Chapter 1

Linear Systems of Equations

Introduction

Linear Systems of Equations: Example

- Consider an open economy with two very basic industries: **goods** and **services**.

- To produce €1 of their products ($\rightsquigarrow$ **internal demand**),
  - the **goods** industry must spend €0.40 on goods and €0.20 on services
  - the **services** industry must spend €0.30 on goods and €0.30 on services

- Assume also that during a period of one week, the economy has an **external demand** of **€75,000 in goods** and **€50,000 in services.**

- **Question:** How much should each sector produce to meet both **internal and external demand?**

Formulating the equations

- Let x_1 **be the Euro value of goods** produced and x_2 **the Euro value of services** produced.
- The total Euro value of **goods consumed** is $\underbrace{0.4x_1 + 0.3x_2}_{\text{internal}} + \underbrace{75000}_{\text{external}}$.
- The total Euro value of **services consumed** is $0.2x_1 + 0.3x_2 + 50000$.
- If we assume that **production equals consumption**, then we get

$$\begin{aligned} x_1 &= 0.4x_1 + 0.3x_2 + 75000 \\ x_2 &= 0.2x_1 + 0.3x_2 + 50000 \end{aligned} \quad \Leftrightarrow \quad \begin{bmatrix} 0.6 & -0.3 \\ -0.2 & 0.7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 75000 \\ 50000 \end{bmatrix}$$

- The **solution** is $x_1 = 187500, \quad x_2 = 125000$. Can be checked easily...

Formal solution

- Main inside: triangular systems can be easily solved by substitution
  $\rightsquigarrow$ transform system to (upper) triangular.

- Do all operations on **augmented matrix** $\begin{bmatrix} A & \boldsymbol{b} \end{bmatrix}$.

$$\begin{bmatrix} 0.6 & -0.3 & 75000 \\ -0.2 & 0.7 & 50000 \end{bmatrix} \Rightarrow \begin{bmatrix} 0.6 & -0.3 & 75000 \\ -0.6 & 2.1 & 150000 \end{bmatrix} \Rightarrow \begin{bmatrix} 0.6 & -0.3 & 75000 \\ 0 & 1.8 & 225000 \end{bmatrix}$$

$$\Rightarrow 1.8x_2 = 225000 \Rightarrow x_2 = 125000 \Rightarrow x_1 = 187500.$$

- **Elimination step:** subtract a multiple of eq. 2 from eq. 1.
  $\rightsquigarrow$ **Gaussian elimination**

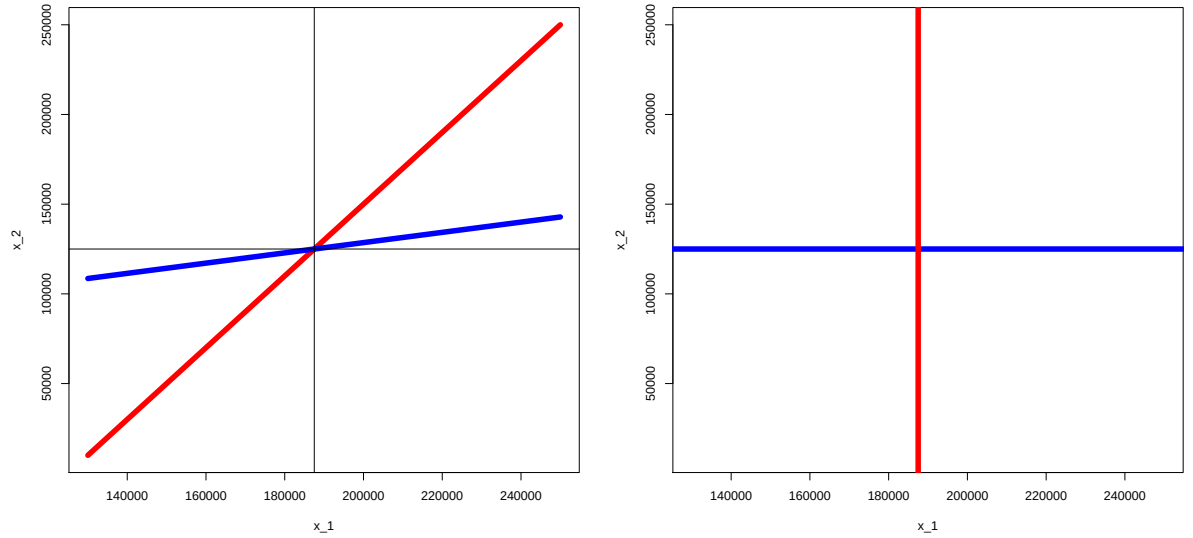
Formal solution

Instead of substituting, we could have continued with the elimination:

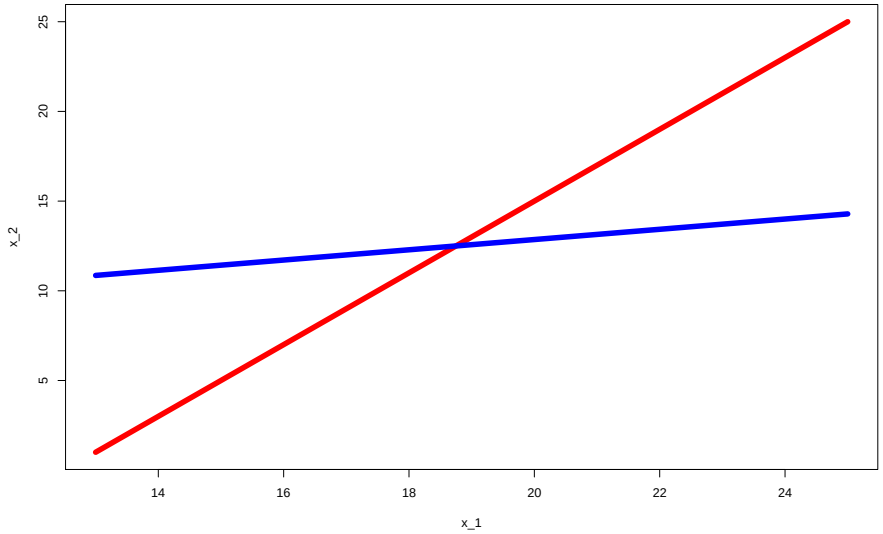
$$\begin{bmatrix} 0.6 & -0.3 & 75000 \\ 0 & 1.8 & 225000 \end{bmatrix} \Rightarrow \begin{bmatrix} 3.6 & -1.8 & 450000 \\ 0 & 1.8 & 225000 \end{bmatrix} \Rightarrow \begin{bmatrix} 3.6 & 0 & 675000 \\ 0 & 1.8 & 225000 \end{bmatrix}$$

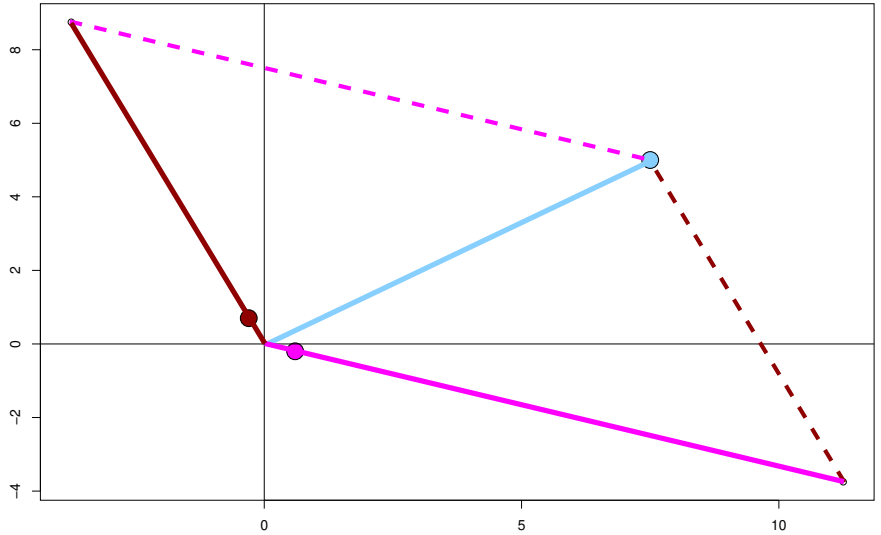
$\rightsquigarrow$ **Gauss-Jordan elimination**

Geometric interpretation: have transformed original equations into a new space in which they are aligned with the coordinate axis:



Row and column view

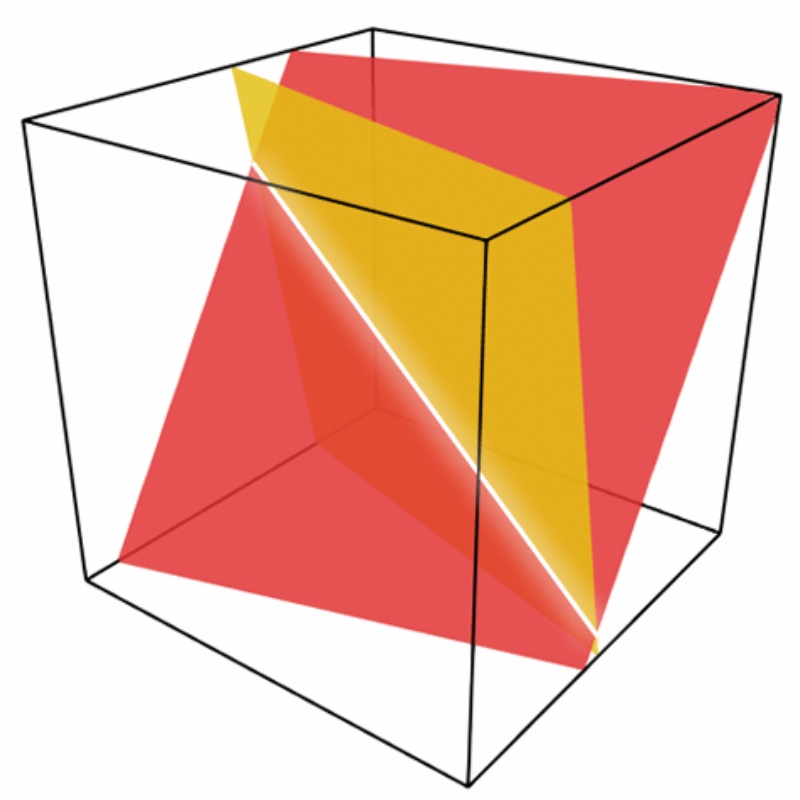




$$\begin{aligned} 0.6x_1 - 0.3x_2 &= 7.5 \\ -0.2x_1 + 0.7x_2 &= 5 \end{aligned} \quad \Leftrightarrow \quad \begin{bmatrix} 0.6 & -0.3 \\ -0.2 & 0.7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 7.5 \\ 5 \end{bmatrix}$$

Column view (right): $\begin{bmatrix} 0.6 \\ -0.2 \end{bmatrix} x_1 + \begin{bmatrix} -0.3 \\ 0.7 \end{bmatrix} x_2 = \begin{bmatrix} 7.5 \\ 5 \end{bmatrix}$

Some examples and concepts



The solution set for two equations in three variables is usually a line.

This is an example of an **underdetermined** system.

Chapter 1

Linear Systems of Equations

Linear Algebra I

Definition: The **vector space** $\mathbb{R}^n$ consists of all column vectors v with n real components.

Vector spaces and subspaces

A **subspace** of a vector space is a **nonempty subset** that satisfies the

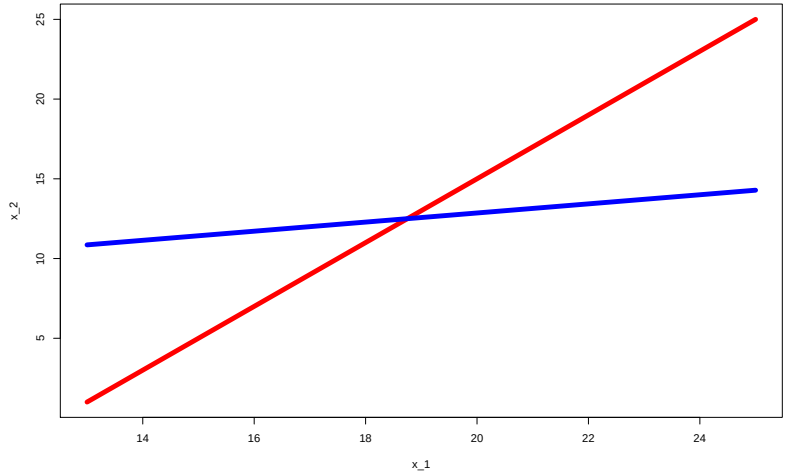
Requirements for a **vector space:**
"Linear combinations stay in the subspace"
(i) If we add any vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ in the subspace,
$\boldsymbol{x} + \boldsymbol{y}$ is in the subspace.
(ii) If we multiply any vector $\boldsymbol{x}$ in the subspace by **any scalar** c,
$c\boldsymbol{x}$ is in the subspace.

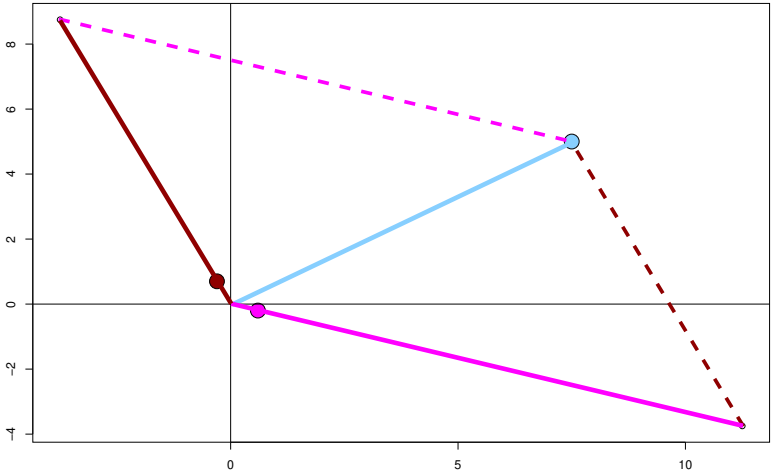
Rule (ii) with $c = 0 \rightsquigarrow$ **Every subspace contains the zero vector.**

The smallest subspace Z contains only the zero vector.
Why? Rules (i) and (ii) are satisfied:
$\mathbf{0} + \mathbf{0}$ is in this one-point space, and so are all multiples $c\mathbf{0}$.

The **largest subspace** is the whole of the original space.

The column space of a matrix





Column view (right): $\begin{bmatrix} 0.6 \\ -0.2 \end{bmatrix} x_1 + \begin{bmatrix} -0.3 \\ 0.7 \end{bmatrix} x_2 = \begin{bmatrix} 7.5 \\ 5 \end{bmatrix}$

The **column space** $C(A)$ contains all linear combinations of the columns of $A_{m \times n} \rightsquigarrow$ subspace of $\mathbb{R}^m$.

The system $Ax = b$ is solvable iff b is in the column space of A.

Nullspace

A system with right-hand side $\boldsymbol{b} = \mathbf{0}$ always allows the solution $\boldsymbol{x} = \mathbf{0}$, but there may be **infinitely many other solutions.**

The solutions to $A\boldsymbol{x} = \mathbf{0}$ form the **nullspace of A.**

The **nullspace** $N(A)$ of a matrix A consists of all vectors $\boldsymbol{x}$ such that $A\boldsymbol{x} = \mathbf{0}$. It is a subspace of $\mathbb{R}^n$:
(i) If $A\boldsymbol{x} = \mathbf{0}$ and $A\boldsymbol{x}' = \mathbf{0}$, then $A(\boldsymbol{x} + \boldsymbol{x}') = \mathbf{0}$.
(ii) If $A\boldsymbol{x} = \mathbf{0}$ then $A(c\boldsymbol{x}) = cA\boldsymbol{x} = \mathbf{0}$.

For an invertible matrix A:

- $N(A)$ **contains only** $\boldsymbol{x} = \mathbf{0}$ (multiply $A\boldsymbol{x} = \mathbf{0}$ by A^{-1}).
- **The column space is the whole space.**
  ($A\boldsymbol{x} = \boldsymbol{b}$ has a solution for every $\boldsymbol{b}$)
- **The columns of A are independent.**

Nullspace

Singular matrix example:

$$A = \begin{bmatrix} 1 & 2 \\ 3 & 6 \end{bmatrix}.$$

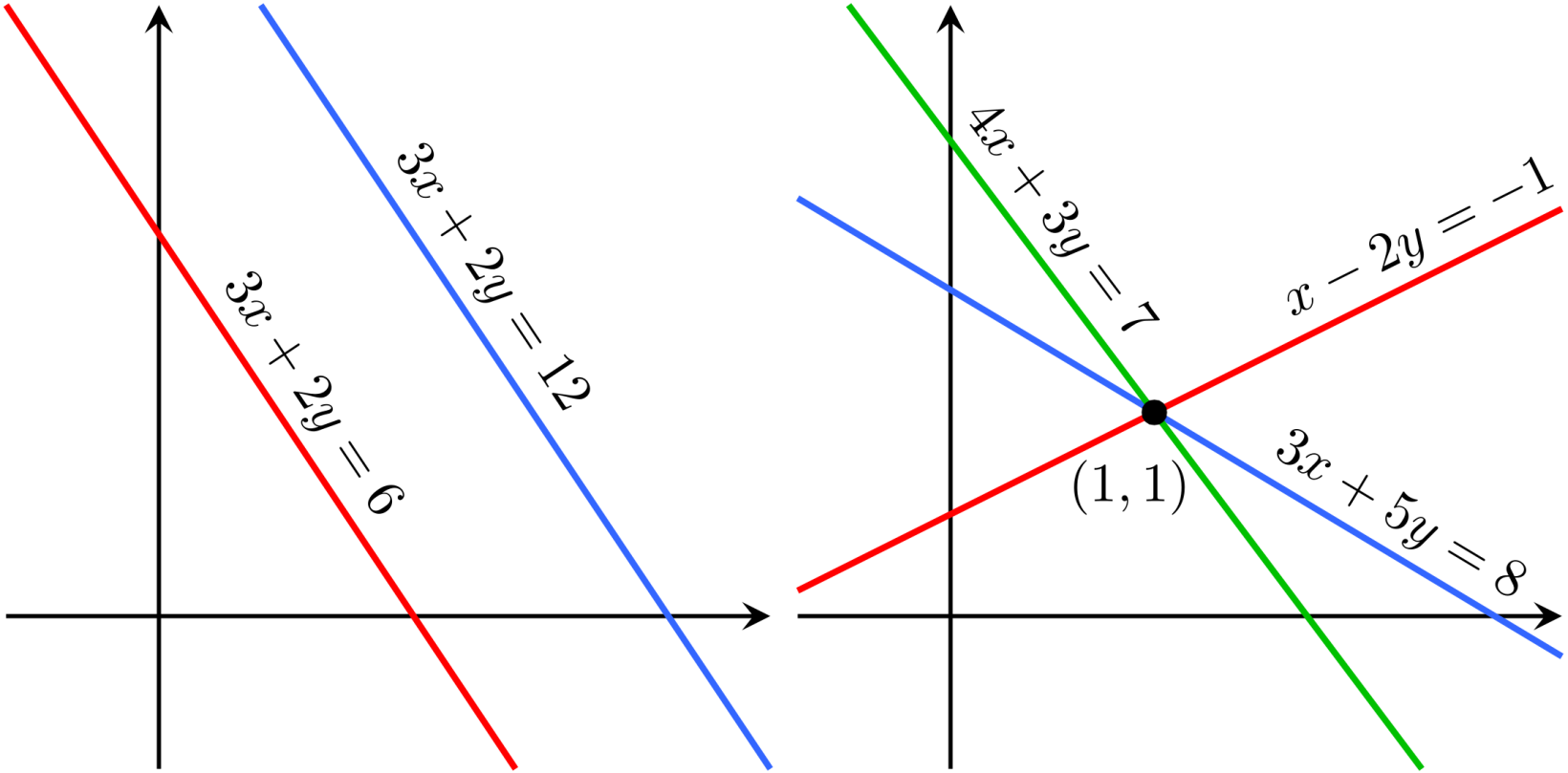
Consider $A\boldsymbol{x} = \mathbf{0}$: Any pair that fulfills $x_1 + 2x_2 = 0$ is a solution.
This line is the **one-dimensional nullspace** $N(A)$.

Choose one point on this line as a "special" solution
$\rightsquigarrow$ all points on the line are multiples.

Let $\boldsymbol{x}_p$ be a particular solution and $\boldsymbol{x}_n \in N(A)$:
The solutions to all linear equations have the form $\boldsymbol{x} = \boldsymbol{x}_p + \boldsymbol{x}_n$.

Proof: $A\boldsymbol{x}_p = \boldsymbol{b}$ and $A\boldsymbol{x}_n = \mathbf{0}$ produce $A(\boldsymbol{x}_p + \boldsymbol{x}_n) = \boldsymbol{b}$.

Inconsistent equations and linear dependency



The equations $3x + 2y = 6$ and $3x + 2y = 12$ are **inconsistent**:
$\boldsymbol{b}$ is **not** in the $C(A)$ $\rightsquigarrow$ no solution exists!

$x - 2y = -1$, $3x + 5y = 8$, and $4x + 3y = 7$ are **linearly dependent**:
$\boldsymbol{b} \in C(A)$ $\rightsquigarrow$ solution exists, but two equations are sufficient.

Linear Dependence

A sequence of vectors $\{\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_k\}$ from a vector space V is said to be **linearly dependent**, if there exist scalars $a_1, a_2, \ldots, a_k$, **not all zero**, such that

$$a_1\boldsymbol{v}_1 + a_2\boldsymbol{v}_2 + \cdots + a_k\boldsymbol{v}_k = \mathbf{0}.$$

Linear dependence:

Not all of the scalars are zero $\rightsquigarrow$ at least one is non-zero (say a_1):

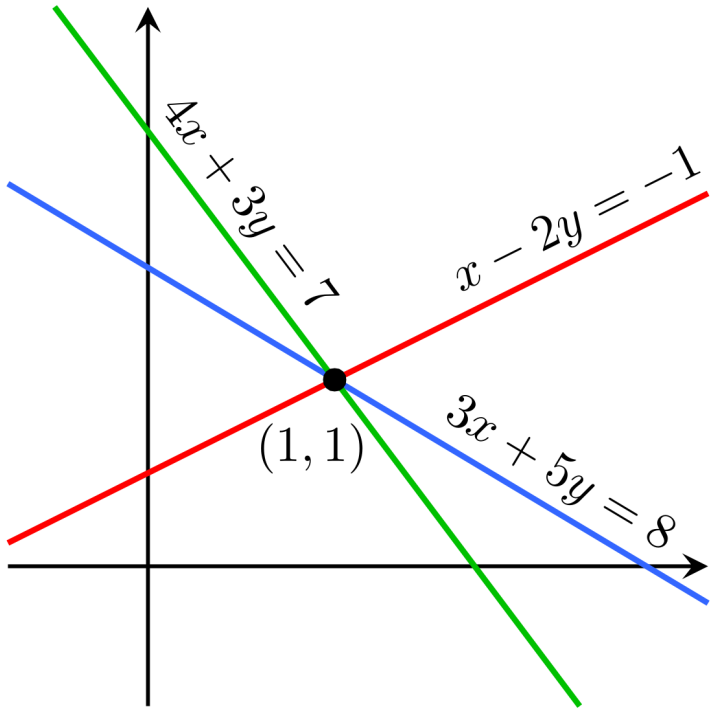
$$\boldsymbol{v}_1 = \frac{-a_2}{a_1}\boldsymbol{v}_2 + \cdots + \frac{-a_k}{a_1}\boldsymbol{v}_k.$$

Thus, $\boldsymbol{v}_1$ is a **linear combination of the remaining vectors.**

Linear Dependence Example

Matrix form: $A\boldsymbol{x} = \boldsymbol{b}$

$$\begin{bmatrix} 1 & -2 \\ 3 & 5 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} -1 \\ 8 \\ 7 \end{bmatrix}$$



Row vectors of A are linearly dependent

$$\begin{bmatrix} 1 \\ -2 \end{bmatrix} + \begin{bmatrix} 3 \\ 5 \end{bmatrix} - \begin{bmatrix} 4 \\ 3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Linear Independence

The vectors $\{\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_k\}$ are **linearly independent** if the equation

$$a_1\boldsymbol{v}_1 + a_2\boldsymbol{v}_2 + \cdots + a_k\boldsymbol{v}_k = \mathbf{0}$$

can **only** be satisfied by $a_i = 0$ for $i = 1, \ldots, k$.

- This implies that **no vector in the set can be represented as a linear combination of the remaining vectors** in the set.
- In other words: A set of vectors is linearly independent if the only representations of $\mathbf{0}$ as a linear combination of the vectors is the **trivial representation** in which all scalars a_i are zero.
- Any set of $k > m$ vectors in $\mathbb{R}^m$ must be linearly dependent.

Span and Basis

A set of vectors **spans a space** if their linear combinations fill the space.

Special case: the columns of a matrix A span its **column space** $C(A)$.
They might be **independent** $\rightsquigarrow$ **basis of** $C(A)$**.**

A basis for a vector space is a sequence of vectors such that:
(i) the basis vectors are linearly independent, and
(ii) they span the space.

Immediate consequence: There is **one and only one way** to write an element of the space as a combination of the basis vectors.

The dimension of a space is the number of vectors in every basis.

The dimension of $C(A)$ is called the (column-)**rank** of A.

The dimension of $N(A)$ is called the **nullity** of A.

Nullspace and Independence

Example: The columns of this triangular matrix are linearly independent:

$$A = \begin{bmatrix} 3 & 4 & 2 \\ 0 & 1 & 5 \\ 0 & 0 & 2 \end{bmatrix}.$$

Why? Solving $A\boldsymbol{x} = \mathbf{0} \rightsquigarrow$ look for combination of the columns that produces $\mathbf{0}$:

$$c_1 \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix} + c_2 \begin{bmatrix} 4 \\ 4 \\ 0 \end{bmatrix} + c_3 \begin{bmatrix} 2 \\ 5 \\ 2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Independence: show that c_1, c_2, c_3 are all forced to be zero.

Last equation $\rightsquigarrow c_3 = 0$. Next equation gives $c_2 = 0$, substituting into 1st eq.: $c_1 = 0$.

The nullspace of A contains only the zero vector $c_1 = c_2 = c_3 = 0$.

The columns of A are independent exactly when $N(A) = \{\mathbf{0}\}$.

Then, the dimension of the column space (the rank) is n.

We say that the matrix has **full rank**.

Chapter 1

Linear Systems of Equations

Gauss-Jordan Elimination

The invertible case: Gauss-Jordan elimination

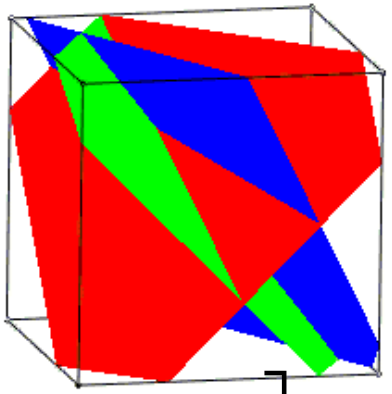
Assume A is invertible $\rightsquigarrow$ a solution is guaranteed to exist: $\boldsymbol{x} = A^{-1}\boldsymbol{b}$.
Sometimes we also want to find the inverse itself.
Then **Gauss-Jordan elimination** is the method of choice.

- **PRO**
  - produces both the solution(s), for (multiple) $\boldsymbol{b}_j$, **and the inverse** A^{-1}
  - numerically stable if **pivoting** is used $\rightsquigarrow$ will be discussed later...
  - **straightforward, understandable** method
- **CON**
  - all right hand sides $\boldsymbol{b}_j$ must be known before the elimination starts.
  - **three times slower** than alternatives when inverse is not required

The invertible case: Gauss-Jordan elimination

- **Augmented matrix** $A' = [A, \boldsymbol{b}_1, \ldots, \boldsymbol{b}_j, I_n]$

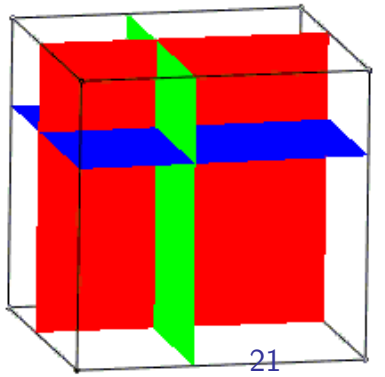
- Idea:
  Define $B = [\boldsymbol{b}_1, \ldots, \boldsymbol{b}_j] \quad X = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_j]$
  $[A, B, I] \Rightarrow A^{-1}[A, B, I] = [IXA^{-1}]$.



- Example:

$$A = \begin{bmatrix} 1 & 3 & -2 \\ 3 & 5 & 6 \\ 2 & 4 & 3 \end{bmatrix}, \quad B = \begin{bmatrix} 5 \\ 7 \\ 8 \end{bmatrix} \Rightarrow [A, B, I] = \begin{bmatrix} 1 & 3 & -2 & 5 & 1 & 0 & 0 \\ 3 & 5 & 6 & 7 & 0 & 1 & 0 \\ 2 & 4 & 3 & 8 & 0 & 0 & 1 \end{bmatrix}$$

$$\Rightarrow [I, X, A^{-1}] = \begin{bmatrix} 1 & 0 & 0 & -15 & \frac{9}{4} & \frac{17}{4} & -7 \\ 0 & 1 & 0 & 8 & -\frac{3}{4} & -\frac{7}{4} & 3 \\ 0 & 0 & 1 & 2 & -\frac{1}{2} & -\frac{1}{2} & 1 \end{bmatrix}$$



Gauss-Jordan: Simplest Form

Main idea: Cycle through columns of A ($\rightsquigarrow$ pivot column) and select entry on diagonal ($\rightsquigarrow$ pivot element).

Then normalize pivot row and introduce zeros below and above.

Pivot column: 1, pivot element = 1. Divide pivot row by pivot element

$$\begin{bmatrix} 1 & 3 & -2 & 5 & 1 & 0 & 0 \\ 3 & 5 & 6 & 7 & 0 & 1 & 0 \\ 2 & 4 & 3 & 8 & 0 & 0 & 1 \end{bmatrix}$$

For all other rows: (i) store element in pivot column,
(ii) subtract pivot row multiplied with this element

$$\begin{bmatrix} 1 & 3 & -2 & 5 & 1 & 0 & 0 \\ 0 & -4 & 12 & -8 & -3 & 1 & 0 \\ 0 & -2 & 7 & -2 & -2 & 0 & 1 \end{bmatrix}$$

Proceed to pivot column 2 with pivot element = -4

Gauss-Jordan: Simplest Form

Proceed to pivot column 2 with pivot element = -4

$$\begin{bmatrix} 1 & 0 & 7 & -1 & -1.25 & 0.75 & 0 \\ 0 & 1 & -3 & 2 & 0.75 & -0.25 & 0 \\ 0 & 0 & 1 & 2 & -0.5 & -0.5 & 1 \end{bmatrix}$$

After elimination in column 3 with pivot = 1

$$\begin{bmatrix} 1 & 0 & 0 & -15 & 2.25 & 4.25 & -7 \\ 0 & 1 & 0 & 8 & -0.75 & -1.75 & 3 \\ 0 & 0 & 1 & 2 & -0.5 & -0.5 & 1 \end{bmatrix}$$

Now we have transformed A to the identity matrix I.

This is a special case of the **reduced row Echelon form** (more on this later).

The **solution vector** is the 4th column $\boldsymbol{x} = (-15, 8, 2)^t$.

Note that we have overwritten the original $\boldsymbol{b} \rightsquigarrow$ no need to allocate further memory.

The **inverse** A^{-1} is the right 3×3 block.

Gauss-Jordan elimination

Elementary operations (they **do not change** the solution):

1. **Replace a row** by a linear combination of itself and any other row(s).
2. **Interchange two rows**.
3. **Interchange two columns** and **corresponding rows** of x.

Basic G-J elimination uses **only operation #1** but...
Elimination **fails mathematically** when a **zero pivot** is encountered
$\rightsquigarrow$ pivoting is essential to avoid **total failure** of the algorithm.

Example: Try $Ax = b$ with

$$A = \begin{bmatrix} 2 & 4 & -2 & -2 \\ 1 & 2 & 4 & -3 \\ -3 & -3 & 8 & -2 \\ -1 & 1 & 6 & -3 \end{bmatrix}, \quad b = \begin{bmatrix} -4 \\ 5 \\ 7 \\ 7 \end{bmatrix}$$

Chapter 1

Linear Systems of Equations

Linear Systems: Numerical Issues

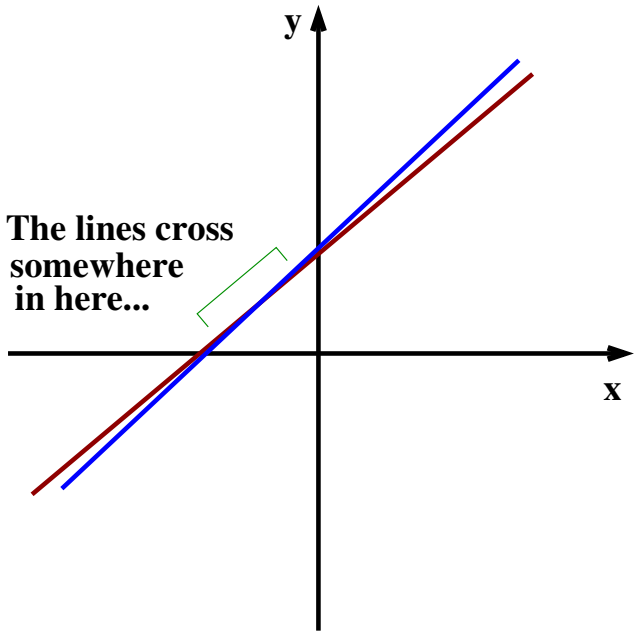
The need for pivoting

- Elimination **fails mathematically** when a **zero pivot** is encountered
- and **fails numerically** with a **too-close-to-zero pivot** (we will see why in a minute...)
- The fix is **partial pivoting**
  - use **operation #2** to place a **desirable** pivot entry in the current row
  - **usually sufficient** for stability
- Using **operation #3** as well gives **full pivoting**

Linear systems: numerical issues

If a system is **too close to linear dependence**

- an algorithm may **fail altogether** to get a solution
- **round off errors** can produce apparent linear dependence at some point in the solution process
  $\rightsquigarrow$ **accumulated roundoff errors**
  can dominate in the solution
  $\rightsquigarrow$ an algorithm may still work
  but **produce nonsense**.



When is sophistication necessary?

- Sophisticated methods can **detect and correct** numerical pathologies
- Rough guide for a **"not-too-singular"** $n \times n$ system:
  - $n < 20...50$ **single** precision
  - $n < 200...300$ **double** precision
  - $n = 1000$ OK if equations are **sparse**
    (special techniques take advantage of sparsity)
- **Close-to-singular** can be a problem even for **very small** systems
- But...what is the underlying reason for these numerical problems?

Floating Point Numbers: float, double

- `float` similar to **scientific notation**
  $\pm$ D.DDDD $\times 10^{\mathsf{E}}$
  - D.DDDD has leading mantissa digit $\neq 0$
  - D.DDDD has **fixed** number of mantissa digits.
  - E is **signed integer**.

- **Precision varies:** precision of 1.000×10^{-2} is 100 times higher than precision of 1.000×10^{0}.

- The **bigger the number**, the **less precise**:
  $1.000 \times 10^{4} + 1.000 \times 10^{0} = 1.000 \times 10^{4}$!!!

