Computational Physics (PHYS6350)

Lecture 5: Linear algebra and matrices: Part II

- Matrix inversion
- Tri- and band-diagonal systems
- QR decomposition
- Eigenvalue problem

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Course materials: https://github.com/vlvovch/PHYS6350-ComputationalPhysics

Matrix inversion

Inverse of matrix **A**, if it exists, satisfies

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}.$$

Let us denote the columns of the inverse matrix $\mathbf{A}^{-1}$ by $\mathbf{x}_k$, i.e. $\mathbf{A}^{-1}=(\mathbf{x}_1,\ldots,\mathbf{x}_n)$

The vectors $\mathbf{x}_k$ satisfy the following *N* systems of non-linear equations

$$\mathbf{A}\mathbf{x}_k = \mathbf{v}_k, \qquad k = 1 \ldots N$$

where $\mathbf{v}_{k,j} = \delta_{kj}$

Since the matrix **A** is always the same, these systems can be efficiently solved with LU-decomposition to find all $\mathbf{x}_k$ and thus the inverse matrix $\mathbf{A}^{-1}$

Complexity: 1 LU-decomposition $O(N^3)$
+ N backsubstitutions [each one is $O(N^2)$]
~ **$O(N^3)$ overall**

Matrix inversion

```
def matrix_inverse_with_ludecomp(A):
    # First step: LU decomposition of matrix A
    L, U, row_map = lu_decomp_partialpivot(A)
    N = len(row_map)

    Ainv = A.copy()
    for c in range(N):
        v = np.zeros(N, float)
        v[c] = 1.
        x = solve_using_lu_partialpivot(L,U,row_map,v)
        Ainv[:,c] = x

    return Ainv
```

```
A = np.array([[ 0,  1,  4,  1 ],
              [ 3,  4, -1, -1 ],
              [ 1, -4,  1,  5 ],
              [ 2, -2,  1,  3 ]],float)

Ainv = matrix_inverse_with_ludecomp(A)
print("A*A^{-1} = \n", tabulate(A.dot(Ainv)))
```

```
A*A^{-1} =
 ------------  ------------  ------------  ------------
 1             -5.55112e-17   1.11022e-16  -1.11022e-16
-2.77556e-17    1            -1.11022e-16   3.33067e-16
 2.77556e-17    5.55112e-17   1             4.44089e-16
-2.77556e-17   -5.55112e-17  -5.55112e-16   1
 ------------  ------------  ------------  ------------
```

Tridiagonal systems

Tridiagonal system of equation is a special case when the matrix **A** is tridiagonal

$$\mathbf{A} = \begin{pmatrix} d_1 & u_1 & & & 0 \\ l_2 & d_2 & u_2 & & \\ & l_3 & \ddots & \ddots & \\ & & \ddots & \ddots & u_{n-1} \\ 0 & & & l_n & d_n \end{pmatrix}$$

Tridiagonal systems of linear equations often appear in physics, e.g.

- **Nearest-neighbor interaction** (linear chain of springs)
- **Finite differences applied to partial differential equations** (heat equation)

$$\frac{\partial u(t,x)}{\partial t} = \alpha \frac{\partial^2 u(t,x)}{\partial x^2}$$

$$\begin{pmatrix} \frac{\partial u_1(t)}{\partial t} \\ \frac{\partial u_2(t)}{\partial t} \\ \vdots \\ \frac{\partial u_N(t)}{\partial t} \end{pmatrix} = \frac{\alpha}{\Delta x} \begin{pmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & 1 & -2 & 1 \\ 0 & \dots & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} u_1(t) \\ u_2(t) \\ \vdots \\ u_1(t) \end{pmatrix}$$

Solving tridiagonal systems

$$\mathbf{A} = \begin{pmatrix} d_1 & u_1 & & & 0 \\ l_2 & d_2 & u_2 & & \\ & l_3 & \ddots & \ddots & \\ & & \ddots & \ddots & u_{n-1} \\ 0 & & & l_n & d_n \end{pmatrix}$$

Tridiagonal system can be solved in linear time [O(*N*)] with Gaussian elimination an

1. **Gaussian elimination:** at each step need to subtract only one row below the current one, and at most two elements
2. **Backsubstitution:** subtract only single element from the upper superdiagonal

$$\begin{aligned} x_n &= \tilde{v}_n, \\ x_k &= \tilde{v}_k - \tilde{u}_k x_{k+1}, \qquad k = 1 \ldots N-1. \end{aligned}$$

