Lectures IIT Kanpur, India
Lecture 2: Discrete Physics

Numerics without basis functions

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Outline of this lecture

This short course on mimetic spectral elements consists of 6 lectures:

Lecture 1: In this lecture we will review some basic concepts from differential geometry

Lecture 2: Generalized Stokes Theorem and geometric integration

Lecture 3: Connection between continuous and discrete quantities. The Reduction operator and the reconstruction operator.

Lecture 4: The Hodge-$\star$ operator. Finite volume, finite element methods and least-squares methods.

Lecture 5: Application of mimetic schemes to elliptic equations. Poisson and Stokes problem

Lecture 6: Open research questions. Collaboration.

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What we did yesterday

Yesterday we looked at:

- The vector as a tangent vector along curves, although the interpretation in terms of derivations seems more natural for mimetic discretizations.
- Differential forms as alternating tensors on the linear vector space.
- The wedge product to construct higher order tensors.
- The relation between differential forms and integration.
- The exterior derivative which is a linear map between spaces of differential forms
- The resemblance between the exterior derivative and the grad, curl and div from vector calculus.

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Today we are going to take a look at the generalized Stokes Theorem which will make the connection between the exterior derivative and the geometry of space.

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The Mother of all equations

Let Ω_k be a k-dimensional sub-variety of the manifold $\mathcal{M}$ with boundary $\partial\Omega_k$ and let $\boldsymbol{\alpha}^{(k-1)}$ be a differential $(k-1)$-form, then the following identity holds:

$$\int_{\partial\Omega_k} \boldsymbol{\alpha}^{(k-1)} = \int_{\Omega_k} \mathrm{d}\boldsymbol{\alpha}^{(k-1)} \, .$$

Using the notation we introduced yesterday this identity reads

$$\left\langle \boldsymbol{\alpha}^{(k-1)}, \partial\Omega_k \right\rangle = \left\langle \mathrm{d}\boldsymbol{\alpha}^{(k-1)}, \Omega_k \right\rangle$$

Generalized Stokes Theorem

Stokes Theorem: Let Ω_{k+1} be a $k+1$-dimensional manifold and $a \in \Lambda^k$ then

$$\int_{\partial\Omega_{k+1}} a^{(k)} = \int_{\Omega_{k+1}} \mathrm{d}a^{(k)} \qquad \Leftrightarrow \qquad \left\langle a^{(k)}, \partial\Omega_{k+1} \right\rangle = \left\langle \mathrm{d}a^{(k)}, \Omega_{k+1} \right\rangle$$

$$k = 0: \quad \int_{\mathcal{L}} \mathrm{grad}\ \phi\ \mathrm{d}l = \phi(l_{\mathrm{end}}) - \phi(l_{\mathrm{begin}}), \quad \mathrm{grad}: H_p \mapsto H_L$$

$$k = 1: \quad \int_{\mathcal{S}} \mathrm{curl}\ \xi\ \mathrm{d}S = \int_{\partial\mathcal{S}} \xi\ \mathrm{d}l, \quad \mathrm{curl}: H_L \mapsto H_S$$

$$k = 2: \quad \int_{\mathcal{V}} \mathrm{div}\ F\ \mathrm{d}V = \int_{\partial\mathcal{V}} F\ \mathrm{d}S, \quad \mathrm{div}: H_S \mapsto H_V$$

Exact sequence (De Rham complex):

$$\mathbb{R} \hookrightarrow H_p \xrightarrow[\mathrm{grad}]{\mathrm{d}} H_L \xrightarrow[\mathrm{curl}]{\mathrm{d}} H_S \xrightarrow[\mathrm{div}]{\mathrm{d}} H_V \to 0$$