Simple Data Types: float, double (2)

Technical Realization (IEEE Standard 754)

- 32 bit (`float`) or 64 bit (`double`)
- `float`:

  1 bit *sign* ($s \in \{0, 1\}$)
  8 bit *exponent* ($e \in \{0, 1, \ldots, 255\}$) (like before, but basis 2!)
  23 bit *mantissa* ($m \in \{0, 1, \ldots, 2^{23} - 1\}$)

S	EEEEEEEE	MMMMMMMMMMMMMMMMMMMMMMM

- `double`: 1 bit sign, 11 bit exponent, 52 bit mantissa

S	EEEEEEEEEEE	MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM

Floating Point Arithmetic: Problems

- **Fixed number of mantissa bits $\Rightarrow$ limited precision:**
  If `a` $\gg$ `b` $\Rightarrow$ `a+b = a`.

- Iterated addition of small numbers (like `a=a+b` with `a` $\gg$ `b`) can lead to a **huge error**: at some point, `a` does not increase anymore, **independent of the number of additions**.

- `double` is better, but needs **two times more memory**.

- **Machine epsilon** (informal definition): The smallest number ϵ_m which when added to 1 gives something different than 1.
  Float (23 mantissa bits): $\epsilon_m \approx 2^{-23} \approx 10^{-7}$,
  Double (52 mantissa bits): $\epsilon_m \approx 2^{-52} \approx 10^{-16}$.

Chapter 1

Linear Systems of Equations

Elementary Matrices

Elementary matrices: Row-switching transformations

Switches row i and row j. Example:

$$R_{35}A = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{0} & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{1} & 0 & \mathbf{0} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \\ a_{41} & a_{42} \\ a_{51} & a_{52} \\ a_{61} & a_{62} \\ a_{71} & a_{72} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{51} & a_{52} \\ a_{41} & a_{42} \\ a_{31} & a_{32} \\ a_{61} & a_{62} \\ a_{71} & a_{72} \end{bmatrix}$$

The inverse of this matrix is itself: $R_{ij}^{-1} = R_{ij}$

Elementary matrices: Row-multiplying transformations

Multiplies all elements on row i by $m \neq 0$.

$$R_i(m) = \begin{bmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & 1 & & & & \\ & & & m & & & \\ & & & & 1 & & \\ & & & & & \ddots & \\ & & & & & & 1 \end{bmatrix}$$

The inverse of this matrix is: $R_i(m)^{-1} = R_i(1/m)$.

Elementary matrices: Row-addition transformations

Subtracts row j multiplied by m from row i.

$$R_{ij}(m) = \begin{bmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & & & \\ & & & \ddots & & \\ & & -m & & 1 & \\ & & & & & \ddots \\ & & & & & & 1 \end{bmatrix}$$

The inverse of this matrix is: $R_{ij}(m)^{-1} = R_{ij}(-m)$.

Row operations

- Elementary row operations correspond to **left-multiplication** by elementary matrices:

$$A \cdot \boldsymbol{x} = \boldsymbol{b}$$
$$(\cdots R_3 \cdot R_2 \cdot R_1 \cdot A) \cdot \boldsymbol{x} = \cdots R_3 \cdot R_2 \cdot R_1 \cdot \boldsymbol{b}$$
$$(I_n) \cdot \boldsymbol{x} = \cdots R_3 \cdot R_2 \cdot R_1 \cdot \boldsymbol{b}$$
$$\boldsymbol{x} = \cdots R_3 \cdot R_2 \cdot R_1 \cdot \boldsymbol{b}$$

- x can be built-up **in stages** since the R matrices are multiplied in the **order of acquisition**.

- **Inverse** matrix A^{-1} and **solution** $\boldsymbol{x}$ can be built up in the storage locations of A and $\boldsymbol{b}$ respectively.

Column operations

Elementary column operations correspond to **right-multiplication**: transform rows of A^t, then transpose: $(RA^t)^t = AR^t = AC \rightsquigarrow C = R^t$.
Note that $(AB)^t = B^t A^t$.

$$
\begin{aligned}
A \cdot \boldsymbol{x} &= \boldsymbol{b} \\
A \cdot C_1 \cdot C_1^{-1} \cdot \boldsymbol{x} &= \boldsymbol{b} \\
A \cdot C_1 \cdot C_2 \cdot C_2^{-1} \cdot C_1^{-1} \cdot \boldsymbol{x} &= \boldsymbol{b} \\
(A \cdot C_1 \cdot C_2 \cdot C_3 \cdots) \cdot (\cdots C_3^{-1} \cdot C_2^{-1} \cdot C_1^{-1}) \cdot \boldsymbol{x} &= \boldsymbol{b} \\
(I_n) \cdot (\cdots C_3^{-1} \cdot C_2^{-1} \cdot C_1^{-1}) \cdot \boldsymbol{x} &= \boldsymbol{b} \\
\boldsymbol{x} &= C_1 \cdot C_2 \cdot C_3 \cdots \cdot \boldsymbol{b}
\end{aligned}
$$

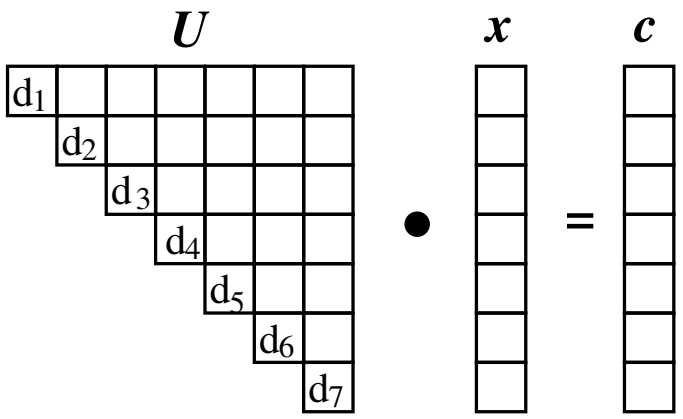
The C matrices must be **stored until the last step:**
they are applied to $\boldsymbol{b}$ in the **reverse order of acquisition.**

Gaussian Elimination with Backsubstitution

- Like Gauss-Jordan, but (i) don't normalize pivot row,
  and (ii) introduce zeros only in rows **below the current pivot element.**

- Example: a_{22} is current **pivot** element
  $\rightsquigarrow$ use pivot row to zero only $a_{32}, a_{42}, \ldots$

- Suppose we use partial pivoting (never change columns)
  $\rightsquigarrow$ Original system $A\boldsymbol{x} = \boldsymbol{b}$ transformed to
  upper triangular system $U\boldsymbol{x} = \boldsymbol{c}$.
  $\rightsquigarrow$ Pivots $d_1, \ldots, d_n$ on diagonal of U.



- Solve with **backsubstitution**.

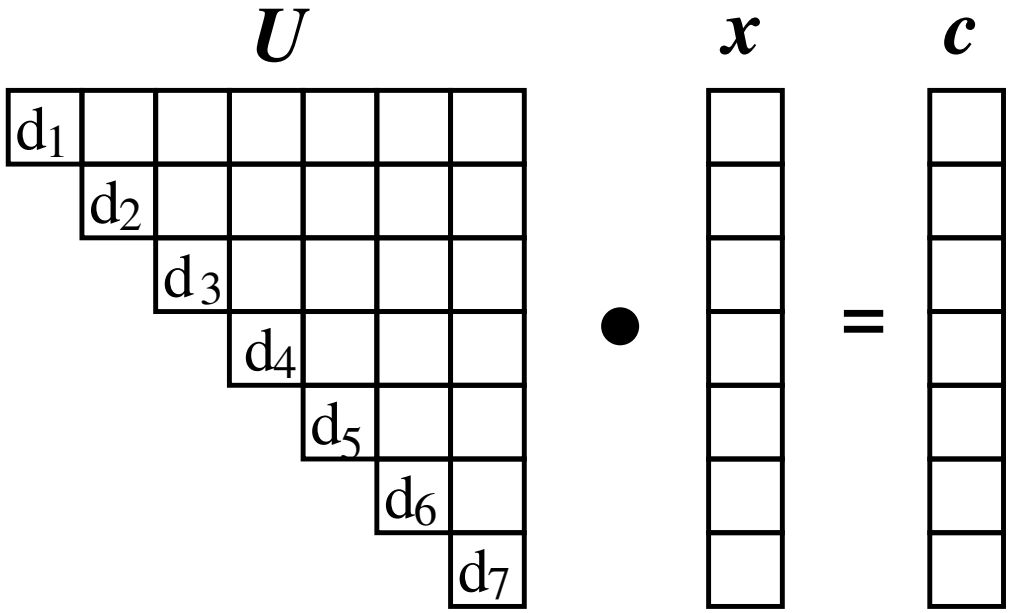
- **Triangular** systems are
  computationally and numerically straightforward.

Gaussian Elimination with Backsubstitution

$$A\boldsymbol{x} = \boldsymbol{b}$$

$$R_1 A\boldsymbol{x} = R_1\boldsymbol{b}$$

$$\underbrace{(\cdots R_2 \cdot R_1)A}_{U}\boldsymbol{x} = \underbrace{(\cdots R_2 \cdot R_1)\boldsymbol{b}}_{\boldsymbol{c}}$$



The invertible case: Summary

- $\boldsymbol{b}$ is in the column space of $A_{n\times n}$, the columns of A are a basis of $\mathbb{R}^n$ (so $C(A) = \mathbb{R}^n$), the rank of A is n.
- G-J: $A \to I$ by multiplication with elementary row matrices:

$$(\cdots R_3 \cdot R_2 \cdot R_1) \cdot A = I = R_E.$$

  $R_E = rref(A)$ is the **reduced row Echelon matrix**,
  and $A\boldsymbol{x} = \boldsymbol{b} \to R_E\boldsymbol{x} = \boldsymbol{d} \Leftrightarrow \boldsymbol{x} = (\cdots R_3 \cdot R_2 \cdot R_1)\boldsymbol{b}$.
- A invertible $\rightsquigarrow$ $R_E = I$ $\rightsquigarrow$ columns are standard basis of $\mathbb{R}^n$.
- Gaussian elim.: Zeros only below diagonal: $A\boldsymbol{x} = \boldsymbol{b} \to U\boldsymbol{x} = \boldsymbol{c}$.
- Representation of floating-point numbers $\rightsquigarrow$ numerical problems $\rightsquigarrow$ round-off errors $\rightsquigarrow$ nonsense results possible.
- Solution: Partial (rows) and full pivoting (columns).

Chapter 1

Linear Systems of Equations

Singular Systems

The singular case

Recall: Let $\boldsymbol{x}_p$ be a particular solution and $\boldsymbol{x}_n \in N(A)$.
The solutions to all linear equations have the form $\boldsymbol{x} = \boldsymbol{x}_p + \boldsymbol{x}_n$.

How to find $\boldsymbol{x}_p$ and $\boldsymbol{x}_n$? $\rightsquigarrow$ Elimination. Start with the nullspace.

Example: $A_{3\times 4}$: 4 columns, but how many pivots?

$$A = \begin{bmatrix} 1 & 2 & 2 & 2 \\ 2 & 4 & 6 & 8 \\ 3 & 6 & 8 & 10 \end{bmatrix}$$

Initial observations:
- 2nd column is a multiple of first one
- 1st and 3rd column are linearly independent.

$\rightsquigarrow$ **We expect to find pivots for column 1 and 3.**

- 3rd row is linear combination of other rows.

The singular case

$$A = \begin{bmatrix} 1 & 2 & 2 & 2 \\ 2 & 4 & 6 & 8 \\ 3 & 6 & 8 & 10 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 2 & 2 & 2 \\ 0 & \mathbf{0} & 2 & 4 \\ 0 & \mathbf{0} & 2 & 4 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 2 & 2 & 2 \\ 0 & 0 & 2 & 4 \\ 0 & 0 & 0 & \mathbf{0} \end{bmatrix} = U$$

U is called the **Echelon** (staircase) form of A.

Note that elimination uses only elementary operations that do not change the solutions, so $A\boldsymbol{x} = \mathbf{0}$ **exactly when** $U\boldsymbol{x} = \mathbf{0}$.

U Gives us important information about A:

- 2 pivots, associated with columns 1, 3
  $\rightsquigarrow$ **pivot columns** (not combinations of earlier columns.)
- 2 free columns (these are combinations of earlier columns)
  $\rightsquigarrow$ can assign x_2, x_4 to arbitrary values.

The Reduced Row Echelon Form

Idea: Simplify U further: Elimination also above the pivots.

$$U = \begin{bmatrix} 1 & 2 & 2 & -2 \\ 0 & 0 & 2 & 4 \\ 0 & 0 & 0 & 0 \end{bmatrix} \to \begin{bmatrix} 1 & 2 & 0 & -2 \\ 0 & 0 & 2 & 4 \\ 0 & 0 & 0 & 0 \end{bmatrix} \to \begin{bmatrix} 1 & 2 & 0 & -2 \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & 0 \end{bmatrix} = R_E.$$

A, U and R_E all have 2 independent columns:
$pivcol(A) = pivcol(U) = pivcol(R_E) = (1, 3) \rightsquigarrow$ same rank 2.

Obviously, the **rank equals the number of pivots!** This is equivalent to the algebraic definition **rank** $=$ **dim**$(C(A))$, but maybe more intuitive.

Pivot cols: independent, span the column space $\rightsquigarrow$ basis of $C(A)$.
Pivot rows: independent, span row space $\rightsquigarrow$ basis of $C(A^t)$.

The special solutions

Solutions to $A\boldsymbol{x} = \mathbf{0}$ and $R_E\boldsymbol{x} = \mathbf{0}$ can be obtained by setting the free variables to arbitrary values and solving for the pivot variables.

"Special" solutions are linear independent:
set one free variable equal to 1, and all other free variables to 0.

$$R_E\boldsymbol{x} = \begin{bmatrix} 1 & 2 & 0 & -2 \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \mathbf{0}. \quad s_1 = \begin{bmatrix} x_1 \\ 1 \\ x_3 \\ 0 \end{bmatrix}, \quad s_2 = \begin{bmatrix} x_1 \\ 0 \\ x_3 \\ 1 \end{bmatrix}$$

Set 1st free variable $x_2 = 1$, with $x_4 = 0 \rightsquigarrow x_1 + 2 = 0, x_3 = 0$.
Pivot variables are $x_1 = -2, x_3 = 0 \rightsquigarrow s_1 = (-2, 1, 0, 0)^t$.

2nd special solution has $x_2 = 0, x_4 = 1 \rightsquigarrow x_1 - 2 = 0, x_3 + 2 = 0$
$\rightsquigarrow s_2 = (2, 0, -2, 1)^t$.

The nullspace matrix

The nullspace matrix N contains the two special solutions in its columns, so $AN = 0$.

$$R_E = \begin{bmatrix} 1 & 2 & 0 & -2 \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad N = \begin{bmatrix} -2 & 2 \\ 1 & 0 \\ 0 & -2 \\ 0 & 1 \end{bmatrix}$$

The linear combinations of these two columns give all vectors in the nullspace $\rightsquigarrow$ basis of null-space $\rightsquigarrow$ complete solution to $A\boldsymbol{x} = \mathbf{0}$.

Consider the dimensions: $n = 4, r = 2$. One special solution for every free variable. r columns have pivots $\rightsquigarrow n - r = 2$ free variables:

$A\boldsymbol{x} = \mathbf{0}$ has r pivots and $n - r$ free variables. The nullspace matrix N contains the $n - r$ special solutions, and $AN = R_E N = 0$.

General form

General form: Suppose that the fist r columns are the pivot columns:

$$R_E = \begin{bmatrix} I & F \\ 0 & 0 \end{bmatrix} \begin{matrix} r \\ m-r \end{matrix} \quad \begin{matrix} \text{pivot rows} \\ \text{zero rows} \end{matrix}$$

The **upper left block** is the $r \times r$ **identity matrix**.
There are $n - r$ **free columns**
$\rightsquigarrow$ **upper right block** F has dimension $r \times (n - r)$

Nullspace matrix:

$$N = \begin{bmatrix} -F \\ I \end{bmatrix} \begin{matrix} r \\ n-r \end{matrix} \quad \begin{matrix} \text{pivot variables} \\ \text{free variables} \end{matrix}$$

From this definition, we directly see that $R_E N = I(-F) + FI = 0$.

The Complete Solution

- So far: $A\boldsymbol{x} = \mathbf{0}$ converted by elimination to $R_E\boldsymbol{x} = \mathbf{0}$
  $\rightsquigarrow$ solution $\boldsymbol{x}$ is in the nullspace of A.

- Now: $\boldsymbol{b}$ nonzero $\rightsquigarrow$ consider column-augmented matrix $[A\boldsymbol{b}]$.
  We will reduce $A\boldsymbol{x} = \boldsymbol{b}$ to $R_E\boldsymbol{x} = \boldsymbol{d}$.

- Example:

$$\begin{bmatrix} 1 & 3 & 0 & 2 \\ 0 & 0 & 1 & 4 \\ 1 & 3 & 1 & 6 \end{bmatrix} \boldsymbol{x} = \begin{bmatrix} 1 \\ 6 \\ 7 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 3 & 0 & 2 & 1 \\ 0 & 0 & 1 & 4 & 6 \\ 1 & 3 & 1 & 6 & 7 \end{bmatrix} = [A\boldsymbol{b}]$$

Elimination: $\begin{bmatrix} 1 & 3 & 0 & 2 & 1 \\ 0 & 0 & 1 & 4 & 6 \\ 0 & 0 & 1 & 4 & 6 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 3 & 0 & 2 & 1 \\ 0 & 0 & 1 & 4 & 6 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} = [R_E\boldsymbol{d}]$

The Complete Solution

- Particular solution $\boldsymbol{x}_p$: set free variables $x_2 = x_4 = 0$
  $\rightsquigarrow \boldsymbol{x}_p = (1, 0, 6, 0)^t$. By definition, $\boldsymbol{x}_p$ solves $A\boldsymbol{x}_p = \boldsymbol{b}$.

- The $n - r$ special solutions $\boldsymbol{x}_n$ solve $A\boldsymbol{x}_n = \boldsymbol{0}$.

- The complete solution is

$$\boldsymbol{x} = \boldsymbol{x}_p + \boldsymbol{x}_n = \begin{bmatrix} 1 \\ 0 \\ 6 \\ 0 \end{bmatrix} + x_2 \begin{bmatrix} -3 \\ 1 \\ 0 \\ 0 \end{bmatrix} + x_4 \begin{bmatrix} -2 \\ 0 \\ -4 \\ 1 \end{bmatrix}$$

Chapter 1

Linear Systems of Equations

Linear Algebra II: The Fundamental Theorem

The Four Fundamental Subspaces

Assume A is $(m \times n)$.

1. The **column space is $C(A)$**, a subspace of $\mathbb{R}^m$.
   It is spanned by the columns of A or R_E.
   Its dimension is the rank $r = \#(\text{independent columns}) = \#(\text{pivots})$.
2. The **row space is $C(A^t)$**, a subspace of $\mathbb{R}^n$. It is spanned by the rows of A or R_E. There is one nonzero row in R_E for every pivot
   $\rightsquigarrow$ dimension is also r.
3. The **nullspace is $N(A)$**, a subspace of $\mathbb{R}^n$.
   It is spanned by the $n-r$ special solutions (one for every free variable), they are independent $\rightsquigarrow$ they form a basis
   $\rightsquigarrow$ dimension of $N(A)$ ("nullity") is $n-r$.
4. The **left nullspace is $N(A^t)$**, a subspace of $\mathbb{R}^m$.
   It contains all vectors $\boldsymbol{y}$ such that $A^t\boldsymbol{y} = \mathbf{0}$. Its dimension is $m-r$.

The Fundamental Theorem of Linear Algebra (I)

1.), 2.) and 3.) are part one of the

Fundamental Theorem of Linear Algebra.
For any $m \times n$ matrix A:

- Column space and row space both have dimension r.
  In other words: column rank $=$ row rank $=$ rank.
- Rank $+$ Nullity $= r + (n - r) = n$.

4.) additionally defines the "left nullspace": it contains any left-side row vectors $\boldsymbol{y}^t$ that are mapped to the zero (row-)vector: $\boldsymbol{y}^t A = \mathbf{0}^t$.
$A^t := B$ is a $(n \times m)$ matrix

$$\rightsquigarrow \quad \underbrace{\dim(C(B))}_{r} + \underbrace{\dim(N(B))}_{m-r} = m.$$

$\rightsquigarrow$ **Rank + "Left Nullity" $= m$.**

The Fundamental Theorem of Linear Algebra (II)

Part two of the Fundamental Theorem of Linear Algebra concerns orthogonal relations between the subspaces. Two definitions:

Two vectors $\boldsymbol{v}, \boldsymbol{w} \in V$ are **perpendicular** if their scalar product is zero. The **orthogonal complement** $V^\perp$ of a subspace V contains **every** vector that is perpendicular to V.

The nullspace is the orthogonal complement of the row space.

Proof: Every $\boldsymbol{x}$ perpendicular to the rows satisfies $A\boldsymbol{x} = \boldsymbol{0}$.
Reverse is also true: If $\boldsymbol{v}$ is orthogonal to $N(A)$, it must be in the row space. Otherwise we could add $\boldsymbol{v}$ as an extra independent row of the matrix (thereby increasing the rank) without changing the nullspace
$\rightsquigarrow$ row space would grow, contradicting $r + \dim(N(A)) = n$.

The Fundamental Theorem of Linear Algebra (II)

Same reasoning holds true for the left nullspace:

Part two of the Fundamental Theorem of Linear Algebra:

- $N(A)$ is the orthogonal complement of $C(A^t)$ (in $\mathbb{R}^n$).
- $N(A^t)$ is the orthogonal complement of $C(A)$ (in $\mathbb{R}^m$).

Immediate consequences:

Every $\boldsymbol{x} \in \mathbb{R}^n$ can be split into $\boldsymbol{x} = \boldsymbol{x}_{\text{row}} + \boldsymbol{x}_{\text{nullspace}}$.

Thus, the action of A on $\boldsymbol{x}$ is as follows:

$$A\boldsymbol{x}_n = \mathbf{0},$$
$$A\boldsymbol{x}_r = A\boldsymbol{x}$$

The 4 subspaces

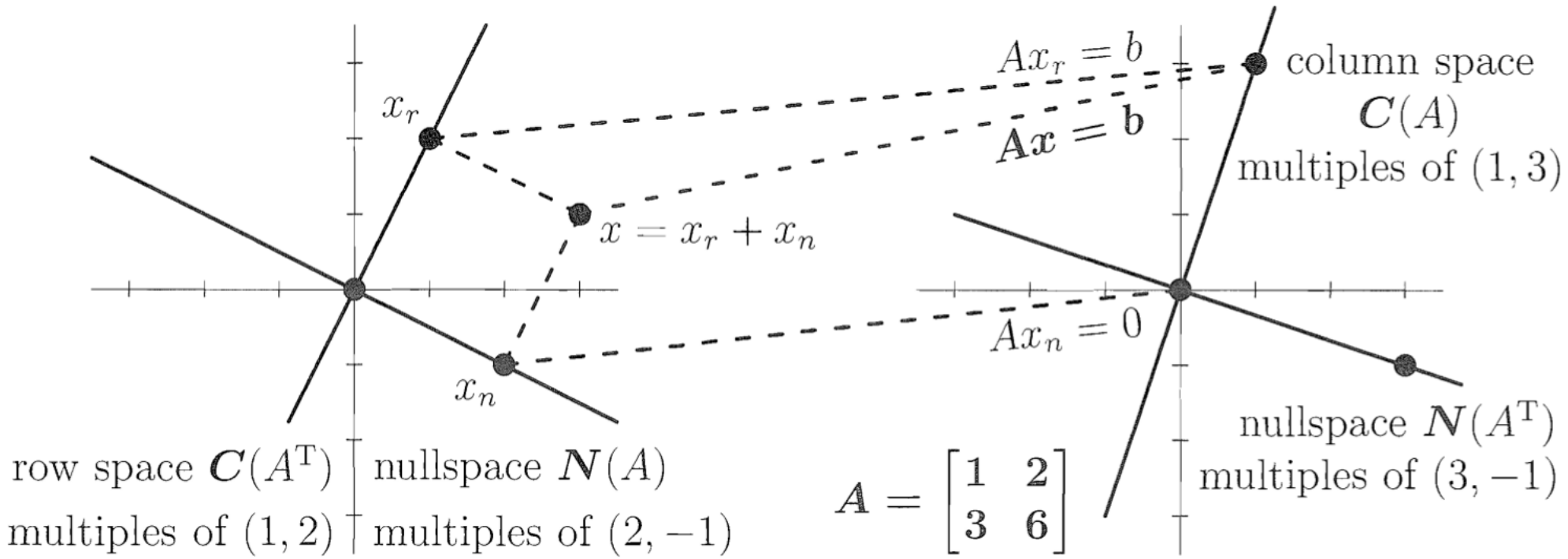


Figure 2.5: The four fundamental subspaces (lines) for the singular matrix A.

Fig. 2.5 in Gilbert Strang: Linear Algebra and Its Applications

Invertible part of a matrix

Every vector in $C(A)$ comes from **one and only one vector** in the row space. Every vector in $C(A^t)$ comes from **one and only one vector** in the column space.

Proof (first assertion):
(i) $A\boldsymbol{x}_r = A\boldsymbol{x}'_r \;\Rightarrow\; A(\boldsymbol{x}_r - \boldsymbol{x}'_r) = \mathbf{0} \;\Rightarrow\; \boldsymbol{\delta} := \boldsymbol{x}_r - \boldsymbol{x}'_r \in N(A)$.
(ii) $\boldsymbol{x}_r \in C(A^t), \boldsymbol{x}'_r \in C(A^t) \;\Rightarrow\; \boldsymbol{\delta} \in C(A^t)$.
But $N(A)$ and $C(A^t)$ are orthogonal $\Rightarrow \boldsymbol{\delta} = \mathbf{0}$.

Conclusion: From the row space to the column space, A is invertible.
In other words: **There is a $r \times r$ invertible matrix "hidden" inside A.**

This will be explored later in this course in the context of the **pseudoinverse** and the **SVD**.

Chapter 1

Linear Systems of Equations

Alternatives to Gaussian Elimination

Further Methods for Linear Systems

- **Direct solution methods**
  - Gauss-Jordan elimination with pivoting
  - Matrix factorization (LU, Cholesky)
  - **Predictable number of steps**
- **Iterative solution methods**
  - Jacobi, Newton etc.
  - **converge in as many steps as necessary**
- **Combination**
  - direct solution, then improved by iterations
  - useful for close-to-singular systems

Factorization methods

- **Disadvantage of Gaussian elimination:**
  all righthand sides $\boldsymbol{b}_j$ must be known in advance.

- LU decomposition keeps track of the steps in Gaussian elimination
  $\rightsquigarrow$ The result can be applied to **any future $\boldsymbol{b}$** required.

- A is **decomposed** or factorized as $A = LU$:
  - L lower triangular,
  - U upper triangular.

- **Example:** For a 3×3 matrix, this becomes:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}.$$

LU factorization

- $A = LU$, L lower triangular, U upper triangular.

- $A\boldsymbol{x} = \boldsymbol{b}$ becomes $LU\boldsymbol{x} = \boldsymbol{b}$. Define $\boldsymbol{c} = U\boldsymbol{x}$.
  $L\boldsymbol{c} = \boldsymbol{b}$ solved by **forward-substitution**, followed by
  $U\boldsymbol{x} = \boldsymbol{c}$ solved by **back-substitution**.

- The two interim systems are **trivial to solve** since both are triangular.

- Work effort goes into the **factorization** steps to get L and U.

- U can be computed by **Gaussian elimination**,
  L records the information necessary to **undo the elimination steps**.

LU factorization: the book-keeping

- Steps in Gaussian elimination involve **pre-multiplication** by elementary R-matrices $\rightsquigarrow$ These are trivially invertible.

$$\begin{aligned} A &= (R_1^{-1} \cdot R_1) \cdot A = \cdots = \\ &= (R_1^{-1} \cdot R_2^{-1} \cdot R_3^{-1} \cdots R_3 \cdot R_2 \cdot R_1) \cdot A \\ &= \underbrace{(R_1^{-1} \cdot R_2^{-1} \cdot R_3^{-1} \cdots)}_{L} \cdot \underbrace{(\cdots R_3 \cdot R_2 \cdot R_1 \cdot A)}_{U} \end{aligned}$$

- Entries for L are the inverses (i.e. negatives) of the multipliers in the row transformation for each step: $R_{ij}(m)$ Subtracts row j multiplied by m from row i. **Inverse:** $R_{ij}(m)^{-1} = R_{ij}(-m)$.

$$\underset{A}{\begin{bmatrix} 2 & 1 \\ 6 & 8 \end{bmatrix}} = \underset{R^{-1}}{\begin{bmatrix} 1 & 0 \\ 3 & 1 \end{bmatrix}} \underset{R}{\begin{bmatrix} 1 & 0 \\ -3 & 1 \end{bmatrix}} \underset{A}{\begin{bmatrix} 2 & 1 \\ 6 & 8 \end{bmatrix}} = \underset{L}{\begin{bmatrix} 1 & 0 \\ 3 & 1 \end{bmatrix}} \underset{U}{\begin{bmatrix} 2 & 1 \\ 0 & 5 \end{bmatrix}}$$

LU factorization via Gaussian elimination

- **LU is not unique:**
  - Decomposition is multiplicative
    $\rightsquigarrow$ factors can be re-arranged between L and U.

- LU **may not exist at all**, if there is a **zero pivot**. **Pivoting:**
  - Can factorize as $A = P^{-1}LU = P^tLU$.
  - P records the effects of row permutations, so $PA = LU$.
    Need to **keep track of permutations** in P.

$$\text{Permutation } \pi = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 1 & 4 & 2 & 5 & 3 \end{pmatrix} \Rightarrow P_\pi = \begin{bmatrix} \boldsymbol{e}_1^t \\ \boldsymbol{e}_4^t \\ \boldsymbol{e}_2^t \\ \boldsymbol{e}_5^t \\ \boldsymbol{e}_3^t \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix}.$$

Crout's algorithm

- Alternative method to find the L and U matrices
- Write out $A = LU$ with unknowns for the non-zero elements of L, U.
- Equate entries in the $n \times n$ matrix equation
  $\rightsquigarrow n^2$ equations in $n^2 + n$ unknowns.
- **Underdetermined** $\rightsquigarrow n$ unknowns are arbitrary
  (shows that the LU decomposition is **not unique**)
  $\rightsquigarrow$ choose the diagonal entries $l_{ii} = 1$.
- **Crout's algorithm:**
  - re-write the n^2 equations in a carefully chosen order so that elements of L and U can be found **one-by-one**.

Crout's algorithm

$$\begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

Multiplying out gives:

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

Red indicates where an element is used for the first time.

Only one red entry in each equation!

Crout's method fills in the combined matrix

$$\begin{bmatrix} u_{11} & u_{12} & u_{13} & u_{14} & \cdots \\ l_{21} & u_{22} & u_{23} & u_{24} & \cdots \\ l_{31} & l_{32} & u_{33} & u_{34} & \cdots \\ l_{41} & l_{42} & l_{43} & u_{44} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

by columns from left to right, and from top to bottom.

A small example

$$\begin{bmatrix} 4 & 3 \\ 6 & 3 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ l_{21} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} \\ 0 & u_{22} \end{bmatrix}$$

Solve the linear equations:

$$\begin{aligned} u_{11} &= 4 \\ l_{21} \cdot u_{11} &= 6 \\ u_{12} &= 3 \\ l_{21} \cdot u_{12} + u_{22} &= 3 \end{aligned}$$

Substitution yields: $\begin{bmatrix} 4 & 3 \\ 6 & 3 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1.5 & 1 \end{bmatrix} \begin{bmatrix} 4 & 3 \\ 0 & -1.5 \end{bmatrix}$

Chapter 1

Linear Systems of Equations

Positive Definite Matrices and the Cholesky Decomposition

Positive definite matrices

An $n \times n$ **symmetric real matrix** A is positive-definite if $\boldsymbol{x}^t A \boldsymbol{x} > 0$ for all vectors $\boldsymbol{x} \neq \mathbf{0}$.

Simple tests for positive definiteness?

- A positive definite matrix A has **all positive entries** on the main diagonal (use $\boldsymbol{x}^t A \boldsymbol{x} > 0$ with vectors $(1, 0, ..., 0)^t$, $(0, 1, 0, ..., 0)^t$ etc.)
- A is **diagonally dominant** if $|a_{ii}| > \sum_{i \neq j} |a_{ij}|$.
- A diagonally dominant matrix is positive definite if it is **symmetric** and has **all main diagonal entries positive**. Follows from the **Gershgorin circle theorem** (details will follow...). Note that the **converse is false**.

There are many applications of pos. def. matrices:

- **Linear regression** models ($\rightsquigarrow$ chapter 2).
- Solution of **partial differential equations** $\rightsquigarrow$ heat conduction, mass diffusion, wave equation etc.

Example: Heat equation

- $u = u(x,t)$ is **temperature as a function of space and time**. This function will change over time as heat spreads throughout space.
- $u_t := \frac{\partial u}{\partial t}$ is the **rate of change** of temperature at a point over time.
- $u_{xx} := \frac{\partial^2 u}{\partial x^2}$ is the second spatial derivative of temperature.
- **Heat equation:** $u_t \propto u_{xx}$. **The rate of change of temperature over time is proportional to the local difference of temperature**. Proportionality constant: diffusivity of the (isotropic) medium.
- **Discretization** $u_j^{(m)} = u(x_j, t_m)$ at grid points x_j and time points t_m:

$$x_j := j \cdot \underbrace{h}_{\text{spatial step size}} \quad \text{and} \quad t_m := m \cdot \underbrace{\tau}_{\text{temporal step size}}$$

- Assume $h = \tau = 1$, and also diffusivity $= 1$.

Example: Heat equation

- Approximate derivative on grid ($\rightsquigarrow$ **finite differences**):

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}.$$

- Second order (**central difference approximation**):

$$f''(x) \approx \frac{\frac{f(x+h)-f(x)}{h} - \frac{f(x)-f(x-h)}{h}}{h} = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$

- Approximate equation $u_t = u_{xx}$ by (we assumed step size $=1$)

$$\underbrace{u_j^{(m+1)} - u_j^{(m)}}_{\text{rate of change over time}} = \underbrace{u_{j-1}^{(m+1)} - 2u_j^{(m+1)} + u_{j+1}^{(m+1)}}_{\text{local temperature difference}}$$

Example: Heat equation

- Solve this **implicit scheme** for $u^{(m+1)}$:

$$(1+2)u_j^{(m+1)} - u_{j-1}^{(m+1)} - u_{j+1}^{(m+1)} = u_j^{(m)}, \quad \text{for } j = 1, \ldots, n-1, \text{ and } m \geq 0.$$

- With $A =$ tri-diagonal with $(a_{j,j-1}, a_{j,j}, a_{j,j+1}) = (-1, 2, -1)$:

$$(I + A)u^{(m+1)} = \begin{bmatrix} . & . & . & . & . & . & . \\ 0 & -1 & \mathbf{3} & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & \mathbf{3} & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & \mathbf{3} & -1 & 0 \\ . & . & . & . & . & . & . \end{bmatrix} u^{(m+1)} = u^{(m)}$$

- $(I + A)$ is diagonal dominant and symmetric, and has positive diagonal entries $\rightsquigarrow$ **positive definite**! It is also **sparse** $\rightsquigarrow$ efficient elimination possible: per column only 1 zero needs to be produced below the pivot.

