

Computational Physics I - Lecture 3, part 1

Adam Foster, Dorothea Golze, Patrick Rinke
Levi Keller, Yashasvi Ranawat, Ygor Morais Jaques

Aalto University
School of Science
Department of Applied Physics

Solutions of linear and non-linear equations

Linear equation: $ax + b = c$

- sets of linear equations are very common in physics
- they can be solved with matrix algebra
- matrix algebra is one of the most important applications in computational physics

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Non linear equation: $x = f(x)$

- non-linear equations are even more common than linear
- they are much harder to solve than linear equations
- numeric approaches for non-linear eqns are very important

Solutions of linear and non-linear equations

Linear equation: $ax + b = c$ today

- sets of linear equations are very common in physics
- they can be solved with matrix algebra
- matrix algebra is one of the most important applications in computational physics

Non linear equation: $x = f(x)$ next week

- non-linear equations are even more common than linear
- they are much harder to solve than linear equations
- numeric approaches for non-linear eqns are very important

Simultaneous linear equations

set of linear equations:

$$2w + x + 4y + z = -4$$
$$3w + 4x - y - z = 3$$
$$w - 4x + y + 5z = 9$$
$$2w - 2x + y + 3z = 7$$

- techniques for solving simultaneous sets of equations are well understood and straightforward,
- but humans are slow and prone to error in such calculations
- computers are perfectly suited for this, in particular for large systems with many variables

Simultaneous linear equations

- cast the set of equations into matrix form:

$$\begin{pmatrix} 2 & 1 & 4 & 1 \\ 3 & 4 & -1 & -1 \\ 1 & -4 & 1 & 5 \\ 2 & -2 & 1 & 3 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -4 \\ 3 \\ 9 \\ 7 \end{pmatrix} \quad \text{or in short } \mathbf{Ax} = \mathbf{v}$$

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$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{v}$$

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- algebraically, inversion seems easiest solution:

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{v}$$

- But numerically matrix inversion is not the best solution!
- There are more efficient ways.

Gaussian elimination and back substitution

- suppose we could transform the equations into this form:

$$\begin{pmatrix} 1 & a_{01} & a_{02} & a_{03} \\ 0 & 1 & a_{12} & a_{13} \\ 0 & 0 & 1 & a_{23} \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} v_0 \\ v_1 \\ v_2 \\ v_3 \end{pmatrix}$$

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- then the solution is simple:

$$z = v_3$$



$$y = v_2 - a_{23}z$$

$$x = v_1 - a_{12}y - a_{13}z$$

$$w = v_0 - a_{01}x - a_{02}y - a_{03}z$$

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back substitution

Gaussian elimination and back substitution

Gaussian elimination

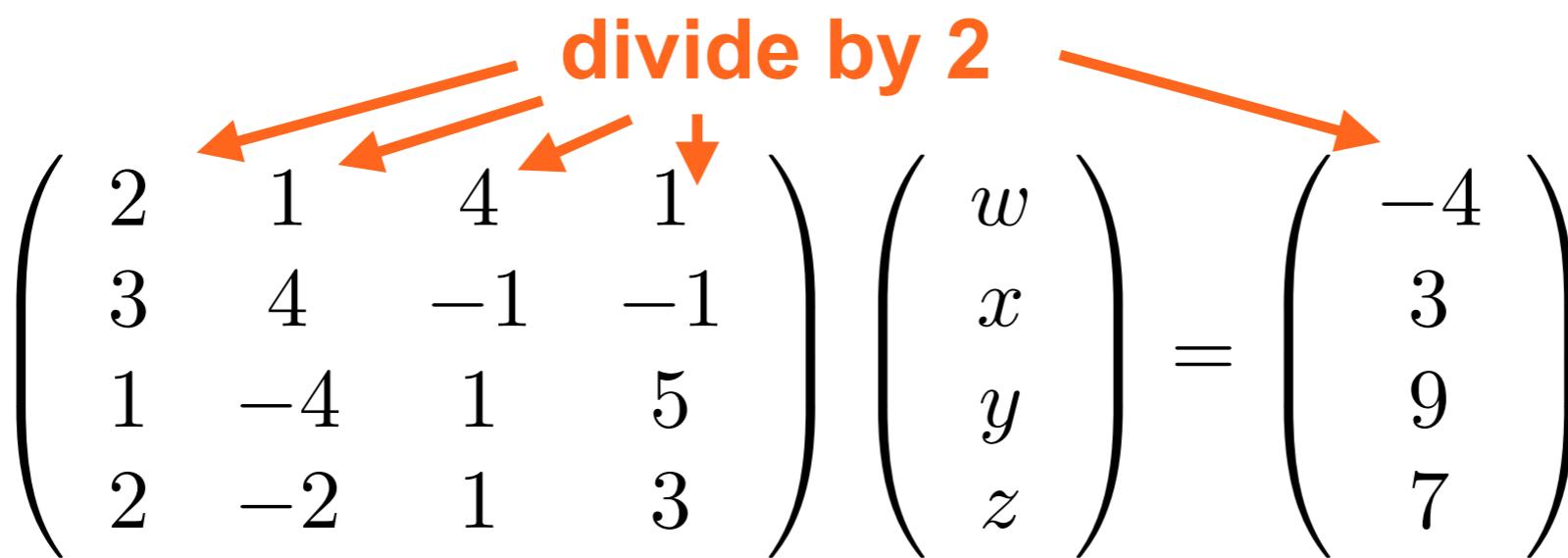
- To arrive at the upper tridiagonal form we apply two rules consecutively:
 1. If we multiply any row of \mathbf{A} and the corresponding row of \mathbf{v} by a constant, the solution does not change.
 2. If we add to or subtract from any row of \mathbf{A} a multiple of any other row, and we do the same for \mathbf{v} , then the solution does not change.