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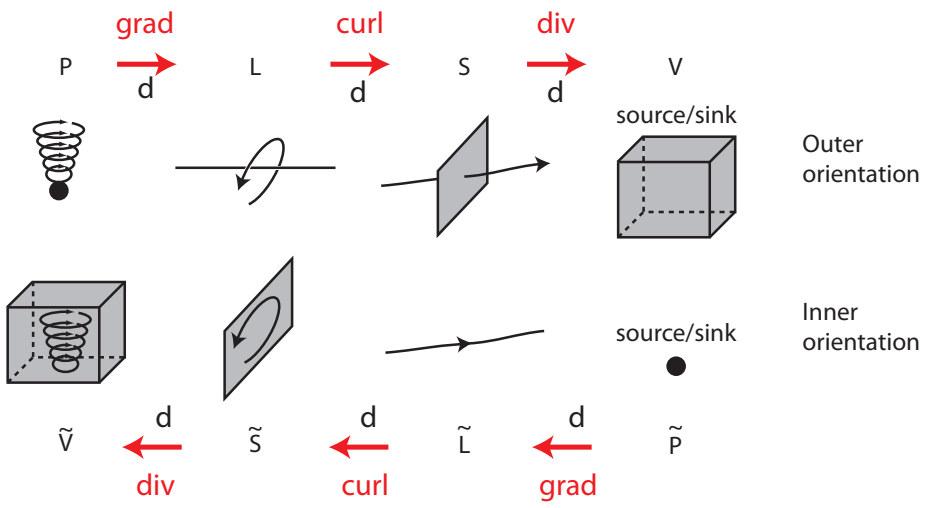

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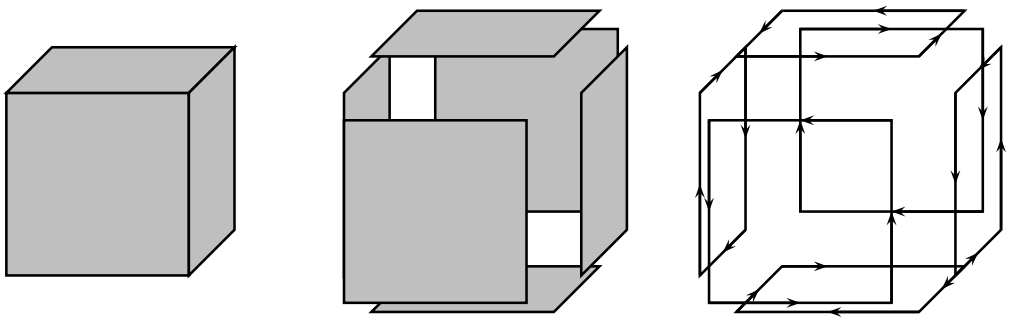
Vector identities

For all geometric objects we have: The boundary of the boundary is empty.



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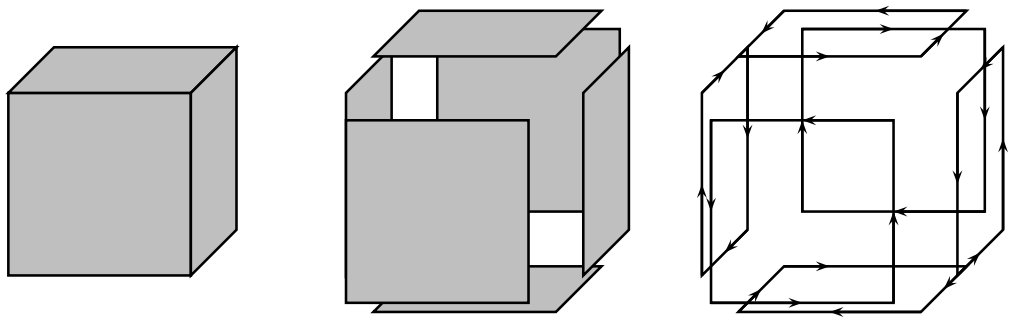

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This implies that $\mathrm{dd} \equiv 0$

$$0 = \left\langle a^{(k)}, \partial\partial\Omega_{k+2} \right\rangle = \left\langle \mathrm{d}a^{(k)}, \partial\Omega_{k+2} \right\rangle = \left\langle \mathrm{dd}a^{(k)}, \Omega_{k+2} \right\rangle$$