Cholesky LU decomposition

- **The Cholesky LU factorization of a pos. def. matrix A is $A = LL^t$.**
- Use it to solve a pos. def. system $A\boldsymbol{x} = \boldsymbol{b}$.
- Cholesky algorithm: Partition matrices in $A = LL^t$ as

$$\begin{pmatrix} a_{11} & \boldsymbol{a}_{21}^t \\ \boldsymbol{a}_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} l_{11} & 0 \\ \boldsymbol{l}_{21} & L_{22} \end{pmatrix} \begin{pmatrix} l_{11} & \boldsymbol{l}_{21}^t \\ 0 & L_{22}^t \end{pmatrix} = \begin{pmatrix} l_{11}^2 & l_{11}\boldsymbol{l}_{21}^t \\ l_{11}\boldsymbol{l}_{21} & \boldsymbol{l}_{21}\boldsymbol{l}_{21}^t + L_{22}L_{22}^t \end{pmatrix}$$

  Recursion:

  – step 1: $l_{11} = \sqrt{a_{11}}, \quad \boldsymbol{l}_{21} = \frac{1}{l_{11}}\boldsymbol{a}_{21}$.
  – step 2: compute L_{22} from $S := A_{22} - \boldsymbol{l}_{21}\boldsymbol{l}_{21}^t = L_{22}L_{22}^t$.
  This is a Cholesky factorization of $S_{(n-1)\times(n-1)}$.

Cholesky: Proof

Proof that the algorithm works for positive definite $A_{n\times n}$ **by induction:**

1. If A is positive definite then $a_{11} > 0$,
   $\rightsquigarrow l_{11} = \sqrt{a_{11}}$ **and** $\boldsymbol{l}_{21} = \frac{1}{l_{11}}\boldsymbol{a}_{21}$ **are well-defined.**
2. If A is positive definite, then
   $S = A_{22} - \boldsymbol{l}_{21}\boldsymbol{l}_{21}^t = A_{22} - \frac{1}{a_{11}}\boldsymbol{a}_{21}\boldsymbol{a}_{21}^t$ **is positive definite.**

   Proof: take any $(n-1)$ vector $\boldsymbol{v} \neq 0$ and $w = -(1/a_{11})\boldsymbol{a}_{21}^t\boldsymbol{v} \in \mathbb{R}$.

$$\boldsymbol{v}^t S \boldsymbol{v} = \begin{pmatrix} w & \boldsymbol{v}^t \end{pmatrix} \begin{pmatrix} a_{11} & \boldsymbol{a}_{21}^t \\ \boldsymbol{a}_{21} & A_{22} \end{pmatrix} \begin{pmatrix} w \\ \boldsymbol{v} \end{pmatrix} = \begin{pmatrix} w & \boldsymbol{v}^t \end{pmatrix} A \begin{pmatrix} w \\ \boldsymbol{v} \end{pmatrix} > 0.$$

- **Induction step:** Algorithm works for $n = k$ if it works for $n = k - 1$.
- **Base case:** It obviously works for $n = 1$; **therefore it works for all** n**.**

Chapter 1

Linear Systems of Equations

Iterative Methods

Iterative improvement

- Floating point arithmetic **limits the precision of calculated solutions**.
- For large systems and "close-to-singular" small systems, precision is generally **far worse than machine precision** ϵ_m.
  - Direct methods **accumulate roundoff errors**.
  - **Loss of some significant digits** isn't unusual even for well-behaved systems.
- **Iterative improvement:** Start with direct solution method (Gauss, LU, Cholesky etc.), followed by some post-iterations.
  It will get your solution **back to machine precision** efficiently.

Iterative improvement

- Suppose $\boldsymbol{x}$ is the (unknown) **exact solution** of $A\boldsymbol{x} = \boldsymbol{b}$ and $\boldsymbol{x} + \delta\boldsymbol{x}$ is a calculated (**inexact**) solution with **unknown error** $\delta\boldsymbol{x}$.
- Substitute calculated solution in original equation:

$$A(\boldsymbol{x} + \delta\boldsymbol{x}) = \boldsymbol{b} + \delta\boldsymbol{b}, \tag{1}$$

- Subtract $A\boldsymbol{x}$ (or $\boldsymbol{b}$) from both sides:

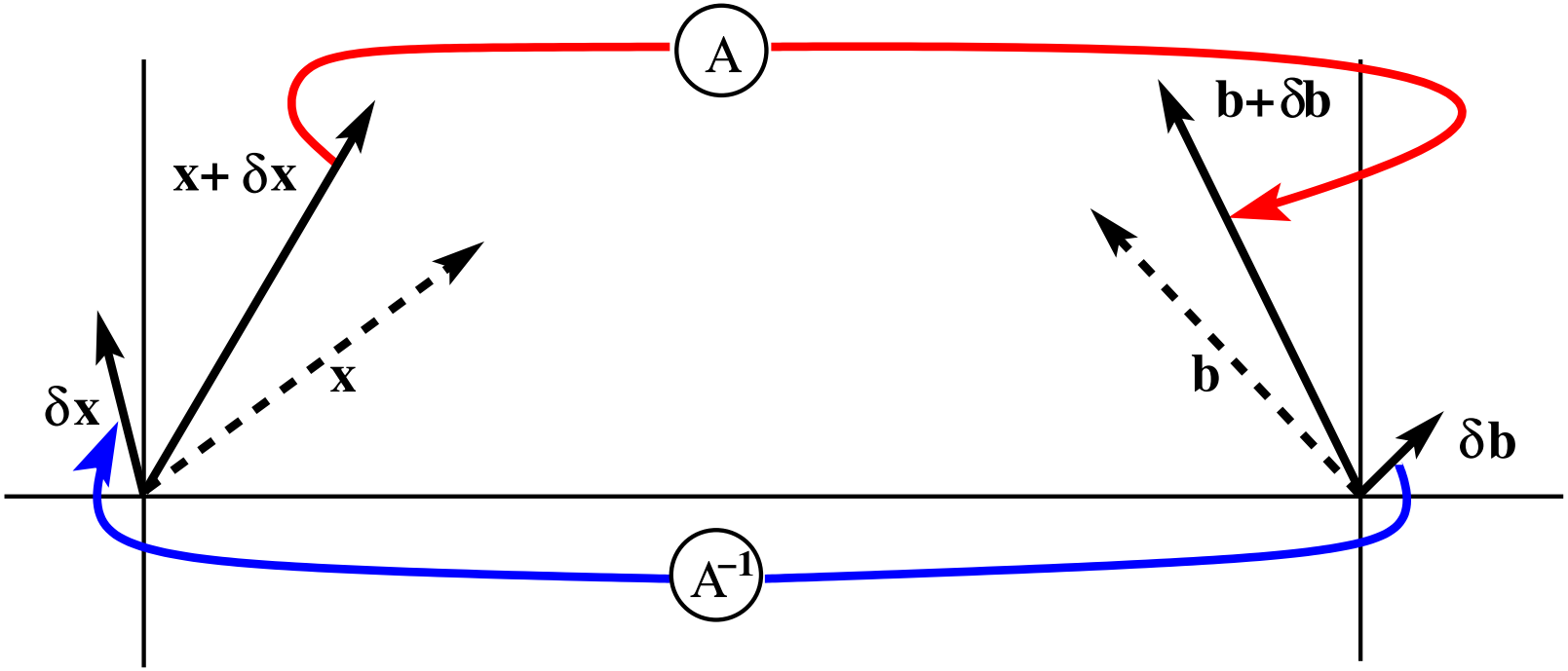
$$A\delta\boldsymbol{x} = \delta\boldsymbol{b}. \tag{2}$$

- Eqn. (1) gives:

$$\delta\boldsymbol{b} = A \underbrace{(\boldsymbol{x} + \delta\boldsymbol{x})}_{\text{calculated solution}} - \boldsymbol{b}. \tag{3}$$

- Right hand side of eqn. (3) is known
  $\rightsquigarrow$ get $\delta\boldsymbol{b}$ and use this in (2) to solve for $\delta\boldsymbol{x}$.

Iterative improvement



Iterative improvement: first guess $\boldsymbol{x} + \delta\boldsymbol{x}$ is multiplied by A to produce $\boldsymbol{b} + \delta\boldsymbol{b}$.
Known vector $\boldsymbol{b}$ is subtracted $\rightsquigarrow \delta\boldsymbol{b}$.
Inversion gives $\delta\boldsymbol{x}$ and subtraction gives an improved solution $\boldsymbol{x}$.

LU factorization of A can be used to solve $A\delta\boldsymbol{x} = LU\delta\boldsymbol{x} = \delta\boldsymbol{b}$ to get $\delta\boldsymbol{x}$.

Repeat until $\|\delta\boldsymbol{x}\| \approx \epsilon_m$.

Iterative methods: Jacobi

- Assume that all diagonal entries of A are nonzero.
- Write $A = D + L + U$

  where $D = \begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ 0 & a_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{bmatrix}$ and $L+U = \begin{bmatrix} 0 & a_{12} & \cdots & a_{1n} \\ a_{21} & 0 & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & 0 \end{bmatrix}$
- So $A\boldsymbol{x} = \boldsymbol{b} \quad \rightsquigarrow \quad (L + D + U)\boldsymbol{x} = \boldsymbol{b}$.
- The solution is then obtained iteratively via

$$D\boldsymbol{x} = \boldsymbol{b} - (L + U)\boldsymbol{x}.$$

Iterative methods: Jacobi

- The solution is obtained iteratively via

$$D\boldsymbol{x} = \boldsymbol{b} - (L + U)\boldsymbol{x}. \tag{4}$$

- Given $\boldsymbol{x}_{(i)}$ obtain $\boldsymbol{x}_{(i+1)}$ by solving (4) with $\boldsymbol{x} = \boldsymbol{x}_{(i)}$:

$$\boldsymbol{x}_{(i+1)} = -D^{-1}(L + U)\boldsymbol{x}_{(i)} + D^{-1}\boldsymbol{b}.$$

- Define $J = D^{-1}(L + U)$ as the **iteration matrix.**
  $\rightsquigarrow \boldsymbol{x}_{(i+1)} = -J\boldsymbol{x}_{(i)} + D^{-1}\boldsymbol{b}.$
- From (4): $D^{-1}\boldsymbol{b} = \boldsymbol{x} + D^{-1}(L + U)\boldsymbol{x} = \boldsymbol{x} + J\boldsymbol{x}$
  $\Rightarrow \boldsymbol{x}_{(i+1)} = -J\boldsymbol{x}_{(i)} + \boldsymbol{x} + J\boldsymbol{x}.$
- $(i + 1)$-th error term: $\boldsymbol{\epsilon}_{(i+1)} = \boldsymbol{x}_{(i+1)} - \boldsymbol{x} = -J(\boldsymbol{x}_{(i)} - \boldsymbol{x}) = -J\boldsymbol{\epsilon}_{(i)}$.
- **Convergence guaranteed** if J is "contracting".

Calculating the error, revisited

- Error in $(i+1)$-th iteration: $\boldsymbol{\epsilon}_{(i+1)} = -J\boldsymbol{\epsilon}_{(i)}$.
- $\boldsymbol{\epsilon}_{(i+1)} = -J(-J\boldsymbol{\epsilon}_{(i-1)}) = J^2\boldsymbol{\epsilon}_{(i-1)} = \cdots = (-1)^{i+1}J^{i+1}\boldsymbol{\epsilon}_{(0)}$.
- So if $J^i \to 0$ (zero matrix) for $i \to \infty$ then $\boldsymbol{\epsilon}_{(i)} \to \mathbf{0}$.
- The key to understanding this condition is the **eigenvalue decomposition** $J = V\Lambda V^{-1}$ (details next section)
  - the columns of V consist of **eigenvectors** of J and
  - Λ is a diagonal matrix of **eigenvalues** of J.
- Then $J^2 = V\Lambda V^{-1}V\Lambda V^{-1} = V\Lambda^2 V^{-1} \rightsquigarrow J^n = V\Lambda^n V^{-1}$.

  If all the eigenvalues of J have magnitude < 1,
  then $\Lambda^n \to 0$ and consequently $J^n \to 0 \rightsquigarrow$ convergence.
- **A diagonally dominant $\rightsquigarrow$ Jacobi method converges.**
  Follows from the **Gershgorin circle theorem**.

Chapter 1

Linear Systems of Equations

Linear Algebra III: Eigenvalues and Eigenvectors

Eigenvalues and eigenvectors

- Consider a square matrix A. A vector $\boldsymbol{v}$ for which $A\boldsymbol{v} = \lambda\boldsymbol{v}$ for some (possibly complex) scalar λ is an **eigenvector** of A, and λ is the associated **eigenvalue.**
- **The eigenvectors span the nullspace** of $(A - \lambda I)$: They are the solutions of $(A - \lambda I)\boldsymbol{v} = \mathbf{0}$.
- A **non-zero solution** $\boldsymbol{v} \neq \mathbf{0}$ exists if and only if the matrix $(A - \lambda I)$ is **not invertible**:

  otherwise we could invert $(A - \lambda I)$ and get the unique solution $\boldsymbol{v} = (A - \lambda I)^{-1}\mathbf{0} = \mathbf{0}$, i.e. only the zero solution.
- Equivalently we have **non-zero eigenvectors** if and only if the rank of $(A - \lambda I) < n$.
- Equivalently we want: $det(A - \lambda I) = 0$. Why?

Determinants

- The **determinant of a square matrix** is a single number.
  It contains a lot of information about the matrix.
- But is is not a "simple" function...
  Explicit formulas are complicated, but its properties are simple.

Three rules completely determine the number $det(A)$:

1. **The determinant of the identity matrix is 1:** $det(I) = |I| = 1$.
2. **The determinant changes sign when two rows are exchanged.**
3. **The determinant is a linear function in each row separately**
   (all other rows stay fixed): 2d-example for first row

$$\begin{vmatrix} ta & tb \\ c & d \end{vmatrix} = t \begin{vmatrix} a & b \\ c & d \end{vmatrix}$$

$$\begin{vmatrix} a+a' & b+b' \\ c & d \end{vmatrix} = \begin{vmatrix} a & b \\ c & d \end{vmatrix} + \begin{vmatrix} a' & b' \\ c & d \end{vmatrix}$$

Determinants

Further rules can be deduced:

4. **If two rows of A are equal, then $det(A) = 0$.**
   Rule 2: Exchange of the equal rows $\rightsquigarrow$ $det(A)$ changes sign.
   But matrix stays the same, so det cannot change $\rightsquigarrow$ $det(A) = 0$.
5. **Subtracting a multiple of one row from another row leaves the same determinant.**

$$\begin{vmatrix} a - lc & b - ld \\ c & d \end{vmatrix} = \begin{vmatrix} a & b \\ c & d \end{vmatrix} - l \underbrace{\begin{vmatrix} c & d \\ c & d \end{vmatrix}}_{=0 \text{ (rule 4)}}$$

   Usual elimination steps do not affect the determinant!

6. **If A has a row of zeros, then $det(A) = 0$.**
   Add some other row to zero row $\rightsquigarrow$ $det(A)$ is unchanged (rule 5).
   But now there are two identical rows $\rightsquigarrow$ $det(A) = 0$ by rule 4.

Determinants

7. **If A is triangular then $det(A) = \prod_i a_{ii}$.**
   Suppose the diagonal entries are nonzero. Then elimination can remove all the off-diagonal entries, without changing $det(A)$ (rule 5).
   Factoring out the diagonal elements gives
   $det(A) = \prod_i a_{ii} \cdot det(I) = \prod_i a_{ii}$ (rules 3 and 1).
   Zero diagonal entry $\rightsquigarrow$ elimination produces a zero row.
   Rule 5: elimination steps do not change $det(A)$.
   Rule 6: zero row $\rightsquigarrow det(A) = 0$.
8. **If A is singular, then $det(A) = 0$. If A is invertible, $det(A) \neq 0$.**
   A singular: Elimination $\rightsquigarrow$ zero row in U $\rightsquigarrow det(A) = det(U) = 0$.
   A nonsingular: Elimination puts the nonzero pivots $d_1, \ldots, d_n$ on the diagonal. Sign depends on whether the number of row exchanges is even or odd: $det(A) = \pm det(U) = \pm \prod_i d_i \neq 0$**.**

Determinants

9. **The determinant of AB is the product $det(A) \cdot det(B)$.**
   Proof sketch: When $|B| \neq 0$, consider ratio $D(A) := |AB|/|B|$.
   Check that this ratio has properties
   1: $A = I$ implies $D(A) = 1$,
   2: exchange of two rows of A gives a sign reversal of $D(A)$,
   3: linearity in each row
   $\rightsquigarrow D(A)$ must be the determinant of A: $D(A) = |A| = |AB|/|B|$.
10. **Formula for 2×2 case:**

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = LU = \underbrace{\begin{bmatrix} 1 & 0 \\ c/a & 1 \end{bmatrix}}_{det=1} \underbrace{\begin{bmatrix} a & b \\ 0 & (ad-bc)/a \end{bmatrix}}_{det=ad-bc}$$

Eigenvalues and eigenvectors

- $det(A - \lambda I) = 0$ is the **characteristic polynomial** of A.
  - it's a **polynomial of degree** n for $A_{(n \times n)}$,
  - its solutions give **all the eigenvalues** λ_i.

$$\text{Example:} \quad \begin{vmatrix} a - \lambda & b \\ c & d - \lambda \end{vmatrix} = (a - \lambda)(d - \lambda) - bc = 0.$$

- Once we know all the $\lambda_1, \lambda_2, \ldots, \lambda_n$ we take each one in turn and find the **corresponding eigenvectors** $\boldsymbol{v}_i$ by solving the **linear system**

$$(A - \lambda_i I)\boldsymbol{v}_i = \mathbf{0}.$$

- All eigenvectors fulfill $A\boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i$. In matrix form: $AV = V\Lambda$, where $\boldsymbol{v}_i$ is the i-th column of V and Λ is the diagonal matrix

$$\Lambda = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}$$

Eigenvalues, pivots and determinants

- Suppose that $\lambda_1, \ldots \lambda_2$ are eigenvalues of A. Then the λ_i are the roots of the characteristic polynomial, and this polynomial of degree n always separates into n factors involving the (possibly complex) eigenvalues (**fundamental theorem of algebra**), i.e.

$$det(A - \lambda I) = (\lambda_1 - \lambda)(\lambda_2 - \lambda) \cdots (\lambda_n - \lambda).$$

- Holds for every $\lambda \rightsquigarrow$ can set $\lambda = 0$:

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

- We already showed that $det(A) = \pm det(U) = \pm \prod_i d_i$, so **Determinant = $\pm$ (product of pivots) = product of eigenvalues.**

Diagonalization

- **Not all** linear operators can be represented by diagonal matrices with respect to some basis.

- A square matrix A for which there is some (invertible) P so that $P^{-1}AP = D$ is a diagonal matrix is called **diagonalizable**.

Theorem. *Suppose that $A_{(n\times n)}$ has n **linearly independent** eigenvectors $v_1, \ldots, v_n$, arranged as columns in the matrix V. Then*

$$V^{-1}AV = \Lambda = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}$$

Proof. $Av_i = \lambda_i \boldsymbol{v}_i \;\Rightarrow\; AV = V\Lambda \;\Rightarrow\; V^{-1}AV = \Lambda$ □

Diagonalization

Theorem. *Eigenvectors corresponding to distinct (all different) eigenvalues are linearly independent.*

Proof. Suppose $c_1\boldsymbol{v}_1 + c_2\boldsymbol{v}_2 = \mathbf{0}$.
Then $A(c_1\boldsymbol{v}_1 + c_2\boldsymbol{v}_2) = c_1\lambda_1\boldsymbol{v}_1 + c_2\lambda_2\boldsymbol{v}_2 = \mathbf{0}$.
Also $\lambda_2(c_1\boldsymbol{v}_1 + c_2\boldsymbol{v}_2) = c_1\lambda_2\boldsymbol{v}_1 + c_2\lambda_2\boldsymbol{v}_2 = \mathbf{0}$.
Subtraction gives:

$$(\lambda_1 - \lambda_2)c_1\boldsymbol{v}_1 = \mathbf{0} \;\Rightarrow\; c_1 = 0 \text{ , since } \boldsymbol{v}_1 \neq \mathbf{0} \text{ and } \lambda_1 \neq \lambda_2.$$

Similarly, $c_2 = 0$. Thus, no other combination $c_1\boldsymbol{v}_1 + c_2\boldsymbol{v}_2 = \mathbf{0}$, and the eigenvectors must be independent. Proof directly extends to any number of eigenvectors. □

Orthogonal Diagonalization

- If P is also orthogonal ($PP^t = I$), A is **orthogonally** diagonalizable.
- Columns of $P =$ linearly independent eigenvectors of A.
- Diagonal entries of D are the corresponding eigenvalues.

Theorem. *If a matrix is orthogonally diagonalizable, then it is symmetric*

Proof. We assume that $P^tAP = D$ holds, with $P^t = P^{-1}$.
Thus, $A = PDP^t$ and $A^t = (PDP^t)^t = PDP^t = A$. □

Orthogonal Diagonalization

Theorem. *Eigenvectors of a symmetric matrix corresponding to different eigenvalues are orthogonal.*

Proof. Let $A^t = A$ have eigenvectors $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ for eigenvalues $\lambda_1 \neq \lambda_2$.

$$(A\boldsymbol{v}_1)^t\boldsymbol{v}_2 = \boldsymbol{v}_1^t(A\boldsymbol{v}_2) = \lambda_1\boldsymbol{v}_1^t\boldsymbol{v}_2 = \lambda_2\boldsymbol{v}_1^t\boldsymbol{v}_2.$$

Since $\lambda_1 \neq \lambda_2$, we must have $\boldsymbol{v}_1^t\boldsymbol{v}_2 = 0$. □

More general version (without explicit proof): Spectral Theorem

Theorem. *Suppose the $n \times n$ matrix A is symmetric.*
Then it has n orthogonal eigenvectors with real eigenvalues.

A square matrix A is orthogonally diagonalizable
if and only if it is symmetric.

Chapter 1

Linear Systems of Equations

Matrix Powers and Markovian Matrices

Matrix Powers

- Consider a square matrix A with eigenvector decomposition $A_{(n\times n)} = V\Lambda V^{-1}$.

- What are the eigenvectors of $A^2 = AA$?
  Substitution gives: $A^2 = V\Lambda V^{-1}V\Lambda V^{-1} = V\Lambda^2 V^{-1}$.
  So A^2 **has the same eigenvectors and squared eigenvalues.**

- General form: $A^n = V\Lambda^n V^{-1}$.

- When does $A^k \to 0$ (zero matrix)?
  All $|\lambda_i| < 1$ (cf. convergence analysis of Jacobi iterations).

- Are there other interesting applications of matrix powers? Yes, **many!**

Matrix Powers: Fibonacci numbers

- The Fibonacci sequence $0, 1, 1, 2, 3, 5, 8, 13, \ldots$ comes from $F_{k+2} = F_{k+1} + F_k$.
- Assume you want to compute F_{100}. **Can it be done directly?** Yes, with the help of matrix powers...
- Define $\boldsymbol{u}_k = \begin{bmatrix} F_{k+1} \\ F_k \end{bmatrix}$ and the **transition matrix** $A = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}$.
- The rule $\begin{matrix} F_{k+2} &=& F_{k+1} + F_k \\ F_{k+1} &=& F_{k+1} \end{matrix}$ is $\boldsymbol{u}_{k+1} = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} \boldsymbol{u}_k$.
- After 100 steps we reach $\boldsymbol{u}_{100} = A^{100}\boldsymbol{u}_0$, with $\boldsymbol{u}_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$.

Matrix Powers: Fibonacci numbers

1. Find **eigenvectors** $\boldsymbol{v}_1, \boldsymbol{v}_2$ and associated **eigenvalues** of A.

2. Express $\boldsymbol{u}_0$ as **combination of eigenvectors:**
   $\boldsymbol{u}_0 = c_1\boldsymbol{v}_1 + c_2\boldsymbol{v}_2 \rightsquigarrow \boldsymbol{c} = V^{-1}\boldsymbol{u}_0$.

3. Now $A^{100}\boldsymbol{u}_0 = V\Lambda^{100}V^{-1}\boldsymbol{u}_0 = V\Lambda^{100}\boldsymbol{c}$. Thus, multiply each eigenvector $\boldsymbol{v}_i$ with λ_i^{100} and **add up the results with weights c_i.**

In our case:

$$A - \lambda I = \begin{bmatrix} 1-\lambda & 1 \\ 1 & -\lambda \end{bmatrix} \rightsquigarrow det(A - \lambda I) = \lambda^2 - \lambda - 1 \stackrel{!}{=} 0$$

$$\rightsquigarrow \lambda = \tfrac{1}{2} \pm \sqrt{\tfrac{1}{4} + 1} \rightsquigarrow \lambda_1 = \tfrac{1+\sqrt{5}}{2} \approx 1.618, \quad \lambda_2 = \tfrac{1-\sqrt{5}}{2} \approx -0.618.$$

$$(A - \lambda I)\boldsymbol{v} = \boldsymbol{0} \rightsquigarrow \boldsymbol{v}_1 = \begin{bmatrix} \lambda_1 \\ 1 \end{bmatrix}, \quad \boldsymbol{v}_2 = \begin{bmatrix} \lambda_2 \\ 1 \end{bmatrix}.$$

Matrix Powers: Fibonacci numbers

Weights: $c_1 = 1/(\lambda_1 - \lambda_2), \quad c_2 = -1/(\lambda_1 - \lambda_2)$

After 100 steps: $\boldsymbol{u}_{100} = c_1\lambda_1^{100}\boldsymbol{v}_1 + c_2\lambda_2^{100}\boldsymbol{v}_2 = \frac{\lambda_1^{100}\boldsymbol{v}_1 - \lambda_2^{100}\boldsymbol{v}_2}{\lambda_1 - \lambda_2}$.

- We want F_{100} = second component of $\boldsymbol{u}_{100}$.
  Second components of eigenvectors are 1, and $\lambda_1 - \lambda_2 = \sqrt{5}$. Thus,

$$F_{100} = \frac{\lambda_1^{100} - \lambda_2^{100}}{\lambda_1 - \lambda_2} = \frac{1}{\sqrt{5}}\left[\left(\frac{1+\sqrt{5}}{2}\right)^{100} - \left(\frac{1-\sqrt{5}}{2}\right)^{100}\right] \approx 3.54{\cdot}10^{20}.$$

- **Note:** $\lambda_2^k/(\lambda_1 - \lambda_2) < 1/2$ and result must be an integer,
  so $F_k = \frac{\lambda_1^k - \lambda_2^k}{\lambda_1 - \lambda_2}$ must be the **nearest integer to** $\frac{1}{\sqrt{5}}\left(\frac{1+\sqrt{5}}{2}\right)^k$**.**

- The ratio $\frac{F_{k+1}}{F_k}$ approaches the **golden ratio** $\frac{1+\sqrt{5}}{2} \approx 1.618$ for large k.

Matrix Powers: Markov matrices

- A matrix is a **Markov matrix** iff the following holds:
  1. Every entry is non-negative, 2. Every column adds to 1.

- A Markov matrix is called **column-stochastic:**
  entries in every column can be interpreted as probabilities.

- Suppose A is Markovian, and start with probability vector $\boldsymbol{u}_0$.

- **Observation:** if we make a sequence of update steps, $\boldsymbol{u}_k = A^k \boldsymbol{u}_0$, we will approach a **steady state** for $k \to \infty$, and this steady state **does not depend on the starting vector $\boldsymbol{u}_0$!**

- **Asymptotic loss of memory:** Markov chain "forgets" where it started. The question is why...

Matrix Powers: Markov matrices

- **Intuition:** Since the eigenvalues of A are raised to larger and larger powers, a non-trivial steady state can only occur for $\lambda = 1$.
  The **steady state equation** $A\boldsymbol{u}_\infty = \boldsymbol{u}_\infty$ then makes $\boldsymbol{u}_\infty$ an eigenvector of A with eigenvalue $\lambda = 1$.
- **A^2 is also a Markov matrix:**

$$A^2 = \begin{bmatrix} p_1^2 + p_2 q_1 & p_1 q_1 + q_1 q_2 \\ p_1 p_2 + p_2 q_2 & p_2 q_2 + q_2^2 \end{bmatrix}$$

  Note that this matrix is also column-stochastic: Sum of first column is

$$p_1^2 + p_2 q_1 + p_1 p_2 + p_2 q_2 = p_1(p_1 + p_2) + p_2(q_1 + q_2) = p_1 + p_2 = 1.$$

- By induction, **all matrices A^k are Markov matrices!**
  $\rightsquigarrow$ they all have the eigenvalue $\lambda = 1$.
- This argument holds true for any $n \times n$ Markov matrix A.

Matrix Powers: Markov matrices

Theorem. *A positive Markov matrix (entries $a_{ij} > 0$) has one eigenvalue $\lambda_1 = 1$, all other eigenvalues have $|\lambda| < 1$.*

Proof part 1: Existence of $\lambda_1 = 1$ follows from this observation: Consider $A = \begin{bmatrix} p_1 & q_1 \\ p_2 & q_2 \end{bmatrix}$. A is column-stochastic, so every column of $A - 1I$ adds to $1 - 1 = 0 \rightsquigarrow$ the **row vectors add up to zero**, $(p_1 - 1, q_1)^t + (p_2, q_2 - 1)^t = (0, 0)^t$, so they are **linearly dependent** $\rightsquigarrow det(A - 1I) = 0 \rightsquigarrow$ **$\lambda = 1$ is an eigenvalue of A.**

Proof part 2: No eigenval. can have $|\lambda| > 1$: With such a λ, powers A^k would grow without bound as $k \to \infty \rightsquigarrow$ contradiction to observation that A^k is a Markov matrix (non-negative entries in columns add to 1)!

Markov matrices: Rental cars example

Rental cars in Denver. Every month, 80% of the Denver cars stay in Denver, 20% leave. 5% of outside cars come in, 95% stay outside. Fraction of cars in Denver starts at $1/50 = 0.02 \rightsquigarrow \boldsymbol{u}_0 = (0.02, 0.98)^t$.

First month: $\boldsymbol{u}_1 = \begin{bmatrix} 0.8 & 0.05 \\ 0.2 & 0.95 \end{bmatrix} \begin{bmatrix} 0.02 \\ 0.98 \end{bmatrix} = \begin{bmatrix} 0.065 \\ 0.935 \end{bmatrix}$

k-th month: $\boldsymbol{u}_k = A^k \boldsymbol{u}_0 = V \Lambda^k V^{-1} \boldsymbol{u}_0$

Eigenvalues and eigenvectors:

$$A \begin{bmatrix} 0.2 \\ 0.8 \end{bmatrix} = 1 \begin{bmatrix} 0.2 \\ 0.8 \end{bmatrix}, \quad A \begin{bmatrix} -1 \\ 1 \end{bmatrix} = 0.75 \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

Weights: $\boldsymbol{u}_0 = c_1 \boldsymbol{v}_1 + c_2 \boldsymbol{v}_2 = \begin{bmatrix} 0.02 \\ 0.98 \end{bmatrix} = 1 \begin{bmatrix} 0.2 \\ 0.8 \end{bmatrix} + 0.18 \begin{bmatrix} -1 \\ 1 \end{bmatrix}$

Markov matrices: Rental cars example

After k months: $\boldsymbol{u}_k = A^k \boldsymbol{u}_0 = V\Lambda^k \boldsymbol{c} = 1^k \cdot 1 \begin{bmatrix} 0.2 \\ 0.8 \end{bmatrix} + (0.75)^k \cdot 0.18 \begin{bmatrix} -1 \\ 1 \end{bmatrix}$

Thus, the eigenvector $\boldsymbol{v}_1 = \begin{bmatrix} 0.2 \\ 0.8 \end{bmatrix}$ with $\lambda_1 = 1$ is the steady state,

i.e. in the limit, **20% of the cars are in Denver** and 80% outside.

Initial vector $\boldsymbol{u}_0$ **is asymptotically irrelevant.**

Other eigenvector v_2 disappears because $|\lambda_2| < 1$.

Magnitude of λ_2 controls the **speed of convergence** to the steady state.

Markov matrices: Google example

Idea: for n websites, columns in $A_{n\times n}$ contain pairwise transition probabilities from one website to all other ones, computed from the **number of links between the sites.**

Then find $\boldsymbol{u}_\infty$ by a **random walk** that follows links (i.e. random surfing).

This steady state vector gives the **limit fraction of time at each site.**

The **ranking** of sites is then based on $\boldsymbol{u}_\infty$.

According to Google, the Markov matrix A has $2.7 \cdot 10^9$ rows and cols. Probably the largest eigenvalue problem ever solved!

Non-negative matrices: Perron-Frobenius

Theorem (Perron-Frobenius).
Assume $A > 0$. *All numbers in* $A\boldsymbol{x} = \lambda_{\max}\boldsymbol{x}$ *are strictly positive.*

Note that there is no requirement that columns add to 1.

Proof part 1: For some non-negative $\boldsymbol{x}$, look at all $t : A\boldsymbol{x} \geq t\boldsymbol{x}$. Then, for the largest value $t_{\max}$, equality holds: $A\boldsymbol{x} = t_{\max}\boldsymbol{x}$.
Why? Otherwise, multiplication by A gives $A^2\boldsymbol{x} > t_{\max}A\boldsymbol{x}$ (because A is strictly positive) $\rightsquigarrow$ the strictly positive vector $\boldsymbol{y} = A\boldsymbol{x}$ satisfies $A\boldsymbol{y} > t_{\max}\boldsymbol{y}$, and $t_{\max}$ could be increased.
So $A\boldsymbol{x} = t_{\max}\boldsymbol{x}$ and $t_{\max}$ is an eigenvalue. Its eigenvector $\boldsymbol{x}$ is positive, because on the left side of the equality, $A\boldsymbol{x}$ is positive.

Non-negative matrices and population models

Proof part 2: No eigenvalue can be larger than $t_{\max}$: Suppose $A\boldsymbol{z} = \lambda\boldsymbol{z}$ for some (genrerally complex) eigenvalue and eigenvector.
Take absolute values: $|\lambda||\boldsymbol{z}| = |A\boldsymbol{z}| \leq A|\boldsymbol{z}|$ (triangle inequality).
Now $|\boldsymbol{z}|$ is non-negative, so $|\lambda|$ is one of the possible candidates t
$\rightsquigarrow |\lambda| \leq t_{\max} \rightsquigarrow t_{\max} = \lambda_{\max}$.

Simple population model:

- Divide the population into three age groups (generations):
  age < 20, age 20 to 39, and age 40 to 59.
- At year T the sizes of those groups are n_1, n_2, n_3.
  Twenty years later, the sizes have changed for two reasons:
  - Reproduction $n_1^{\text{new}} = F_1 n_1 + F_2 n_2 + F_3 n_3$ gives a new generation (F_i are fertility rates)
  - Survival $n_2^{\text{new}} = P_1 n_1$ and $n_3^{\text{new}} = P_2 n_2$ gives the older generations

Population Models

In matrix form (with the **Leslie matrix** A):

$$\begin{bmatrix} n_1 \\ n_2 \\ n_3 \end{bmatrix}_{(T+\Delta)} = \begin{bmatrix} F_1 & F_2 & F_3 \\ P1 & 0 & 0 \\ 0 & P_2 & 0 \end{bmatrix} \begin{bmatrix} n_1 \\ n_2 \\ n_3 \end{bmatrix}_{(T)} = \begin{bmatrix} .04 & \mathbf{1.1} & .01 \\ .98 & \mathbf{0} & 0 \\ 0 & \mathbf{.92} & 0 \end{bmatrix} \begin{bmatrix} n_1 \\ n_2 \\ n_3 \end{bmatrix}_{(T)}$$

Note: In a more realistic model, A will change with time (from the environment or internal factors).