Solving tridiagonal systems

```python
# Solve tridiagonal system of linear equations
#  d: vector of diagonal elements
#  l: vector of elements on the lower subdiagonal
#  u: vector of elements on the upper superdiagonal
# v0: right-hand-side vector
def linsolve_tridiagonal(d, l, u, v0):
    # Initialization
    N = len(v0)
    a = d.copy() # Current diagonal elements
    b = u.copy() # Current upper diagonal elements
    v = v0.copy()

    # Gaussian elimination
    for r in range(N):
        if (a[r] == 0.):
            print("Diagonal element is zero! Cannot solve
            return None
        b[r] /= a[r]
        v[r] /= a[r]
        a[r] = 1.
        if (r < N - 1):
            a[r + 1] -= l[r+1] * b[r]
            v[r + 1] -= l[r+1] * v[r]

    # Backsubstitution
    x = np.empty(N,float)

    x[N - 1] = v[N - 1]
    for r in range(N-2,-1,-1):
        x[r] = v[r] - b[r] * x[r + 1]

    return x
```

Test for a random tridiagonal matrix

```python
def random_tridiagonal(n):
    A = np.random.rand(n, n)
    for r in range(n):
        for c in range(0,r-1):
            A[r][c] = 0.
        for c in range(r + 2, n):
            A[r][c] = 0.
    return A
```

```python
n = 8
A = random_tridiagonal(n)
print("A =\n", tabulate(A))
v = np.random.rand(n)
x = linsolve_tridiagonal(*(get_tridiagonal(A)),v)
print(" x = ", x)
print("Ax = ", A.dot(x))
print(" v = ", v)
```

```
A =
 --------  --------  ---------  --------  --------  --------  ----------  --------
0.258085  0.365256  0          0         0         0         0           0
0.598828  0.60432   0.0777664  0         0         0         0           0
0         0.839862  0.209281   0.418171  0         0         0           0
0         0         0.730628   0.406732  0.789413  0         0           0
0         0         0          0.597044  0.627719  0.575418  0           0
0         0         0          0         0.639515  0.293871  0.737697    0
0         0         0          0         0         0.74846   0.477541    0.704847
0         0         0          0         0         0         0.00826684  0.109495
--------  --------  ---------  --------  --------  --------  ----------  --------
 x =  [ 2.2288744  -0.6670926  -5.72667763  5.03759801  3.51116171 -7.41798625
  1.22249979  8.40485586]
Ax =  [0.33158055 0.48623086 0.34782961 0.63663712 0.94324165 0.96734828
 0.9558695  0.93039484]
 v =  [0.33158055 0.48623086 0.34782961 0.63663712 0.94324165 0.96734828
 0.9558695  0.93039484]
```

Band-diagonal systems

Band-diagonal system: in each row

- at most m_{lower} non-zero elements to the left of the main diagonal
- at most m_{upper} non-zero elements to the right of the main diagonal

$$\mathbf{A} = \begin{pmatrix} d_1 & u_{1,1} & u_{2,1} & & & & \\ l_{1,2} & d_2 & u_{1,2} & u_{2,2} & & 0 & \\ l_{2,3} & l_{1,3} & d_3 & u_{1,3} & u_{2,3} & & \\ & l_{2,4} & l_{1,4} & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & u_{1,n-2} & u_{2,n-2} \\ & 0 & & \ddots & \ddots & \ddots & u_{1,n-1} \\ & & & & l_{2,n} & l_{1,n} & d_n \end{pmatrix}$$

Generalization of tridiagonal systems ($m_{lower} = m_{upper} = 1$)

- *k*-nearest-neighbor interaction (linear chain of springs)
- High-order finite difference applied to partial differential equations (heat equation)

Solving band-diagonal systems

$$\mathbf{A} = \begin{pmatrix} d_1 & u_{1,1} & u_{2,1} & & & & \\ l_{1,2} & d_2 & u_{1,2} & u_{2,2} & & 0 & \\ l_{2,3} & l_{1,3} & d_3 & u_{1,3} & u_{2,3} & & \\ & l_{2,4} & l_{1,4} & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & u_{1,n-2} & u_{2,n-2} \\ & 0 & & \ddots & \ddots & \ddots & u_{1,n-1} \\ & & & & l_{2,n} & l_{1,n} & d_n \end{pmatrix}$$