Gaussian elimination and back substitution

Rule 1:

$$\left(\begin{array}{cccc} 2 & 1 & 4 & 1 \\ 3 & 4 & -1 & -1 \\ 1 & -4 & 1 & 5 \\ 2 & -2 & 1 & 3 \end{array} \right) \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -4 \\ 3 \\ 9 \\ 7 \end{pmatrix}$$

divide by 2



Gaussian elimination and back substitution

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divide by 2

now equal to 1

$$\left(\begin{array}{cccc} 1 & 0.5 & 2 & 0.5 \\ 3 & 4 & -1 & -1 \\ 1 & -4 & 1 & 5 \\ 2 & -2 & 1 & 3 \end{array} \right) \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -2 \\ 3 \\ 9 \\ 7 \end{pmatrix}$$

Gaussian elimination and back substitution

Rule 2:

subtract 3 times first row from 2nd

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Gaussian elimination and back substitution

Rule 2:

now equal to 0

$$\begin{pmatrix} 1 & 0.5 & 2 & 0.5 \\ 0 & 2.5 & -7 & -2.5 \\ 1 & -4 & 1 & 5 \\ 2 & -2 & 1 & 3 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -2 \\ 9 \\ 9 \\ 7 \end{pmatrix}$$

subtract 3 times first row from 2nd

$$\begin{pmatrix} 1 & 0.5 & 2 & 0.5 \\ 3 & 4 & -1 & -1 \\ 1 & -4 & 1 & 5 \\ 2 & -2 & 1 & 3 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -2 \\ 3 \\ 9 \\ 7 \end{pmatrix}$$

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$$\begin{pmatrix} 1 & 0.5 & 2 & 0.5 \\ 0 & 2.5 & -7 & -2.5 \\ 1 & -4 & 1 & 5 \\ 2 & -2 & 1 & 3 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -2 \\ 9 \\ 9 \\ 7 \end{pmatrix}$$

- By applying Rule 1 and Rule 2 successively, we can set all diagonal elements to 1 and the lower triangle to 0.

Linear equations - Exercise 1

Solve:
$$\begin{pmatrix} 2 & 1 & 4 & 1 \\ 3 & 4 & -1 & -1 \\ 1 & -4 & 1 & 5 \\ 2 & -2 & 1 & 3 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -4 \\ 3 \\ 9 \\ 7 \end{pmatrix}$$

1. Complete the Gaussian elimination part of the program.
2. Add a print statement that prints the matrix at every step to check that the program is eliminating correctly.
3. Check your final solution for the vector $\mathbf{x} = (w, x, y, z)$

Talking points:

1. **What do you observe?**
2. **Is your solution correct?**

Linear equations - Example 1

Show model solution.

Linear equations - Example 1

Show model solution.

Key concept: Gaussian elimination

With *Gaussian elimination* and *back substitution* we can solve a set of linear equations efficiently.

Gaussian elimination - Pivoting

Pivoting in Gaussian elimination

- suppose the set is slightly different:

$$\begin{pmatrix} 0 & 1 & 4 & 1 \\ 3 & 4 & -1 & -1 \\ 1 & -4 & 1 & 5 \\ 2 & -2 & 1 & 3 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -4 \\ 3 \\ 9 \\ 7 \end{pmatrix}$$

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- The solution is to swap this row with another one to make that the first row. Then Gaussian elimination and back substitution can be applied again. Care has to be taken, however, to not introduce problems elsewhere.

Linear equations - LU decomposition

Sets of equations: $\mathbf{Ax} = \mathbf{v}_1, \mathbf{Ax} = \mathbf{v}_2, \dots, \mathbf{Ax} = \mathbf{v}_n$

Question:

If we want to apply A to different vectors v , Gauss Elimination is wasteful, because it has to be carried out over and over again. Is there a better way?

Linear equations - LU decomposition

- We wish to transform a general matrix \mathbf{A}

$$\mathbf{A} = \begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{pmatrix}$$

so that it can be applied to any vector \mathbf{v} .

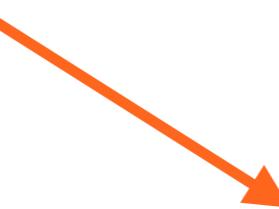
- We are looking for matrix operations that transform \mathbf{A} .

Linear equations - LU decomposition

- The operations that turn the first row into its correct form can be encapsulated in the following matrix multiplication

$$\frac{1}{a_{00}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ -a_{10} & a_{00} & 0 & 0 \\ -a_{20} & 0 & a_{00} & 0 \\ -a_{30} & 0 & 0 & a_{00} \end{pmatrix} \begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{pmatrix} = \begin{pmatrix} 1 & b_{01} & b_{02} & b_{03} \\ 0 & b_{11} & b_{12} & b_{13} \\ 0 & b_{21} & b_{22} & b_{23} \\ 0 & b_{31} & b_{32} & b_{33} \end{pmatrix}$$

lower triangular
matrix


$$L_0 A = B$$

Linear equations - LU decomposition

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lower triangular matrix

$$L_0 A = B$$

now we have to continue with B

Linear equations - LU decomposition

- Operating on \mathbf{B} with a new matrix

$$\frac{1}{b_{11}} \begin{pmatrix} b_{11} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -b_{21} & b_{11} & 0 \\ 0 & -b_{31} & 0 & b_{11} \end{pmatrix} \begin{pmatrix} 1 & b_{01} & b_{02} & b_{03} \\ 0 & b_{11} & b_{12} & b_{13} \\ 0 & b_{21} & b_{22} & b_{23} \\ 0 & b_{31} & b_{32} & b_{33} \end{pmatrix} = \begin{pmatrix} 1 & c_{01} & c_{02} & c_{03} \\ 0 & 1 & c_{12} & c_{13} \\ 0 & 0 & c_{22} & c_{23} \\ 0 & 0 & c_{32} & c_{33} \end{pmatrix}$$

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$$\mathbf{L}_1 \mathbf{B} = \mathbf{L}_1 \mathbf{L}_0 \mathbf{A} = \mathbf{C}$$

Linear equations - LU decomposition

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$$\frac{1}{b_{11}} \begin{pmatrix} b_{11} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -b_{21} & b_{11} & 0 \\ 0 & -b_{31} & 0 & b_{11} \end{pmatrix} \begin{pmatrix} 1 & b_{01} & b_{02} & b_{03} \\ 0 & b_{11} & b_{12} & b_{13} \\ 0 & b_{21} & b_{22} & b_{23} \\ 0 & b_{31} & b_{32} & b_{33} \end{pmatrix} = \begin{pmatrix} 1 & c_{01} & c_{02} & c_{03} \\ 0 & 1 & c_{12} & c_{13} \\ 0 & 0 & c_{22} & c_{23} \\ 0 & 0 & c_{32} & c_{33} \end{pmatrix}$$

lower triangular
matrix

$$L_1 B = L_1 L_0 A = C$$

we need two
more operations
for C

Linear equations - LU decomposition

- The final two operations are:

$$\mathbf{L}_2 = \frac{1}{c_{22}} \begin{pmatrix} c_{22} & 0 & 0 & 0 \\ 0 & c_{22} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -c_{32} & c_{22} \end{pmatrix} \quad \text{and} \quad \mathbf{L}_3 = \frac{1}{d_{33}} \begin{pmatrix} d_{33} & 0 & 0 & 0 \\ 0 & d_{33} & 0 & 0 \\ 0 & 0 & d_{33} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