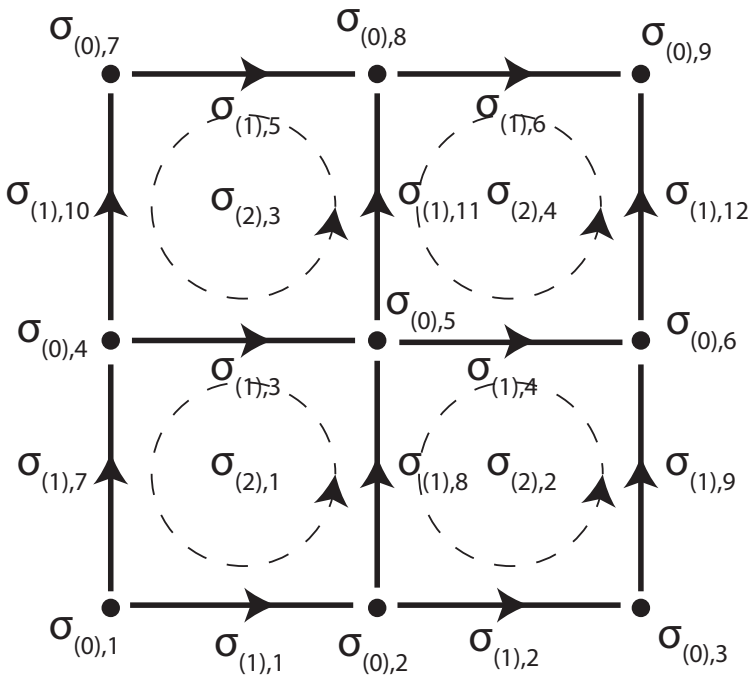
Exact sequence (De Rham complex):

$$\mathbb{R} \hookrightarrow H_p \xrightarrow[\text{grad}]{\mathrm{d}} H_L \xrightarrow[\text{curl}]{\mathrm{d}} H_S \xrightarrow[\text{div}]{\mathrm{d}} H_V \to 0 \qquad \text{curl grad} = \text{div curl} \equiv 0$$

The computational grid

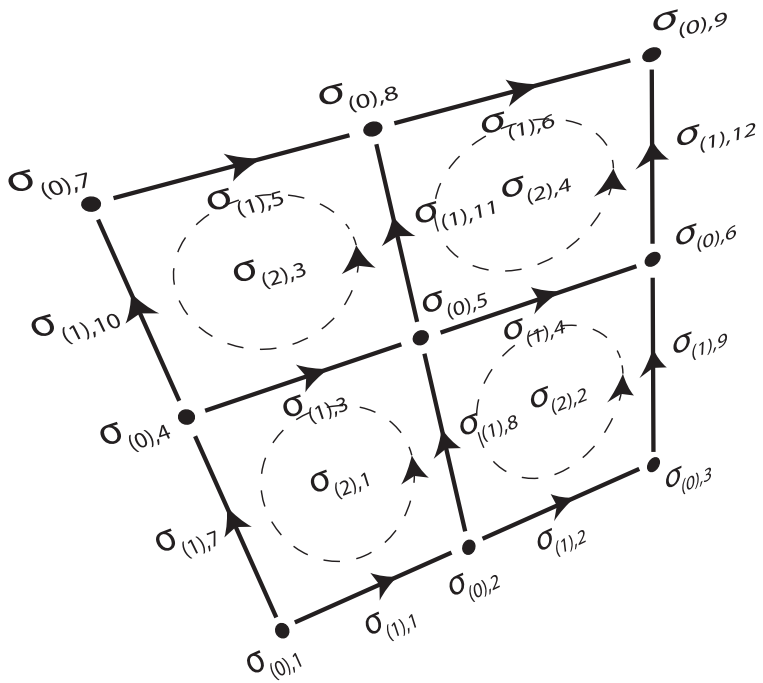
Consider the very simple 2-dimensional grid on the right. This grid consists of:

- 9 points
- 12 line segments
- 4 surfaces



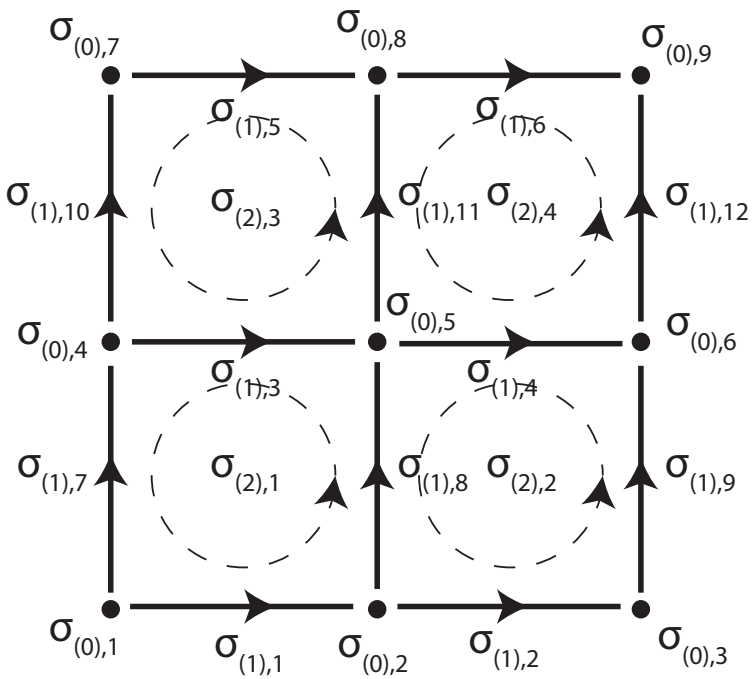
The computational grid

The actual size and shape is irrelevant in what follows. We can stretch, twist, deform the grid as much as we want, as long as we do not change the connectivity between the points, lines and surfaces



The computational grid

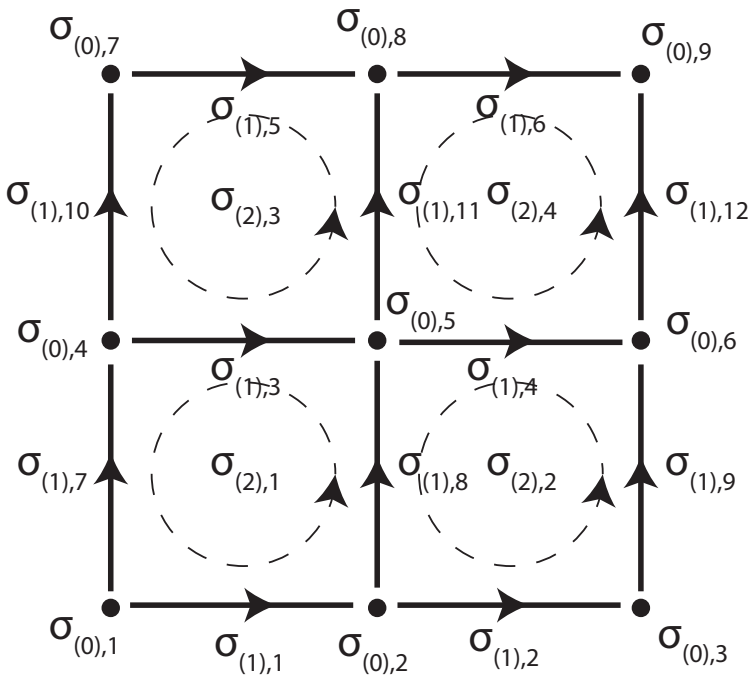
- We will call the points in the grid 0-cells, denoted by $\sigma_{(0),i}$. The subscript (0) indicates that it is a 0-dimensional object (a point) and the i is a label to distinguish different points.
- We will call the line segments in the grid 1-cells, denoted by $\sigma_{(1),i}$. The subscript (1) indicates that it is a 1-dimensional object (a line segment) and the i is a label to distinguish different points.
- We will call the surfaces in the grid 2-cells, denoted by $\sigma_{(2),i}$. The subscript (2) indicates that it is a 2-dimensional object (a surface) and the i is a label to distinguish different points.