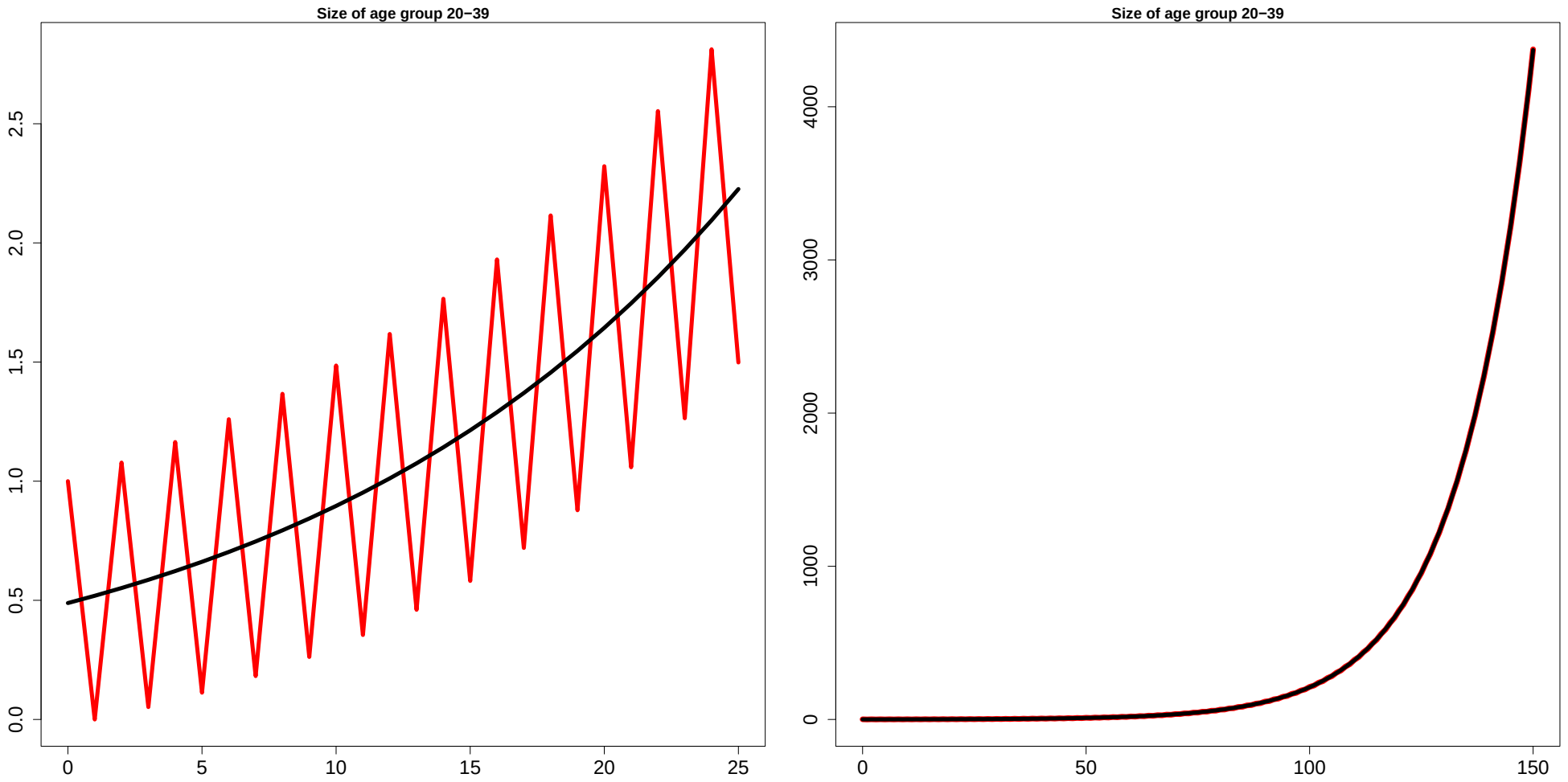
The matrix has $A \geq 0$ but not $A > 0$. The Perron-Frobenius theorem still applies because $A^3 > 0$. The largest eigenvalue is $\lambda_{\max} \approx 1.06$.

$$\boldsymbol{\lambda}(A) = \begin{bmatrix} \mathbf{1.06} \\ -1.01 \\ -0.01 \end{bmatrix}, A^2 = \begin{bmatrix} 1.08 & \mathbf{0.05} & .00 \\ 0.04 & \mathbf{1.08} & .01 \\ 0.90 & \mathbf{0} & 0 \end{bmatrix}, A^3 = \begin{bmatrix} 0.10 & \mathbf{1.19} & .01 \\ 0.06 & \mathbf{0.05} & .00 \\ 0.04 & \mathbf{0.99} & .01 \end{bmatrix}$$

Population Models

- Assume $\boldsymbol{u}_{(0)} = (0, 1, 0)$. That middle group will reproduce 1.1 and also survive .92. The newest and oldest generations are in $\boldsymbol{u}_1 = A\boldsymbol{u}_0 = (1.1, 0, .92) =$ column 2 of A.
- Then $\boldsymbol{u}_2 = A\boldsymbol{u}_1 = A^2\boldsymbol{u}_0$ is the second column of A^2.
- The early numbers (transients) depend a lot on $\boldsymbol{u}_0$, but the asymptotic growth rate $\lambda_{\max}$ is the same from every start.
- Solution in terms of eigenvalues/vectors:
  - Express initial values as linear combinations of eigenvectors, i.e. find coefficients $\boldsymbol{c}$ that solve $\boldsymbol{u}_0 = V\boldsymbol{c}$.
  - Solution at time k : $\boldsymbol{u}_k = V\Lambda^k\boldsymbol{c}$.
  - For large k, the leading eigenvalue λ_1 dominates $\rightsquigarrow$ numbers asymptotically grow like $\boldsymbol{v}_1\lambda_1^k c_1$, i.e. multiples of leading eigenvector $\boldsymbol{v}_1 \approx (.63, .58, .51)$

Population Models



Size of age group 20-39 years. X-axis represents index of generation (1 generation = 20 years). Red: exact values, Black: Asymptotic model using only the leading eigenvalue. The red curve starts according to $\boldsymbol{u}_0 = c(0, 1, 0)$.

Population Models: Sensitivity analysis

Model are never exactly right. If the F's or P's in the matrix change by 10%, does $\lambda_{\max}$ go below 1 (which means extinction)?

$\rightsquigarrow$ **Analyze the sentivity of eigenvalues to changes ΔA in matrix A.**

Consider changes in eigenvalues of perturbed matrix:

$$(A + \Delta A)(V + \Delta V) = (V + \Delta V)(\Lambda + \Delta\Lambda)$$

Ignore "quadratic" terms $(\Delta A)(\Delta V)$ and $(\Delta V)(\Delta\Lambda)$:

$$\begin{aligned} A(\Delta V) + (\Delta A)V &= V(\Delta\Lambda) + (\Delta V)\Lambda \\ V^{-1}A(\Delta V) + V^{-1}(\Delta A)V &= (\Delta\Lambda) + V^{-1}(\Delta V)\Lambda \\ \underbrace{V^{-1}A(\Delta V) - V^{-1}(\Delta V)\Lambda}_{\text{Diagonal elements are } 0} + V^{-1}(\Delta A)V &= \underbrace{\Delta\Lambda}_{\text{Diagonal matrix}} \\ \text{diag}(V^{-1}(\Delta A)V) &= \Delta\Lambda \end{aligned}$$

Population Models: Sensitivity analysis

$$\underbrace{V^{-1}A(\Delta V) - V^{-1}(\Delta V)\Lambda}_{\text{Diagonal elements are } 0}$$

Why? Note that $AV = V\lambda$ implies $V^{-1}A = \Lambda V^{-1}$, so the statement follows if

$$\text{diag}(\Lambda B) = \text{diag}(B\Lambda), \text{ with } B := V^{-1}(\Delta V),$$

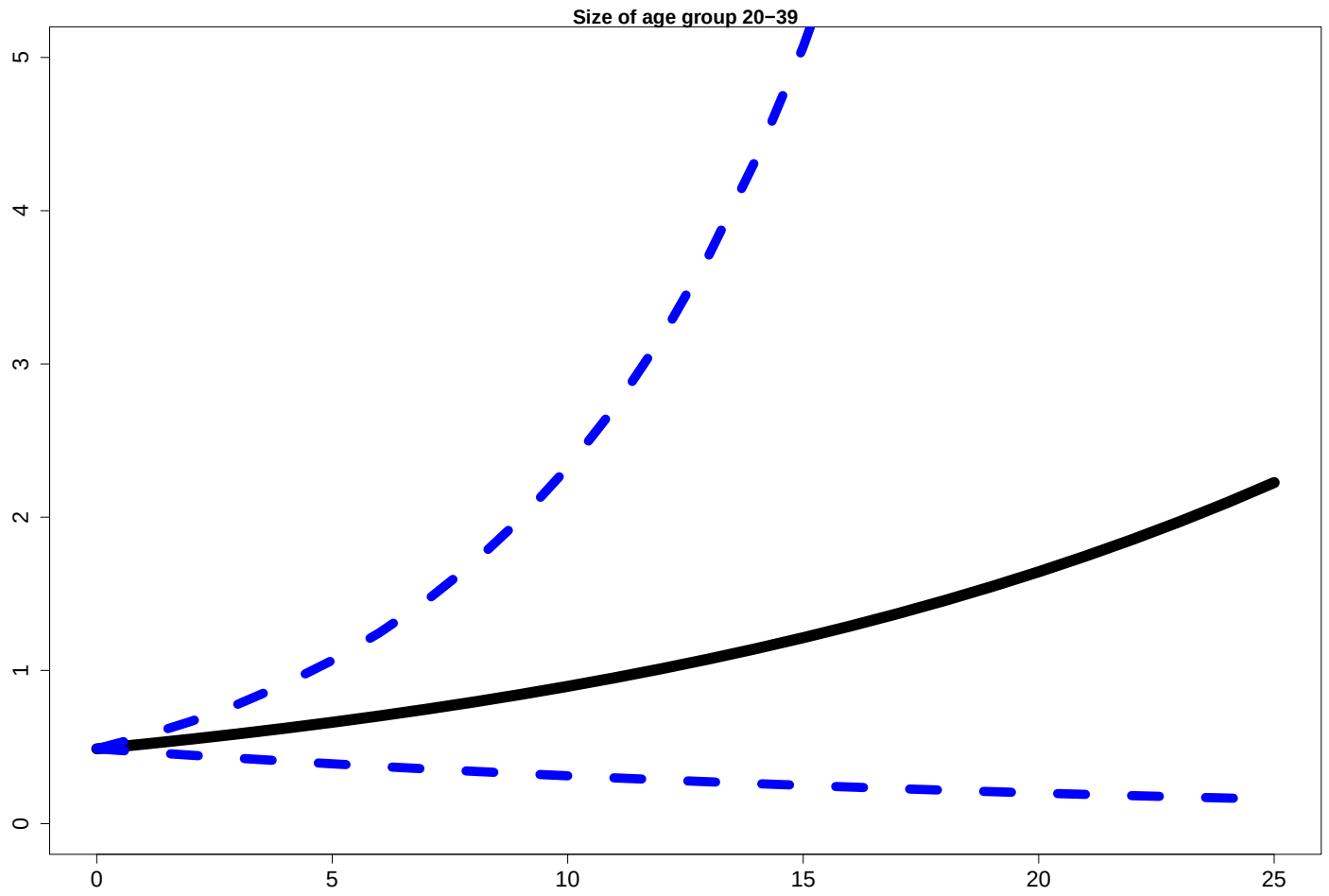
but this is the case for any B, because Λ is diagonal!

In our case for $\Delta A = \pm 0.1\, A$:

$$\begin{aligned} \Lambda &= (1.063, -1.014, -0.008) \\ \Delta\Lambda &= \pm(0.106, -0.101, -0.001) \end{aligned}$$

So there might be a huge uncertainty...

Population Models: Sensitivity analysis



Size of age group 20-39 years. X-axis represents index of generation (1 generation = 20 years). Black: Asymptotic model using only the leading eigenvalue. Dashed blue lines: perturbed matrix with $\Delta A = \pm 0.1\, A$.

Linear Algebra in Economics

- We have n industries like chemicals, food, and oil.
- To produce a unit of chemicals may require .2 units of chemicals, .3 units of food, and .4 units of oil.
- **Consumption matrix:**

$$\begin{bmatrix} \text{chemical output} \\ \text{food output} \\ \text{oil output} \end{bmatrix} = \begin{bmatrix} .2 & .3 & .4 \\ .4 & .4 & .1 \\ .5 & .1 & .3 \end{bmatrix} \begin{bmatrix} \text{chemical input} \\ \text{food input} \\ \text{oil input} \end{bmatrix}$$

- Note: The "real" matrix for the United States in 1958 contained 83 industries. Modern models are much larger and more precise.
- **Question: Can this economy meet demands** y_1, y_2, y_3 for chemicals, food, and oil?
- To do that, the inputs p_1, p_2, p_3 will have to be higher, because **part of p is consumed in producing y.**

Linear Algebra in Economics

- The input is $\boldsymbol{p}$ and the consumption is $A\boldsymbol{p}$, which leaves the output $\boldsymbol{p} - A\boldsymbol{p}$. This net production is what meets the demand $\boldsymbol{y}$.
- **Problem:** Find $\boldsymbol{p}$ such that $\boldsymbol{p} - A\boldsymbol{p} = \boldsymbol{y}$ **or** $\boldsymbol{p} = (I - A)^{-1}\boldsymbol{y}$, **assuming the inverse exists.**
- The demand vector $\boldsymbol{y}$ is **nonnegative**, and so is A.
  Production levels in $\boldsymbol{p} = (I - A)^{-1}\boldsymbol{y}$ must also be **nonnegative.**
- The **real question is:** When is $(I - A)^{-1}$ **a nonnegative matrix?**
  Answer: If $\lambda_{\max} < 1$ then $(I - A)^{-1}$ is nonnegative as desired.
- Why? Series expansion $(I - A)^{-1} = I + A + A^2 + \cdots$. Analog to geometric series $1 + x + x^2x^2 + \cdots = (1 - x)^{-1}$, for $x \in [-1, 1]$. When $x = 1$ the series is $1 + 1 + \cdots = \infty$. When $|x| > 1$ the series diverges.
- If you multiply the series $S = 1 + A + A2 + \cdots$ by A, you get the same series except for I. Therefore $S - AS = I$, which is $(I - A)S = I$. The series adds to $S = (I - A)^{-1}$ if it converges.
  And it converges if all eigenvalues of A have $|\lambda| < 1$.

Linear Algebra in Economics

- Our case: $A > 0 \rightsquigarrow$ **All terms in series** $\geq 0 \rightsquigarrow$ **sum is** $(I - A)^{-1} \geq 0$.
- $A = \begin{bmatrix} .2 & .3 & .4 \\ .4 & .4 & .1 \\ .5 & .1 & .3 \end{bmatrix}$ has $\lambda_{\max} = 0.9$ and $(I - A)^{-1} = \frac{1}{93} \begin{bmatrix} 41 & 25 & 27 \\ 33 & 36 & 24 \\ 34 & 23 & 36 \end{bmatrix}$.
- **This economy is productive:** A is small compared to I, because $\lambda_{\max} = 0.9$. To meet the demand $\boldsymbol{y}$, start from $\boldsymbol{p} = (1 - A)^{-1}\boldsymbol{y}$.
  Then $A\boldsymbol{p}$ is consumed in production, leaving $\boldsymbol{p} - A\boldsymbol{p}$.
  This is $(1 - A)\boldsymbol{p} = \boldsymbol{y}$**, and the demand is met.**
- Other example: $A = \begin{bmatrix} 0 & 4 \\ 1 & 0 \end{bmatrix}$ has $\lambda_{\max} = 2$ and $(I - A)^{-1} = -\frac{1}{3} \begin{bmatrix} 1 & 4 \\ 1 & 1 \end{bmatrix}$.
- This consumption matrix A is too large. **Demands can't be met**, because **production consumes more than it yields.**
  The series does not converge to $(I - A)^{-1}$ because $\lambda_{\max} > 1$.

Chapter 1

Linear Systems of Equations

Singular Value Decomposition

Singular value decomposition

- Remember matrix diagonalization: $V^{-1}AV = \Lambda$. Three problems:
  - A must be square.
  - There are not always enough eigenvectors.
  - Only for symmetric matrices, the $\boldsymbol{v}_i$ are orthogonal.

- The SVD solves these problems, but at an additional price: we now have **two sets of singular vectors** $\boldsymbol{u}_i$ and $\boldsymbol{v}_i$.
  Denoting by σ_i the **singular values**, they are related as:

$$A\boldsymbol{v}_i = \sigma_i \boldsymbol{u}_i \quad \text{and} \quad A^t \boldsymbol{u}_i = \sigma_i \boldsymbol{v}_i.$$

- If r is the rank of A, there will be r positive singular values, say $\sigma_1, \ldots, \sigma_r > 0$. All remaining ones will be zero.

Calculating the SVD

- Combine the two equations that define a pair $\boldsymbol{u}, \boldsymbol{v}$:

$$A^t(A\boldsymbol{v}) = A^t(\sigma\boldsymbol{u}) = \sigma(A^t\boldsymbol{u}) = \sigma(\sigma\boldsymbol{v}) = \sigma^2\boldsymbol{v}.$$

- So $A^tA\boldsymbol{v} = \sigma^2\boldsymbol{v}$.
  Singular values: **square roots of the eigenvalues of** A^tA (note that A^tA is positive semi-definite).
  Singular vectors $\boldsymbol{v}$: **eigenvectors of** A^tA.
- We can always choose orthonormal eigenvectors: Orthonormal basis always exists, because A^tA is symmetric $\rightsquigarrow$ orthogonally diagonalizable.
- Given $\boldsymbol{v}_i, \sigma_i$, compute $\boldsymbol{u}_i$ according to $\boldsymbol{u}_i = \sigma_i^{-1}A\boldsymbol{v}_i, \quad i = 1, \ldots, r$.
- Arrange singular values on **diagonal of a matrix** S and singular vectors as the columns of **orthogonal matrices** U **and** V.
- Then we have $AV = US$ and $A^tU = VS$.

Calculating the SVD: starting with U

- So far: Start with eigenvector decomposition of $A^tA \rightsquigarrow V$ and S, then compute $\boldsymbol{u}_i = \sigma_i^{-1} A\boldsymbol{v}_i$.
- Can also start with $AA^t \rightsquigarrow U$ and S:

$$AA^t\boldsymbol{u} = A\sigma\boldsymbol{v} = \sigma(A\boldsymbol{v}) = \sigma(\sigma\boldsymbol{u}) = \sigma^2\boldsymbol{u}.$$

  Singular values are also the **square roots of the eigenvalues of** AA^t, and the **eigenvectors of** AA^t are the columns of U.
- Then $\boldsymbol{v}_i = \sigma_i^{-1} A^t\boldsymbol{u}_i, \quad i = 1, \ldots, r.$
- **BUT:** Don't mix the two methods. Problem: Eigenvectors only determined **up to the direction**: if $\boldsymbol{v}$ is eigenvector of A^tA, then also $-\boldsymbol{v}$ is one: $A^tA\boldsymbol{v} = \lambda\boldsymbol{v} \;\Rightarrow\; A^tA(-\boldsymbol{v}) = \lambda(-\boldsymbol{v})$.
  So if you compute both $\boldsymbol{u}_i$ and $\boldsymbol{v}_i$ as eigenvectors of AA^t and A^tA, the signs can be arbitrary $\rightsquigarrow$ not necessarily a correct SVD.

Singular value decomposition

Orthogonality implies $AV = US \rightsquigarrow AVV^t = A = USV^t$.

Economy version of the **singular value decomposition** (SVD) of A:
U is $m \times r$, S is $r \times r$, V is $n \times r$.

$$A = USV^t = \begin{bmatrix} | & | & | & | \\ \boldsymbol{u}_1 & \boldsymbol{u}_2 & \dots & \boldsymbol{u}_r \\ | & | & | & | \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_r \end{bmatrix} \begin{bmatrix} - & \boldsymbol{v}_1^t & - \\ - & \boldsymbol{v}_2^t & - \\ & \vdots & \\ - & \boldsymbol{v}_r^t & - \end{bmatrix}$$

What about the remaining $n - r$ vectors $\boldsymbol{v}_i$ and the $m - r$ vectors $\boldsymbol{u}_i$ with $\sigma_i = 0$? They span the nullspaces of A and A^t:

$$A\boldsymbol{v}_j = \boldsymbol{0}, \quad \text{for } j > r$$

$$A^t\boldsymbol{u}_j = \boldsymbol{0}, \quad \text{for } j > r$$

Singular value decomposition

Full singular value decomposition (SVD) of A:
U is $m \times m$, S is $m \times n$, V is $n \times n$.

$$\begin{bmatrix} | & | & | & | & | & & | \\ \boldsymbol{u}_1 & \boldsymbol{u}_2 & \dots & \boldsymbol{u}_r & \boldsymbol{u}_{r+1} & \dots & \boldsymbol{u}_m \\ | & | & | & | & | & & | \end{bmatrix} \begin{bmatrix} \sigma_1 & & & & & & \\ & \sigma_2 & & & & & \\ & & \ddots & & & & \\ & & & \sigma_r & & & \\ & & & & 0 & & \\ & & & & & \ddots & \\ & & & & & & 0 \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 \end{bmatrix} \begin{bmatrix} - & \boldsymbol{v}_1^t & - \\ - & \boldsymbol{v}_2^t & - \\ & \vdots & \\ - & \boldsymbol{v}_r^t & - \\ - & \boldsymbol{v}_{r+1}^t & - \\ & & \\ & \vdots & \\ - & \boldsymbol{v}_n^t & - \end{bmatrix}$$

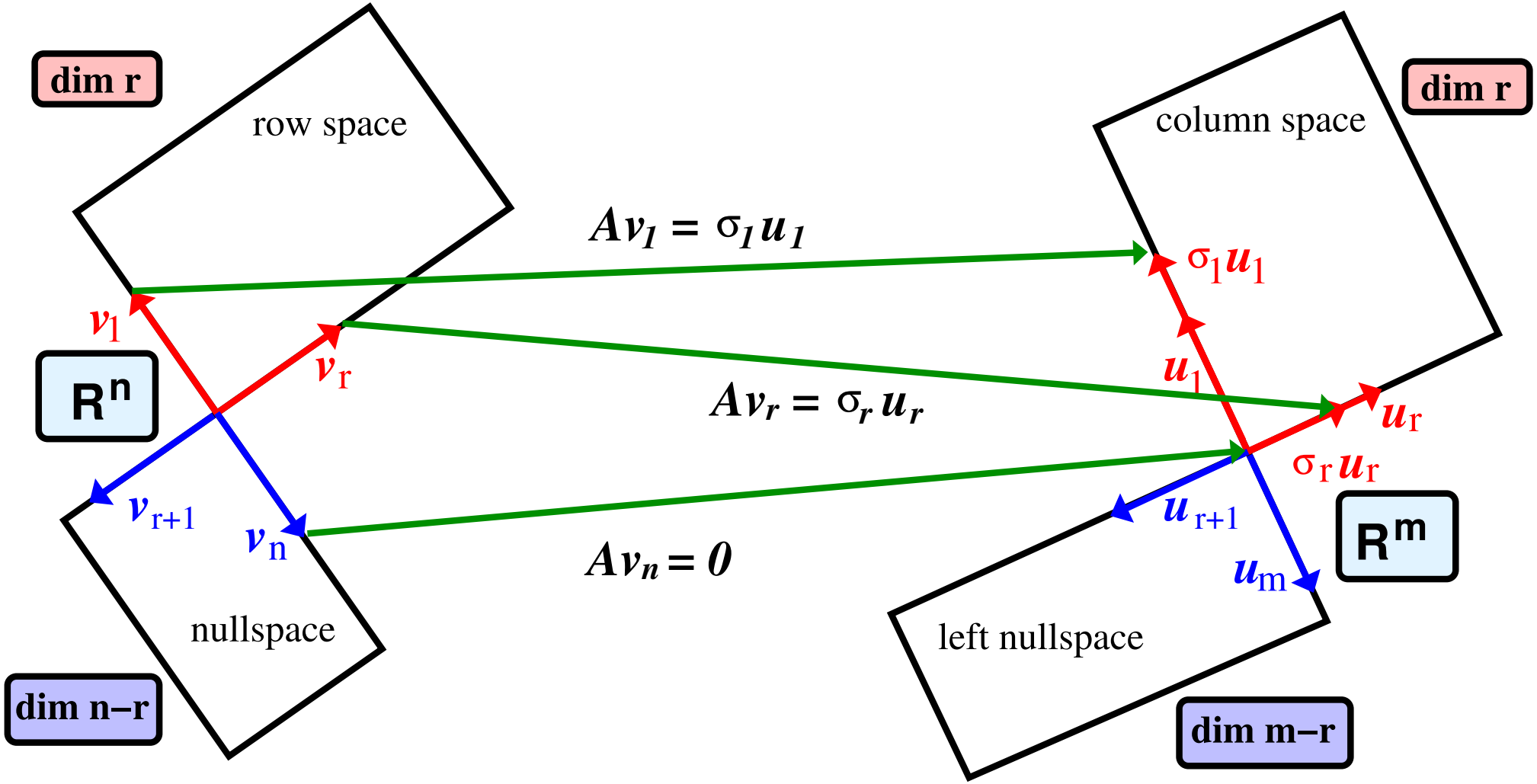
SVD and bases for the 4 subspaces

$$A\boldsymbol{v}_j = \sigma_j \boldsymbol{u}_j, \quad \text{for } j \le r. \qquad A^t\boldsymbol{u}_j = \sigma_j \boldsymbol{v}_j, \quad \text{for } j \le r.$$

$$A\boldsymbol{v}_j = \boldsymbol{0}, \quad \text{for } j > r. \qquad A^t\boldsymbol{u}_j = \boldsymbol{0}, \quad \text{for } j > r.$$

- **Columns of V with $\sigma_j > 0$ are an orthonormal basis for $C(A^t)$.**
  Diagonal elements in S scale the columns in V: $A^t\boldsymbol{y} = VS^tU^t\boldsymbol{y}$, so the columns of V with nonzero σ span the row space.
- **Last $n-r$ columns of V are an orthonormal basis for $N(A)$.**
- **Columns of U with $\sigma_j > 0$ are an orthonormal basis for $C(A)$.**
  Diagonal elements in S scale the columns in U: $A\boldsymbol{x} = USV^t\boldsymbol{x}$, so the columns of U with nonzero σ span the column space.
- **Last $m-r$ columns of U are an orthonormal basis for $N(A^t)$.**

SVD and bases for the 4 subspaces



SVD and linear systems

Assume A is a $n \times n$ matrix. With the SVD decomposition:

$$\begin{aligned} A\boldsymbol{x} &= \boldsymbol{b} \\ USV^t\boldsymbol{x} &= \boldsymbol{b} \\ SV^t\boldsymbol{x} &= U^t\boldsymbol{b} \\ S\boldsymbol{z} &= \boldsymbol{d}, \text{ where } \boldsymbol{z} = V^t\boldsymbol{x} \text{ and } \boldsymbol{d} = U^t\boldsymbol{b}. \end{aligned}$$

Written in blocks this is

$$\begin{bmatrix} \sigma_1 & & & & & & \\ & \sigma_2 & & & & & \\ & & \ddots & & & & \\ & & & \sigma_r & & & \\ & & & & \sigma_{r+1} = 0 & & \\ & & & & & \ddots & \\ & & & & & & \sigma_n = 0 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_r \\ z_{r+1} \\ \vdots \\ z_n \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_r \\ d_{r+1} \\ \vdots \\ d_n \end{bmatrix}$$

Solution: $z_i = d_i/\sigma_i, \quad i = 1, \ldots, r$. What about the remaining entries?

SVD and linear systems

Recall: $\boldsymbol{b}$ must be in $C(A)$ (otherwise no solution exists),
last $m - r$ columns of U form basis of orthogonal complement $N(A^t)$.

Right hand side is

$$\boldsymbol{d} = U^t \boldsymbol{b} = \begin{bmatrix} - & \boldsymbol{u}_1^t & - \\ - & \boldsymbol{u}_2^t & - \\ & \vdots & \\ - & \boldsymbol{u}_r^t & - \\ - & \boldsymbol{u}_{r+1}^t & - \\ - & \boldsymbol{u}_{r+2}^t & - \\ & \vdots & \\ - & \boldsymbol{u}_m^t & - \end{bmatrix} \boldsymbol{b} = \begin{bmatrix} d_1 \\ \vdots \\ d_r \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

For $r + 1 \leq i \leq n$: $0 \cdot z_i = 0 \rightsquigarrow$ can choose them arbitrarily.

Pseudoinverse

Alternative formalism for SVD solution:

- Write S^+ to denote the matrix obtained by replacing each σ_k in S^t by its reciprocal, so $S^+S = \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix}$
- Then compute:

$$\begin{aligned} USV^t\boldsymbol{x} &= \boldsymbol{b} \\ SV^t\boldsymbol{x} &= U^t\boldsymbol{b} \\ S\boldsymbol{z} &= U^t\boldsymbol{b} \\ \tilde{\boldsymbol{z}} = (\boldsymbol{z}_{[1:r]}, \mathbf{0})^t &= S^+U^t\boldsymbol{b} \\ \boldsymbol{x} = V\tilde{\boldsymbol{z}} &= \underbrace{VS^+U^t}_{A^+}\boldsymbol{b}. \end{aligned}$$

A^+ is the **pseudoinverse** of A: it maps $\boldsymbol{b} \in C(A)$ back to $\boldsymbol{x} \in C(A^t)$.

SVD and linear systems

Homogeneous equations:

- Zero right hand side: $\boldsymbol{b} = \mathbf{0}$
- Columns of V with $\sigma_j = 0$ are an orthonormal basis for the $N(A)$.
- **Solved immediately by SVD:**
  Any column of V whose corresponding $\sigma_j = 0$ yields a solution.

General case:

- Consider arbitrary $\boldsymbol{b}$. **Two cases: does $\boldsymbol{b}$ lie in $C(A)$ or not?**
- If **YES**, there exists a solution $\boldsymbol{x}$; in fact more than one,
  since any vector in the nullspace can be added to $\boldsymbol{x}$.
- SVD solution $\boldsymbol{x} = A^+ \boldsymbol{b}$ is the "purest" solution: the one with smallest length $\|\boldsymbol{x}\|^2$. Why? $\boldsymbol{x} \in C(A^t)$, any nonzero component in the orthogonal nullspace would only increase the length.

General case

Consider arbitrary b. **Two cases: does b lie in $C(A)$ or not?**

NO: If b is not in $C(A)$, there is **no solution**.

But: can compute **compromise** solution: Among all possible x, it will minimize the **sum of squared errors** between left- and right hand side

$\rightsquigarrow$ **least-squares methods.**

SVD and Zeroing

The SVD can solve further numerical problems:

- Zero a small singular value if σ_j is (too) close to zero.
- This forces a **zero coefficient** instead of a **random large coefficient** that would scale a vector "close to" the nullspace:

$$\boldsymbol{x} = V\boldsymbol{z} = \underbrace{\boldsymbol{v}_1\frac{d_1}{\sigma_1} + \cdots + \boldsymbol{v}_r\frac{d_r}{\sigma_r}}_{\text{rowspace}} + \underbrace{\boldsymbol{v}_{r+1}z_{r+1} + \cdots + \boldsymbol{v}_n z_n}_{\text{nullspace}}$$

- Rule of thumb: if the ratio $\sigma_j/\sigma_1 < \epsilon_m$ then **zero the entry in the pseudo-inverse matrix**, since the value is probably **corrupted by roundoff** anyway.

Chapter 1

Linear Systems of Equations

The condition number

Conditioning

- **Conditioning** is a measure of the **sensitivity to perturbations**, due to measurement error, statistical fluctuations in the data analysis process, or caused by roundoff errors.
  These perturbations might affect the numerical values in $\boldsymbol{b}$ and/or A.

- Conditioning describes how this **problem error** $\Delta \boldsymbol{b}, \Delta A$ will affect the **solution error** $\Delta \boldsymbol{x}$.

- A function of the **problem itself**, **independent** of the algorithm used. (In practice, however, this separation between the problem and the algorithm might be less clear as it seems...Example: In elimination, the values in A change after every elimination step.)

Vector and matrix norms

- How to compare **closeness** of two vectors $\boldsymbol{x}$ and $\boldsymbol{x} + \Delta\boldsymbol{x}$? Look at relative quantities like $\frac{\|\Delta\boldsymbol{x}\|}{\|\boldsymbol{x}\|} \leq \delta$, or $\frac{\|\Delta\boldsymbol{x}\|}{\|\boldsymbol{x}+\Delta\boldsymbol{x}\|} \leq \delta$.
- **Vector norm properties:**
  (i) $\|\boldsymbol{x}\| > 0$, $\forall \boldsymbol{x} \neq 0$
  (ii) $\|a\boldsymbol{x}\| = |a|\|\boldsymbol{x}\|$
  (iii) $\|\boldsymbol{x} + \boldsymbol{y}\| \leq \|\boldsymbol{x}\| + \|\boldsymbol{y}\|$
- The **vector p-norms (ℓ_p norms)** are defined by

$$\|\boldsymbol{x}\|_p = \left(\sum_{i=1}^{n} |x_i|^p \right)^{1/p}, \quad 1 \leq p \leq \infty,$$

$$\|\boldsymbol{x}\|_\infty = \max(|x_1|, \cdots |x_n|).$$

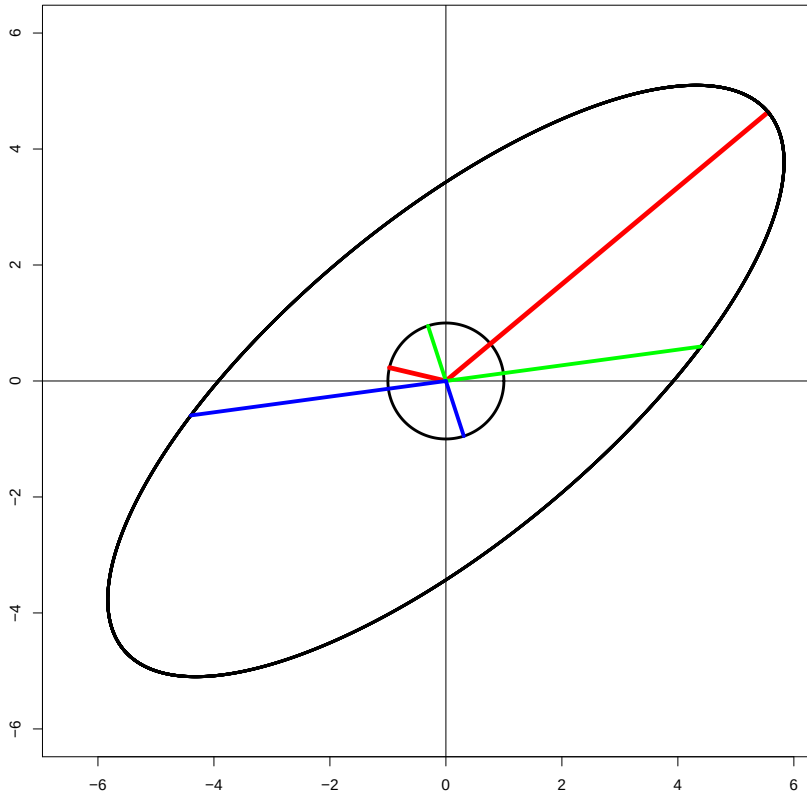
- $\|x\|_2$ is the usual **Euclidean norm.** What about **matrix norms**?

Vector and matrix norms

- $\boldsymbol{y} = A\boldsymbol{x}$ **transforms** vector $\boldsymbol{x}$ into $\boldsymbol{y}$
  $\rightsquigarrow$ A **rotates and/or stretches** $\boldsymbol{x}$.

- Consider the effect of A on a unit vector $\boldsymbol{x}$ (i.e. $\boldsymbol{x}$ so that $\|\boldsymbol{x}\|_2 = 1$).

- The "largest" $A\boldsymbol{x}$ value is a measure of the **geometric effect of the transformation** A.



- The 2-norm is $\|A\|_2 = \max_{\|\boldsymbol{x}\|_2=1} \|A\boldsymbol{x}\|_2$.