- Putting it all together we have:

$$\mathbf{L}_3 \mathbf{L}_2 \mathbf{L}_1 \mathbf{L}_0 \mathbf{A} = \mathbf{L}_3 \mathbf{L}_2 \mathbf{L}_1 \mathbf{L}_0 \mathbf{v} = \mathbf{U} \mathbf{v}$$

Linear equations - LU decomposition

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 upper diagonal matrix

Linear equations - LU decomposition

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- Putting it all together we have:

$$L_3 L_2 L_1 L_0 A = L_3 L_2 L_1 L_0 v = U v$$



now we need to find the inverse of
the left-hand side to obtain an
expression for A



upper diagonal
matrix

Linear equations - LU decomposition

- With the following inverses of L_n

$$L_0^{-1} = \begin{pmatrix} a_{00} & 0 & 0 & 0 \\ a_{10} & 1 & 0 & 0 \\ a_{20} & 0 & 1 & 0 \\ a_{30} & 0 & 0 & 1 \end{pmatrix}, \quad L_1^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b_{11} & 0 & 0 \\ 0 & b_{21} & 1 & 0 \\ 0 & b_{31} & 0 & 1 \end{pmatrix}$$
$$L_2^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & c_{22} & 0 \\ 0 & 0 & c_{32} & 1 \end{pmatrix}, \quad L_3^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & d_{33} \end{pmatrix}$$

- we obtain:

$$L = L_0^{-1} L_1^{-1} L_2^{-1} L_3^{-1} = \begin{pmatrix} a_{00} & 0 & 0 & 0 \\ a_{10} & b_{11} & 0 & 0 \\ a_{20} & b_{21} & c_{22} & 0 \\ a_{30} & b_{31} & c_{32} & d_{33} \end{pmatrix}$$

Linear equations - LU decomposition

- we obtain:

lower triangular matrix **easy to calculate from known elements**

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Linear equations - LU decomposition

LU decomposition: $A = LU$

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Linear equations - LU decomposition

LU decomposition of our problem: $\mathbf{Ax} = \mathbf{v}$

$$\mathbf{Ax} = \mathbf{LUx} = \mathbf{Ly} = \mathbf{v} \quad \text{with} \quad \mathbf{Ux} = \mathbf{y}$$

Linear equations - LU decomposition

LU decomposition of our problem: $Ax = v$

$$Ax = LUx = Ly = v \quad \text{with} \quad Ux = y$$

1st back substitution
gives y from v



Linear equations - LU decomposition

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1st back substitution
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2nd back substitution
gives x from y



Linear equations - LU decomposition

LU decomposition of our problem: $Ax = v$

$$Ax = LUx = Ly = v \quad \text{with} \quad Ux = y$$

1st back substitution
gives y from v

2nd back substitution
gives x from y

With LU decomposition and two back substitutions we can solve $Ax = v$ for any v .

Linear equations - LU decomposition

LU decomp.: $\mathbf{Ax} = \mathbf{LUx} = \mathbf{Ly} = \mathbf{v}$ with $\mathbf{Ux} = \mathbf{y}$

- For the exercises, you will write your own LU decomposition.

Linear equations - LU decomposition

LU decomp.: $Ax = LUx = Ly = v$ with $Ux = y$

- For the exercises, you will write your own LU decomposition.
- Python has a build in solver for simultaneous linear equations that uses LU decomposition and back substitution.

```
from numpy.linalg import solve  
x = solve(A, v)
```

Linear equations - LU decomposition

LU decomp.: $\mathbf{Ax} = \mathbf{LUx} = \mathbf{Ly} = \mathbf{v}$ with $\mathbf{Ux} = \mathbf{y}$

- For the exercises, you will write your own LU decomposition.
- Python has a build in solver for simultaneous linear equations that uses LU decomposition and back substitution.

```
from numpy.linalg import solve  
x = solve(A, v)
```

- In the SciPy package you can find a LU decomposition function under linalg.



Linear equations - Exercise 2

Solve:
$$\begin{pmatrix} 2 & 1 & 4 & 1 \\ 3 & 4 & -1 & -1 \\ 1 & -4 & 1 & 5 \\ 2 & -2 & 1 & 3 \end{pmatrix} \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -4 \\ 3 \\ 9 \\ 7 \end{pmatrix}$$

- For this problem, the LU decomposition is:

$$L = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 3 & 2.5 & 0 & 0 \\ 1 & -4.5 & -13.6 & 0 \\ 2 & -3 & -11.4 & -1 \end{pmatrix} \quad U = \begin{pmatrix} 1 & 0.5 & 2 & 0.5 \\ 0 & 1 & -2.8 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Linear equations - Exercise 2

1. Verify that $L*U$ gives the matrix A . You can use the numpy routine `matmul`.
2. Perform the double back substitution $Ly=v$ and $Ux=y$ with the numpy.linalg routine `solve`.
3. Verify your result.
4. Apply the LU decomposition to the new vectors $v_1=(1,0,0,0)$, $v_2=(0,1,0,0)$, $v_3=(0,0,1,0)$, $v_4=(0,0,0,1)$.
5. Check your result with `solve`.

Talking points:

1. What do you observe?
2. What happens when you apply the LU decomposition to the vectors v_1 to v_4 ?

Linear equations - LU decomposition

Key concept: LU decomposition

The *LU decomposition* is one of several factorisations of a square matrix A. It factors A into a lower and an upper triangular matrix. The LU decomposition is the first step in an efficient solution of linear sets of equations.

Linear equations - Matrix inversion

Matrix inverse: $\mathbf{A}\mathbf{A}^{-1} = \mathbf{1}$

Linear equations - Matrix inversion

Matrix inverse: $\mathbf{A}\mathbf{A}^{-1} = \mathbb{1}$

- LU decomposition is a common way to invert a matrix.

$$\mathbf{AX} = \mathbf{LUX} = \mathbb{1}$$

$\uparrow \quad \uparrow$
 $\mathbf{A}^{-1} \quad \mathbb{1}$

**When \mathbb{V} is the identity,
 \mathbf{X} is the inverse of \mathbf{A} .**

Linear equations - Matrix inversion

Matrix inverse: $\mathbf{A}\mathbf{A}^{-1} = \mathbf{1}$

- LU decomposition is a common way to invert a matrix.

$$\mathbf{AX} = \mathbf{LUX} = \mathbf{1}$$

- With back substitution we can repeatedly solve for the columns of \mathbf{X} and so gradually build up the inverse of \mathbf{A} .

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- This is a good example for different right hand sides \mathbf{v} .

Linear equations - Matrix inversion

Matrix inverse: $\mathbf{A}\mathbf{A}^{-1} = \mathbf{1}$

- LU decomposition is a common way to invert a matrix.

$$\mathbf{AX} = \mathbf{LUX} = \mathbf{1}$$

- numpy has a build in function that inverts a matrix.

```
from numpy.linalg import inv  
X = inv(A)
```

Linear equations - Matrix inversion

Key concept: matrix inversion

The *LU decomposition* provides one way to invert a square matrix numerically.

