PHYSICAL FORMULATION

MATHEMATICS AS THE LANGUAGE OF PHYSICS

A. BÁEZ, F.X. TRIAS AND N. VALLE

OPERATORS

OPERATORS AS THE BRICKS OF EQUATIONS

DISCLAIMER

This is <u>NOT</u> a PDE course.

If interested you can check this:

Introduction to PDE | MIT

So, what will we do today, then?

1) Understand the concept of operator
2) Look at operator properties

Operators: Definition

An operator is a mapping:

It takes an input from a vector space and returns an output in another, not necessarily the same, vector space.

It generalizes the concept of function.

∇, $\nabla\cdot$ and ∇^2 are your breakfast operators!

In mathematical terms:

$$A := U \rightarrow V$$

Operators: Fundamentals

Vector spaces:

A vector space is a set of objects (vectors) over a field of scalars that satisfy **vector addition** and **scalar multiplication.**

We are familiar with n-dimensional vectors:

$$\vec{u}=\left(u_1\hat{\boldsymbol{e}}_{\mathbf{1}}+u_2\hat{\boldsymbol{e}}_{\mathbf{2}}+\ldots+u_n\hat{\boldsymbol{e}}_{\boldsymbol{n}}\right)$$

Where the basis is defined as:

$$\left(\hat{\boldsymbol{e}}_{\mathbf{1}},\hat{\boldsymbol{e}}_{\mathbf{2}},\ldots,\hat{\boldsymbol{e}}_{\boldsymbol{n}}\right)=\left\{\left(1,0,\ldots,0\right),\left(0,1,\ldots,0\right),\left(0,0,\ldots,1\right)\right\}$$

Vector spaces:

As far as we satisfy vector **addition** and **scalar multiplication*** we can choose a different basis such as:

$$(\hat{\boldsymbol{e}}_1, \hat{\boldsymbol{e}}_2, \ldots, \hat{\boldsymbol{e}}_n) = \{\sin(\pi x), \sin(2\pi x), \ldots, \sin(n\pi x)\}$$

*There are actually 8 axions that need to be satisfied to formally prove that a set of vectors and a field form a vector space. More here.

Vector spaces:

You can look at “normal” vectors as a function where the input space is the position of the vector. Like in a tabulated function, every index corresponds with a value. For an *n*-dimensional vector:

$$\hat{\boldsymbol{e}}_{\mathbf{1}} = \{1, 0, \ldots, 0\}$$
$$\hat{\boldsymbol{e}}_{\mathbf{1}} : \{\mathbb{N} \leqslant n\} \rightarrow \mathbb{R}$$

Note that the **<u>size of the input space is *n*</u>**, which is the number of components that the space has.

termofluids FTCM Centre Tecnològic de Transferència de Calor UNIVERSITAT POLITÈCNICA DE CATALUNYA

Vector spaces:

When you have a given vector:

$$\vec{u}=\left(u_1\hat{\boldsymbol{e}}_{\boldsymbol{1}}+u_2\hat{\boldsymbol{e}}_{\boldsymbol{2}}+\ldots+u_n\hat{\boldsymbol{e}}_{\boldsymbol{n}}\right)$$

You end up having something that:

$$\vec{u}:\{\mathbb{N}\leqslant n\}\rightarrow\mathbb{R}$$

Note that the **<u>dimension of *u* is not necessarily the same as *n*</u>** (i.e., a 2D plane in a 3D space)

$$\vec{u}_{plane}=x_{plane}\{1,1,0\}+y_{plane}\{0,0,1\}$$

Vector spaces:

"Function" vectors define a set of values as well, but instead of a "table", they use a function. We say that the independent variable is the input and the dependent one is the output.

$$\hat{\boldsymbol{e}}_{\mathbf{1}} = \sin(\omega_1 t)$$
$$\hat{\boldsymbol{e}}_{\mathbf{1}} : \mathbb{R} \rightarrow \mathbb{R}$$

Note that the input space are the real numbers and thus the **<u>size of the input space is infinity</u>**.

Operators: Fundamentals

Vector spaces:

When you have a given vector:

$$\vec{u} = \left(u_1 \hat{\boldsymbol{e}}_{\mathbf{1}} + u_2 \hat{\boldsymbol{e}}_{\mathbf{2}} + \ldots + u_n \hat{\boldsymbol{e}}_{\boldsymbol{n}} \right)$$

You end up having something that:

$$\vec{u} : \mathbb{R} \rightarrow \mathbb{R}$$

So we end up with another function!