- Also called the **spectral norm** of A,
  because $\|A\|_2 = \sqrt{\max(\lambda_i)}$ where λ_i is an **eigenvalue** of $A^t A$
  (See handout on matrix norms).

Vector and matrix norms

- Two other **useful and easier-to-calculate** matrix norms:
- $\|A\|_1 = \max_j \sum_{i=1}^{m} |a_{ij}|$ **column sum norm**.
- $\|A\|_\infty = \max_i \sum_{j=1}^{n} |a_{ij}|$ **row sum norm**.
- $\|A\|$ satisfies vector norm properties **PLUS**
  $\|AB\| \leq \|A\|\|B\|$ and, in particular, $\|A\boldsymbol{x}\| \leq \|A\|\|\boldsymbol{x}\|$.

Sensitivity to perturbations

- Original system is $A\boldsymbol{x} = \boldsymbol{b}$. Assume that right hand side is changed to $\boldsymbol{b} + \Delta\boldsymbol{b}$ because of roundoff or measurement error.

- Then the solution is changed to $\boldsymbol{x} + \Delta\boldsymbol{x}$.
  Goal: Estimate the change in the solution from the change $\Delta\boldsymbol{b}$.
  Subtract $A\boldsymbol{x} = \boldsymbol{b}$ from $A(\boldsymbol{x} + \Delta\boldsymbol{x}) = \boldsymbol{b} + \Delta\boldsymbol{b}$
  to find $A(\Delta\boldsymbol{x}) = \Delta\boldsymbol{b} \quad \Leftrightarrow \quad \Delta\boldsymbol{x} = A^{-1}\Delta\boldsymbol{b}$

$$\begin{aligned} \Delta\boldsymbol{x} = A^{-1}\Delta\boldsymbol{b} \quad &\Rightarrow \quad \|\Delta\boldsymbol{x}\| \leq \|A^{-1}\|\|\Delta\boldsymbol{b}\| \\ A\boldsymbol{x} = \boldsymbol{b} \quad &\Rightarrow \quad \|\boldsymbol{b}\| \leq \|A\|\|\boldsymbol{x}\| \end{aligned}$$

  Multiplication and division of both sides by $(\|\boldsymbol{b}\|\|\boldsymbol{x}\|)$ gives

$$\frac{\|\Delta\boldsymbol{x}\|}{\|\boldsymbol{x}\|} \leq \underbrace{\|A\|\|A^{-1}\|}_{k(A)} \frac{\|\Delta\boldsymbol{b}\|}{\|\boldsymbol{b}\|}.$$

Sensitivity to perturbations

- Error can also be in the matrix: we have $A + \Delta A$ instead of the true matrix A.
- Subtract $A\boldsymbol{x} = \boldsymbol{b}$ from $(A + \Delta A)(\boldsymbol{x} + \Delta \boldsymbol{x}) = \boldsymbol{b}$
  to find $A(\Delta \boldsymbol{x}) = -(\Delta A)(\boldsymbol{x}+\Delta \boldsymbol{x}) \quad \Leftrightarrow \quad \Delta \boldsymbol{x} = -A^{-1}(\Delta A)(\boldsymbol{x}+\Delta \boldsymbol{x})$

$$\|\Delta \boldsymbol{x}\| \le \|A^{-1}\|\|\Delta A\|\|\boldsymbol{x} + \Delta \boldsymbol{x}\|$$

$$\frac{\|\Delta \boldsymbol{x}\|}{\|\boldsymbol{x} + \Delta \boldsymbol{x}\|} \le \underbrace{\|A\|\|A^{-1}\|}_{k(A)} \frac{\|\Delta A\|}{\|A\|}.$$

- Conclusion: Errors can be in the matrix or in the r.h.s.
  This **problem error** is amplified into the **solution error Δx**.
  Rel. solution error is bounded by $k(A)$ times rel. problem error.

Condition number

- $k(A) = \|A\|\|A^{-1}\|$ is called the **condition number** of A.
- $1 \leq k(A) \leq \infty$.
- An **ill-conditioned problem has a large condition number.**
- Small residual does **not** guarantee accuracy for ill-conditioned problems:
  $\hat{\boldsymbol{x}}$ is a numerical solution to $A\boldsymbol{x} = \boldsymbol{b}$, and $\Delta\boldsymbol{x} = \boldsymbol{x} - \hat{\boldsymbol{x}}$.
  Define **residual** $\boldsymbol{r}$ to represent the error $\boldsymbol{r} = \boldsymbol{b} - A\hat{\boldsymbol{x}} = \boldsymbol{b} - \hat{\boldsymbol{b}} = \Delta\boldsymbol{b}$:

$$\frac{\|\Delta\boldsymbol{x}\|}{\|\boldsymbol{x}\|} \leq k(A)\frac{\|\boldsymbol{r}\|}{\|\boldsymbol{b}\|}.$$

- $k(A)$ is a **mathematical property of the coefficient matrix** A.
- In **exact** math a singular matrix has $k(A) = \infty$. $k(A)$ indicates how close a matrix is to being **numerically** singular.

Condition number

- $k(A)$ can be measured with any matrix p-norm.
- Spectral norm $\|A\|_2 = \sqrt{\lambda_{\max}(A^t A)} = \sigma_{\max}(A)$

  For an invertible matrix M we have:

$$M\boldsymbol{v} = \lambda \boldsymbol{v} \;\Rightarrow\; \boldsymbol{v} = \lambda M^{-1}\boldsymbol{v} \;\Rightarrow\; M^{-1}\boldsymbol{v} = \lambda^{-1}\boldsymbol{v},$$

  so M^{-1} has the same eigenvectors but inverse eigenvalues, and

$$\|A^{-1}\|_2 = \sqrt{\lambda_{\min}(A^t A)} = \sigma_{\min}(A) \rightsquigarrow \quad k(A) = \frac{\sigma_{\max}}{\sigma_{\min}}.$$

- Can be generalized to singular/rectangular matrices: $k(A) = \|A\|\|A^+\|$ = ratio of largest and smallest positive singular value.

Chapter 1

Linear Systems of Equations

Matrix Exponentials and Differential Equations

Applications to Differential Equations

Main Idea: **Convert constant-coefficient DEs into linear algebra.**

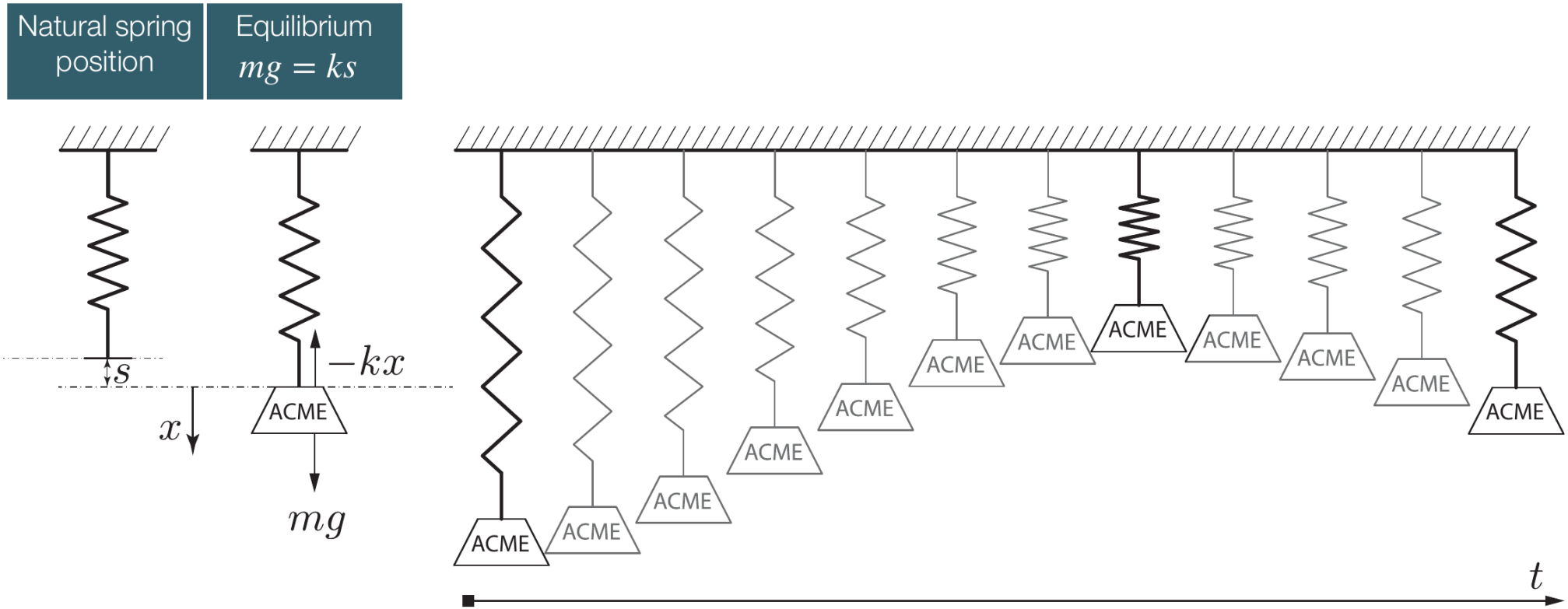
- One equation: $\frac{du}{dt} = \lambda u$ has solutions $u(t) = ce^{\lambda t}$.
- **Initial conditions:** Choose $c = u(0)$ (since $e^0 = 1$).
- n equations: $\frac{d\boldsymbol{u}}{dt} = A\boldsymbol{u}$, starting from $\boldsymbol{u}(0)$ at $t = 0$.
- **Equations are linear:**
  If $\boldsymbol{u}(t)$ and $\boldsymbol{v}(t)$ are solutions $\rightsquigarrow$ $c\boldsymbol{u}(t) + d\boldsymbol{v}(t)$ is solution.
- Here, A is a constant matrix
  $\rightsquigarrow$ compute eigen-vectors and -values satisfying $A\boldsymbol{v} = \lambda\boldsymbol{v}$.
- Substitute $\boldsymbol{u}(t) = e^{\lambda t}\boldsymbol{v}$ into $\frac{d\boldsymbol{u}}{dt} = A\boldsymbol{u}$:

$$\rightsquigarrow \ \lambda e^{\lambda t}\boldsymbol{v} = Ae^{\lambda t}\boldsymbol{v} \ \Leftrightarrow \ A\boldsymbol{v} = \lambda\boldsymbol{v}.$$

First Order Equations

- All components of this **special solution** $\boldsymbol{u}(t) = e^{\lambda t}\boldsymbol{v}$ share the same time-dependent scalar $e^{\lambda t}$.
- Real eigenvalues: $\lambda > 0 \rightsquigarrow$ solution grows, $\lambda < 0 \rightsquigarrow$ solution decays.
- **Complex eigenvalues:** Real part describes **growth/decay**, imaginary part ω gives **oscillation** like a sine wave: $e^{i\omega t} = \cos(\omega t) + i\sin(\omega t)$.
- Complete solution is **linear combination of special solutions** for each $(\boldsymbol{v}, \lambda)$-pair. Coefficients are determined by initial conditions.
- **Recipe** (assuming no repeated eigenvalues $\rightsquigarrow n$ eigenvectors):
  - Write $\boldsymbol{u}(0)$ as combination of eigenvectors $c_1\boldsymbol{v}_1 + \cdots + c_n\boldsymbol{v}_n$
  - Multiply $\boldsymbol{v}_i$ by $e^{\lambda_i t}$
  - Solution is $\boldsymbol{u}(t) = c_1 e^{\lambda_1 t}\boldsymbol{v}_1 + \cdots + c_n e^{\lambda_n t}\boldsymbol{v}_n$.

Second Order Equations



$$F_G = mg \qquad F_S = -k(s+x)$$

Spring-Mass Systems: Equilibrium

- The mass comes to an equilibrium position because the force of gravity, F_G, balances the restoring force of the spring, F_S.
- Hooke's law: the force needed to extend or compress a spring by some distance scales linearly with respect to that distance: $F_S = -k(s + x)$, where s is the equilibrium position. k is the spring constant, or "stiffness" parameter.
- **Newton's first law of motion**:
  The sum of the forces acting on a body at rest must equal zero

$$\begin{aligned} \sum F = F_{\text{tot}} &= F_G + F_S = 0 \\ &= mg - ks = 0 \end{aligned}$$

Spring-Mass Systems: Equilibrium

- **Newton's Second law:**
  The change of momentum is proportional to the force impressed

$$F_{\text{tot}} = m\dot{v} = m\ddot{x} = \underbrace{mg - ks}_{=0} - kx.$$

- Second order equation:

$$m\ddot{x} + b\dot{x} + kx = 0.$$

- In real systems, there will always be an additional damping term, proportional to the velocity:

$$\overset{\text{mass}}{m}\ \underset{\text{acceleration}}{\ddot{x}} + \underset{\text{damping}}{b\dot{x}} + \underset{\text{restoring force}}{kx} = 0$$

Second Order Equations

- **Mechanics** is dominated by

$$\underset{\text{mass}}{m}\ \underset{\text{acceleration}}{\ddot{x}} + \underset{\text{damping}}{b\dot{x}} + \underset{\text{restoring force}}{kx} = 0$$

Linear second-order equation with constant coefficients m, b, k.

- Assume $m = 1$. define $\boldsymbol{u} = (x, \dot{x})^t$. The two eqs.

$$\frac{dx}{dt} = \dot{x} \text{ and } \frac{d\dot{x}}{dt} = -kx - b\dot{x}$$

convert to

$$\frac{d}{dt}\boldsymbol{u} = A\boldsymbol{u} \rightsquigarrow \frac{d}{dt}\begin{bmatrix} x \\ \dot{x} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -k & -b \end{bmatrix}\begin{bmatrix} x \\ \dot{x} \end{bmatrix}$$

- **Reduction to first-order system!**

Second Order Equations: No damping

- Special case: No damping $(b = 0)$. Define $k = \omega^2$
- Determinant $|A - \lambda I| = \lambda^2 + \omega^2 \stackrel{!}{=} 0$
  $\rightsquigarrow$ two distinct eigenvalues $\lambda_1, \lambda_2 = \pm i\omega$

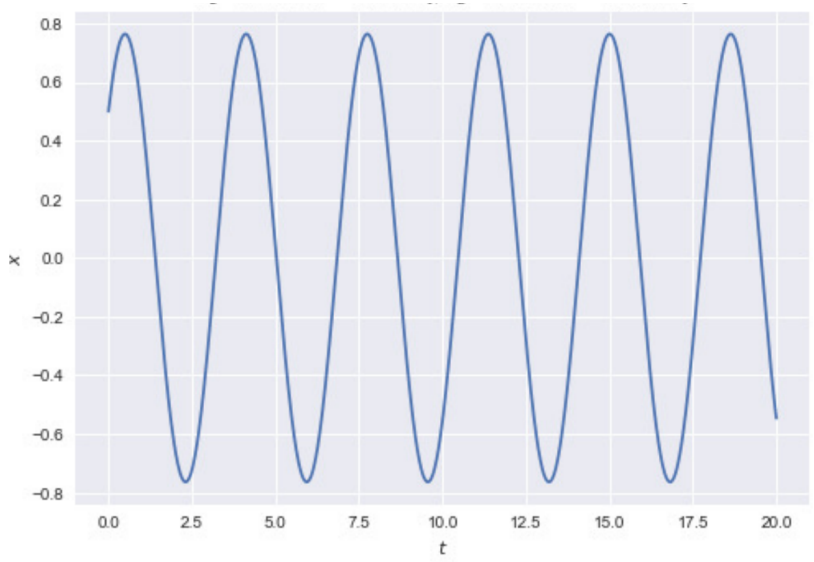
- Solving $|A - \lambda I| = 0 \rightsquigarrow$ two eigenvectors, $\boldsymbol{v}_1 = (1, i\omega)^t, \boldsymbol{v}_2 = (1, -i\omega)^t$.
- Solution:
  $\boldsymbol{u}(t) = c_1 e^{\lambda_1 t}\boldsymbol{v}_1 + c_2 e^{\lambda_2 t}\boldsymbol{v}_2$.
  First component: $x(t)$ (position),
  Second component: $\dot{x}(t)$ (velocity).
- Constants $c_{1,2}$ can be determined from initial conditions $x(0)$ and $\dot{x}(0)$.

Second Order Equations

- With the identity $e^{ix} = \cos(x) + i\,\sin(x)$, we finally get the familiar harmonic oscillations:

$$x(t) = A\,\cos(\omega t) + B\,\sin(\omega t) = \alpha\,\sin(\omega t + \phi),$$

for some **real** constants A, B, α, ϕ, determined by the initial conditions.



Stability

Consider general ODE problem $\frac{d}{dt}\boldsymbol{u} = A\boldsymbol{u}$

Q.: Does the solution approach $\boldsymbol{u} = \mathbf{0}$ as $t \to \infty$?
I.e. Is the problem **stable**, by dissipating energy?
A.: Depends on eigenvalues!

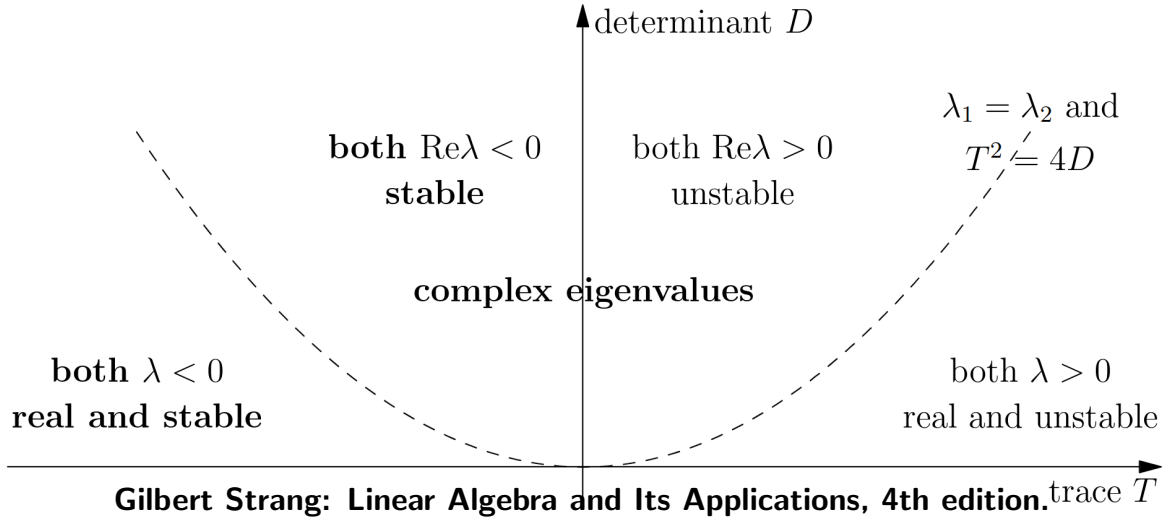
- Solutions are linear combinations of $e^{\lambda_i t}\boldsymbol{x}$.
- If λ is real, then we need $\lambda < 0$ for stability.
- In general, eigenvalues are complex, i.e. $\lambda = \mathcal{R} + i\mathcal{I} \rightsquigarrow e^{\lambda t} = e^{\mathcal{R}t}e^{i\mathcal{I}t}$.
- The factor $e^{i\mathcal{I}t}$ has absolute value $= 1$:

$$e^{i\mathcal{I}t} = \cos(\mathcal{I}t) + i\sin(\mathcal{I}t) \Rightarrow |e^{i\mathcal{I}t}|^2 = \cos^2(\mathcal{I}t) + \sin^2(\mathcal{I}t) = 1.$$

- The factor $e^{\mathcal{R}t}$ controls **growth ($\mathcal{R} > 0$, instability)**
  or **decay ($\mathcal{R} < 0$, stability)**

Stability

- For a 2×2 matrix $A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$, two conditions guarantee that all eigenvalues have negative real part: The trace $T = a + d$ must be negative, and the determinant $D = ad - bc$ must be positive: Why?
- $|A - \lambda I| = \lambda^2 - T\lambda + D = 0 \rightsquigarrow 2\lambda_{1,2} = T \pm \sqrt{T^2 - 4D}$ Assume eigenvalues are complex, i.e. $T^2 < 4D$. Both T and D are real, which implies $\mathcal{R}(\lambda_1) = \mathcal{R}(\lambda_2) = T$, $\mathcal{I}(\lambda_1) = -\mathcal{I}(\lambda_2)$.
- Thus, $T < 0$ implies that the real part $\mathcal{R}$ is negative $\rightsquigarrow$ stable.
- Parabola $T = 4D$ separates real from complex eigenvalues.



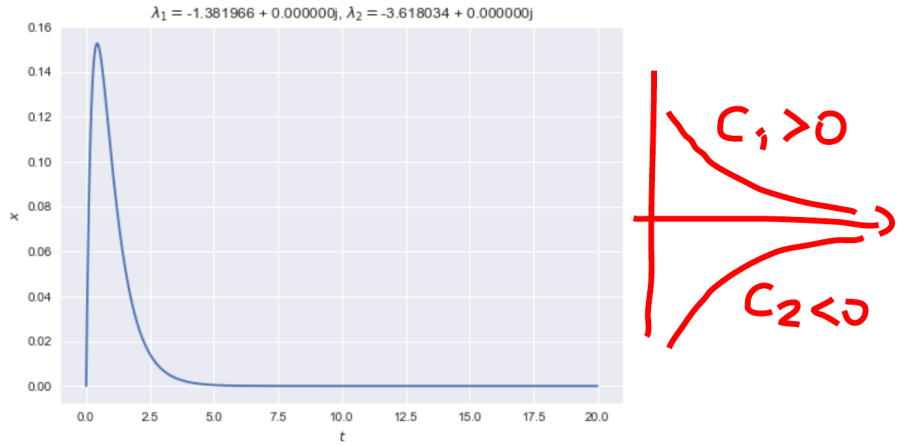
Gilbert Strang: Linear Algebra and Its Applications, 4th edition.

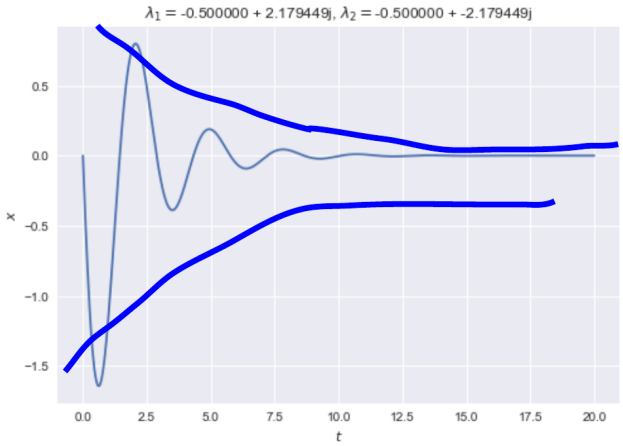
Damped oscillations

- $F_D = -b\dot{x}$ describes damping, or friction, proportional to velocity.

$$\frac{d}{dt}\boldsymbol{u} = \frac{d}{dt}\begin{bmatrix} x \\ \dot{x} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -k & -b \end{bmatrix}\begin{bmatrix} x \\ \dot{x} \end{bmatrix}$$

- Solving $|A - \lambda I| = 0 \rightsquigarrow \lambda_{1,2} = \frac{-b \pm \sqrt{b^2 - 4mk}}{2m}$
- Two different regimes: Overdamped: $b^2 > 4mk$
  $\rightsquigarrow \sqrt{b^2 - 4mk} < b \rightsquigarrow \lambda_{1,2} < 0$, $x(t) = c_1 e^{\lambda_1 t} + c_2 e^{\lambda_2 t}$
  Underdamped: $b^2 < 4mk \quad \rightsquigarrow \quad \mathcal{R}(\lambda_1) = \mathcal{R}(\lambda_2) = -\frac{b}{2m} < 0.$





Forced Oscillations

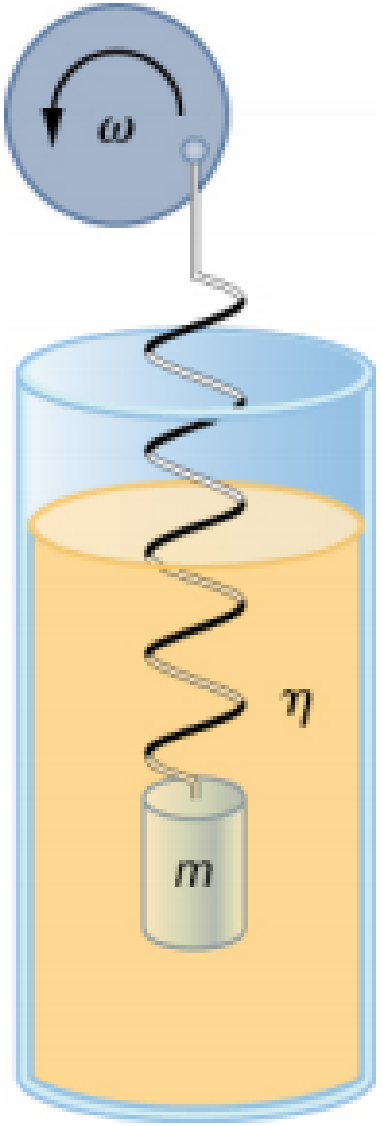
- So far: the right-hand side of the ODE is zero: natural modes of the spring-mass system
- In many applications there is an external forcing

$$\underbrace{m}_{\text{mass}}\underbrace{\ddot{x}}_{\text{acceleration}} + \underbrace{b\dot{x}}_{\text{damping}} + \underbrace{kx}_{\text{restoring force}} = f(t)$$

- A general solution can be written as

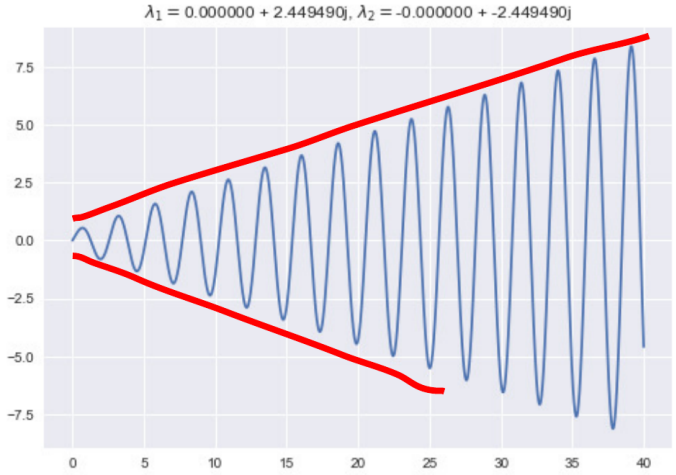
$$x(t) = \underbrace{x_h(t)}_{\text{solves } m\ddot{x}+b\dot{x}+kx=0} + \underbrace{x_p(t)}_{\text{A particular solution}}$$

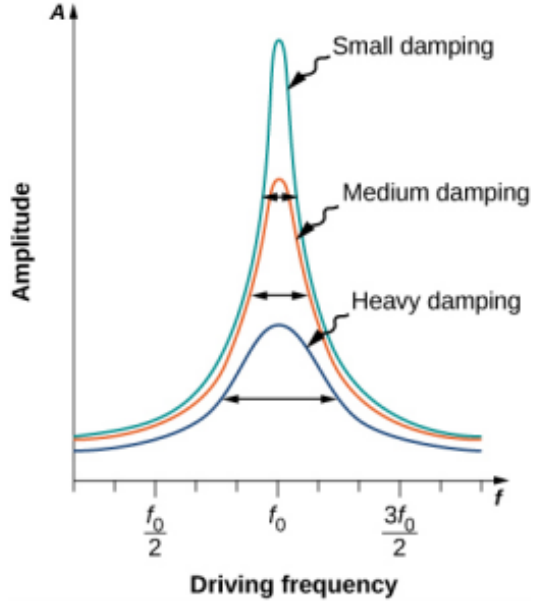
- In a damped system, x_h vanishes over time and x_p dictates the long-term behavior
  $\rightsquigarrow$ steady-state solution



Resonance

- Systems that are not overdamped have their own natural modes or resonant frequencies
- Example $\ddot{x}(t) + x(t) = 5\cos(t)$.
  Homogeneous solution is $x_h(t) = A\sin(t+\phi)$.
  Particular solution is $x_p(t) = \frac{1}{2}t\sin(t)$ (can be easily checked).
  Total solution: $x(t) = x_h + x_p(t) = A\sin(t+\phi) + \frac{1}{2}t\sin(t)$.





Happens in real systems with damping, too...

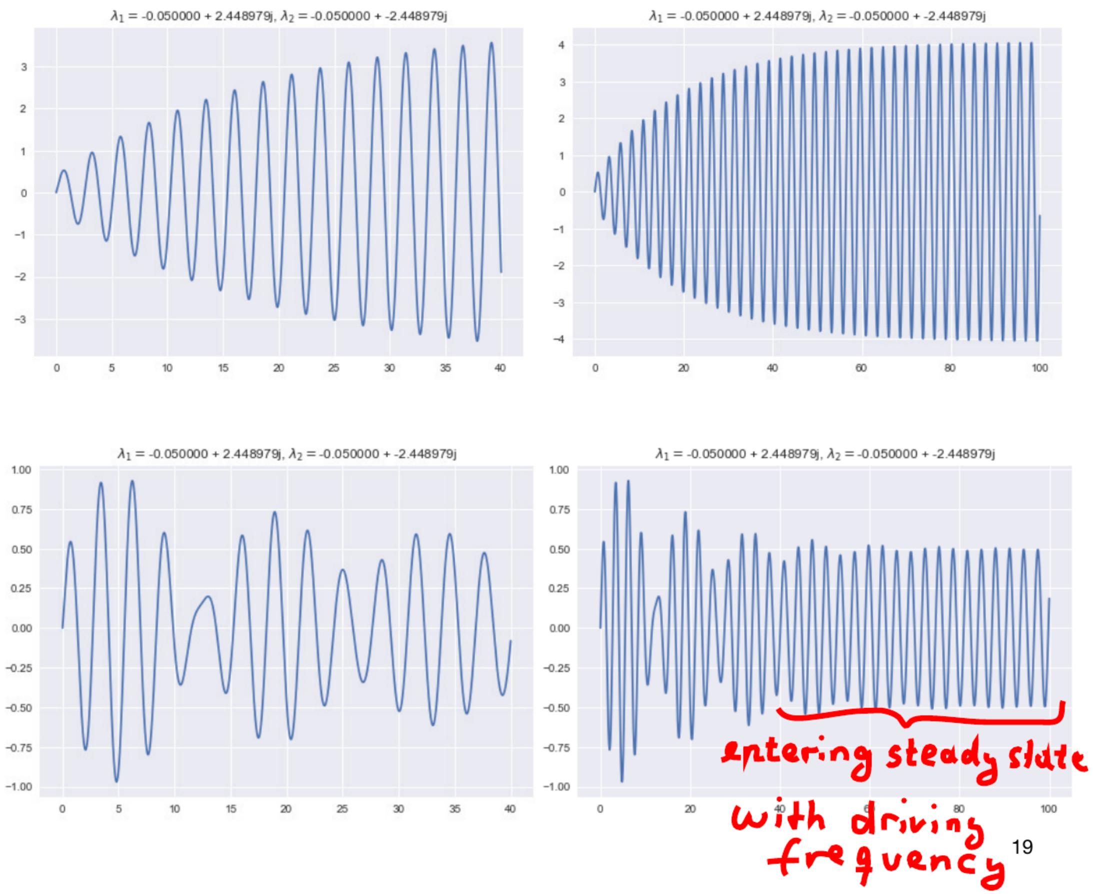
x = u

```python
def f_osc(x, t, m=1, b=1, k=6, c=1, alpha=0, omega=1):
    A = np.array([[ 0,  1],
                  [-k/m, -b/m]])

    dydt = A.dot(x) + [0,
                       c * t**alpha * np.cos(omega*t)
                       ]
    return dydt

m = 1
b = 0.1
k = 6
u_0 = [0, 1]

A = np.array([[ 0,  1],
              [-k/m, -b/m]])
lam, V = np.linalg.eig(A)

T = 100
dt = 0.01
tspan = np.arange(0.0, T, dt)

f_osc_kb = lambda x, t : f_osc(x, t, b=b, k=k,
                               omega=np.abs(lam[0].imag))

u = odeint(f_osc_kb, u_0, tspan)
```

A·x + F

$\frac{du}{dt} = F(u,t)$

drive system with natural modes



Higher Order Systems

- Consider a 3rd-order equation with constant coefficients

$$\dddot{x} + B\ddot{x} + C\dot{x} + Dx = 0$$

- Define $\boldsymbol{u} = (x, \dot{x}, \ddot{x})^t$. The three eqs.

$$\frac{dx}{dt} = \dot{x}, \quad \frac{d\dot{x}}{dt} = \ddot{x}, \quad \text{and} \quad \frac{d\ddot{x}}{dt} = -Dx - C\dot{x} - B\ddot{x}$$

  convert to

$$\frac{d}{dt}\boldsymbol{u} = A\boldsymbol{u} \rightsquigarrow \frac{d}{dt}\begin{bmatrix} x \\ \dot{x} \\ \ddot{x} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -D & -C & -B \end{bmatrix} \begin{bmatrix} x \\ \dot{x} \\ \ddot{x} \end{bmatrix}$$

- **Again a reduction to a first-order system!**

The exponential of a matrix

- If there are n independent eigenvectors: Complete solution is **linear combination of special solutions** for each $(\boldsymbol{v}, \lambda)$-pair.
  More general & compact version?
- **Taylor series** of function $f(x)$ is $\sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n$, where $f^{(n)}(a)$ is the n-th derivative of f at point a.
- Exponential function, $a = 0$: $e^x = 1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 + \cdots$
- Substitute square matrix At for x:

$$e^{At} = I + At + \frac{1}{2}(At)^2 + \frac{1}{6}(At)^3 + \cdots$$

$$\frac{d}{dt}e^{At} = A + A^2t + \frac{1}{2}A^3t^2 + \cdots = Ae^{At}$$

$\rightsquigarrow$ we immediately see that $\boldsymbol{u} = e^{At}\boldsymbol{u}(0)$ **solves** $\frac{d}{dt}\boldsymbol{u} = A\boldsymbol{u}$**.**

The exponential of a matrix

Simple case: n indep. eigenvectors $\rightsquigarrow$ A is diagonalizable $\rightsquigarrow$ $A = V\Lambda V^{-1}$:

$$\begin{aligned} e^{At} &= I + V\Lambda V^{-1}t + \frac{1}{2}(V\Lambda V^{-1}t)^2 + \cdots \\ &= V\left[I + \Lambda t + \frac{1}{2}(\Lambda t)^2 + \cdots\right]V^{-1} \\ &= Ve^{\Lambda t}V^{-1} = V\begin{bmatrix} e^{\lambda_1 t} & & \\ & \ddots & \\ & & e^{\lambda_n t} \end{bmatrix}V^{-1}. \end{aligned}$$

Substitute in general form of solution:

$$\begin{aligned} \boldsymbol{u}(t) = e^{At}\boldsymbol{u}(0) &= Ve^{\Lambda t}\underbrace{V^{-1}\boldsymbol{u}(0)}_{=\boldsymbol{c},\text{ since } V\boldsymbol{c}=\boldsymbol{u}_0} \\ &= c_1 e^{\lambda_1 t}\boldsymbol{v}_1 + \cdots + c_n e^{\lambda_n t}\boldsymbol{v}_n. \end{aligned}$$

The exponential of a matrix

What if there are **not enough eigenvectors?** Example:

$$\frac{d}{dt}\boldsymbol{u} = A\boldsymbol{u} \rightsquigarrow \frac{d}{dt}\begin{bmatrix} y \\ \dot{y} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 2 \end{bmatrix}\begin{bmatrix} y \\ \dot{y} \end{bmatrix}$$

$det(A-\lambda I) = \lambda^2-2\lambda+1 = (\lambda-1)^2 = 0 \rightsquigarrow$ repeated e.value $\lambda_1 = \lambda_2 = 1$
$\rightsquigarrow$ only one eigenvector $\rightsquigarrow$ **diagonalization not possible.**

Idea: Use Taylor series directly. **Series ends after linear term!**

$$e^{At} = e^{It}e^{(A-I)t} = e^t[I + (A-I)t + \frac{1}{2}\underbrace{(A-I)^2}_{0}t^2 + 0 + \cdots]$$

$$\boldsymbol{u}(t) = e^{At}\boldsymbol{u}(0) = e^t\left[I + \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}t\right]\boldsymbol{u}(0)$$

First component: $y(t) = e^t\,y(0) - te^t\,y(0) + te^t\,\dot{y}(0)$.