Tridiagonal and banded matrices

Tridiagonal matrix: $A = \begin{pmatrix} a_{00} & a_{01} & & & \\ a_{10} & a_{11} & a_{12} & & \\ & a_{21} & a_{22} & a_{23} & \\ & & a_{32} & a_{33} & a_{34} \\ & & a_{43} & a_{44} & \end{pmatrix}$

- Gaussian elimination is especially efficient as we do not need to go through all the rows of the matrix, but only the row immediately below the current one.

Tridiagonal and banded matrices

- Gaussian elimination is more efficient than LU decomposition. The result is:

$$\begin{pmatrix} 1 & b_{01} & 0 & 0 \\ 0 & 1 & b_{12} & 0 \\ 0 & 0 & 1 & b_{23} \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \end{pmatrix}$$

- Back substitution is also simple:

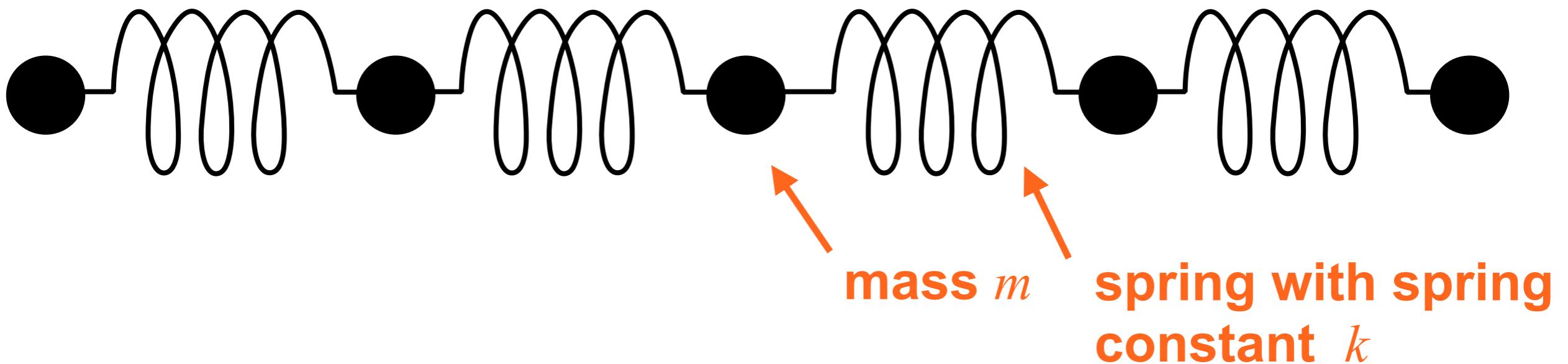
$$x_3 = y_3$$

$$x_2 = y_2 - b_{23}x_3$$

$$x_1 = y_1 - b_{12}x_2$$

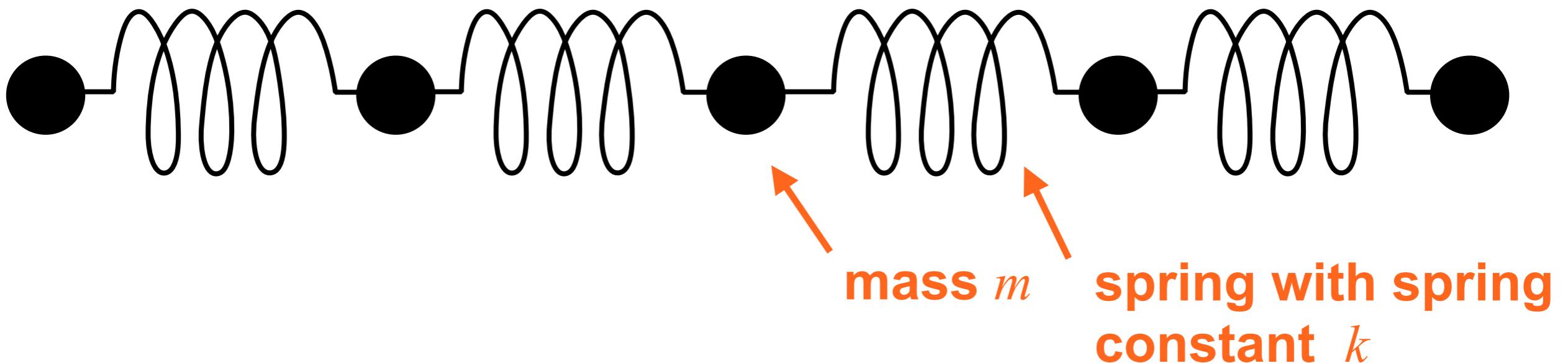
$$x_0 = y_0 - b_{01}x_1$$

Example 1 - Vibration in a 1D system



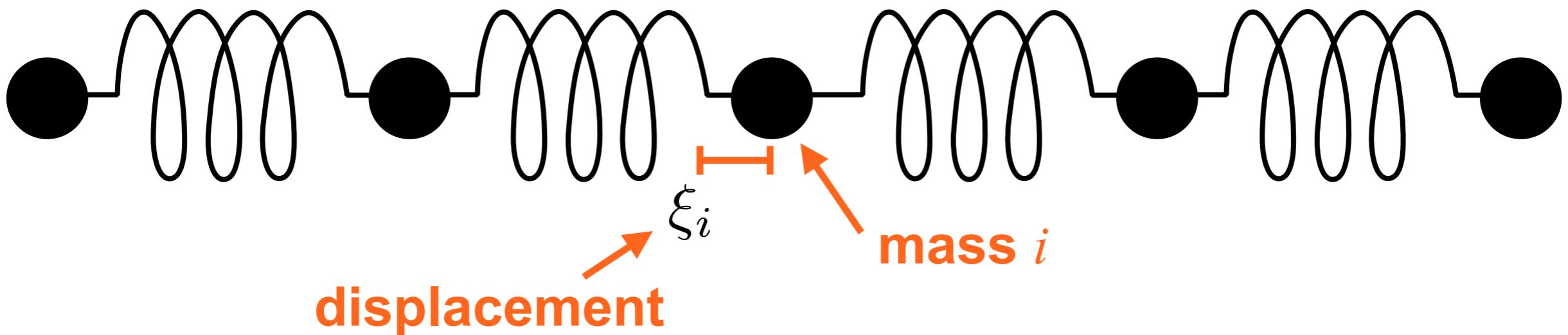
- N masses m in a row joint my identical springs
- We ignore gravity and perturb the system with a force.