Note that, like in the Fourier series, we **<u>may need an infinite sum of base functions</u>** to represent a particular one.

termofluids FTCM CTTC UPC Centre Tecnològic de Transferència de Calor UNIVERSITAT POLITÈCNICA DE CATALUNYA

Vector spaces:

Finally, note that you **already knew** several examples of this: **Fourier and Taylor** series are just ways to **represent a particular function in a different basis**!!!

$$f(x)=\sum_{n=0}^{\infty} a_n \sin(\omega_n x)+b_n \cos(\omega_n x)$$

$$f(x)=\sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!}(x-x_0)^n$$

Operators: Examples

Matrix multiplication

$$Mx$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

$$A = M \quad U = \mathbb{R}^3 \quad V = \mathbb{R}^2$$

Power

$$(x)^n$$

$$x^{1/2} = \sqrt{x}$$

$$A = (\,)^n \quad U = \mathbb{R} \quad V = \mathbb{C}$$

Operators: Examples

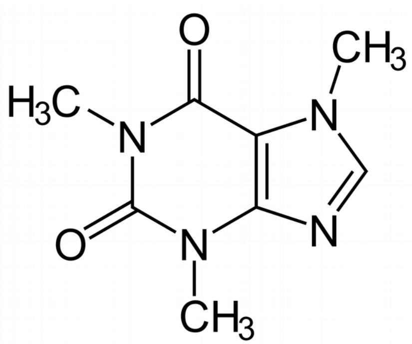
Integration	Differentiation
$\int_{\Omega} f\,dx$	∇f
$\int \sin(n\pi x)\,dx = \frac{-1}{n\pi}\cos(n\pi x)$	$\nabla \sin(n\pi x) = n\pi\cos(n\pi x)$
$A = \int dx$	$A = \nabla$
$U = \sin(n\pi x) \quad V = \cos(n\pi x)$	$U = \sin(n\pi x) \quad V = \cos(n\pi x)$
$\forall n \in \mathbb{Z}$	$\forall n \in \mathbb{Z}$

Operators: Examples

termofluids
FTCM
Fundació per al Progrés de la Transferència de Calor i Massa
CTTC
UPC
Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

PhD Student

Thesis Operator



→


Journal of Computational Physics

$$A = you \quad U = substances \quad V = science\,(?)$$

Disclaimer: Mind blowing risk!

Hold on, am I an operator?

A particular operator may require particular properties of either *U* or *V*.

Most of the times we will require our spaces to be equipped with a ***dot product,*** to have a ***metric*** (measure) and to be ***differentiable*** spaces (manifolds).

We will see how this plays a role in the coming slides and avoid mathematical formalism.

Operators: Examples

Quantum Mechanics	Fluid Mechanics
$\hat{H}\Psi$	$NS\begin{bmatrix} u \\ P \end{bmatrix}$
$\left(\frac{-\hbar}{2m}\nabla^2+V\right)\Psi=Ek+Ep$	$\nabla\cdot u=0$ $\rho\frac{Du}{Dt}+\nabla P=\nabla\cdot\sigma$
$A=\hat{H}$ $U=\mathbb{C}\quad V=\mathbb{R}$	$A=NS$ $U=\mathbb{R}^3\times\mathbb{R}\quad V=\mathbb{R}\times\mathbb{R}^3$

Operators: Properties

Operator properties provide **qualitative insight into the output**.

Is this something you want to preserve? Or not?

We will look at:

- Linearity
- Kernel
- Symmetry
- Normalization
- Conservation
- Norm-conservation
- Definitiveness

Operators: Properties

Preliminary concepts

Endomorphism: $A: U \to U$

Dot product: $(\,)\cdot(\,): U \times U \to \mathbb{R}$

Norm: $\|\cdot\|: U \to \mathbb{R}$

A dot product induces a norm!

Operators: Properties

Linearity

Conditions:

$$A(x+y)=A(x)+A(y)$$

$$A(\alpha x)=\alpha A(x)$$

Linear operator

Example: variables

$$M(x+y)=Mx+My \rightarrow OK$$

$$(x+y)^n \neq x^n+y^n \rightarrow NOT\ linear\,!$$

Example: functions

$$\int (f+g)\,dx=\int f\,dx+\int g\,dx \rightarrow OK$$

$$\nabla (f+g)=\nabla f+\nabla g \rightarrow OK$$

Kernel

Definition:

$$ker(A) = \{u \mid Au = \emptyset\}$$

Tells us what is the space that maps to 0.