The computational grid

We also give all k-cells an orientation as shown in the figure on the right

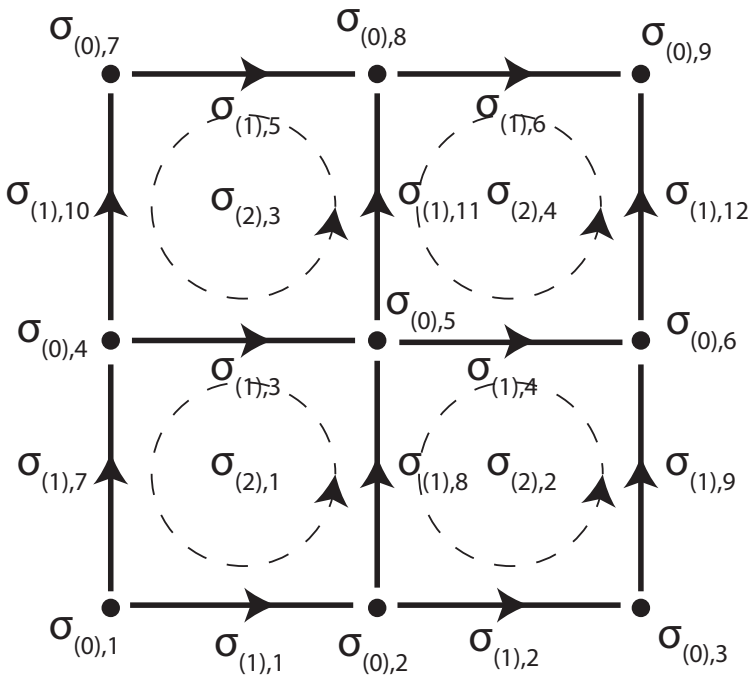
We also need to orient points. A point has 2 orientations, either you move towards a point (sink) or you move away from a point (source). We choose sinks as default orientation.



The computational grid

Now we are in a position to define the boundary operator. The boundary of the points is the empty set, so

$$\partial \sigma_{(0),i} = 0 \quad \forall i$$

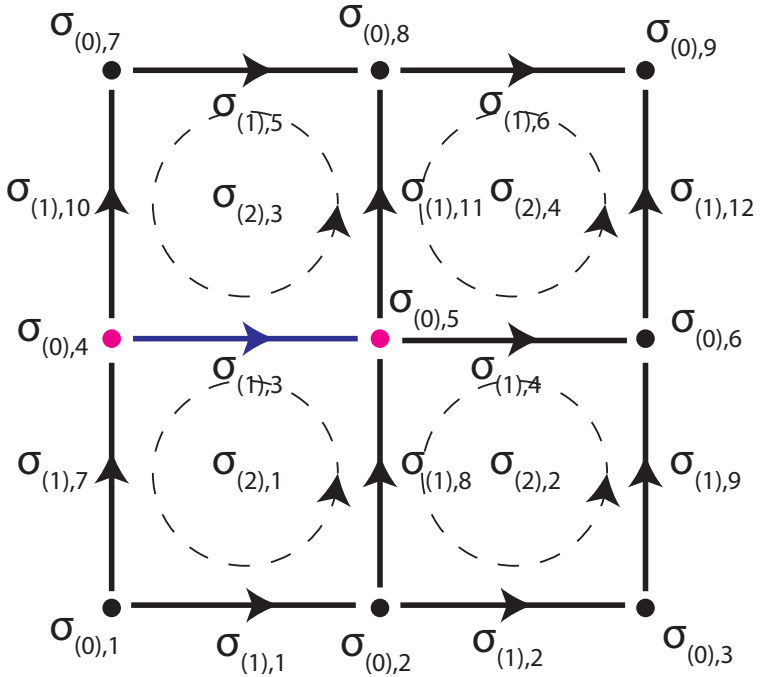


The computational grid

The boundary of a line segment consists of the 2 end points

$$\partial\sigma_{(1),3} = +\sigma_{(0),5} - \sigma_{(0),4}$$

Note that since line segment $\sigma_{(1),3}$ points towards $\sigma_{(0),5}$ (sink) it has a plus sign. The line segment emanates from the point $\sigma_{(0),4}$ (source) and therefore has a minus sign.