Example 1 - Vibration in a 1D system



- N masses m in a row joint my identical springs
- We ignore gravity and perturb the system with a force.
- The masses will start to vibrate relative to each other, which gives a good model for atoms in a solid.

Example 1 - Vibration in a 1D system

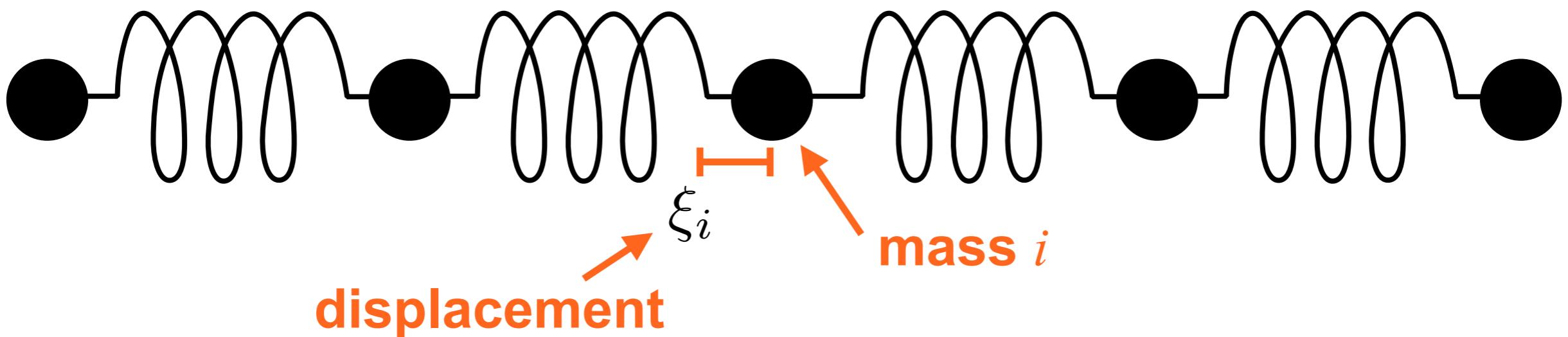


- The equations of motion for the masses are given by Newton's second law:

$$m \frac{d^2 \xi_i}{dt^2} = k(\xi_{i+1} - \xi_i) + k(\xi_{i-1} - \xi_i) + F_i$$

external
force

Example 1 - Vibration in a 1D system

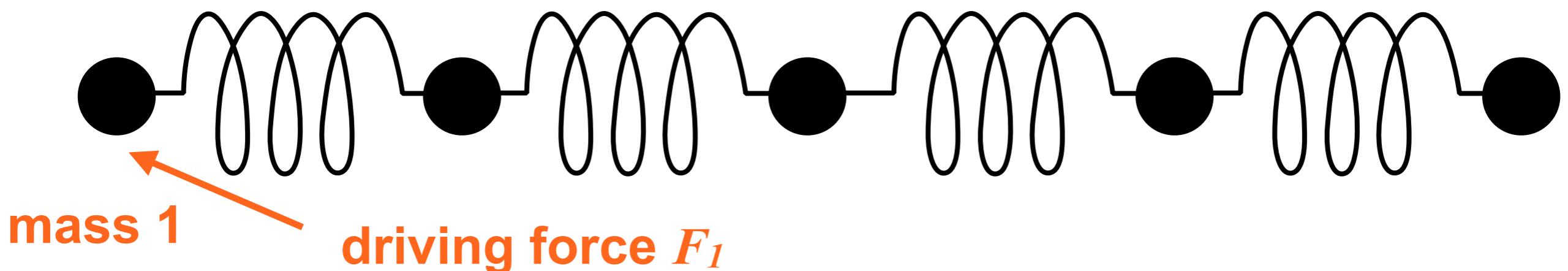


- The chain is finite so that mass 1 and N satisfy the following condition:

$$m \frac{d^2 \xi_1}{dt^2} = k(\xi_2 - \xi_1) + F_1$$

$$m \frac{d^2 \xi_N}{dt^2} = k(\xi_{N-1} - \xi_N) + F_N$$

Example 1 - Vibration in a 1D system

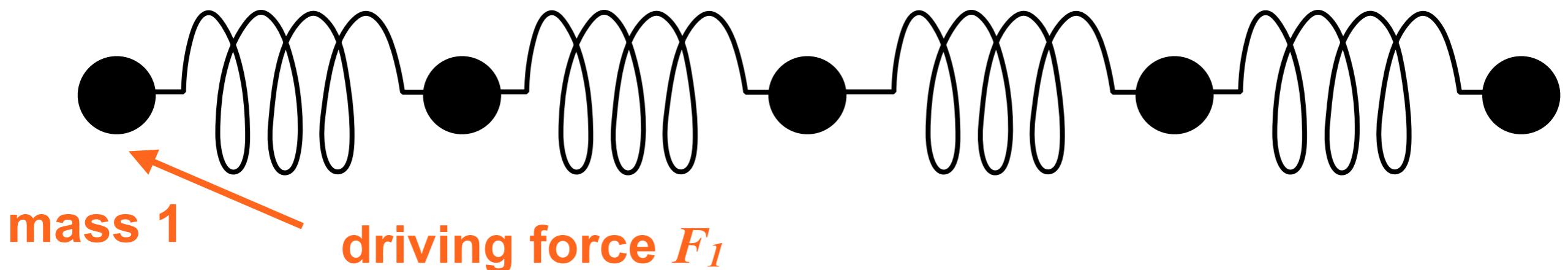


- We apply a harmonic (i.e. sinusoidal) driving force where C is a complex constant:

$$F_1 = C e^{i\omega t}$$

- This could for instance be an electromagnetic wave.

