Computing Fundamentals

Salvatore Filippone

salvatore.filippone@uniroma2.it

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Matrices

Recall arithmetic operators on arrays:

- Unary minus - (change sign);
- Addition/subtraction by a scalar `v+1`;
- Multiplication/division by a scalar `alpha*v, v/beta`;
- Element-by-element operators `+ - .* ./ .^`
- Comparison and logical operators `< > <= >= any find | &`

Matrices

Look again: *Matrix Operators*
Matrix-matrix: product.

C = A∗B

This is the classical multiplication of matrices as defined in linear algebra

$$C = AB \Longleftrightarrow C_{ij} = \sum_k A_{ik} B_{kj}$$

- Map a linear space into another;
- Special cases: rotations, axis scaling, etc.

Rule: number of columns of first matrix must be same as number of rows of second.
The product is *not* commutative, given `A*B`, `B*A` will be different or may not even exist at all!

Matrix transpose: $B_{ij} = A_{ji}$

```
B = A'
```

Matrix exponentiation (by an integer):

```
B = A^n
```

requires A to be square.

Properties of matrix operators:

- Addition is commutative and associative:

$$A + B = B + A, \quad A + (B + C) = (A + B) + C$$

- Multiplication is associative but *not* commutative:

$$A * B \neq B * A, \quad A * (B * C) = (A * B) * C$$

- Multiplication is distributive on both sides:

$$A * (B + C) = A * B + A * C, \quad (A + B) * C = A * C + B * C$$

- Transpose and inversion of products:

$$(A * B)^T = (B^T) * (A^T), \quad (A * B)^{-1} = (B^{-1}) * (A^{-1})$$

Matrices

Predefined matrices:

- `eye(m,n)` The identity (neutral element of multiplication);
- `zeros(m,n)` (neutral element of addition);
- `ones(m,n)`
- `rand(m,n)` (uniform distribution)
- `magic(n)` $N \times N$ magic square

Division: what is division, anyway?

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Division is the inverse of the multiplication operation

So, if we have

$$AB = C,$$

we can think of division as the operator that combines A and C to give back B. When A is square and non singular, this is *formally* equivalent to the multiplication by the inverse

$$B = A^{-1}C,$$

and this is in turn equivalent to the Octave/Matlab statement:

```
B = A\C
```

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- The inverse is well-defined for (non-singular) square matrices;

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- Inverting a multiplication is equivalent to solving a linear system.

The last point is key to understanding the behaviour of Octave/Matlab matrix division operator, so we state it again:

- `X=A\B` is the same as computing the solution to $AX = B$; and therefore
- `X=B/A` is the same as computing the solution to $XA = B$; but we also have $B^T = (XA)^T = A^T X^T$, that is `X'= A'\B'`; therefore `B/A = (A'\B')'`

Matrices

Let us keep going: from a formal point of view the left division

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In practice you should *never* compute the inverse explicitly:

- It is slower, much slower;
- It is less accurate.

The second point would require a long digression into numerical analysis. For the first point, we need to understand how `A\B` is actually computed.

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The second point would require a long digression into numerical analysis. For the first point, we need to understand how `A\B` is actually computed. First step: if `A\B` is equivalent to solving

$$AX = B$$

are there any matrices A that are easy to handle?

If a coefficient matrix is lower triangular it is easy to solve $Lx = b$ by forward substitution:

Triangular linear systems

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```
n=size(L,1);
for i=1:n
   x(i) = b(i) - L(i,1:i-1)*x(1:i-1);
   x(i) = x(i) / L(i,i);
end
```

If the diagonal is unitary, the division steps can be skipped. The total number of operations executed is $\approx n^2$.
Same reasoning applies to an *upper* triangular matrix U with back substitution.

Suppose we are able to decompose

$$A = LU$$

where L is lower triangular and U is upper triangular; then we have

$$Ax = b \Rightarrow x = U^{-1}L^{-1}b$$

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```
y = L\b;
x = U\y;
```

for a cost (after the decomposition) of $\approx 2n^2$ operations. (Remember: solving a triangular system is easy).

LU Factorization

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$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} = \begin{pmatrix} l_{11} & & \\ l_{21} & l_{22} & \\ l_{31} & l_{32} & l_{33} \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ & u_{22} & u_{23} \\ & & u_{33} \end{pmatrix}$$

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Writing down the products and imposing equality:

$$\begin{pmatrix} a_{11} \\ a_{21} \\ a_{31} \end{pmatrix} = \begin{pmatrix} l_{11} \\ l_{21} \\ l_{31} \end{pmatrix} (u_{11}) \qquad \begin{pmatrix} a_{12} & a_{13} \end{pmatrix} = (l_{11}) \begin{pmatrix} u_{12} & u_{13} \end{pmatrix}$$

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n^2 equations in $n^2 + n$ unknowns; need additional constraints.

- Factor the diagonal (auxiliary constraint: $l_{ii} = 1$)

$$\text{Compute}\left(\;a_{11}\;\right) \rightarrow \left(\;l_{11}\;\right)\left(u_{11}\right)$$

The total cost is $\approx \frac{2}{3}n^3$.

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LU Factorization: the algorithm

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- Update the lower-right submatrix;

$$\begin{pmatrix} \hat{a}_{22} & \hat{a}_{23} \\ \hat{a}_{32} & \hat{a}_{33} \end{pmatrix} \leftarrow \begin{pmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{pmatrix} - \begin{pmatrix} l_{21} \\ l_{31} \end{pmatrix} \begin{pmatrix} u_{12} & u_{13} \end{pmatrix}$$

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- Apply recursively to lower-right submatrix;

The total cost is $\approx \frac{2}{3}n^3$.