Example: variables

Matrix:

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \end{bmatrix}$$

$$ker(A) = c \begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix} \quad \forall c \in \mathbb{R}$$

Operators: Properties

Kernel

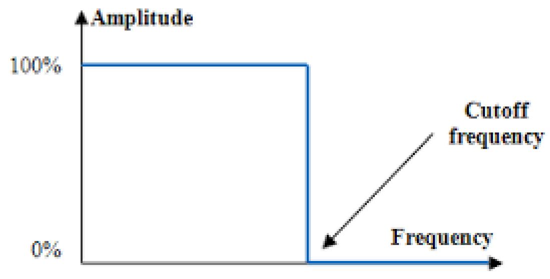
Definition:

$$ker(A)=\{u|Au=\emptyset\}$$

Tells us what is the space that maps to 0.

Example: functions

Low pass filter:



$$F:S\rightarrow S$$
$$S=\{\sin(\omega_i t)\}$$
$$ker(F)=\{S|\omega_i>\omega_{cutoff}\}$$

Operators: Properties

Symmetry

Conditions:

$$A : U \rightarrow U$$

$$\langle Ax | y \rangle = \langle x | Ay \rangle$$

Bracket notation!!

Literally means:

DOT PRODUCT!!

$$\langle Ax | y \rangle := (Ax) \cdot y$$

Example: variables

Matrix multiplication

$$(M\,x) \cdot y = x \cdot (M\,y)\,?$$

We note that:

$$a \cdot b = a^T b \quad (Ax)^T = x^T A^T$$

So:

$$x^T M^T y = x^T M\,y \Leftrightarrow M^T = M$$

Standard matrix transpose!

Operators: Properties

Symmetry

We need to define a DOT product for functions!

$$\langle u|v\rangle := \int_\Omega uv$$

IMPORTANT:

REMEMBER!!!

Example: functions

Laplacian

$$\langle \nabla^2 f|g\rangle = \langle f|\nabla^2 g\rangle \,?$$

We note that:

$$\int_\Omega \nabla^2 f\, g = [\nabla fg]_{\partial\Omega} - \int_\Omega \nabla f\, \nabla g$$

What if $[\nabla fg]_{\partial\Omega} = 0\,?$

Can we do that?

Operators: Properties

Symmetry

We need to define a DOT product for functions!

$$\langle u|v\rangle := \int_{\Omega} uv\, dx$$

IMPORTANT:

REMEMBER!!!

Example: functions

Laplacian

In that case:

$$\int_{\Omega} \nabla^2 f\, g = -\int_{\Omega} \nabla f\, \nabla g$$

Which is the same as:

$$\int_{\Omega} f\, \nabla^2 g = -\int_{\Omega} \nabla f\, \nabla g$$

Symmetric!

Operators: Properties

Normalization

Conditions:

$$A : U \rightarrow U$$

$$A 1_U = 1_U$$

Constants are preserved!

Example: variables

Average matrix:

$$A 1_U = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/3 & 1/3 & 1/3 \\ 0 & 1/2 & 1/2 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

Matrices whose rows sum 1

Operators: Properties

Normalization

Conditions:

$$A : U \rightarrow U$$

$$A\, 1_U = 1_U$$

Constants are preserved!

Example: functions

Helmholtz filter:

$$HF = I + \alpha \nabla^2$$

$$HF\, 1_U = I\, 1_U + \underbrace{\cancel{\alpha \nabla^2 1_U}}_{=0} = 1_U$$

$$1_U \in ker\left(\nabla^2\right)$$

Operators: Properties

Conservation

Conditions:

$$A : U \rightarrow U$$

$$\langle Ax | 1_U \rangle = \langle x | 1_U \rangle$$

Conserves dot product over unitary space vector.

Example: variables

Shift matrix

$$\Gamma x = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$\langle \Gamma x | 1_U \rangle = x^T \Gamma 1_U = x^T 1_U$$

Operators: Properties

Conservation

Conditions:

$$A : U \rightarrow U$$

$$\langle Ax | 1_U \rangle = \langle x | 1_U \rangle$$

Conserves integral.

Example: function

Shift operator:

$$\Gamma x = \exp(\theta) x \quad \forall x \in \exp(i \omega_j t)$$

$$\int_\Omega \exp(i \omega_j t + \theta) 1_U = \int_\Omega \exp(i \omega_j t + \theta)$$

$$\int_\Omega \exp(i \omega_j t) 1_U = \int_\Omega \exp(i \omega_j t) 1_U$$

$$\int_\Omega \exp(i \omega_j t + \theta) = \int_\Omega \exp(i \omega_j t) 1_U$$

termofluids FTCM Fundació per al Progrés de la Transferència de Calor i Massa CTTC UPC Centre Tecnològic de Transferència de Calor UNIVERSITAT POLITÈCNICA DE CATALUNYA

Conservation

We can actually prove that a normalized and symmetric operator is conservative:

$$A: U \to U \quad A 1_U = 1_U \quad \langle Ax | y \rangle = \langle x | Ay \rangle$$

$$\langle Ax | 1_U \rangle = \langle x | A 1_U \rangle = \langle x | 1_U \rangle$$

$$\langle Ax | 1_U \rangle = \langle x | 1_U \rangle$$

Operators: Properties

Norm - Conservation

Conditions:

$$A : U \rightarrow U$$

$$\|Ax\| = \|x\| \quad \forall\, x$$

$$\langle Ax | Ax \rangle = \langle x | x \rangle$$

Conserves the norm of the input!