The incidence matrix

$$\partial\sigma_{(1),3} = +\sigma_{(0),5} - \sigma_{(0),4}$$

$$\partial\sigma_{(1),3} = \begin{pmatrix} \sigma_{(0),1} & \sigma_{(0),2} & \sigma_{(0),3} & \sigma_{(0),4} & \sigma_{(0),5} & \sigma_{(0),6} & \sigma_{(0),7} & \sigma_{(0),8} & \sigma_{(0),9} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

The incidence matrix

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$$=$$

$$\begin{pmatrix} \sigma_{(0),1} & \sigma_{(0),2} & \sigma_{(0),3} & \sigma_{(0),4} & \sigma_{(0),5} & \sigma_{(0),6} & \sigma_{(0),7} & \sigma_{(0),8} & \sigma_{(0),9} \end{pmatrix} \cdot$$

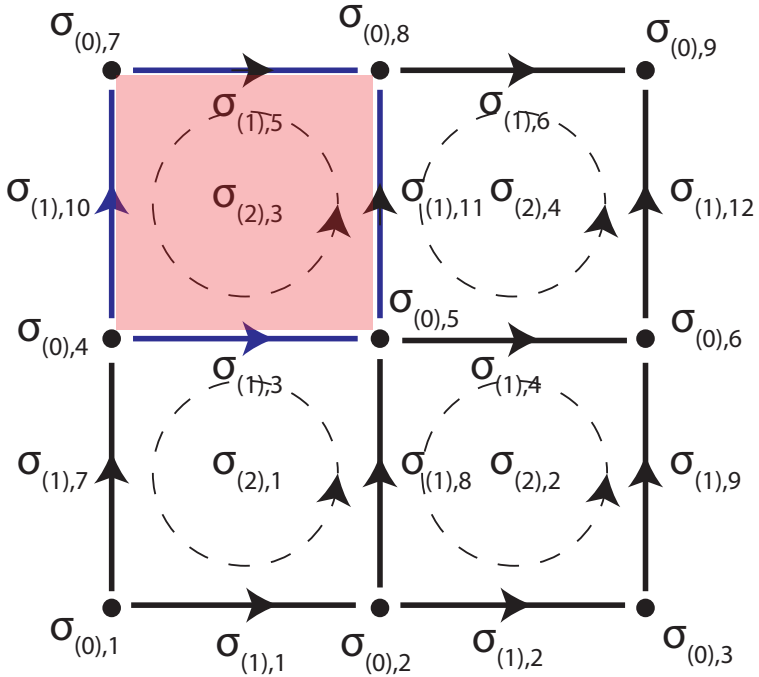
$$\begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

This matrix is called the incidence matrix $\mathbb{E}_{0,1}$. It relates the line segments with its boundary points. $\mathbb{E}_{0,1}$ is a matrix representation of the boundary operator.

The computational grid

The boundary of a surface consists of the 4 line segments, for example

$$\begin{aligned}\partial\sigma_{(2),3} &= +\sigma_{(1),3} + \sigma_{(1),11} \\ &\quad -\sigma_{(1),5} - \sigma_{(1),10}\end{aligned}$$



The incidence matrix

$$\partial\sigma_{(2),3} = +\sigma_{(1),3} + \sigma_{(1),11} - \sigma_{(1),5} - \sigma_{(1),10}$$

$$\partial\sigma_{(2),3} = \begin{pmatrix} \sigma_{(1),1} & \cdots & \cdots & \sigma_{(1),12} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \\ -1 \\ 1 \\ 0 \end{pmatrix}$$

The incidence matrix

$$\partial \begin{pmatrix} \sigma_{(2),1} & \sigma_{(2),2} & \sigma_{(2),3} & \sigma_{(2),4} \end{pmatrix}$$
$$=$$
$$\begin{pmatrix} \sigma_{(1),1} & \cdots & \cdots & \sigma_{(1),12} \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

This matrix is called the incidence matrix $\mathbb{E}_{1,2}$. It relates the surfaces with its boundary line segments. $\mathbb{E}_{1,2}$ is a matrix representation of the boundary operator.

The incidence matrix

Note that

$$\partial\partial\begin{pmatrix} \sigma_{(2),1} & \sigma_{(2),2} & \sigma_{(2),3} & \sigma_{(2),4} \end{pmatrix} =$$

$$\partial\begin{pmatrix} \sigma_{(1),1} & \cdots & \cdots & \sigma_{(1),12} \end{pmatrix}\mathbb{E}_{1,2} =$$

$$\begin{pmatrix} \sigma_{(0),1} & \cdots & \cdots & \sigma_{(0),9} \end{pmatrix}\mathbb{E}_{0,1}\mathbb{E}_{1,2} = 0$$

Since the incidence matrix is just the matrix representation of the boundary operator, $\mathbb{E}_{0,1}\mathbb{E}_{1,2}$ is the matrix representation of $\partial\partial$ and it is a geometric fact that this is always zero as we saw.