Example 1 - Vibration in a 1D system

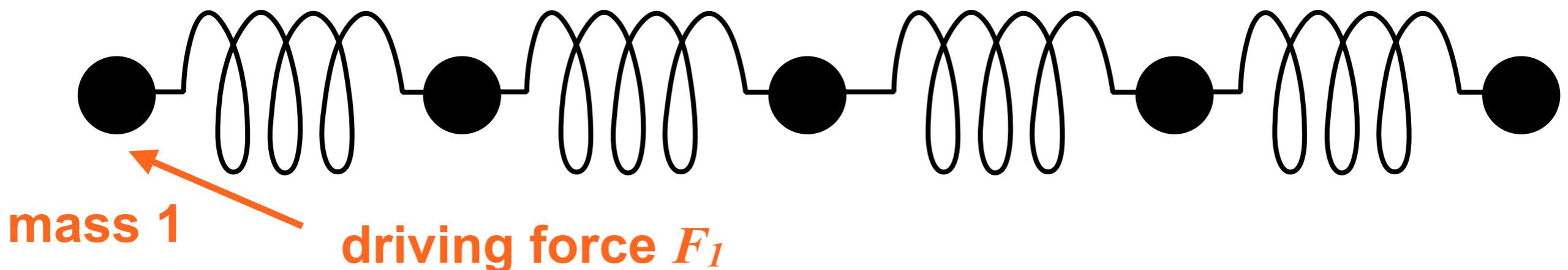


- The masses (atoms) will oscillate in with angular frequency ω :

$$\xi_i(t) = x_i e^{i\omega t}$$

amplitude

Example 1 - Vibration in a 1D system



- Substituting this into our set of Newton's equations gives:

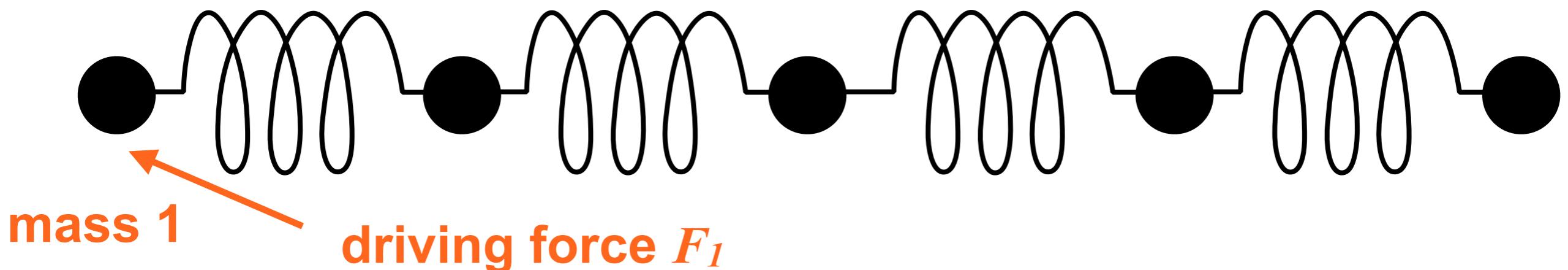
$$-m\omega^2 x_1 = k(x_2 - x_1) + C$$

$$-m\omega^2 x_i = k(x_{i+1} - x_i) + k(x_{i-1} - x_i)$$

$$-m\omega^2 x_N = k(x_{N-1} - x_N)$$

where i ranges from 2 to $N-1$.

Example 1 - Vibration in a 1D system



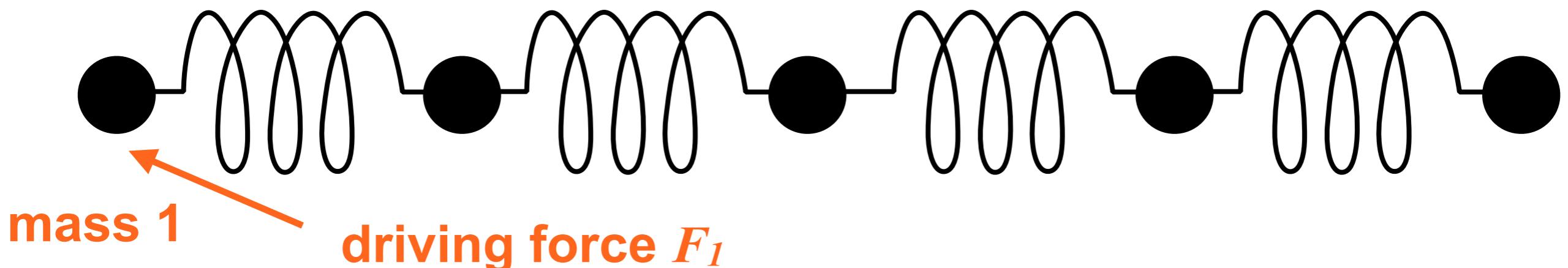
- With $\alpha = 2k - m\omega^2$ we can rearrange to:

$$(\alpha - k)x_1 - kx_2 = C$$

$$\alpha x_i - kx_{i-1} - kx_{i+1} = 0$$

$$(\alpha - k)x_N - kx_{N-1} = 0$$

Example 1 - Vibration in a 1D system



- But this is nothing else than a set of linear equations in tridiagonal form:

$$\begin{pmatrix} (\alpha - k) & -k & & & \\ -k & \alpha & -k & & \\ & -k & \alpha & -k & \\ & & \ddots & \ddots & \ddots \\ & & & -k & \alpha & -k \\ & & & & -k & (\alpha - k) \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{N-1} \\ x_N \end{pmatrix} = \begin{pmatrix} C \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}$$

Linear equations - Exercise 3

Solve the connected linear spring model for 26 masses with $C=1$, $m=1$, $k=2$ and $\omega=2$.

