are functions to create frequently used \(m \times n\) matrices. If \(m = n\), only one argument is necessary.

- `eye(m,n)` produces a matrix with ones on the main diagonal and zeros elsewhere. When \(m = n\), the identity matrix is generated.
- `zeros(m,n)` generates the zero matrix of dimension \(m \times n\).
- `ones(m,n)` generates an \(m \times n\) matrix where all entries are 1.
- `rand(m,n)` generates a random matrix whose entries are uniformly distributed in the interval \((0, 1)\).

### 2.3 Basic matrix arithmetic

- `+`, `−`, and `∗` denote matrix addition, subtraction, and multiplication.
- `A'` transposes and conjugates `A`.
- `A.'` transposes `A`.

**Examples:**

```octave
octave:1> A = [1 2; 3 4]; B = 2*ones(2,2);
octave:2> A+B, A-B, A*B
ans =
  3   4  
  5   6  
ans =
-1   0  
  1   2  
ans =
  6   6  
 14  14  
```

### 2.4 Element-wise operations

While `∗` refers to the usual matrix multiplication, `.∗` denotes element-wise multiplication. Similarly, `/` and `.^` denote the element-wise division and power operators.

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Examples:

octave:1> A = [1 2; 3 4]; A.^2 % Element-wise power
ans =
     1     4
     9    16

octave:2> A^2 % Proper matrix power: A^2 = A*A
ans =
     7    10
    15    22

2.5 Indexing and slicing

- \( v(k) \) is the \( k \)-th element of the row or column vector \( v \).
- \( A(k,l) \) is the matrix element \( a_{kl} \).
- \( v(m:n) \) is the “slice” of the vector \( v \) from its \( m \)-th to its \( n \)-th entry.
- \( A(k,:) \) is the \( k \)-th row of matrix \( A \).
- \( A(:,l) \) is the \( l \)-th column of matrix \( A \).

Querying dimensions:

- \( \text{length}(v) \) returns the number of elements of the vector \( v \).
- \( [\text{Rows},\text{Columns}] = \text{size}(A) \) returns the number of rows and columns of the matrix \( A \).

Reshaping:

- \( \text{reshape}(A,m,n) \) transforms \( A \) into an \( m \times n \)-matrix.
- \( \text{diag}(A) \) creates a column vector containing the diagonal elements \( a_{jj} \) of the matrix \( A \).
- \( \text{diag}(v) \) generates a matrix with the elements from the vector \( v \) on the diagonal.
- \( \text{diag}(v,k) \) generates a matrix with the elements from the vector \( v \) on the \( k \)-th diagonal.
- \( A(k,:) = rv \) assigns to the \( k \)-th row of \( A \) the row vector \( rv \).
- \( A(k,:) = [] \) deletes the \( k \)-th row of \( A \).
- \( A(:,j) = cv \) assigns to the \( j \)-th column of \( A \) the column vector \( cv \).
- \( A(:,j) = [] \) deletes the \( j \)-th column of \( A \).
Examples:

```octave
octave:1> A = [1 2 3; 4 5 6]; v = [7; 8];
octave:2> A(2,3) = v(2)
    A =
        1  2  3
        4  5  8
```

```octave
octave:3> A(:,2) = v
    A =
        1  7  3
        4  8  8
```

```octave
octave:4> A(1,1:2) = v'
    A =
        7  8  3
        4  8  8
```

### 2.6 Solving linear systems of equations

- `A\b` solves the equation $Ax = b$.

### 2.7 Inverses, decompositions, eigenvalues

- `B = inv(A)` computes the inverse of $A$.
- `[L,U,P] = lu(A)` computes the LU-decomposition $LU = PA$.
- `[Q,R] = qr(A)` computes the QR-decomposition $QR = A$.
- `R = chol(A)` computes the Cholesky decomposition of $A$.
- `S = svd(A)` computes the singular values of $A$.
- `H = hess(A)` brings $A$ into Hessenberg form.
- `E = eig(A)` computes the eigenvalues of $A$.
- `[V,D] = eig(A)` computes a diagonal matrix $D$, containing the eigenvalues of $A$, and a matrix $V$ containing the corresponding eigenvectors such that $AV =VD$.
- `norm(X,p)` calculates the $p$-norm of vector $X$. If $X$ is a matrix, $p$ can only take the values 1, 2 or inf. The default is $p = 2$.
- `cond(A)` computes the condition number of $A$ with respect to the 2-norm.

A lot of these commands support further options. They can be listed by typing `help funcname`. 