LU Factorization

```
function [L, U]=lufact1(A)
  (nargin() == 1) ||  usage("[L,U] = lufact1(A)");

  m=size(A,1);   n=size(A,2);
  if ((m==0)||(n==0))
    return
  end

  mn=min(m,n);
  for j=1:mn
%     A(j,j+1:n) = (1.0)\A(j,j+1:n);
    A(j+1:m,j) = A(j+1:m,j)/(A(j,j));
    A(j+1:m,j+1:n) = A(j+1:m,j+1:n) - A(j+1:m,j)*A(j,j+1:n);
  end

  if (nargout() < 1)
    ans = A
  elseif (nargout() == 1)
    L=A;
  elseif (nargout() > 1)
    L=tril(A,-1)+eye(mn);
    U=triu(A);
  end

end
```

LU Factorization: Pivoting

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> *When an element on the diagonal is zero, search for a nonzero in its column, and swap the relevant rows*

This is equivalent to applying P

$$PA = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1.5 \\ 2 & 0 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 1.5 \end{pmatrix}$$

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Thus we are computing $PA = LU$ to get at the solution

$$Ax = b \Rightarrow x = U^{-1}L^{-1}Pb$$

Extension: what is zero? *Always* search for the coefficient with largest absolute value!

LU Factorization: Pivoting

```
function [L, U, P]=lupfact1(A)
  (nargin() ==1) ||  usage("[L,U,P] = lupfact1(A)");
  m=size(A,1);  n=size(A,2);
  if ((m==0)||(n==0))
    return
  end

  mn=min(m,n); Ip=eye(m);
  for j=1:mn
    [mx,ix] = max(abs(A(j:m,j)));   ix=ix+j-1;
    tmp(1:n)  = A(j,1:n);    A(j,1:n)  = A(ix,1:n);    A(ix,1:n) = tmp(1:n);
    tmp(1:m)  = Ip(j,1:m);  Ip(j,1:m)  = Ip(ix,1:m);  Ip(ix,1:m) = tmp(1:m);

%    A(j,j+1:n) = (1.0)\A(j,j+1:n);
    A(j+1:m,j) = A(j+1:m,j)/(A(j,j));
    A(j+1:m,j+1:n) = A(j+1:m,j+1:n) - A(j+1:m,j)*A(j,j+1:n);
  end

  if (nargout() < 1)
    ans = A
  elseif (nargout() == 1)
    L = A;
  elseif (nargout() >= 2)
    L=tril(A,-1); L(1:mn,1:mn)=L(1:mn,1:mn)+eye(mn);     U=triu(A);
    if (nargout()>2)
      P=Ip;
    end
  end
end
```

LU Factorization: Pivoting

Whenever you apply the division operator

```
x=A\b;
```

this is what Octave/Matlab does internally:

```
[L,U,P] = lu(A);
z=P*b;
y=L\z;
x=U\y;
```

The most expensive part is the invocation of the `lu` function ($2/3n^3$).

If you are solving multiple linear systems with the same matrix, it is more efficient to do:

```
[L,U,P] = lu(A);
for j=1:k
  b = rhs(j); % Create the next RHS
  z=P*b;
  y=L\z;
  x=U\y;
  % do something with x
end
```

What about `inv(A)`? Actually this is computed with

$$A^{-1} = U^{-1}L^{-1}P$$

No wonder it costs more: it *starts* with LU factorization, then goes on with more computations!

Never explicitly form `inv(A)*B`, *always use* `A\B`.

Cases where you *really* need the inverse exist but are (vanishingly) rare.

Matrix division (reloaded)

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```
octave:20> a=[1,2;3,4;5,6;]
a =
   1   2
   3   4
   5   6
octave:21> b=[3,4,5]';
octave:22> x=a\b
```

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x =
  -2.0000
   2.5000
```

What's going on here?

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Go back to the beginning and say it again:

> *Applying the matrix division operator* `x=A\b` *is equivalent to solving the linear system* $Ax = b$

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So, to define division for a *rectangular* matrix we need to know what to do with a linear system:

$$Ax = b$$

when A is $m \times n$ and $m \neq n$ (i.e.: rectangular).

Matrix division (reloaded)

Linear algebra comes to the rescue:

When A is not square, we can minimize the mismatch between RHS and LHS, i.e. we search for a least-squares solution

$$Ax = b \Rightarrow \min_x \|Ax - b\|_2$$

When A is square and non-singular this reduces to a "normal" system solution.
The least squares solution is computed through the QR factorization

$$A = QR$$

where Q is orthogonal (i.e. $QQ^T = Q^T Q = I$) and R is upper triangular (trapezoidal).

```
[Q,R]=qr(A);
```

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- The matrices A and B must have the same number of rows;
- The number of rows of X equals the number of columns of A;
- The number of columns of X equals the number of columns of B;
- The solution always exists in the least squares sense, not necessarily in the usual matrix inversion sense; moreover, it is not necessarily unique;

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The *right* division `X=B/A` is equivalent to

```
X = (A'\B')';
```

from which we can derive the row/columns constraints.

An example: curve fitting

Suppose you are measuring a physical phenomenon: you get a set of points (x_i, y_i) and you make a guess: they lie on a parabola. You should have

$$y_i = ax_i^2 + bx_i + c, \qquad i = 1, \dots n$$

for some (unknown) coefficients a, b, c. However measurements have *noise*, so the equations will *not* be satisfied exactly. What do you do?

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```
C = XX\Y
```

where

$$XX = \begin{pmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ \vdots & \vdots & \vdots \\ x_n^2 & x_n & 1 \end{pmatrix}$$

The coefficients will give the *best fit* parabola. BTW: use the Vandermonde matrix function

```
XX = vander(x,3)
```