Adding a source term

- We now know that when A is constant in time, the solution to $\frac{d}{dt}\boldsymbol{u} = A\boldsymbol{u}$ is $e^{At}\boldsymbol{u}(0)$.

- Now consider an additional source term: $\frac{d}{dt}\boldsymbol{u}(t) = A\boldsymbol{u}(t) + \boldsymbol{f}(t)$.
  Idea: Massage this equation and integrate:

$$\begin{aligned}
\dot{\boldsymbol{u}}(t) - A\boldsymbol{u}(t) &= \boldsymbol{f}(t) \\
e^{At}\underbrace{\frac{d}{dt}\left[e^{-At}\boldsymbol{u}(t)\right]}_{e^{-At}\dot{\boldsymbol{u}} - Ae^{-At}\boldsymbol{u}} &= \boldsymbol{f}(t) \\
\frac{d}{dt}\left[e^{-At}\boldsymbol{u}(t)\right] &= e^{-At}\boldsymbol{f}(t)
\end{aligned}$$

Adding a source term

Integrating both sides gives

$$\int_0^t \frac{d}{ds}\left[e^{-As}\boldsymbol{u}(s)\right] ds = \int_0^t e^{A(-s)}\boldsymbol{f}(s)ds$$

The left side is

$$\int_0^t \frac{d}{ds}\left[e^{-As}\boldsymbol{u}(s)\right] ds = \left[e^{-At}\boldsymbol{u}(t)\right] - \left[e^{-A0}\boldsymbol{u}(0)\right] = e^{-At}\boldsymbol{u}(t) - \boldsymbol{u}(0)$$

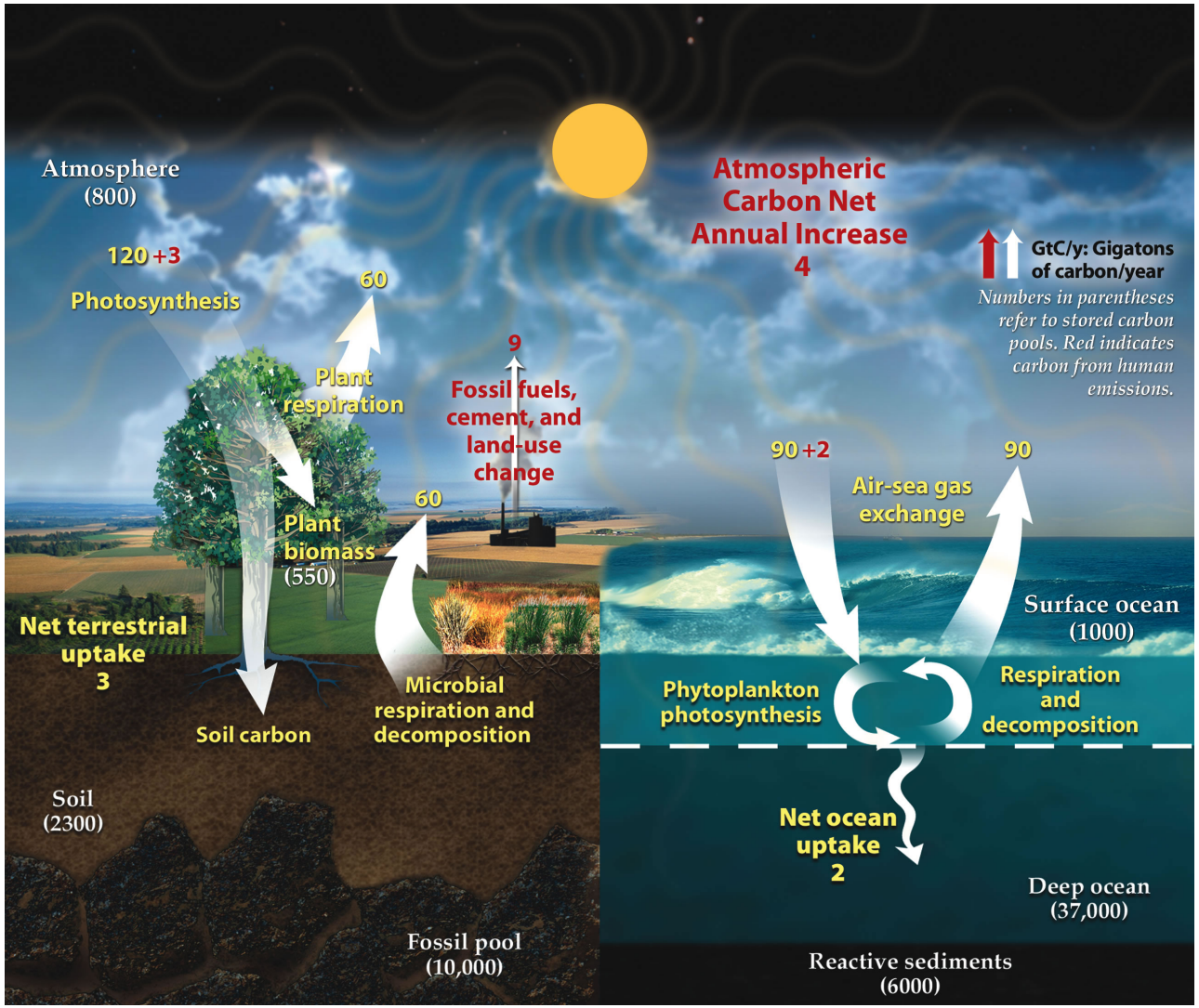
Finally,

$$\boldsymbol{u}(t) = \underbrace{e^{At}\boldsymbol{u}(0)}_{\text{homogenous sol.}} + \underbrace{\int_0^t e^{A(t-s)}\boldsymbol{f}(s)ds}_{\text{particular sol.}}.$$

In a stable system, $\boldsymbol{u}_{\text{hom}}$ vanishes over time and $\boldsymbol{u}_{\text{part}}$ dictates the long-term behavior $\rightsquigarrow$ steady-state solution

Applications of ODEs

Application 1: Modeling the Carbon Cycle



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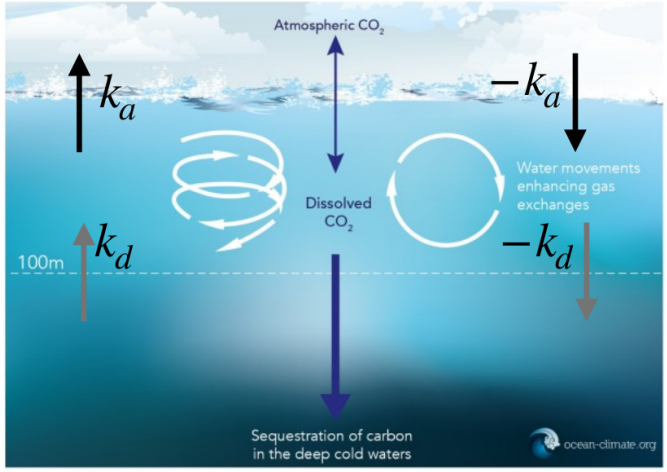
The Carbon Cycle: Box Models

- Most carbon cycle models are **box models:** The total CO_2 is split into boxes. The boxes exchange CO_2 with certain rates (often determined via experimental fitting)
- The simplest non-trivial models of this kind contain 3 boxes: **Atmosphere**, **Upper Ocean** and **Lower Ocean.** More sophisticated models include many more boxes, representing different regimes in the ocean and the biosphere.

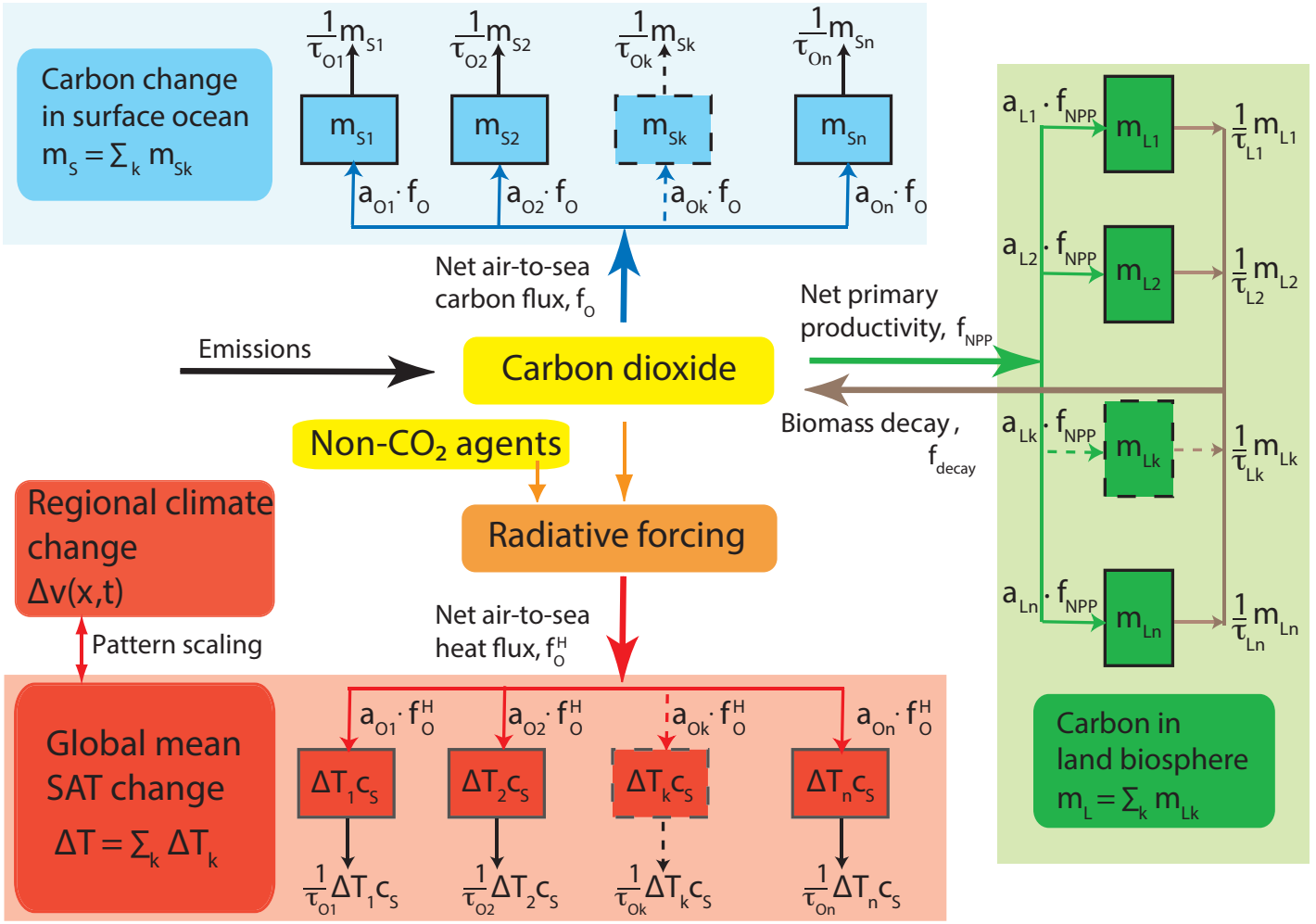


$$\frac{dM_{AT}}{dt} = E(t) - k_a \cdot (M_{AT} - A \cdot B \cdot M_{UP})$$

$$\frac{dM_{UP}}{dt} = k_a \cdot (M_{AT} - A \cdot B \cdot M_{UP}) - k_d \cdot (M_{UP} - \frac{M_{LO}}{\delta})$$

$$\frac{dM_{LO}}{dt} = k_d \cdot (M_{UP} - \frac{M_{LO}}{\delta})$$

The Carbon Cycle: Box Models

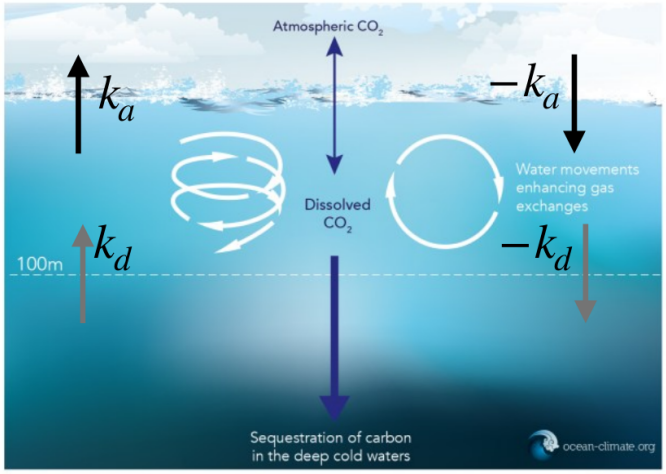


The Bern Simple Climate Model (BernSCM) v1.0: an extensible and fully documented open-source re-implementation of the Bern reduced-form model for global carbon cycle-climate simulations, https://doi.org/10.5194/gmd-11-1887-2018

The BEAM model

- Introduced in (Glotter et al., Climatic Change (2014)) as a simple generalization of classical models.
- Based on a 3-box carbon cycle model first outlined by Bolin and Eriksson (1959)
- BEAM: "Bolin and Eriksson Adjusted Model"
- Taking into account **nonlinearities of CO_2 uptake in the upper ocean.**
- No longer a constant coefficient ODE model: Parameters describing the exchange between boxes vary over time, reflecting different dependencies on environmental conditions.

The BEAM model



$$\frac{dM_{AT}}{dt} = E(t) - k_a \cdot (M_{AT} - A \cdot B \cdot M_{UP})$$

$$\frac{dM_{UP}}{dt} = k_a \cdot (M_{AT} - A \cdot B \cdot M_{UP}) - k_d \cdot (M_{UP} - \frac{M_{LO}}{\delta})$$

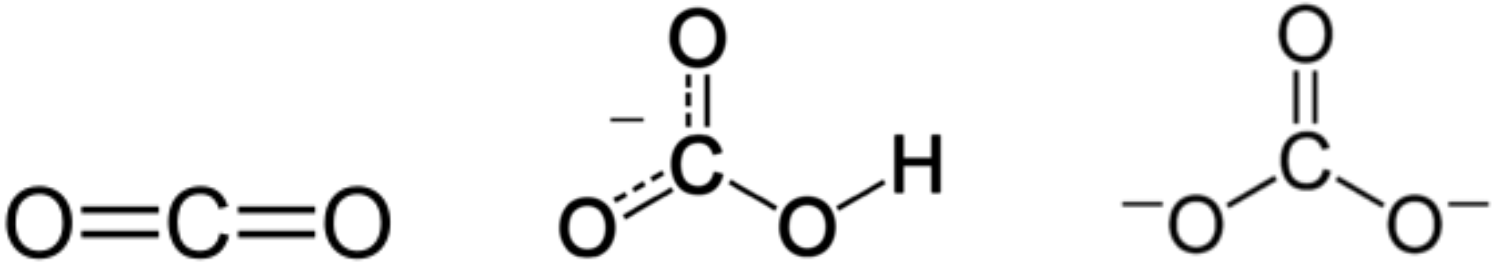
$$\frac{dM_{LO}}{dt} = k_d \cdot (M_{UP} - \frac{M_{LO}}{\delta})$$

- $M_{AT} - A \cdot B \cdot M_{UP}$: disequilibrium between atmospheric and ocean inorganic carbon.
- A is the ratio of atmosphere to ocean CO_2 concentration at equilibrium, which is **weakly dependent on temperature:**
  a warmer ocean holds less dissolved CO_2.
- B is the ratio of dissolved CO_2 to total ocean inorganic carbon at equilibrium, **a strong function of acidity:**
  more acidic seawater stores less inorganic carbon.

The BEAM model

- Variation in B in particular alters uptake rates dramatically
  $\rightsquigarrow$ very different (and more realistic!) model behavior as compared to linear variant of this model: **Dynamic Integrated model of Climate and the Economy (DICE)** (Nordhaus, 1993, 2008, 2010).
- **Uptake of CO_2** proceeds when concentrations in the atmosphere and upper ocean are **out of equilibrium** $(M_{AT} \neq A \cdot B \cdot M_{UP})$.
- Crucial insight from ocean carbon chemistry: dissolved inorganic carbon species are partitioned between

  carbon dioxide CO_2, **bicarbonate (HCO_3^-)**, **carbonate (CO_3^{2-})**.



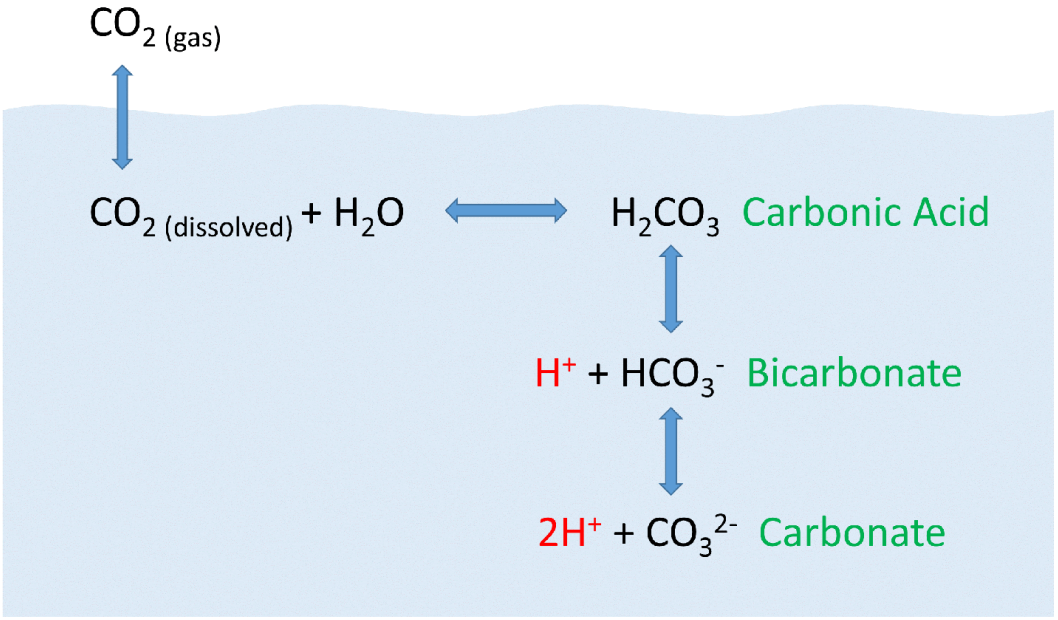
in proportions fixed by the ocean's acidity.

Carbon chemistry

- Assumption: instantaneous repartitioning of **inorganic carbon species:**

$$CO_2 + H_2O \rightleftharpoons HCO_3^- + H^+ \rightleftharpoons CO_3^{2-} + 2\,H^+$$

- Partitioning set by **dissociation coefficients k_1 and k_2 and acidity (pH)** of seawater (pH = neg. log of concentration of hydrogen ions)

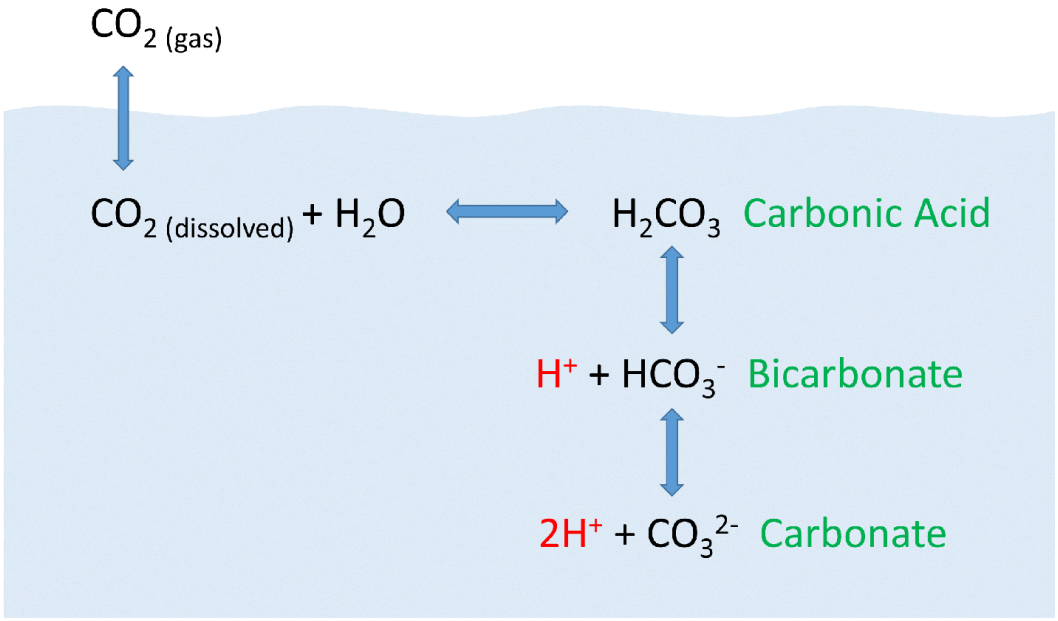


Introduction to Oceanography, Paul Webb, rwu.pressbooks.pub/webboceanography/

Carbon chemistry

- The **carbon storage factor** $1/B$:
  equilibrium ocean total inorganic carbon relative to dissolved CO_2:

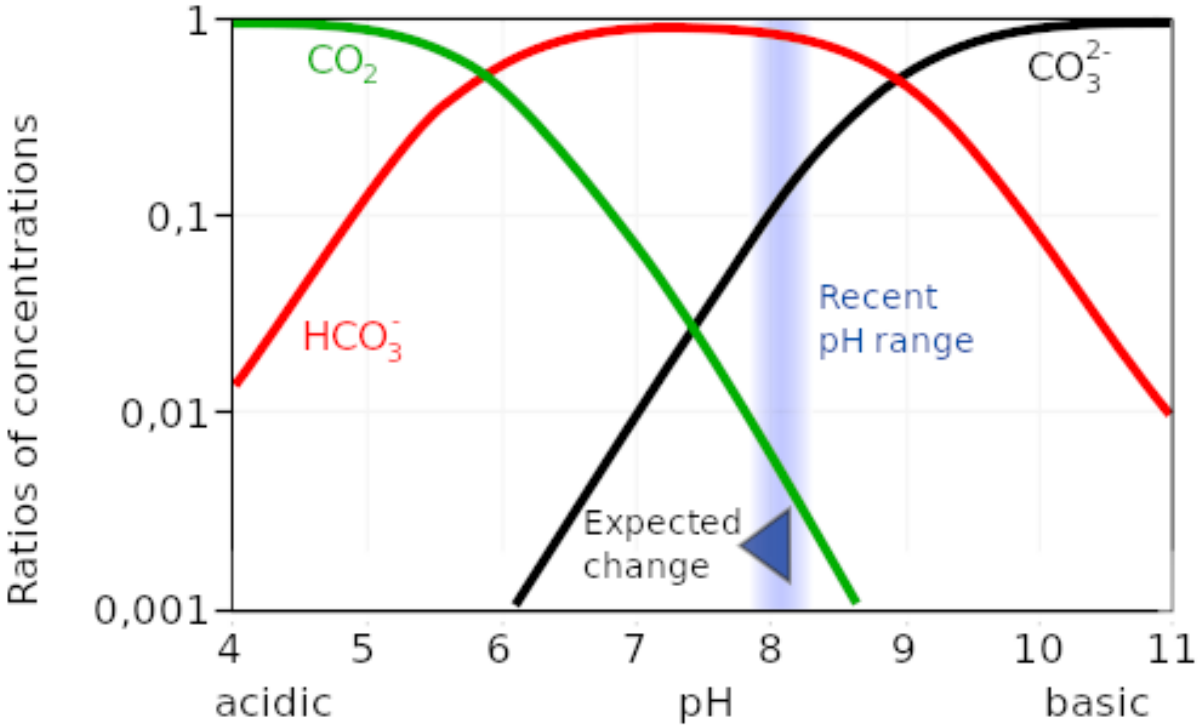
$$\frac{1}{B} = \frac{[CO_2] + [HCO_3^-] + [CO_3^{2-}]}{[CO_2]} = 1 + \frac{k_1}{[H^+]} + \frac{k_2}{[H^+]^2}$$



Introduction to Oceanography, Paul Webb, rwu.pressbooks.pub/webboceanography/

Carbon chemistry

- **Higher acidity reduces the ocean's ability to store carbon.** (higher $[H^+]$, lower pH)
- But: Dissolved CO_2 itself acts a weak acid.
- **Any ocean uptake of CO_2 reduces the efficiency of future uptake.**



At present, bicarbonate dominates DIC and the carbon storage factor is ≈ 170. In a more acidic ocean (lower pH), CO_2 becomes more significant and the carbon storage factor drops. At pH below 5, CO_2 dominates and the carbon storage factor approaches 1.
Glotter et al., Climatic Change (2014), 126:319-335.

Back to the BEAM model...

ODE system with **time dependent coefficient** $A \cdot B = (AB)(t)$**:**

$$\frac{d}{dt}\begin{pmatrix} m_{AT} \\ m_{UP} \\ m_{LO} \end{pmatrix} = \left(\begin{array}{c|c|c} -k_a & k_a \cdot AB & 0 \\ k_a & -(k_a \cdot AB) - k_d & \frac{k_d}{\delta} \\ 0 & k_d & -\frac{k_d}{\delta} \end{array}\right) \begin{pmatrix} m_{AT} \\ m_{UP} \\ m_{LO} \end{pmatrix} + \begin{pmatrix} e \\ 0 \\ 0 \end{pmatrix}$$

No analytic solution possible $\rightsquigarrow$ discretize time and use implicit scheme (cf. slides on the heat equation).

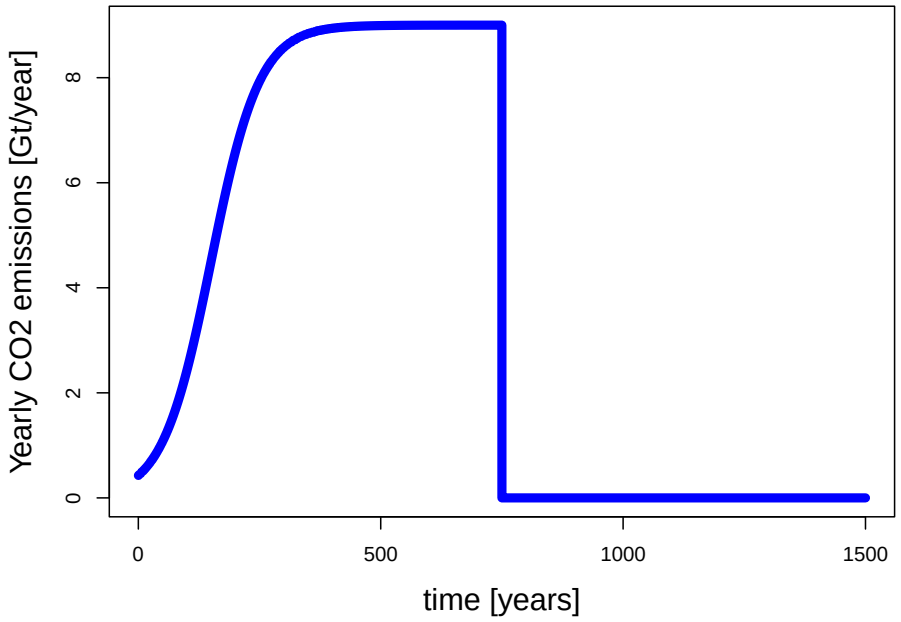
$$\frac{d}{dt}\boldsymbol{m}(t) = D(t)\boldsymbol{m}(t) + \boldsymbol{e}(t) \approx \frac{\boldsymbol{m}^{(t+1)} - \boldsymbol{m}^{(t)}}{\Delta t} = D^{(t)}\boldsymbol{m}^{(t+1)} + \boldsymbol{e}^{(t)}$$

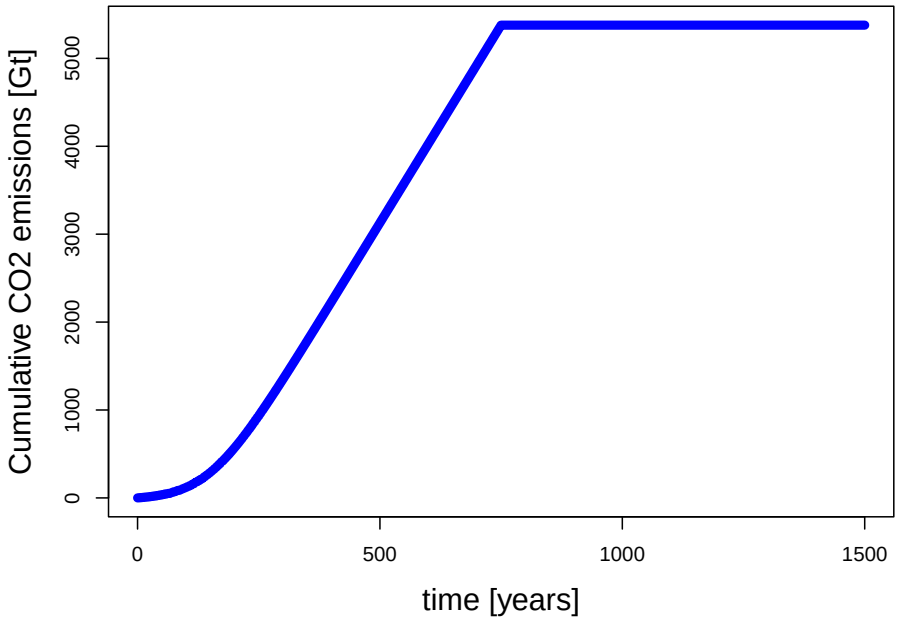
.

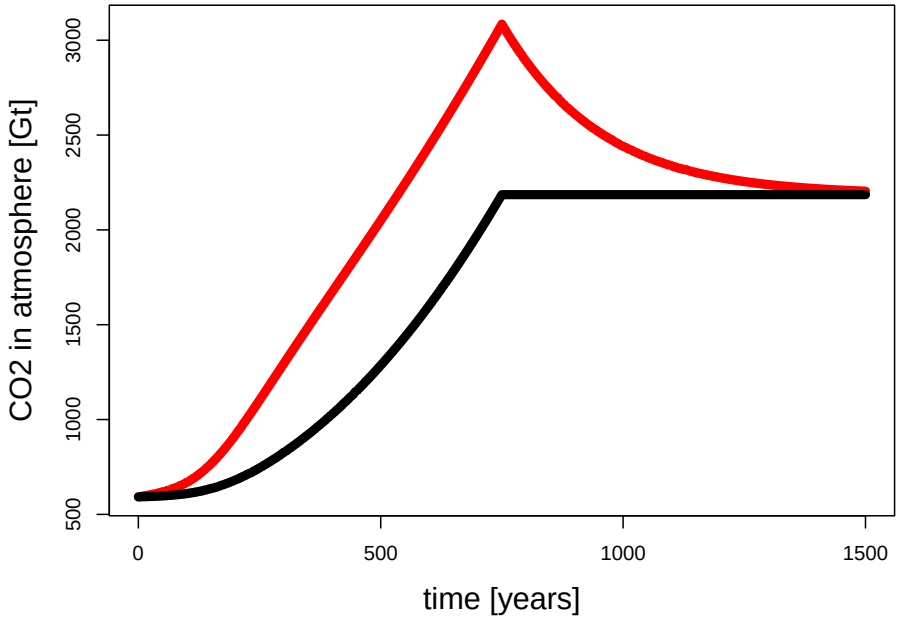
update $\quad \boldsymbol{m}^{(t+1)} = (I - \Delta t \cdot D^{(t)})^{-1}(\boldsymbol{m}^{(t)} + \Delta t \cdot \boldsymbol{e}^{(t)})$.

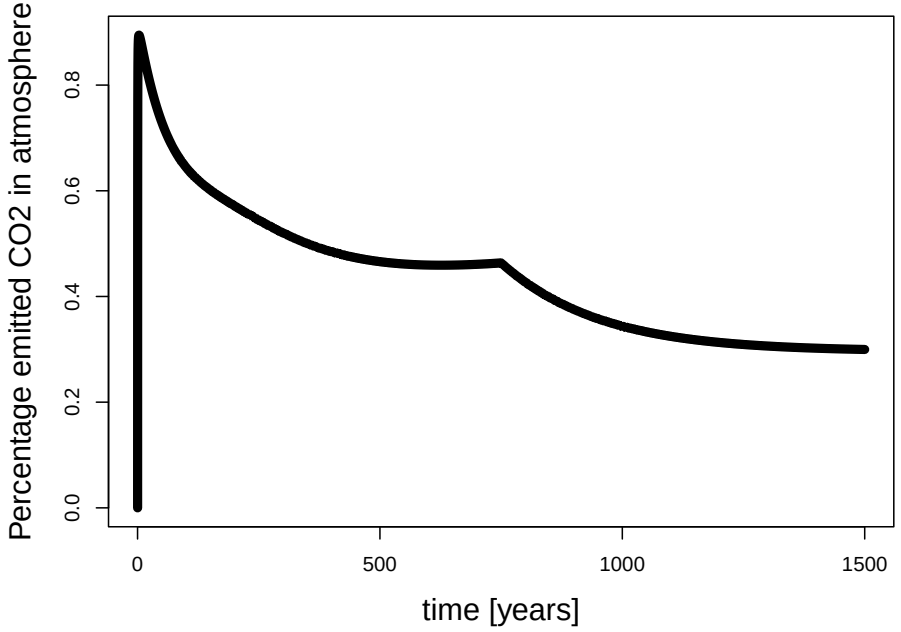
update $\quad D^{(t+1)}$ as a function of new carbon mass $\boldsymbol{m}^{(t+1)}$.

Simulations: Constant emissions









Coupling to Temperature Model

- Just as the ocean takes up CO_2 in response to atmospheric CO_2 perturbations, **it also takes up heat in response to surface warming**, with a **long equilibration time** because of the large thermal inertia of the ocean.
- In BEAM, the **DICE 2007 temperature model** was used:
  Heat uptake is represented by a linear model (which seems to be a realistic assumption for heat uptake).
- Many of the coefficients in DICE 2007 temperature model are calibrated to the MAGICC model (Wigley et al, 2007) or taken from the IPCC (2001) and IPCC (2007).
- **Dynamic Integrated model of Climate and the Economy (DICE)** (Nordhaus, 1993, 2008, 2010): Essentially the same model, but without proper handling of the ocean chemistry.