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2.8 Testing for zero elements
• \([i,j,v] = \text{find}(A)\) finds the indices of all nonzero elements of \(A\). The resulting vectors satisfy \(A_{i(j)},j(i) = v \neq 0\).
• \(\text{any}(v)\) returns 1 if the vector \(v\) contains nonzero elements.
• \(\text{any}(A)\) applies \(\text{any}\) to each of the columns of the matrix \(A\).

3 Control structures
3.1 Functions
Traditionally, functions are also stored in plain text files with suffix \(.m\). In contrast to scripts, functions can be called with arguments, and all variables used within the function are \(local\)—they do not influence variables defined previously.

Example: A function \(f\), saved in the file named \(f.m\).

\[
\begin{align*}
\text{function } y &= f(x) \\
y &= \cos(x/2)+x;
\end{align*}
\]

Remark: In Octave, several functions can be defined in a single script file. Matlab on the other hand, strictly enforces one function per \(.m\) file, where the name of the function must match the name of the file. If compatibility with Matlab is important, this restriction should also be applied to programs written in Octave.

Example with two function values: A function \(\text{dolittle}\), which is saved in the file named \(\text{dolittle.m}\).

\[
\begin{align*}
\text{function } [out1, out2] &= \text{dolittle}(x) \\
out1 &= x^2; \\
out2 &= \text{out1} \times x;
\end{align*}
\]

Calling the function:

\[
\begin{align*}
octave:1> [x1,x2]=\text{dolittle}(2) \\
x1 &= 4 \\
x2 &= 8
\end{align*}
\]

\[
\begin{align*}
octave:2> \text{whos}
\end{align*}
\]

\[
\begin{array}{llll}
<table>
<thead>
<tr>
<th>prot</th>
<th>type</th>
<th>rows</th>
<th>cols</th>
<th>name</th>
</tr>
</thead>
<tbody>
<tr>
<td>wd</td>
<td>user function</td>
<td>-</td>
<td>-</td>
<td>dolittle</td>
</tr>
</tbody>
</table>
\end{array}
\]

\[
\begin{array}{llll}
<table>
<thead>
<tr>
<th>prot</th>
<th>type</th>
<th>rows</th>
<th>cols</th>
<th>name</th>
</tr>
</thead>
<tbody>
<tr>
<td>wd</td>
<td>real scalar</td>
<td>1</td>
<td>1</td>
<td>x1</td>
</tr>
<tr>
<td>wd</td>
<td>real scalar</td>
<td>1</td>
<td>1</td>
<td>x2</td>
</tr>
</tbody>
</table>
\end{array}
\]
Obviously, the variables `out1` and `out2` were local to `dolittle`. Previously defined variables `out1` or `out2` would not have been affected by calling `dolittle`.

### 3.2 Global variables

Global `name` declares `name` as a global variable.

**Example:** A function `foo` in the file named `foo.m`:

```matlab
global N % makes N a global variable; may be set in main file

function out = foo(arg1,arg2)
global N % makes local N refer to the global N
<Computation>
end
```

If you change `N` within the function, it changes in the value of `N` everywhere.

### 3.3 Loops

The syntax of `for`- and `while`-loops is immediate from the following examples:

```matlab
for n = 1:10
    [x(n),y(n)] = dolittle(n);
end

while t<T
    t = t+h;
end
```

*For*-loop backward:

```matlab
for n = 10:-1:1
...
```

### 3.4 Branching

Conditional branching works as follows.

```matlab
if x==0
    error('x is 0!');
else
    y = 1/x;
end

switch pnorm
    case 1
        sum(abs(v))
    case inf
        max(abs(v))
    otherwise
        sqrt(v'*v)
end
```
3.5 Functions of functions

- `eval(string)` evaluates string as Octave code.
- `feval(funcname, arg1, ...)` is equivalent to calling `funcname` with arguments `arg1, ...`.

Example: Approximate an integral by the midpoint rule:

\[
\int_a^b f(x) \, dx \approx \frac{b-a}{N} \sum_{j=0}^{N-1} f \left(a + \frac{j + \frac{1}{2}}{N} (b-a)\right)
\]

We define two functions, `gauss.m` and `mpr.m`, as follows:

```octave
function y = gauss(x)
    y = exp(-x.^2/2);
end

function S = mpr(fun,a,b,N)
    h = (b-a)/N;
    S = h*sum(feval(fun,[a+h/2:h:b]));
end
```

Now the function `gauss` can be integrated by calling:

```octave
octave:1> mpr('gauss',0,5,500)
```

3.6 Efficiency considerations

Loops and function calls, especially through `feval`, have a very high computational overhead. Therefore, if possible, vectorize all operations.