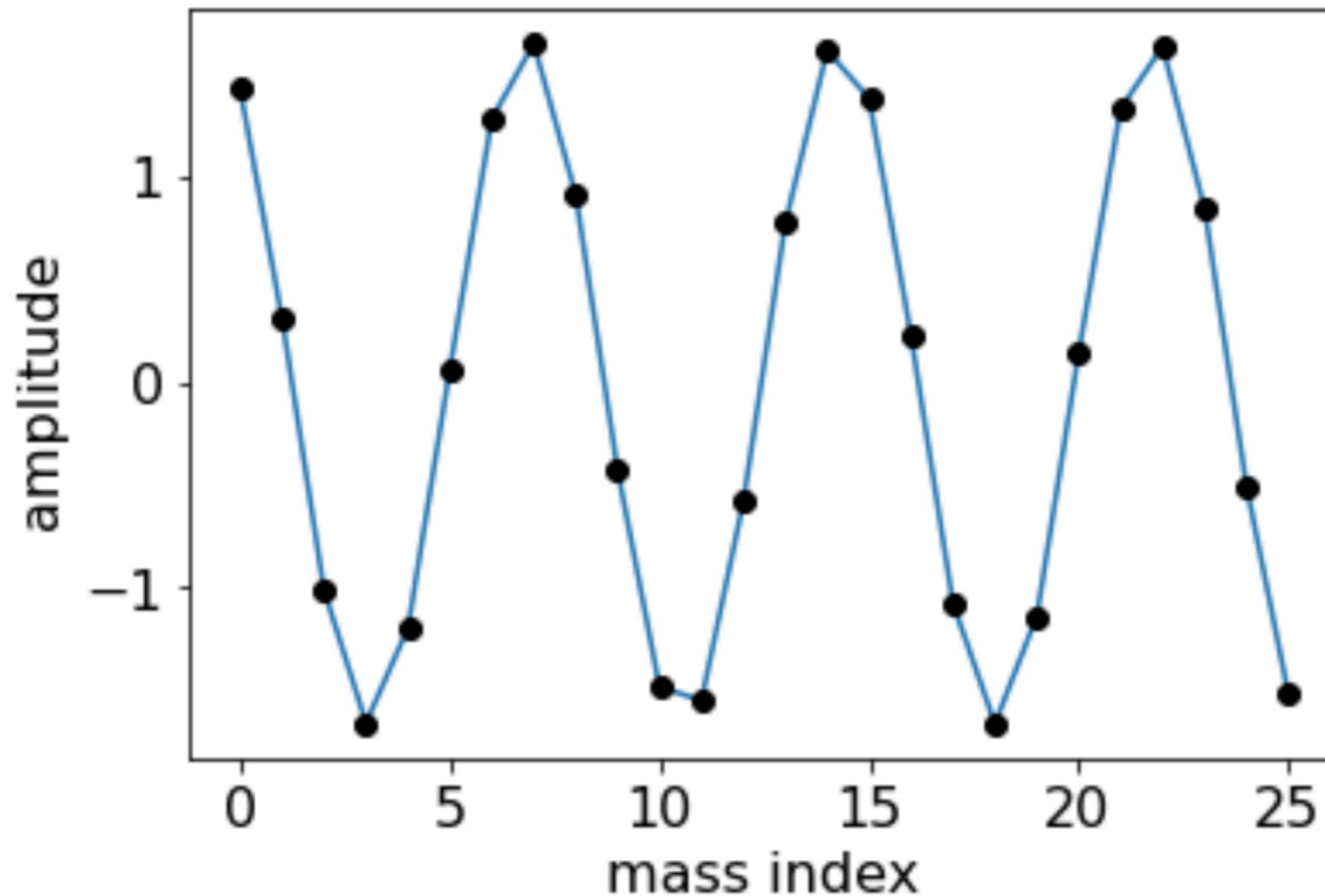
In the `in_class_exercise` notebook you find a skeleton program that calls the subroutine `banded` for the solution of a banded matrix.

1. Download the file `banded.py` from MyCourses.
2. Complete the initialisation part of the program.
3. Add plot statements to plot your results in a graph.

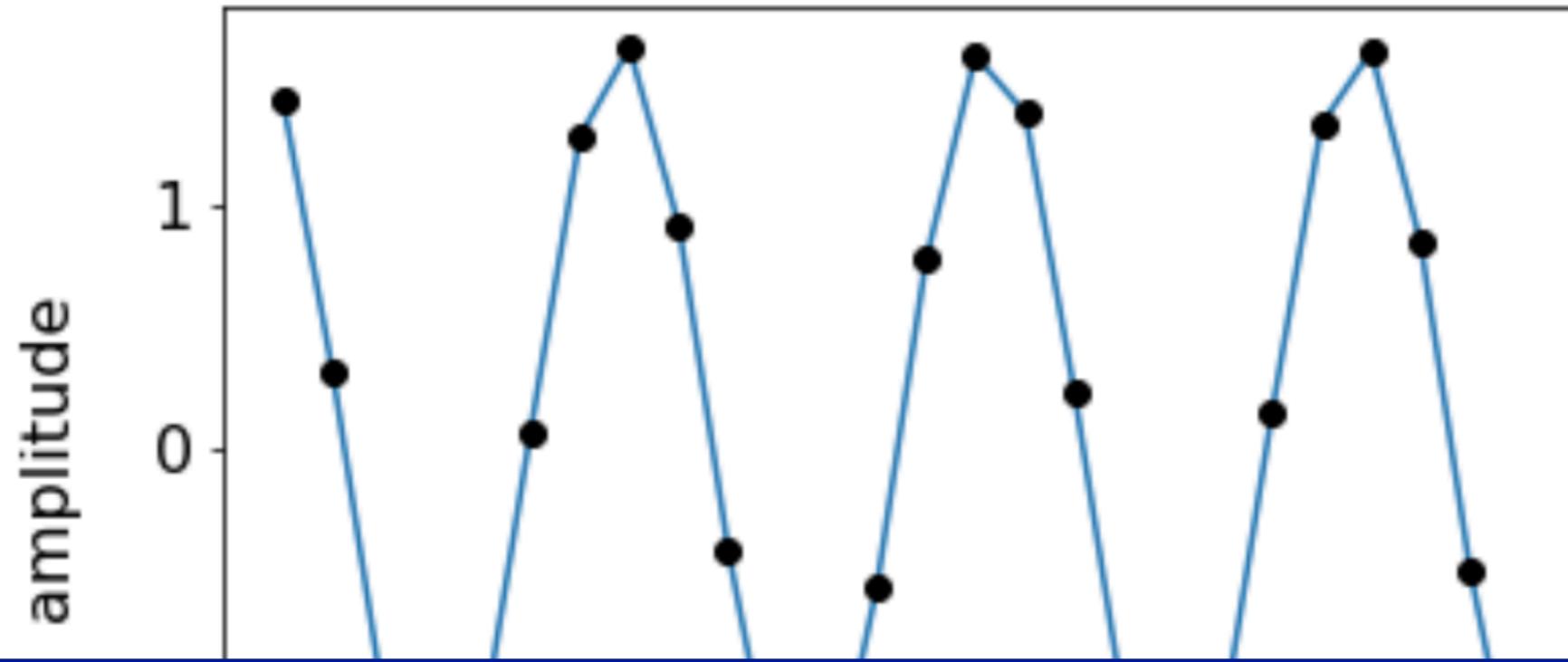
Talking points:

1. **What do you observe?**
2. **What can you say about the amplitudes of the vibrating masses?**

Linear equations - Linear spring model



Linear equations - Linear spring model



Key concept: banded matrices

Many problems in physics result in simplified matrix equations such as banded matrices. Such problems can be solved efficiently with the techniques we just learned.

Linear equations - Eigenvalues and eigenvectors

Eigenvalue problem: $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$

- For a symmetric (or Hermitian) $N \times N$ matrix \mathbf{A} , there are N eigenvalues λ and eigenvectors \mathbf{v} .

Linear equations - Eigenvalues and eigenvectors

Eigenvalue problem: $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$

- For a symmetric (or Hermitian) $N \times N$ matrix \mathbf{A} , there are N eigenvalues λ and eigenvectors \mathbf{v} .
 - We can combine all the solutions for the N many \mathbf{v}_i into one equation:

$$AV = VD$$

orthogonal matrix

diagonal matrix containing the eigenvalues

$$V^T V = VV^T = \mathbb{1}$$

Linear equations - Eigenvalues and eigenvectors

Eigenvalue problem: $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$

- To find the eigenvalues of \mathbf{A} , we use the QR decomposition.