Coupling to Temperature Model

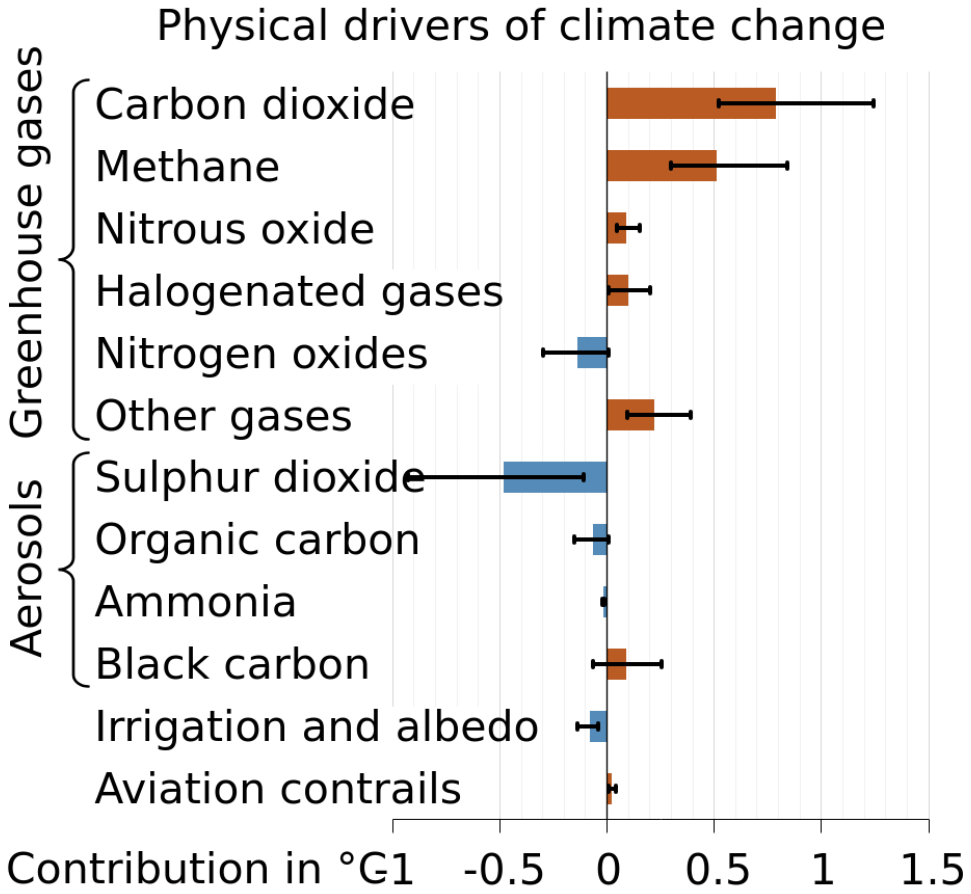
- The temperature model uses **two layers**, the atmosphere and lower ocean; the upper ocean is assumed to follow atmospheric temperature.
- **Radiative forcing F due to increased atmospheric CO_2** warms the atmosphere (and upper ocean), producing a **disequilibrium** with the lower ocean that is eroded with timescales $1/\mu$:

$$\begin{aligned} T_{AT}(t) &= T_{AT}(t-1) \\ &\quad +\mu_{AT} \cdot [\Lambda \cdot (T_{eq}(t) - T_{AT}(t-1)) - \gamma \cdot (T_{AT}(t-1) - T_{LO}(t-1))] \\ T_{LO}(t) &= T_{LO}(t-1) + \mu_{LO} \cdot \gamma \cdot (T_{AT}(t-1) - T_{LO}(t-1)). \end{aligned}$$

  - γ relates atmosphere-ocean heat transfer to temperature anomaly ($\gamma = 0.3\, W/m^2/^\circ C$)
  - Λ is climate sensitivity ($1.3\, W/m^2/^\circ C$);
  - $F(t)$ is the increase in radiative forcing since pre-industrial, in W/m^2;
  - $T_{eq}(t)$ is the equilibrium temperature that would be produced by that forcing: $T_{eq}(t) = F(t)/\Lambda$.

Radiative forcing

- Concept to quantify the change in energy balance in the atmosphere.
- Defined as "the change in the net radiative flux (W/m^2) due to a change in an external driver of climate change."



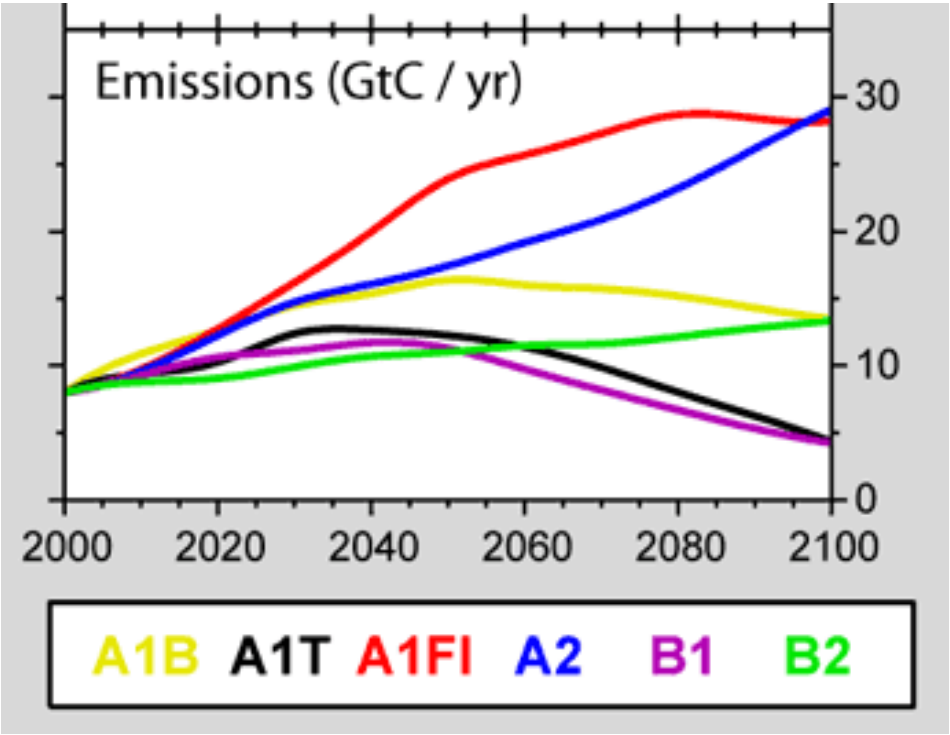
Coupling to Temperature Model

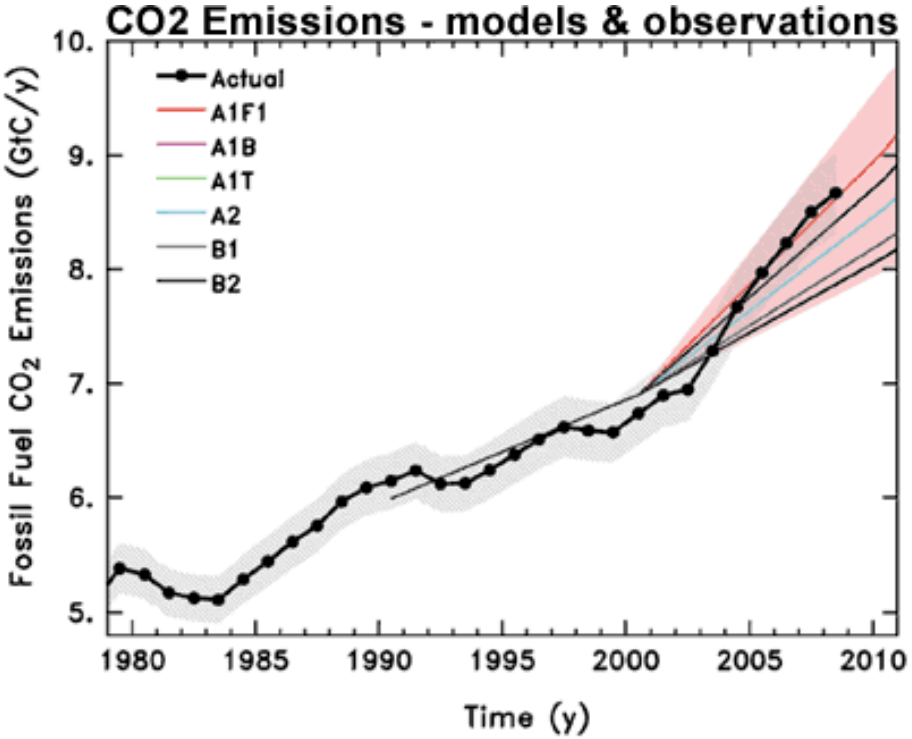
- Forcing $F(t)$ is assumed to be linear with the binary logarithm of the fractional change in CO_2 since pre-industrial times, a standard assumption in climate science:

$$F(t) = \alpha \cdot \log_2(M_{AT}(t)/M_{AT}(PI)),$$

  where $M_{AT}(PI)$ is the mass of pre-industrial atmospheric carbon (596.4 Gt, equivalent to 280 ppm CO_2) and α is the assumed forcing increase per doubling of CO_2 ($\alpha = 3.8\,W/m^2$).
- The climate sensitivity Λ is derived by dividing α by β , the assumed equilibrium warming after doubling of CO_2 ($\beta = 3.0\,°C$ / doubling).

IPCC emission scenarios





Left: Annual Carbon Emissions for the Various IPCC SRES Scenarios. *Credit: Robert A. Rohde / Global Warming Art*

Right: Observed Historic Emissions Compares with the Various IPCC SRES Scenarios. *Credit: The Copenhagen Diagnosis.*

Simulated Carbon and Temperature Anomalies

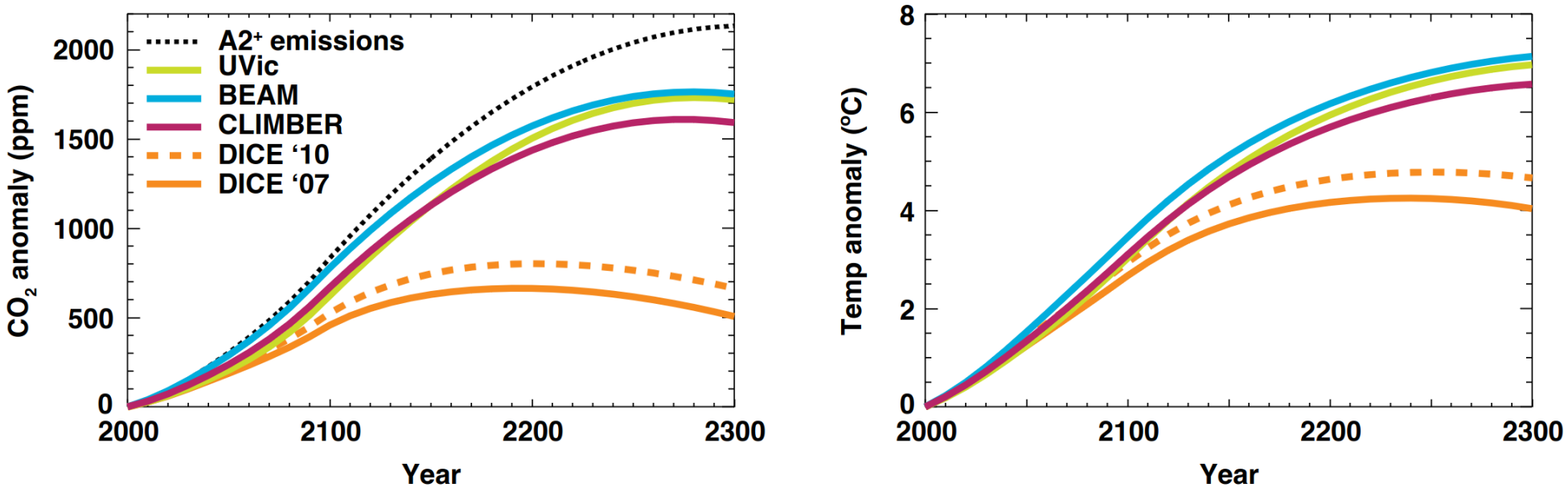
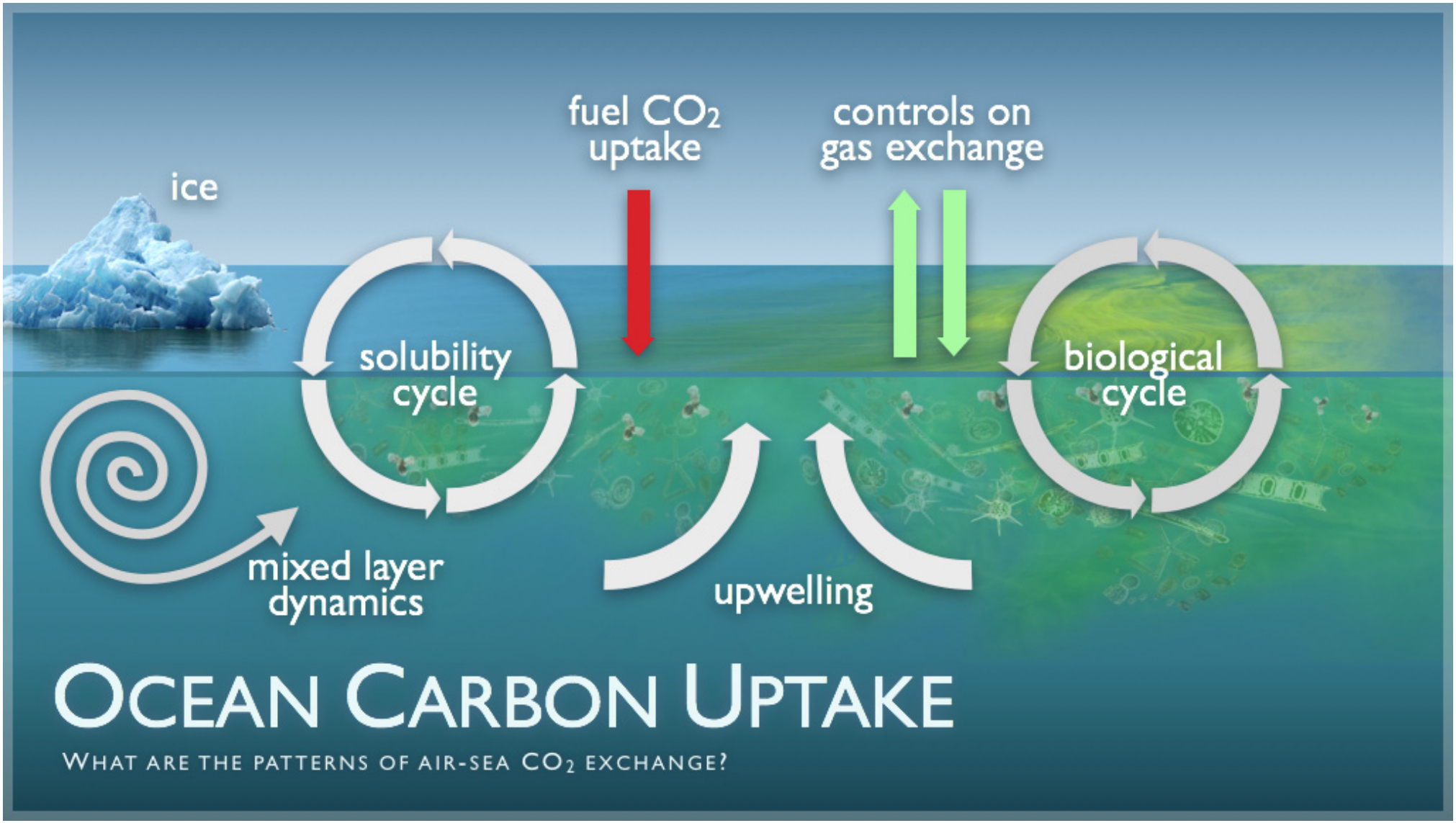


Fig. 3 2000-2300 atmospheric CO_2 anomaly for BEAM and DICE carbon models as compared to intermediate complexity UVic and CLIMBER-2 models for the $A2^+$ emissions scenario (left). Dotted black line shows cumulative emissions, i.e. atmospheric CO_2 concentration if no ocean uptake occurred. BEAM matches the more complex model output well, leading to an accurate projection of warming (right). The DICE carbon model performs adequately for the first several decades, then diverges rapidly. DICE removes 3/4 of all anthropogenic carbon from the atmosphere within 300 years while more realistic models remove only 1/4. Too-low CO_2 in DICE produces underestimation of warming by over 2 °C after 300 years.

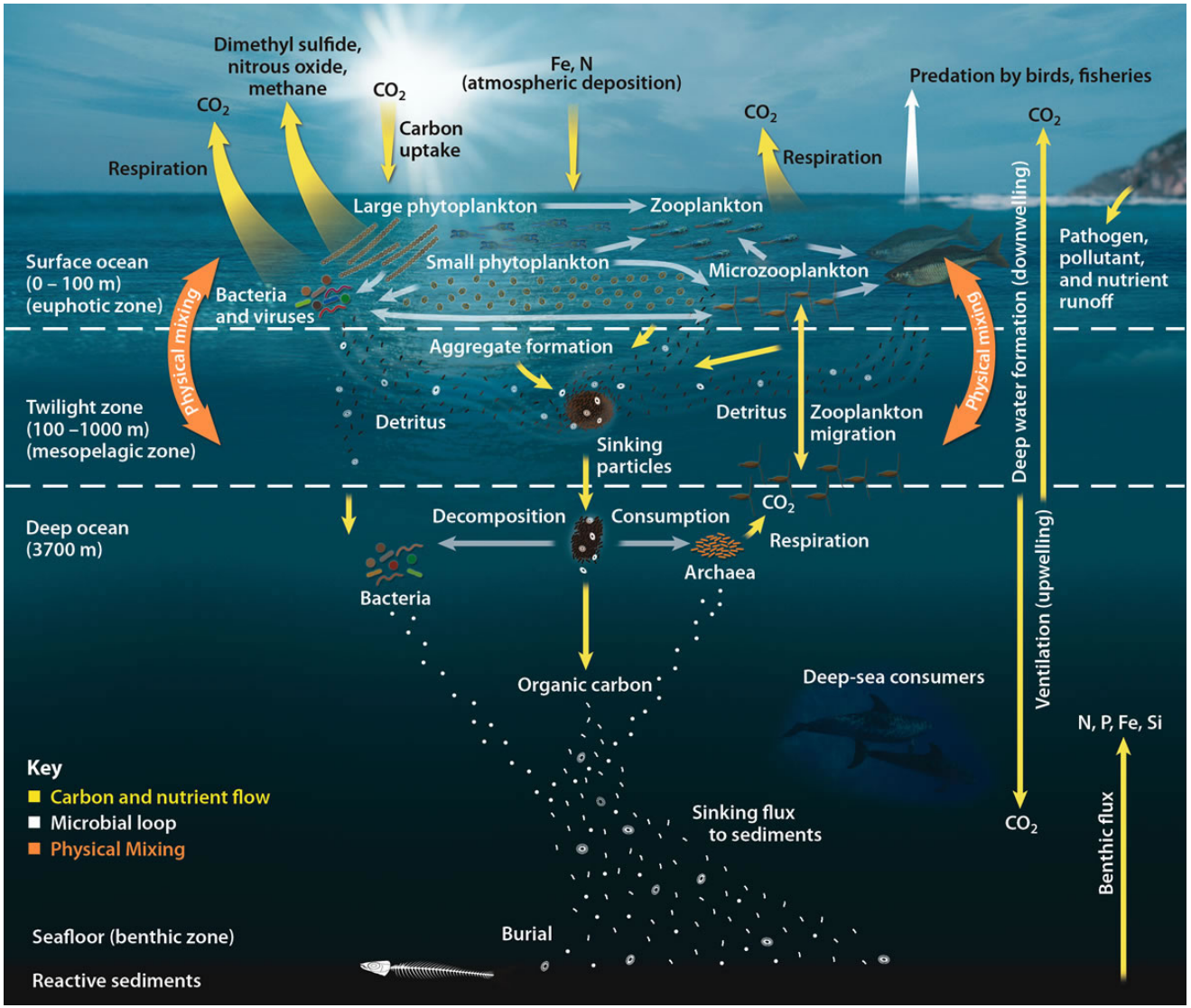
From (Glotter et al., Climatic Change (2014), 126:319-335)

Towards more realistic models



www.pmel.noaa.gov/co2/file/Ocean+Carbon+Uptake+Image

The biological carbon pump



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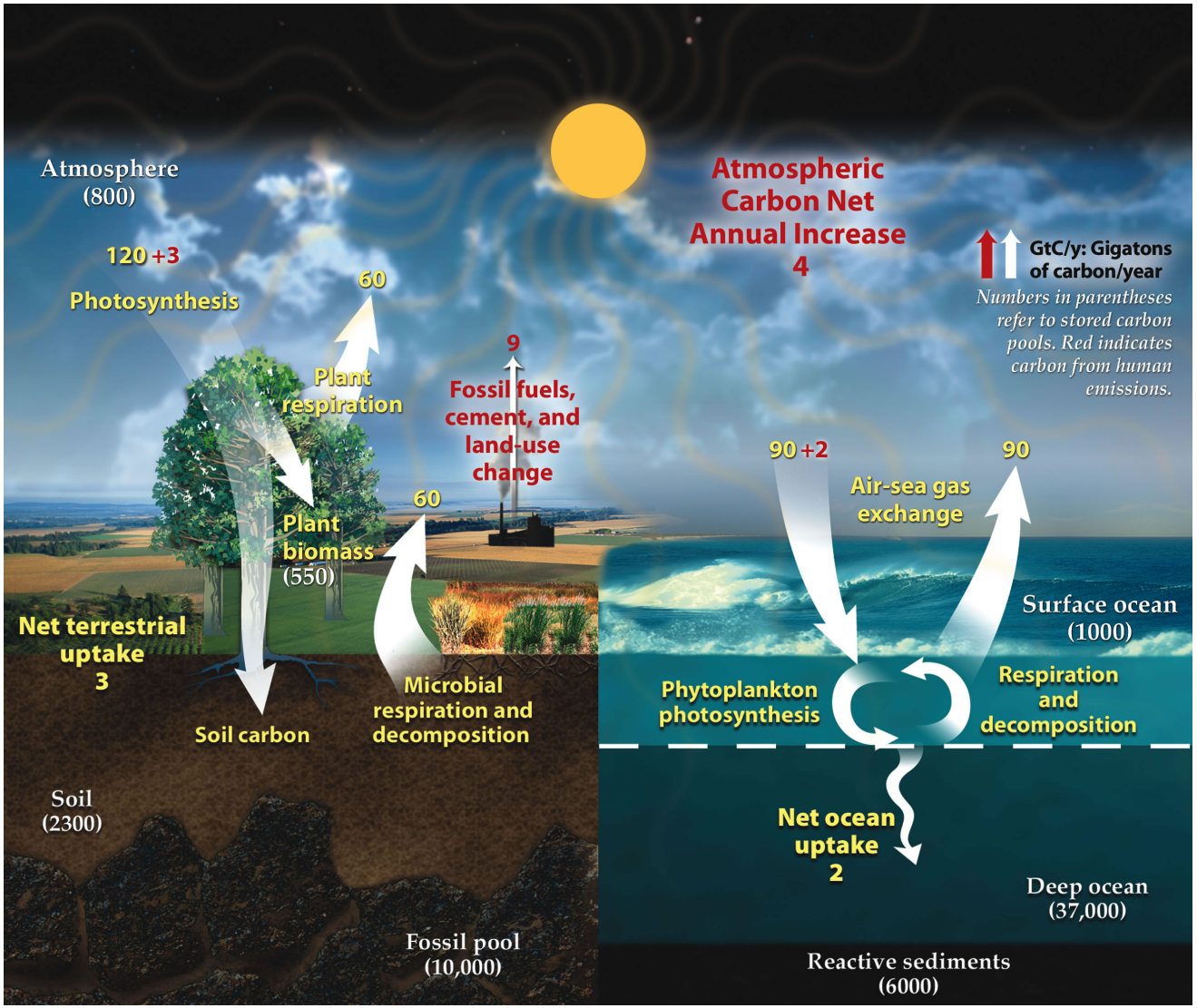
Inclusion of biosphere



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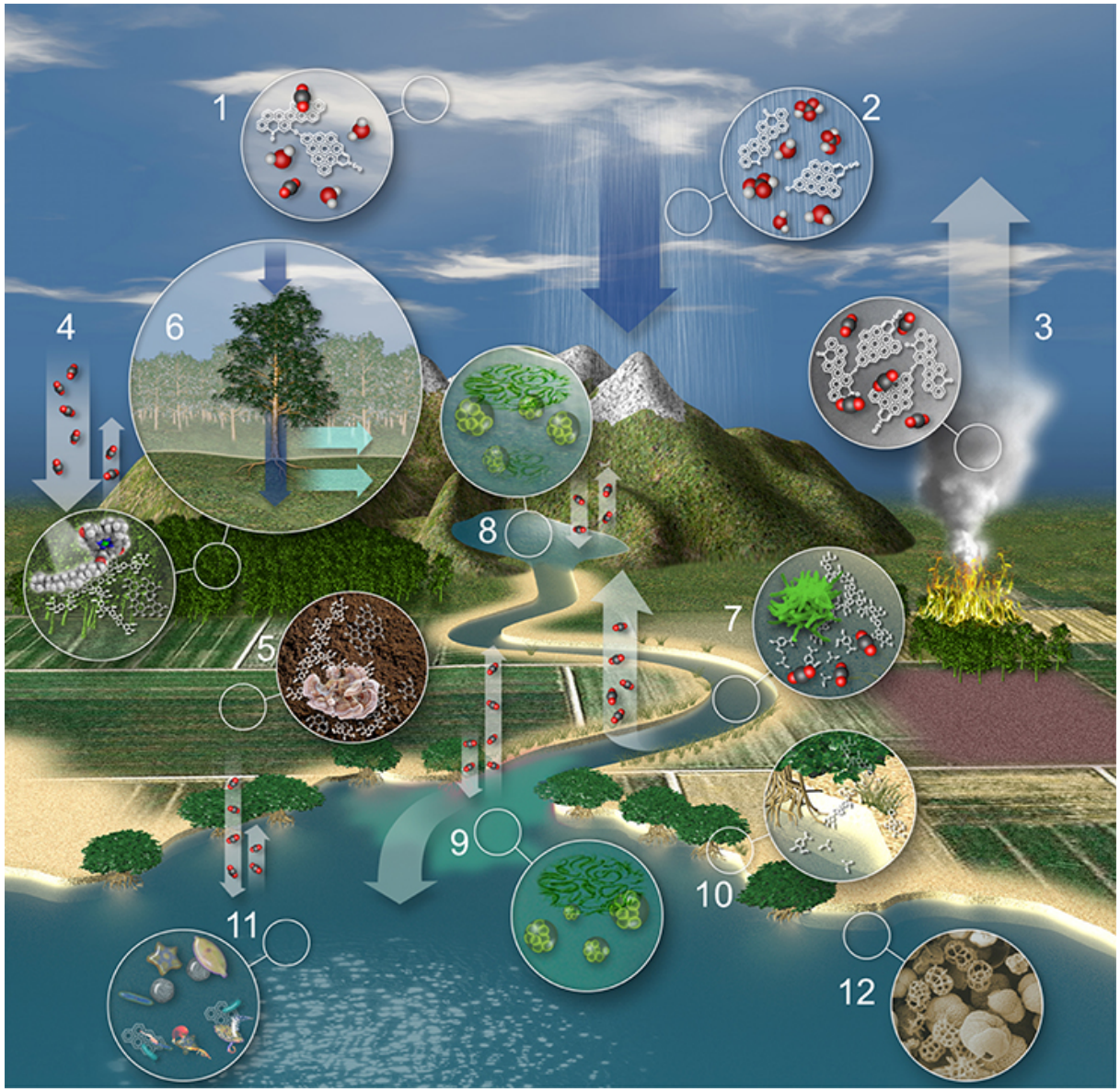
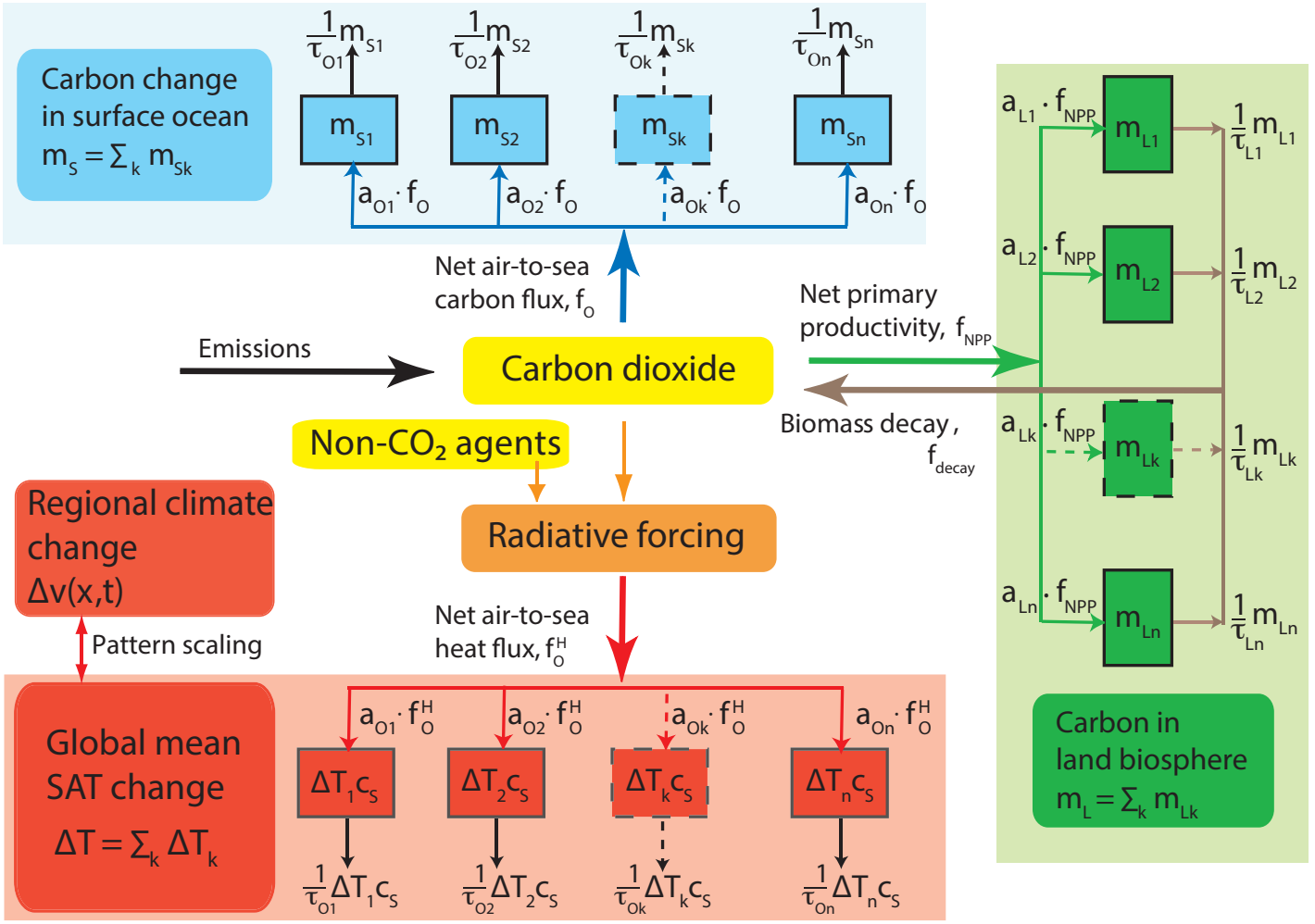
Terrestrial carbon in the water cycle



By Nicholas D. Ward, Thomas S. Bianchi, Patricia M. Medeiros, Michael Seidel, Jeffrey E. Richey, Richard G. Keil and Henrique O. Sawakuchi - [1]

The Bern Simple Climate Model (BernSCM)



The Bern Simple Climate Model (BernSCM) v1.0: an extensible and fully documented open-source re-implementation of the Bern reduced-form model for global carbon cycle-climate simulations, https://doi.org/10.5194/gmd-11-1887-2018

Application 2: Modeling the COVID-19 pandemic

The simplest useful model: SIR

The SIR model [edit]

In 1927, W. O. Kermack and A. G. McKendrick created a model in which they considered a fixed population with only three compartments: susceptible, $S(t)$; infected, $I(t)$; and recovered, $R(t)$. The compartments used for this model consist of three classes:[13]

- $S(t)$ is used to represent the individuals not yet infected with the disease at time t, or those susceptible to the disease of the population.
- $I(t)$ denotes the individuals of the population who have been infected with the disease and are capable of spreading the disease to those in the susceptible category.
- $R(t)$ is the compartment used for the individuals of the population who have been infected and then removed from the disease, either due to immunization or due to death. Those in this category are not able to be infected again or to transmit the infection to others.

(From Wikipedia)

The MSEIR (…) family of models

Idea: divide population into groups according to their status relative to the disease

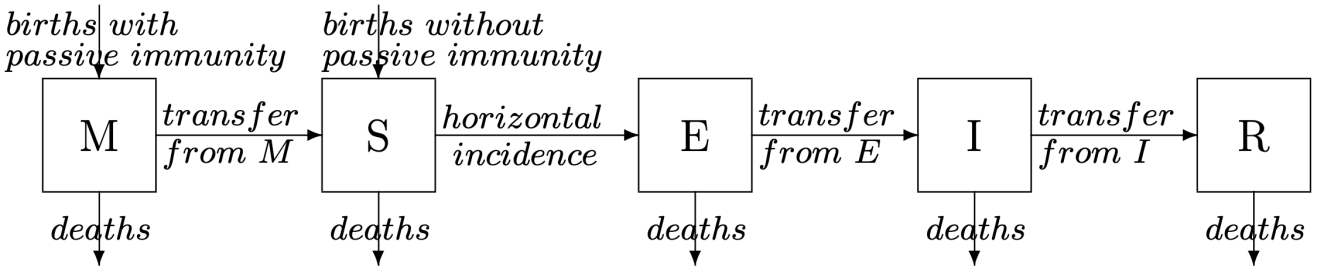


Fig. 1 *The general transfer diagram for the MSEIR model with the passively immune class M, the susceptible class S, the exposed class E, the infective class I, and the recovered class R.*

The simplest useful model: SIR

$$\frac{dS}{dt} = -\beta \frac{I}{N} S \qquad \frac{dI}{dt} = \beta \frac{I}{N} S - \gamma I \qquad \frac{dR}{dt} = \gamma I$$

Fraction of infected $\frac{I(t)}{N}$

λ

Infection rate $\lambda = \beta \frac{I}{N}$ **Recovery rate** γ

Is this a linear algebra problem?

- Letting $\boldsymbol{u}(t) = \begin{bmatrix} S(t) \\ I(t) \\ R(t) \end{bmatrix}$, can we write $\frac{d\boldsymbol{u}(t)}{dt} = A\boldsymbol{u}(t)$ for some matrix A that does not depend on S, I, R?