Example: We are programming the midpoint rule from the previous section with a `for`-loop (file name is `mpr_long.m`):

```octave
function S = mpr_long(fun,a,b,N)
    h = (b-a)/N; S = 0;
    for k = 0:(N-1),
        S = S + feval(fun,a+h*(k+1/2));
    end
    S = h*S;
end
```

We verify that `mpr` and `mpr_long` yield the same answer, and compare the evaluation times.

```octave
octave:1> t = cputime;
> Int1=mprr('gauss',0,5,500); t1=cputime-t;
octave:2> t = cputime;
> Int2=mprr_long('gauss',0,5,500); t2=cputime-t;
octave:3> Int1-Int2, t2/t1
ans = 0
ans = 45.250
```
3.7 Input and output

- **save data** var1 [var2 ...] saves the values of variables var1 etc. into the file *data*.
- **load data** reads the file *data*, restoring the values of the previously saved variables.
- **fprintf(string[,var1,...])** resembles C syntax for formatting output, see `man fprintf` under Unix.
- **format [long|short]** enlarges or reduces the number of decimals displayed. Calling `format` without argument restores the default.
- **pause** Suspends evaluation until a key is pressed.

Example:

```
octave:1> for k = .1:.2:.5,
   > fprintf(’1/%g = %10.2e
’,k,1/k); end
1/0.1 = 1.00e+01
1/0.3 = 3.33e+00
1/0.5 = 2.00e+00
```

4 Graphics

4.1 2D graphics

- **plot(x,y[,fmt])** plots a line through the points \((x_j,y_j)\). With the string `fmt` you can select line style and color; see `help plot` for details.
- **semilogx(x,y[,fmt])** like `plot` with a logarithmic scale for the \(x\) axis.
- **semilogy(x,y[,fmt])** like `plot` with a logarithmic scale for the \(y\) axis.
- **loglog(x,y[,fmt])** like `plot` with a logarithmic scale for both axes.

Procedure for plotting a function \(y = f(x)\):

1. Generate a vector with the \(x\)-coordinates of the points to be plotted.

   \[
   x = x_\text{min}:\text{step}_{-\text{size}}:x_\text{max};
   \]

   (See also Section 2.1.)

2. Generate a vector containing the corresponding \(y\)-values by letting \(f\) act on the vector \(x\) element-wise.

   \[
   y = f(x);
   \]

   *Important:* Since \(f\) operates element-wise, you must use of the operators \(.+,-,\cdot,\cdot^\text{!}\) etc. instead of the usual \(+,-,\cdot\) (See Section 2.4.)

3. Finally you call the plot command.
plot(x,y)

4. To generate a coordinate grid, write:

    plot(x,y)
    grid

Example:

octave:1> x = -10:.1:10;
octave:2> y = sin(x).*exp(-abs(x));
octave:3> plot(x,y)
octave:4> grid

4.2 3D graphics:

- \([xx,yy] = \text{meshgrid}(x,y)\) generates the grid data for a 3D plot—two matrices \(xx\) whose rows are copies of \(x\), and \(yy\) whose columns are copies of \(y\).
- \(\text{mesh}(x,y,z)\) plots a surface in 3D.

Example:

octave:1> x = -2:0.1:2;
octave:2> [xx,yy] = meshgrid(x,x);
octave:3> z = sin(xx.^2-yy.^2);
octave:4> mesh(x,x,z);
4.3 Commands for 2D and 3D graphics

- title(string) writes string as title for the graphics.
- xlabel(string) labels the $x$-axis with string.
- ylabel(string) labels the $y$-axis with string.
- zlabel(string) labels the $z$-axis with string.
- axis(v) sets axes limits for the plot. $v$ is a vector of form $v = (\text{xmin}, \text{xmax}, \text{ymin}, \text{ymax}, \text{zmin}, \text{zmax})$.
- hold [on|off] controls whether the next graphics output should or not clear the previous graphics.
- clg clears the graphics window.

5 Exercises

5.1 Linear algebra

Take a matrix $A$ and a vector $b$ with

$$A = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \quad \text{and} \quad b = \begin{pmatrix} 36 \\ 88 \end{pmatrix}.$$

Solve the system of equations $Ax = b$. Calculate the LU and QR decompositions, and the eigenvalues and eigenvectors of $A$. Compute the Cholesky decomposition of $A^T A$, and verify that $\text{cond}(A^T A) = \text{cond}(A)^2$. 

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Solution:

\[
A = \text{reshape}(1:4,2,2).'; \ b = [36; 88];
A\b
\]
\[
[L,U,P] = \text{lu}(A)
\]
\[
[Q,R] = \text{qr}(A)
\]
\[
[V,D] = \text{eig}(A)
\]
\[
A2 = A.'*A;
R = \text{chol}(A2)
\]
\[
\text{cond}(A)^2 - \text{cond}(A2)
\]

5.2 Timing

Compute the matrix-vector product of a 100×100 random matrix with a random vector in two different ways. First, use the built-in matrix multiplication *.
Next, use for-loops. Compare the results and computing times.