Solving band-diagonal system proceeds also through Gaussian elimination

1. **Gaussian elimination:** At each step one has to normalize $m_{upper}+1$ elements in the current row, then subtract the current row from at most m_{lower} rows below it. ***O(N x m_{upper} x m_{lower})***
2. **Backsubstitution: in** each row subtract up to m_{upper} elements to the right from the main diagonal. ***O(N x m_{upper})***

Overall complexity: O(N x m_{upper} x m_{lower})

Solving band-diagonal systems

```python
# Solving linear system of banded equations
# d: diagonal elements of the banded matrix
# l: lower non-zero diagonals of the banded matrix
# u: upper non-zero diagonals of the banded matrix
# v0: r.h.s. vector
def linsolve_banded(d, l, u, v0):
    # Initialization
    v = v0.copy()
    N = len(v)
    mlower = len(l)
    mupper = len(u)

    a    = d.copy() # Diagonal elements
    dup  = u.copy() # Upper diagonal elements
    dlow = l.copy() # Lower diagonal elements

    # Gaussian elimination
    for r in range(N):
        # Divide row r by diagonal element
        div = a[r]
        if (div == 0.):
            print("Diagonal element is zero! Cannot solve the system with simple
            return None
        for c in range(r+1,min(r + mupper + 1,N)):
            dup[c-r-1,r] /= div
        a[r] /= div
        v[r] /= div

        # Now subtract this row from the lower rows
        # We do not need to go through all the rows
        # but only up to a certain row depending
        # on the number of non-zero elements to right and left of the main diagon
        max_row = min(r + mlower, N - 1)

        # First the vector
        for r2 in range(r+1,max_row + 1):
            v[r2] -= dlow[r2 - r - 1, r2] * v[r]

        # Then the matrix rows
        for c in range(r + 1,min(r + mupper + 1,N)):
            for r2 in range(r+1,max_row + 1):
                if (c == r2):
                    a[r2] -= dlow[r2 - r - 1, r2] * dup[c-r-1,r]
                elif (c < r2 and r2 - c - 1 < mlower):
                    dlow[r2 - c - 1,r2] -= dlow[r2 - r - 1, r2] * dup[c-r-1,r]
                elif (c > r2 and c - r2 - 1 < mupper):
                    dup[c - r2 - 1,r2] -= dlow[r2 - r - 1, r2] * dup[c-r-1,r]

    # Backsubstitution
    x = np.empty(N,float)
    for r in range(N-1,-1,-1):
        x[r] = v[r]
        for c in range(r+1,min(r + mupper + 1,N)):
            x[r] -= dup[c - r - 1,r] * x[c]

    return x
```

```python
def random_banded(n, mlower, mupper):
    A = np.random.rand(n, n)
    for r in range(n):
        for c in range(0,r-mlower):
            A[r][c] = 0.
        for c in range(r + mupper + 1, n):
            A[r][c] = 0.
    return A
```

```python
n = 10
mupper = 4
mlower  = 3
A = random_banded(n, mlower, mupper)
print("A =\n", tabulate(A))
v = np.random.rand(n)
x = linsolve_banded(*(get_banded(A,mlower,mupper)),v)
print(" x = ", x)
print("Ax = ", A.dot(x))
print(" v = ", v)
```

```
A =
 --------  --------  --------  ---------  --------  ----------  ---------  ---------  --------  --------
0.398214  0.972929  0.249665  0.0841269  0.667612  0           0          0          0         0
0.668918  0.27899   0.98081   0.311536   0.395787  0.250914    0          0          0         0
0.103901  0.955985  0.591015  0.178139   0.194452  0.565519    0.207813   0          0         0
0.094764  0.417524  0.401467  0.507737   0.198962  0.872389    0.999096   0.0251162  0         0
0         0.624273  0.727381  0.409819   0.859236  0.00593723  0.68357    0.707848   0.427377  0
0         0         0.304125  0.768458   0.03066   0.322861    0.123774   0.0664194  0.775458  0.117592
0         0         0         0.294081   0.698817  0.82127     0.43601    0.743528   0.107041  0.917906
0         0         0         0          0.642317  0.763591    0.0719641  0.752717   0.223502  0.607639
0         0         0         0          0         0.18334     0.0233041  0.0637123  0.95644   0.420615
0         0         0         0          0         0           0.698929   0.919066   0.824737  0.521482
--------  --------  --------  ---------  --------  ----------  ---------  ---------  --------  --------
 x =  [-0.28014041  0.17110358  1.10225327 -1.21247032  0.14011191  0.26755524
  0.024373   -0.04051962  0.83538165  0.223171  ]
Ax =  [0.32164853 0.68630553 0.75354435 0.15641687 0.87865905 0.1685409
 0.23585233 0.58787029 0.93990131 0.78514492]
 v =  [0.32164853 0.68630553 0.75354435 0.15641687 0.87865905 0.1685409
 0.23585233 0.58787029 0.93990131 0.78514492]
```