- Sadly, no… the expressions contain multiplications between S and I S(t)·I(t)

- A superposition of two solutions is in general **not** a solution

- Perhaps not everything is lost…

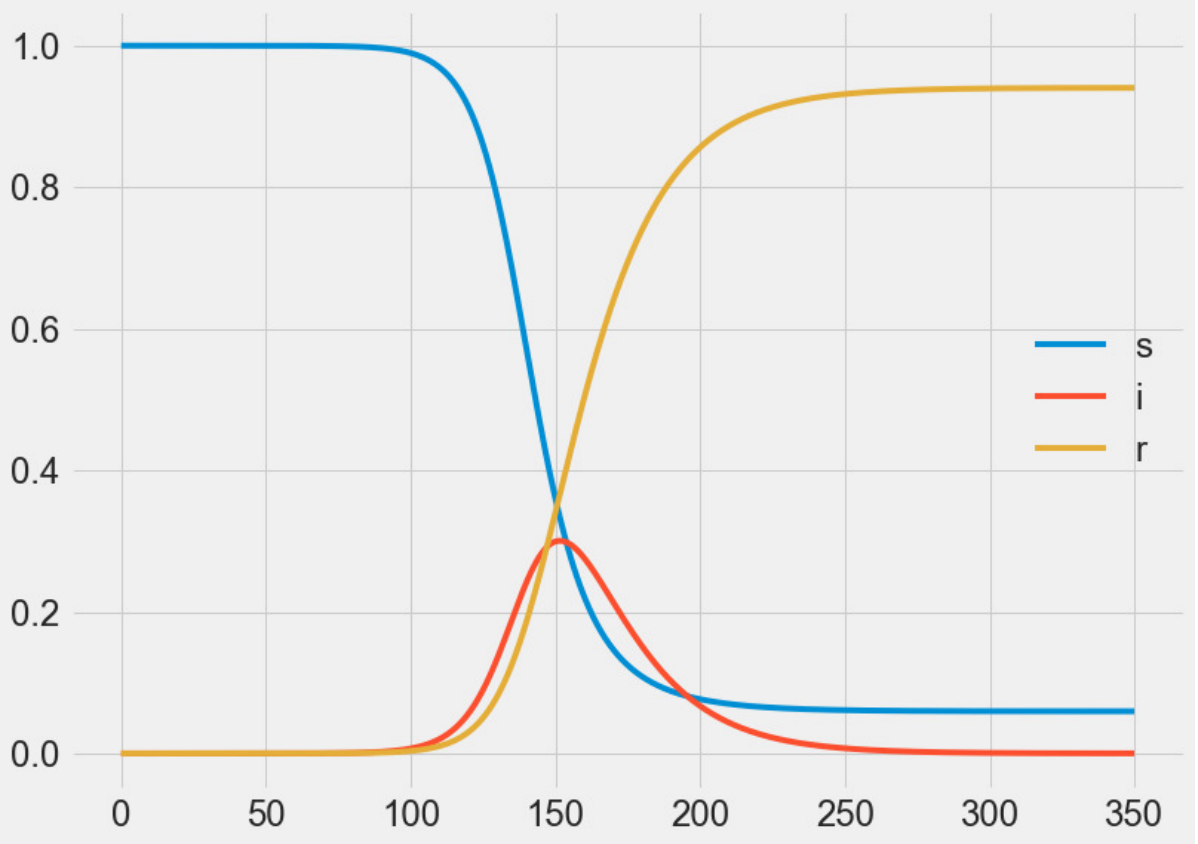
$$\frac{dS}{dt} = -\beta\frac{I(t)}{N}S(t)$$

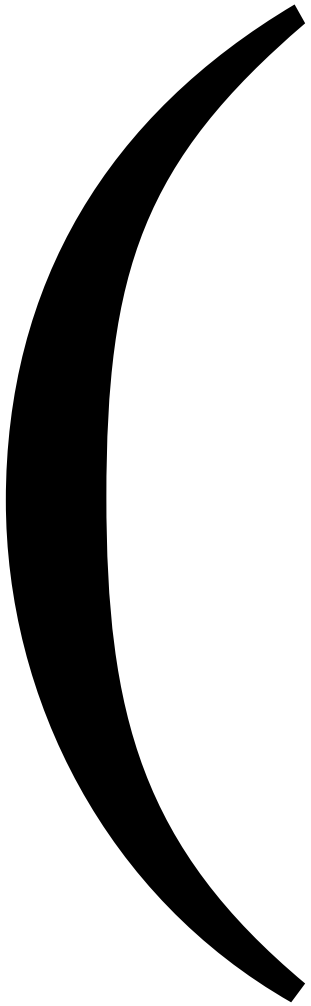
$$\frac{dI}{dt} = \beta\frac{I(t)}{N}S(t) - \gamma I(t)$$

SIR curves

$S + i + r = 1$

```
def f_sir(x, t, gamma=1/18, R0=3):
    s, i, r = x

    dydt = [-gamma*R0*s*i,
             gamma*R0*s*i - gamma*i,
             gamma*i
            ]
    return dydt

# parameters
T = 350
dt = 0.1

i_0 = 1e-7  # 33 = 1E-7 * 330 million
s_0 = 1.0 - i_0
r_0 = 0.0
y_0 = [s_0, i_0, r_0]  # initial condition

tspan = np.arange(0.0, T, dt)

y = odeint(f_sir, y_0, tspan)


ax = plt.plot(tspan, y)
plt.legend(['s', 'i', 'r'], fontsize=24)
```



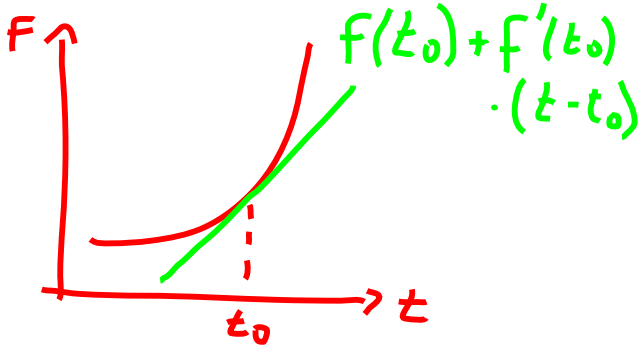


Stability of dynamical systems / ODEs

Key principle When things are non-linear, linearize them!

Taylor series (first two terms)

$$f(t) = f(t_0) + f'(t_0)(t - t_0) + O(|t - t_0|^2)$$



Key question Linearize about which point? How to choose t_0?

Equilibria of dynamical systems

Good choice: **equilibria** of

$$\frac{d\boldsymbol{u}(t)}{dt} = F(t, \boldsymbol{u}(t))$$

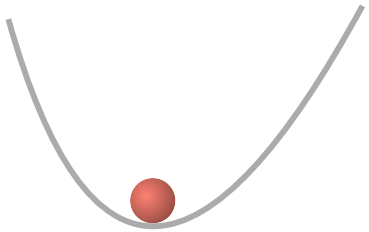
In an equilibrium, $\boldsymbol{u}$ does not change:

$$\frac{d\boldsymbol{u}}{dt} = \mathbf{0} \iff F(t, \boldsymbol{u}(t)) = 0$$

What happens when we tap a system in equilibrium?

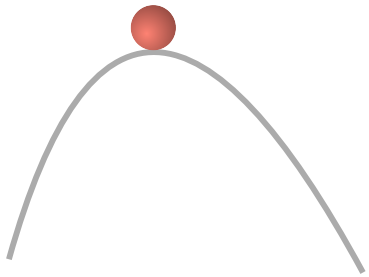
Stable and unstable equilibria

Stable



$$\frac{du}{dt} = 0$$

Unstable



$$\frac{du}{dt} = 0$$

A stability criterion

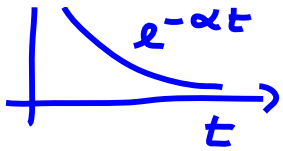
- Let us look at a simple first-order ODE $\frac{du}{dt} = \alpha u$
- Equilibria are at $\frac{du}{dt} = 0$ which is solved by $u = u_0 = 0$

When we **perturb** the system around an **equilibrium**, do we **come back** to the equilibrium or we **go away** from it?

- We know that a general solution is given as $u(t) = ce^{\alpha t}$
- Thus starting from a point $u(0) = u_0 + \epsilon = \epsilon$, do we go back to 0 or not? We already know this!

$\alpha < 0$ **stable**

$\alpha > 0$ **unstable**



A stability criterion

- The key parameter in a linear first-order ODE is α;
  we would like to generalize to $\frac{du}{dt} = f(u)$ with a nonlinear $f(u)$.

- For the linear $f(u) = \alpha u$, the key parameter α equals $f'(u)$.
  Coincidence?

$\alpha = f'(u) = \frac{d}{du}(\alpha u)$

- What happens when we move very slightly out of an equilibrium?

$$\left.\frac{du}{dt}\right|_{u=u_0+\epsilon} = f(u_0+\epsilon) \approx f(u_0) + f'(u_0)\epsilon = f'(u_0)\epsilon$$

$u \Rightarrow u - u_0 = \epsilon$

α

A stability criterion

$$\frac{d(u_0+\epsilon)}{dt} = \frac{d\epsilon}{dt} = f'(u_0)\cdot\epsilon$$

new linear System!

$$\left.\frac{du}{dt}\right|_{u=u_0+\epsilon} = f(u_0+\epsilon) \approx f(u_0) + f'(u_0)\epsilon = f'(u_0)\epsilon$$

A constant scalar

$U = u_0$

- For small ϵ (close to U) the above approximation is accurate: $f'(U)$ plays the role of α!
- Since $\left.\frac{du}{dt}\right|_{u=U+\epsilon} = \frac{d\epsilon}{dt}$, we effectively **linearized** our nonlinear equation around U

Example 1: Simple 1D systems

$f'(u) = \frac{d}{du}(u - u^2) = 1 - 2u$

eq.: $u - u^2 = 0$

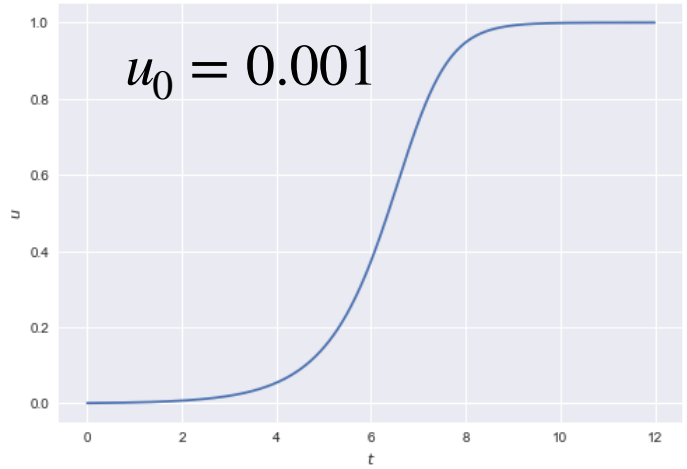
$\Rightarrow u_0 = 0, 1$

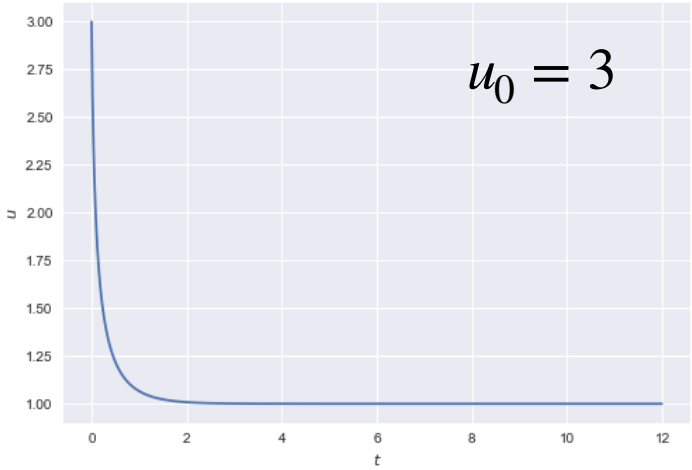
	$\frac{du}{dt} = \alpha u$	$\frac{du}{dt} = u - u^2$	$\frac{du}{dt} = u - u^3$
$\frac{du}{dt} = 0$	$u_0 = 0$	$u_0 = 0,\ 1$	$u_0 = 0, \pm 1$
$\left.\frac{df}{du}\right\|_{u=U}$	α	$f'(0) = 1$ $f'(1) = -1$	$f'(0) = 1$ $f'(\pm 1) = -2$
Stable?	$\alpha < 0$ ✓ $\alpha > 0$ ✗	$U = 0$ ✗ $U = 1$ ✓	$U = 0$ ✗ $U = 1$ ✓ $U = -1$ ✓

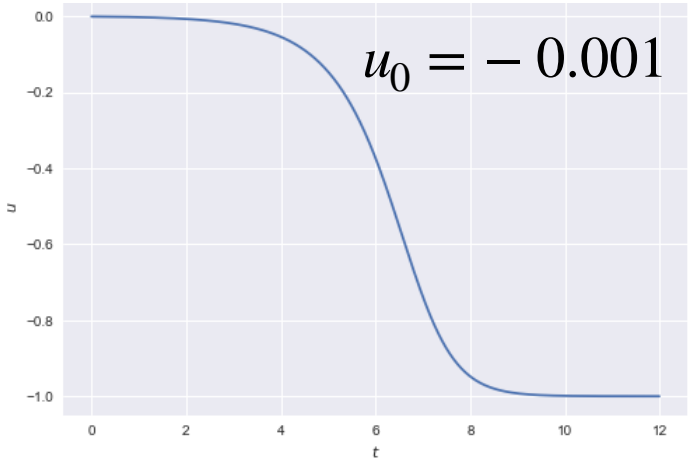
0 : unstable
±1 : stable

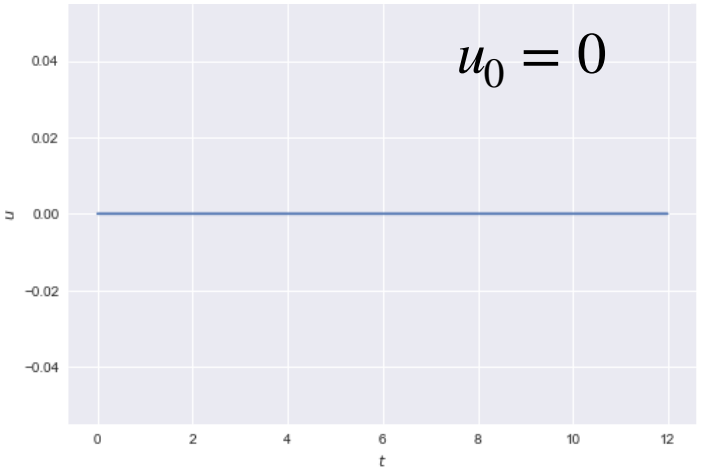
A quick numerical check…

```python
# Simple 1D examples

def f_sys1(x, t, alpha=-1):
    return alpha*x

def f_sys2(x, t):
    return x - x**2

def f_sys3(x, t):
    return x - x**3


T = 12
dt = 0.01
tspan = np.arange(0.0, T, dt)

u_0 = 0.001
u = odeint(f_sys3, u_0, tspan)

plot(tspan, u)
plt.xlabel('$t$')
plt.ylabel('$u$')
```









Example 2: FitzHugh—Nagumo model of a spiking neuron

v = membrane potential $\qquad$ w = recovery variable

$$\frac{dv}{dt} = I_{app} + v - \frac{v^3}{3} - w \qquad \frac{dw}{dt} = \epsilon(v - \alpha w + \beta)$$

$$\boldsymbol{u} = \begin{bmatrix} v \\ w \end{bmatrix} \qquad \frac{d\boldsymbol{u}}{dt} = \boldsymbol{F}(\boldsymbol{u})$$

$$F : \mathbb{R}^2 \to \mathbb{R}^2$$

$$F(v,w) = \begin{pmatrix} F_1(v,w) \\ F_2(v,w) \end{pmatrix}$$

Example 2: FitzHugh—Nagumo model of a spiking neuron

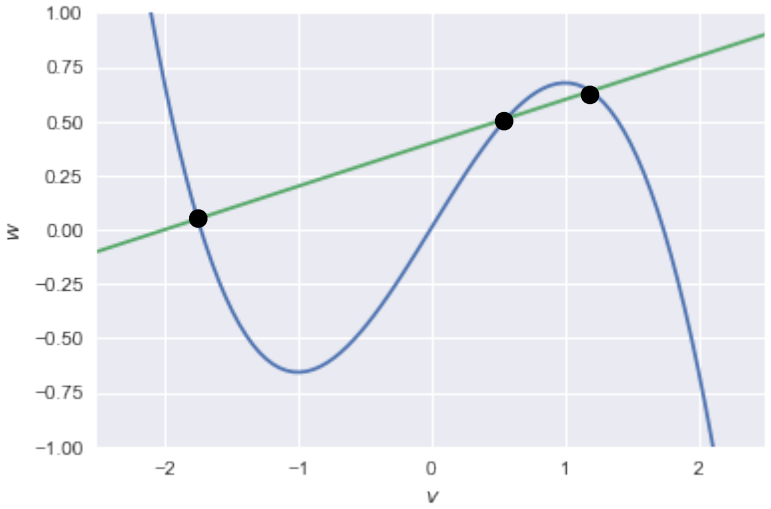
$$I_{app} = 0.01 \text{ A}$$
$$\epsilon = 0.01$$
$$\alpha = 5.00$$
$$\beta = 2.00$$

(Not necessarily a realistic choice of parameters)

r.h.s. ≐ 0

Equilibria

$$I_{app} + v - \frac{v^3}{3} - w = 0$$
$$\epsilon(v - \alpha w + \beta) = 0$$




```
v0 = np.roots([-1.0/3.0, 0, 1.0 - 1.0 / alpha, I_app - beta / alpha])
v0 = np.sort(v0.real)
w0 = 1.0 / alpha * (v0 + beta)

print(v0)
```

v-roots `[-1.75156349  0.56110887  1.19045461]`

Stable or unstable equilibria?

Multivariate Taylor (linear term)

$$\boldsymbol{F}(\boldsymbol{u}) = \boldsymbol{F}(\boldsymbol{u_0}) + \nabla_{\boldsymbol{u}}\boldsymbol{F}(\boldsymbol{u_0})(\boldsymbol{u} - \boldsymbol{u_0}) + O(\|\boldsymbol{u} - \boldsymbol{u_0}\|^2)$$

$\frac{d\epsilon}{dt} = \nabla_u F\big|_{u=u_0} \cdot \epsilon$

$\nabla_{\boldsymbol{u}}\boldsymbol{F}$ is the **Jacobian**

$$\nabla_{\boldsymbol{u}}\boldsymbol{F} = \begin{bmatrix} \frac{dF_1}{dv} & \frac{dF_1}{dw} \\ \frac{dF_2}{dv} & \frac{dF_2}{dw} \end{bmatrix} = \begin{bmatrix} 1 - v^2 & -1 \\ \epsilon & -\epsilon\alpha \end{bmatrix}$$

```
for idx in [0, 1, 2]:
    D = [[1 - v0[idx]**2, -1],
         [epsilon, -alpha*epsilon]
        ]
    evals, _ = np.linalg.eig(D)
    print(evals)
```

```
[-2.06300695 -0.05496769]
[+0.67129284 -0.03613601]
[-0.38755761 -0.07962457]
```

unstable

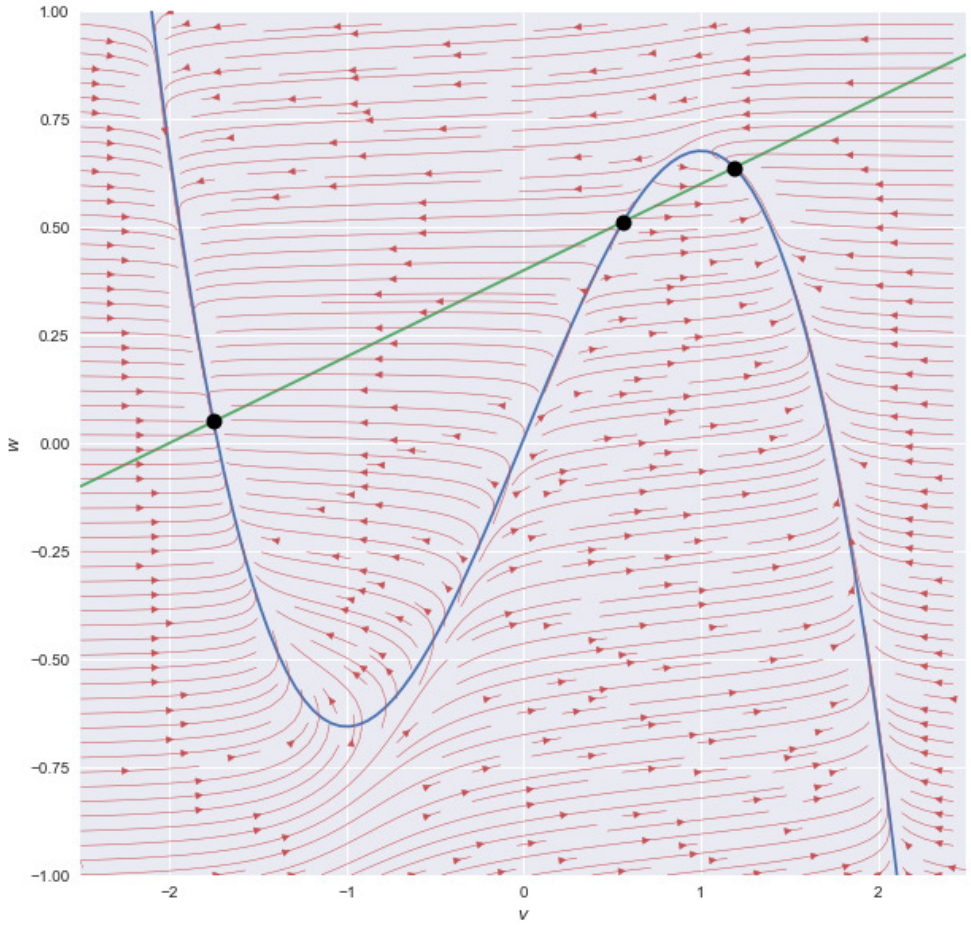
λ_1 λ_2

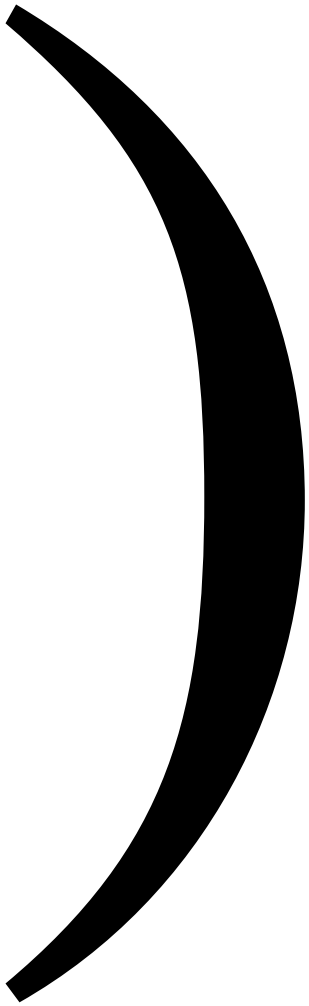
Phase portrait: FitzHugh—Nagumo

- Start the evolution of the system at many points and track where it goes

```
for idx in [0, 1, 2]:
    D = [[1 - v0[idx]**2, -1],
         [epsilon, -alpha*epsilon]
        ]
    evals, _ = np.linalg.eig(D)
    print(evals)
```

```
[-2.06300695 -0.05496769]
[ 0.67129284 -0.03613601]
[-0.38755761 -0.07962457]
```





OK, back to COVID…

Application to the SIR model

$$\frac{dS}{dt} = -\beta \frac{I(t)}{N} S(t)$$
$$\frac{dI}{dt} = \beta \frac{I(t)}{N} S(t) - \gamma I(t)$$

$$\frac{d}{dt}\begin{bmatrix} S \\ I \end{bmatrix} = \boldsymbol{F}(S, I) = \begin{bmatrix} F_1(S, I) \\ F_2(S, I) \end{bmatrix}$$

Since $R = N - S - I$, if $S(t)$ and $I(t)$ don't change, neither does R

$$\frac{dS}{dt} = 0$$
$$\frac{dI}{dt} = 0$$
$$\Longrightarrow$$

Epidemic equilibria

$$(S, I) = (N, 0)$$
$$(S, I) = (0, 0)$$

Linearize around the $(N,0)$ equilibrium

Taylor series (first two terms)

$$\boldsymbol{F}(\boldsymbol{u}) = \boldsymbol{F}(\boldsymbol{u_0}) + \nabla_{\boldsymbol{u}}\boldsymbol{F}(\boldsymbol{u_0})(\boldsymbol{u} - \boldsymbol{u}_0) + O(\|\boldsymbol{u} - \boldsymbol{u}_u\|^2)$$

$$\frac{d}{dt}\begin{bmatrix} S \\ I \end{bmatrix} = \begin{bmatrix} -\beta\frac{I}{N}S \\ \beta\frac{I}{N}S - \gamma I \end{bmatrix}$$

$$\approx \left.\begin{bmatrix} -\beta\frac{I}{N}S \\ \beta\frac{I}{N}S - \gamma I \end{bmatrix}\right|_{S=N,I=0} + \left.\begin{pmatrix} \frac{d}{dS}\left(-\beta\frac{I}{N}S\right) & \frac{d}{dI}\left(-\beta\frac{I}{N}S\right) \\ \frac{d}{dS}\left(\beta\frac{I}{N}S - \gamma I\right) & \frac{d}{dI}\left(\beta\frac{I}{N}S - \gamma I\right) \end{pmatrix}\right|_{S=N,I=0} \left(\begin{bmatrix} S \\ I \end{bmatrix} - \begin{bmatrix} N \\ 0 \end{bmatrix}\right)$$

Finally…

$$\frac{d}{dt}\begin{bmatrix} S \\ I \end{bmatrix} \approx \begin{bmatrix} 0 & -\beta \\ 0 & \beta - \gamma \end{bmatrix} \left(\begin{bmatrix} S \\ I \end{bmatrix} - \begin{bmatrix} N \\ 0 \end{bmatrix} \right)$$

Eigenvalues of the Jacobian matrix

$$\lambda_1 = 0 \qquad \lambda_2 = \beta - \gamma$$

$\beta > \gamma \Rightarrow$ epidemic

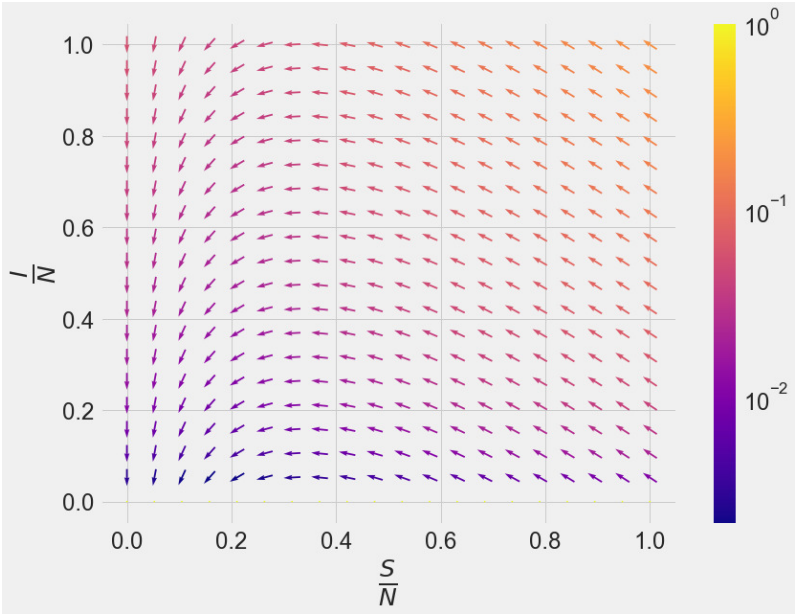
$\beta < \gamma \Rightarrow$ no epidemic

key parameter

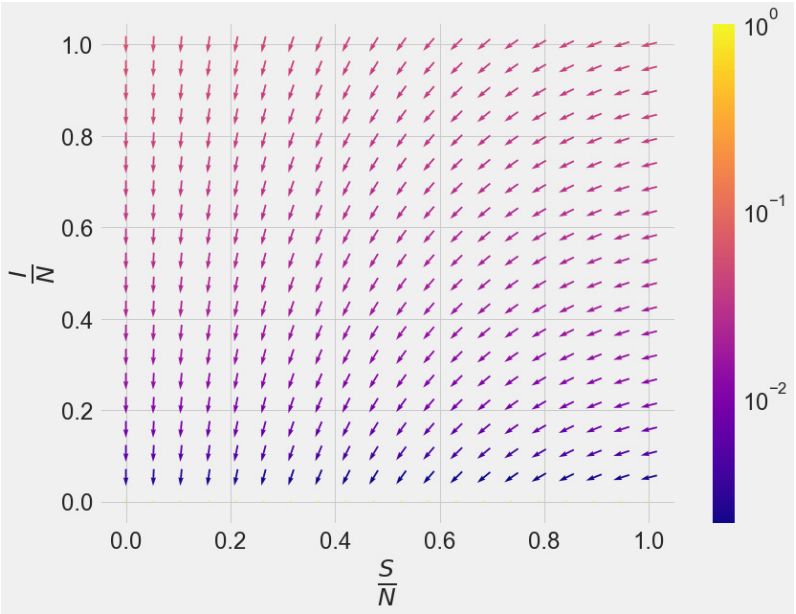
$$R_0 := \frac{\beta}{\gamma}$$

Phase portraits

$R_0 = 3$

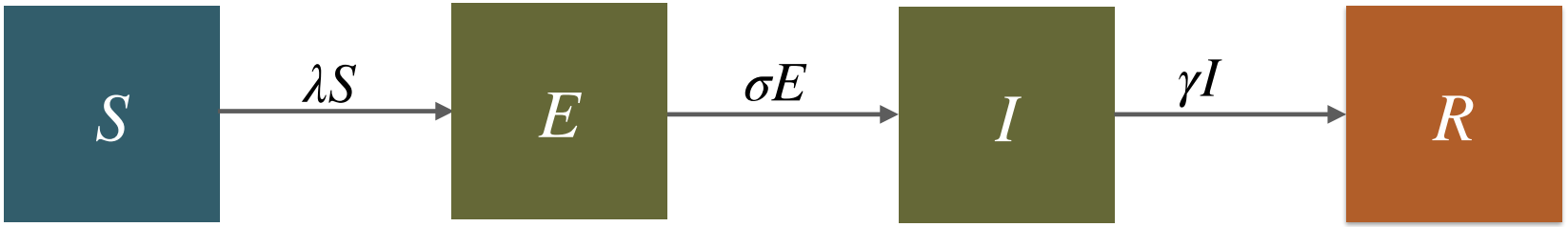


$R_0 = 0.8$



Extending the model

- We can first improve the model by adding a 4th compartment, **E**
- This models *exposed* individuals who will become infected after an **incubation period**



$$\frac{dS}{dt} = -\beta \frac{I}{N} S \qquad \frac{dE}{dt} = \beta S \frac{I}{N} S - \sigma E \qquad \frac{dI}{dt} = \beta \frac{I}{N} S - \gamma I \qquad \frac{dR}{dt} = \gamma I$$

Extending the model

- Next, we normalize everything by the total population, $s = S/N, i = I/N, e = E/N, r = R/N$
- Reparameterize the equations in terms of R_0; here it is defined as $R_0 = \frac{\beta}{\gamma}$

$$\begin{aligned}
\dot{s} &= -\gamma R_0 \, s \, i \\
\dot{e} &= \gamma R_0 \, s \, i - \sigma e \\
\dot{i} &= \sigma e - \gamma i \\
\dot{r} &= \gamma i
\end{aligned}$$

$$s + e + i + r = 1$$

Mitigation

- The idea is that R_0 can be influenced by policy—a lockdown hopefully makes it smaller
- R_0 does not change instantaneously

$$\frac{dR_0}{dt} = \eta(R_{\text{target}} - R_0)$$

- It will be interesting to track the **cumulative caseload** $c = i + r$ and the **number of deaths**

$$\frac{dc}{dr} = \sigma e \qquad \frac{dd}{dt} = \delta\gamma i = \int \frac{dr}{dt}$$

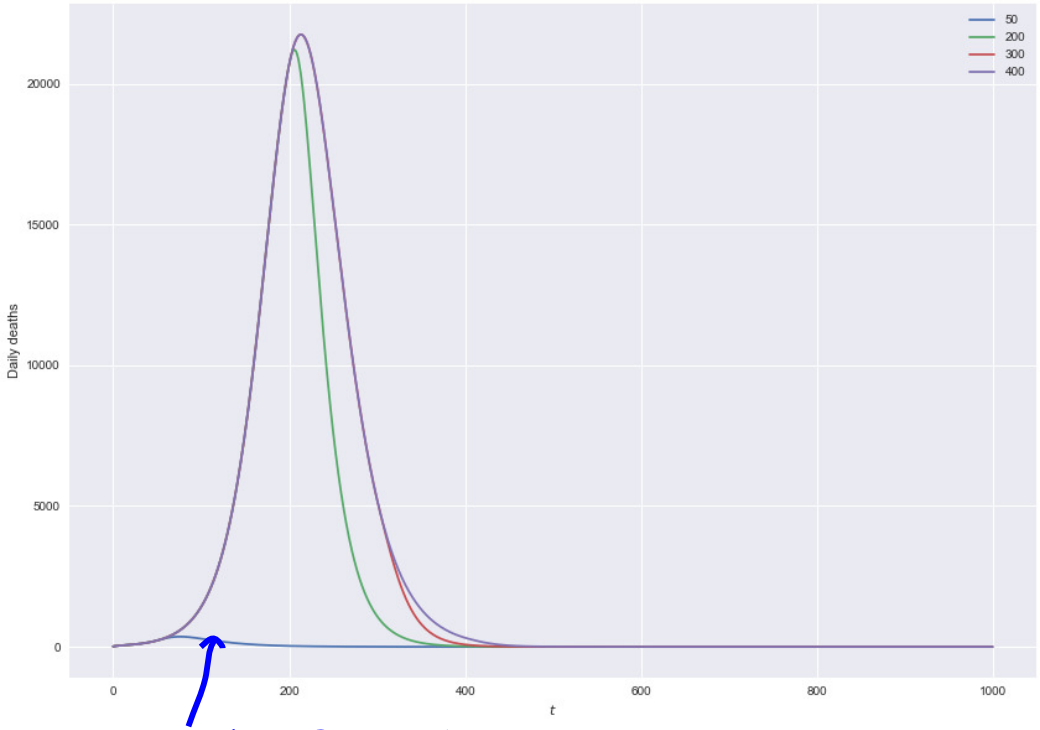
Modeling in python

```
def f_seir_ld(x, t, gamma=1.0/18, sigma=1/5.2, R0_1=2.0,
              R0_2=0.5, t_change=100, eta=1.0/20, delta=0.01):
    s, e, i, r, R0, c, d = x

    R0_inf = R0_1 if t < t_change else R0_2

    dydt = [-gamma*R0*s*i,            # ds/dt = -γR₀si
             gamma*R0*s*i - sigma*e, # de/dt =  γR₀si -σe
             sigma*e  - gamma*i,     # di/dt =         σe -γi
                        gamma*i,     # dr/dt =            γi
             eta*(R0_inf - R0),
             sigma*e,
             delta*gamma*i
            ]
    return dydt
```

Introducing lockdown

```
# lifting or introducing lockdown

lift = False

R0_L = 0.5
R0_NL = 2.0
t_change_list = [50, 200, 300, 400]

R0_1, R0_2 = (R0_L, R0_NL) if lift else (R0_NL, R0_L)

T = 1000
dt = 1
tspan = np.arange(0.0, T, dt)

plt.figure(figsize=(14, 10))
for t_change in t_change_list:
    f_seir_ld_t = lambda x, t : f_seir_ld(x, t, t_change=t_change,
                                          R0_1=R0_1, R0_2=R0_2)

    y_0 = [s_0, e_0, i_0, r_0, R0_1, 0, 0]

    y = odeint(f_seir_ld_t, y_0, tspan)
    deaths = N * delta * gamma * y[:, 2]
    _ = plt.plot(tspan, deaths)
```

target R_0
initial
lockdown at days ...



early lockdown (day 50)

Lifting lockdown

```
# lifting or introducing lockdown

lift = True

R0_L = 0.5
R0_NL = 2.0
t_change_list = [50, 200, 300, 400]

R0_1, R0_2 = (R0_L, R0_NL) if lift else (R0_NL, R0_L)

T = 1000
dt = 1
tspan = np.arange(0.0, T, dt)

plt.figure(figsize=(14, 10))
for t_change in t_change_list:
    f_seir_ld_t = lambda x, t : f_seir_ld(x, t, t_change=t_change,
                                          R0_1=R0_1, R0_2=R0_2)

    y_0 = [s_0, e_0, i_0, r_0, R0_1, 0, 0]

    y = odeint(f_seir_ld_t, y_0, tspan)
    deaths = N * delta * gamma * y[:, 2]
    _ = plt.plot(tspan, deaths)
```