Linear equations - Eigenvalues and eigenvectors

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- The QR decomposition is similar to the LU decomposition.

\mathbf{Q} : **orthogonal matrix** $\mathbf{Q}^T\mathbf{Q} = \mathbf{I}$

\mathbf{R} : **upper triangular matrix**

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- For the graded exercises, you will write your own QR decomposition.
- In Python, SciPy provides a QR decomposition.

Linear equations - Finding eigenvalues

- Suppose we have the QR decomposition of A:

$$A = Q_1 R_1$$

Linear equations - Finding eigenvalues

- Suppose we have the QR decomposition of \mathbf{A} :

$$\mathbf{A} = \mathbf{Q}_1 \mathbf{R}_1$$

- We multiply from the left with \mathbf{Q}_1^T

$$\mathbf{Q}_1^T \mathbf{A} = \mathbf{Q}_1^T \mathbf{Q}_1 \mathbf{R}_1 = \mathbf{R}_1$$

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$$\mathbf{Q}_1^T \mathbf{A} = \mathbf{Q}_1^T \mathbf{Q}_1 \mathbf{R}_1 = \mathbf{R}_1$$

- Then we define a new matrix \mathbf{A}_1 :

$$\mathbf{A}_1 = \mathbf{R}_1 \mathbf{Q}_1 = \mathbf{Q}_1^T \mathbf{A} \mathbf{Q}_1$$



A₁ is an orthogonal transformation of A

Linear equations - Finding eigenvalues

- Next we will repeat the process of forming the QR decomposition of \mathbf{A}_1 and forming a new matrix \mathbf{A}_2 and then decomposing that into its own QR decomposition and so forth:

$$\mathbf{A}_1 = \mathbf{Q}_1^T \mathbf{A} \mathbf{Q}_1$$

$$\mathbf{A}_2 = \mathbf{Q}_2^T \mathbf{Q}_1^T \mathbf{A} \mathbf{Q}_1 \mathbf{Q}_2$$

⋮
⋮

$$\mathbf{A}_k = (\mathbf{Q}_k^T \dots \mathbf{Q}_1^T) \mathbf{A} (\mathbf{Q}_1 \dots \mathbf{Q}_k)$$

Linear equations - Finding eigenvalues

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⋮
⋮

$$\mathbf{A}_k = (\mathbf{Q}_k^T \dots \mathbf{Q}_1^T) \mathbf{A} (\mathbf{Q}_1 \dots \mathbf{Q}_k)$$

- It can be proven, that \mathbf{A}_k becomes eventually diagonal:

$$\mathbf{A}_k = \mathbf{D}$$

Linear equations - Finding eigenvalues

$$\mathbf{A}_k = (\mathbf{Q}_k^T \dots \mathbf{Q}_1^T) \mathbf{A} (\mathbf{Q}_1 \dots \mathbf{Q}_k) = \mathbf{D}$$

- With

$$\mathbf{V} = \mathbf{Q}_1 \mathbf{Q}_2 \mathbf{Q}_3 \dots \mathbf{Q}_k = \prod_{i=1}^k \mathbf{Q}_i$$

this gives us:

$$\mathbf{D} = \mathbf{A}_k = \mathbf{V}^T \mathbf{A} \mathbf{V} \quad \text{or} \quad \mathbf{A} \mathbf{V} = \mathbf{V} \mathbf{D}$$

Linear equations - Finding eigenvalues

$$\mathbf{A}_k = (\mathbf{Q}_k^T \dots \mathbf{Q}_1^T) \mathbf{A} (\mathbf{Q}_1 \dots \mathbf{Q}_k) = \mathbf{D}$$

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↑
eigenvalues

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↑
eigenvectors



This is our eigenvalue equation!

Linear equations - The QR algorithm



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Linear equations - The QR algorithm

The QR algorithm for diagonalizing a matrix (i.e. for calculating its eigenvalues and eigenvectors):

Linear equations - The QR algorithm

The QR algorithm for diagonalizing a matrix (i.e. for calculating its eigenvalues and eigenvectors):

1. Create an $N \times N$ matrix \mathbf{V} and set it to the identity matrix.

Linear equations - The QR algorithm

The QR algorithm for diagonalizing a matrix (i.e. for calculating its eigenvalues and eigenvectors):

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4. Update \mathbf{A} to the new value $\mathbf{A} = \mathbf{R}\mathbf{Q}$.

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5. Multiply \mathbf{V} on the right by \mathbf{Q} .

Linear equations - The QR algorithm

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3. Calculate the QR decomposition $\mathbf{A} = \mathbf{Q}\mathbf{R}$.
4. Update \mathbf{A} to the new value $\mathbf{A} = \mathbf{R}\mathbf{Q}$.
5. Multiply \mathbf{V} on the right by \mathbf{Q} .
6. Check the off-diagonal elements of \mathbf{A} . If they are all less than ε , we are done. Otherwise go back to step 3.

Linear equations - QR decomposition

Key concept: QR decomposition

The *QR decomposition* is another factorisations of a square matrix A. It factors A into an orthogonal and an upper triangular matrix. Successive application of the QR decomposition diagonalises a matrix and finds its eigenvalues and eigenvectors.

Linear equations - Eigenvalues and eigenvectors

- Numpy has build-in routines in its linalg module for finding eigenvalues and eigenvectors:

```
from numpy.linalg import eigh,eigvalsh  
x,v = eigh(A)  
x = eigvalsh(A)
```

eigenvalues and
eigenvectors

returns just eigenvalues

Linear equations - Exercise 4

$$\mathbf{A} = \begin{pmatrix} 2 & 6 & 7 \\ 1 & 0 & -1 \\ 2 & 3 & -2 \end{pmatrix}$$

- The matrix \mathbf{A} has the QR decomposition:

$$\mathbf{Q} = \frac{1}{3} \begin{pmatrix} 2 & 2 & 1 \\ 1 & -2 & 2 \\ 2 & -1 & -2 \end{pmatrix} \quad \mathbf{R} = 3 \begin{pmatrix} 1 & 2 & 1 \\ 0 & 1 & 2 \\ 0 & 0 & 1 \end{pmatrix}$$

- Verify that $\mathbf{Q}^T \mathbf{Q} = \mathbf{I}$
- Check that $\mathbf{QR} = \mathbf{A}$

Linear equations - Exercise 5

Diagonalize: $A = \begin{pmatrix} 2 & 1 & 2 \\ 1 & 0 & 3 \\ 2 & 3 & -2 \end{pmatrix}$

1. Calculate the eigenvalues and eigenvectors of A using the numpy function eigh.
2. Verify that $V^T A V = \mathbb{1}$

Talking points:

1. What do you observe?



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