Depends on the norm!

Example: variables

Rotation matrix:

$$R = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$$

$$x^T R^T R\, x = x^T x \Leftrightarrow R^T R = I$$

$$R^T R = \begin{bmatrix} \cos^2 + \sin^2 & 0 \\ 0 & \sin^2 + \cos^2 \end{bmatrix}$$

Norm - Conservation

Conditions:

$$A : U \rightarrow U$$

$$\|Ax\| = \|x\| \quad \forall\, x$$

$$\langle Ax | Ax \rangle = \langle x | x \rangle$$

Conserves the norm of the input!

Depends on the norm!

Example: function

Shift operator

$$SH : \sin(\omega_i t) \rightarrow \sin(\omega_i t + \theta)$$

$$\int_\Omega \sin^2(\omega_i t) = \int_\Omega \sin^2(\omega_i t + \theta)$$

Operators: Properties

Definitiveness

Definition:

$$A : U \rightarrow U$$

$$\langle Ax | x \rangle = s \| x \| \; \forall \, x \in U$$

$$sign(s) \begin{cases} > 0 \text{ positive} \\ \geqslant 0 \text{ non-negative} \\ \leq 0 \text{ non-positive} \\ < 0 \text{ negative} \end{cases}$$

Example: variables

Rotation matrix:

$$R = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$$

$$x^T R^T x = s \, x^T x$$

$$x^T R \, x = (x_1^2 + x_2^2) \cos(\theta)$$

It will depend on θ!

Operators: Properties

Definitiveness

Definition:

$$A : U \rightarrow U$$

$$\langle Ax | x \rangle = s \|x\| \forall\, x \in U$$

$$sign(s) \begin{cases} > 0 \text{ positive} \\ \geqslant 0 \text{ non-negative} \\ \leq 0 \text{ non-positive} \\ < 0 \text{ negative} \end{cases}$$

Example: functions

Laplacian:

$$\langle \nabla^2 f | f \rangle = -\langle \nabla f | \nabla f \rangle$$

$$\langle \nabla^2 f | f \rangle = -\|\nabla f\|$$

Negative definite!

Operators: Your friends

Review of our every day operators:

name	grad	div	lap
symbol	∇	$\nabla\cdot$	∇^2
linear	yes	yes	yes
kernel			
symm.			yes
norm.			
cons.			
def.			-

Operators: Your friends

Let's fill the gaps!

Note that ***grad*** and ***div*** are ***NOT endomorphisms!***

Symmetry, normalization, conservation, norm-conservation and *definitiveness* ***DO NOT APPLY!***

Operators: Your friends

Let's fill the gaps!

We can, however, find useful relations between them:

$$\langle \nabla \cdot (s\vec{f}) | 1_U \rangle = \langle \nabla \cdot \vec{f} | s \rangle + \langle \vec{f} | \nabla s \rangle$$

1 million $ identity!

$$\int_{\Omega} \nabla \cdot (s\vec{f}) = \int_{\partial\Omega} s\vec{f} = 0$$

$$\langle \nabla \cdot \vec{f} | s \rangle = -\langle \vec{f} | \nabla s \rangle$$

We say that they are negative adjoint!

termofluids
FTCM
Fundació per al Progrés de la Transferència de Calor i Massa
CTTC UPC
Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

Let's fill the gaps!

We have several useful calculus identities as well:

$$\nabla \cdot \nabla \times A = 0 \quad \forall A \in VS \left(Vector\ Space \right)$$

$$\nabla \times \nabla \theta = 0 \quad \forall \theta \in \mathbb{R}$$

$$\nabla \cdot \nabla = \nabla^2$$

Operators: Your friends

Review:

name	grad	div	lap
symbol	∇	$\nabla\cdot$	∇^2
linear	yes	yes	yes
kernel	$f(\vec{x})=C$	$\nabla\times A$	$f(\vec{x})=a\vec{x}+\vec{b}$
symm.	*	*	yes
norm.	*	*	no
cons.	*	*	no
def.	*	*	-

$*$: only apply to endomorphisms