QR decomposition*

Any real square matrix **A** permits a decomposition

$$\mathbf{A} = \mathbf{QR}$$

where

- **Q** is orthogonal, $\mathbf{Q}^{-1}=\mathbf{Q}^{T}$, and thus, $\mathbf{Q}^{T}\mathbf{Q} = \mathbf{I}$
- **R** is upper diagonal

There are many algorithms for constructing the QR decomposition:

- from simple Gram-Schimdt process (numerically unstable)
- to more involved methods using Householder transformation or
- Givens rotations.

`numpy.linalg.qr`

*Has nothing to do with QR codes

QR decomposition and systems of linear equations

System of linear equations

$$\mathbf{Ax} = \mathbf{v}.$$

If **A** = **QR** we can rewrite the system as

$$\mathbf{QRx} = \mathbf{v}.$$

Multiplying each side of the equation by $\mathbf{Q}^T$, we have

$$\mathbf{Rx} = \mathbf{Q}^T\mathbf{v}.$$

The matrix **R** is upper triangular, thus, the system can solved using backsubstitution.

```
def linsolve_using_qr(Q,R,v):
    # Initialization
    N = len(v)
    # Calculate y = Q^T v
    y = np.zeros(N,float)
    for r in range(N):
        for c in range(N):
            y[r] += Q[c][r] * v[c]

    # Backsubstitution for R*x = y
    x = np.empty(N,float)
    for r in range(N-1,-1,-1):
        x[r] = y[r]
        for c in range(r+1,N):
            x[r] -= R[r][c] * x[c]

        x[r] /= R[r][r]
    return x
```

```
A = np.array([[ 0,  1,  4,  1 ],
              [ 3,  4, -1, -1 ],
              [ 1, -4,  1,  5 ],
              [ 2, -2,  1,  3 ]],float)

Q, R = np.linalg.qr(A)
v = np.array([ -4, 3, 9, 7 ],float)
x = linsolve_using_qr(Q,R,v)
print('x  =', x)
print('Ax =', A.dot(x))
print('v  =', v)
```

Eigenvalue problem

A common matrix problem in physics is the calculation of eigenvalues and eigenvectors of a matrix (e.g. classical and quantum mechanics).

The eigenvalue problem corresponds to the equation

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}.$$

Here λ are the eigenvalues and **v** are the eigenvectors

Example:

$$H\psi_n(x) = E_n\psi_n(x)$$

Energy levels in quantum mechanics using matrix form

General approach (not used in practice):

- Eigenvalues are roots of the characteristic polynomial

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

- Once λ are found, the eigenvectors can be computed by solving linear system

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = 0$$

- This approach is impractical: numerically unstable to solve high-degree polynomial roots

Eigenvalue problem

In most cases the matrix **A** is either real symmetric or Hermitian (complex numbers).

In this case, for a NxN matrix there are N eigenvectors $\mathbf{v}_1,\ldots,\mathbf{v}_N$ with real eigenvalues $\lambda_1,\ldots,\lambda_N$. The eigenvectors are orthogonal, i.e. $\mathbf{v}_i\mathbf{v}_j = \delta_{ij}$ with the appropriate normalization.

The eigenvalue problem can thus be cast as a matrix equation

$$\mathbf{AV} = \mathbf{VD}$$

Here **V** is the matrix of eigenvectors, i.e. column *k* corresponds to the eigenvector $\mathbf{v}_k$, and **D** is a diagonal matrix with entries corresponding to eigenvalues, **D** = diag($\lambda_1,\ldots,\lambda_N$).