Solution:

\[
A = \text{rand}(100); \ b = \text{rand}(100,1);
\]
\[
t = \text{cputime};
\]
\[
v = A*b; \ t1 = \text{cputime}-t;
\]
\[
w = \text{zeros}(100,1);
\]
\[
t = \text{cputime};
\]
\[
\text{for} \ n = 1:100,
\text{for} \ m = 1:100
\]
\[
w(n) = w(n)+A(n,m)*b(m);
\text{end}
\text{end}
\]
\[
t2 = \text{cputime}-t;
\]
\[
\text{norm}(v-w), t2/t1
\]

Running this script yields the following output.

\[
\text{ans} = 0
\]
\[
\text{ans} = 577.00
\]

5.3 Stability functions of BDF-integrators

Calculate all the roots of the polynomial

\[
\frac{147}{60} \zeta^6 - 6\zeta^5 + \frac{15}{2} \zeta^4 - \frac{20}{3} \zeta^3 + \frac{15}{4} \zeta^2 - \frac{6}{5} \zeta + \frac{1}{6}.
\]

Hint: Use the command \text{compan}.

Plot these roots as points in the complex plane and draw a unit circle for comparison. (Hint: \text{hold, real, imag}).
Solution:

\[ \text{bdf6} = \begin{bmatrix} 147/60 & -6 & 15/2 & -20/3 & 15/4 & -6/5 & 1/6 \end{bmatrix}; \]

\[ \text{R} = \text{eig} (\text{compan}(\text{bdf6})); \]

plot(\text{companion}(\text{bdf6}));
plot(\text{abs}(\text{R}));
if any(abs(\text{R})>1)
   \text{fprintf}('BDF6 is unstable\n');
else
   \text{fprintf}('BDF6 is stable\n');
end

5.4 3D plot

Plot the graph of the function

\[ f(x, y) = \exp(-x^2 - y^2). \]

Solution:

\[ x = -3:0.1:3; \]
\[ [\text{xx, yy}] = \text{meshgrid}(x, x); \]
\[ z = \exp(-\text{xx}^2 - \text{yy}^2); \]
figure, mesh(x, x, z);
title('exp(-x^2-y^2)');

5.5 Hilbert matrix

For each \( n \times n \) Hilbert matrix \( H \) where \( n = 1, \ldots, 15 \) compute the solution to the linear system \( Hx = b, b = \text{ones}(n, 1) \). Calculate the error and the condition number of the matrix and plot both in semi-logarithmic coordinates. (Hint: hilb, invhilb.)
Solution:

```matlab
err = zeros(15,1); co = zeros(15,1);
for k = 1:15
    H = hilb(k);
    b = ones(k,1);
    err(k) = norm(H\b-invhilb(k)*b);
    co(k) = cond(H);
end
semilogy(1:15,err,'r',1:15,co,'x');
```

5.6 Least square fit of a straight line

Calculate the least square fit of a straight line to the points \((x_j, y_j)\), given as two vectors \(x\) and \(y\). Plot the points and the line.

Solution:

```matlab
function coeff = least_square (x,y)
    n = length(x);
    A = [x ones(n,1)];
    coeff = A\y;
    plot(x,y,'x');
    hold on
    interv = [min(x) max(x)];
    plot(interv,coeff(1)*interv+coeff(2));
end
```

5.7 Trapezoidal rule

Write a program to integrate an arbitrary function \(f\) in one variable on an interval \([a, b]\) numerically using the trapezoidal rule with \(h = (b - a)/N\):

\[
\int_{a}^{b} f(x) \, dx \approx h \left( \frac{f(a) + f(b)}{2} + \sum_{j=1}^{N-1} f(a + jh) \right)
\]

For a function \(f\) of your choice, check, by generating a doubly logarithmic error plot, that the trapezoidal rule is of order 2.

Solution:

```matlab
function S = trapez(fun,a,b,N)
    h = (b-a)/N;
    % fy = feval(fun,[a:h:b]); better:
    fy = feval(fun,linspace(a,b,N+1));
    fy(1) = fy(1)/2;
    fy(N+1) = fy(N+1)/2;
    S = h*sum(fy);
end
```
function y = f(x)
    y = exp(x);
end

for k=1:15;
    err(k) = abs(exp(1)-1-trapez('f',0,1,2^k));
end
loglog(1./2.^[1:15],err);
hold on;
title('Trapezoidal rule, f(x) = exp(x)');
xlabel('Increment');
ylabel('Error');
loglog(1./2.^[1:15],err,'x');