How to solve the matrix equation $\mathbf{AV} = \mathbf{VD}$

QR algorithm

QR algorithm is a method of finding eigenvalues and/or eigenvectors based on an iterative procedure.

1. One starts with matrix $\mathbf{A_1 = A}$ and calculates its QR decomposition $\mathbf{A_1 = Q_1 R_1}$
2. The next matrix is computed as $\mathbf{A_2 = R_1 Q_1}$.
   - This is a similarity transform. Multiplying both sides by $\mathbf{I = Q_1^T Q_1}$ and taking into account $\mathbf{A_1 = Q_1 R_1}$, one gets $\mathbf{A_2 = Q_1^T A_1 Q_1}$.
3. The process is repeated as follows,

$$\mathbf{A_{n+1} = R_n Q_n = Q_n^T A_n Q_n}.$$

4. Matrix $\mathbf{A_n}$ converges to **diagonal form** in the limit $n \to \infty$ (for real symmetric **A**):

$\boldsymbol{A_\infty = QTAQ}$, where $\boldsymbol{Q = \prod_{k=1}^{\infty} Q_k}$ where $\boldsymbol{Q}$ is an orthogonal matrix.

Multiply $\boldsymbol{A_\infty}$ by $\boldsymbol{Q}$ from the right: $\boldsymbol{AQ = QA_\infty}$

Compare with $\boldsymbol{AV = VD}$ ⇒ $\boldsymbol{Q = V}$ (**eigenvector matrix**) $\boldsymbol{A_\infty = D}$ (**eigenvalue matrix**)

In practice, the algorithm stops once non-diagonal elements of $\mathbf{A_n}$ are below a certain threshold ϵ.

QR algorithm

```
def eigen_qr_simple(A, iterations=1000):
    Ak = np.copy(A)
    n = len(A[0])
    QQ = np.eye(n)
    for k in range(iterations):
        Q, R = np.linalg.qr(Ak)
        Ak = np.dot(R,Q)
        QQ = np.dot(QQ,Q)
        if k%100 == 0:
            print("A",k,"=")
            print(tabulate(Ak))
            print("\n")
    return Ak, QQ
```

```
n = 5
A = np.random.rand(n, n)
# Make symmetric
for r in range(n):
    for c in range(r):
        A[r][c] = A[c][r]
```

```
# We call the function
AQ = eigen_qr_simple(A)

# Print A' = D
print("A' =\n",tabulate(AQ[0]))
print("Q  =\n",tabulate(AQ[1]))

# We compare our results with the official numpy algorithm
print(np.linalg.eig(A))

# Check orthogonality
print("v1*v2 = ", P[:,0].dot(P[:,1]))
```

```
A' =
-------  -------------  -------------  ------------  ------------
2.74844  -3.02815e-16    1.6284e-16    -5.32145e-17   2.4959e-16
0        -0.746594       1.15176e-17    4.62374e-17  -1.69369e-17
0         9.02192e-67   -0.643849      -9.85419e-17   1.54078e-16
0        -4.94066e-324  -4.5242e-287    0.331455     -2.97135e-16
0        -4.94066e-324  -7.90505e-323   1.77529e-36  -0.305375
-------  -------------  -------------  ------------  ------------
Q  = V1        V2         V3         V4          V5
 ---------  ---------  ---------  ----------  ----------
-0.537155  -0.550458   0.199338   0.418962   -0.439541
-0.445186  -0.37513    0.179416  -0.561737    0.559775
-0.483201   0.62303    0.264306  -0.365474   -0.418235
-0.457385   0.126918  -0.871099   0.0886914   0.0894995
-0.265687   0.38987    0.315282   0.606205    0.557247
---------  ---------  ---------  ----------  ----------
v1*v2 =  -2.513426757818653e-16
```

Linear algebra: Summary

$$\mathbf{A}\mathbf{x} = \mathbf{v}.$$

System of N linear equations

- General case: use LU-decomposition [$O(N^3)$] + forward/back-substitution [$O(N^2)$] ~ $O(N^3)$]
- No need to repeat LU-decomposition when **v** (but not **A**) changes
- Tridiagonal system: Can be solve in linear O(N) time
- Band-diagonal: $O(N \times m_{upper} \times m_{lower})$

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}.$$

Eigenvalue problem

- General case: use QR-decomposition and QR algorithm (iterative)
- Specialized algorithms for sparse matrices (e.g. **Lanczos algorithm**)

final project idea(?)