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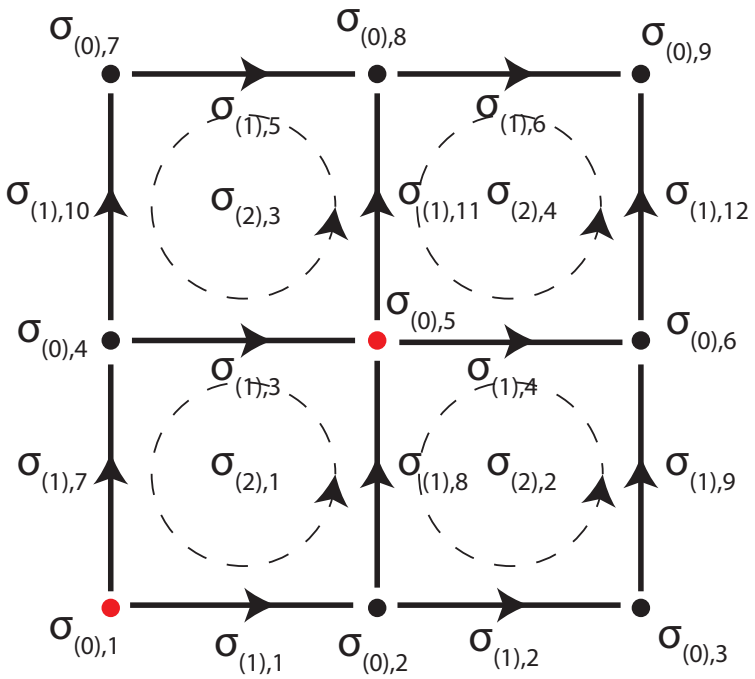
k-chains

A chain is a collection of k-cells with weights. For instance we can have the 0-chain, $\mathbf{c}_{(0)}$

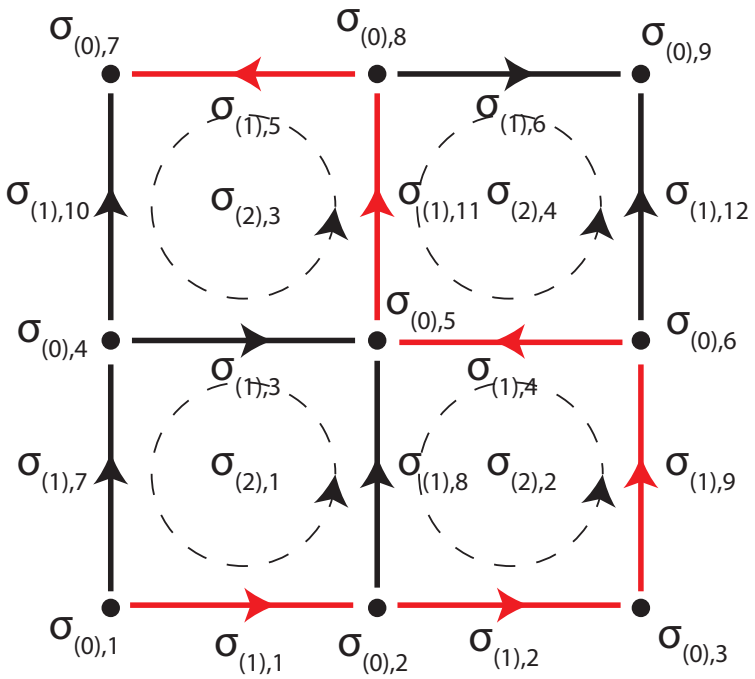
$$\mathbf{c}_{(0)} = -\sigma_{(0),1} + \sigma_{(0),5}$$



k-chains

An example of a 1-chain, $\mathbf{c}_{(1)}$ is given by (see figure on the right)

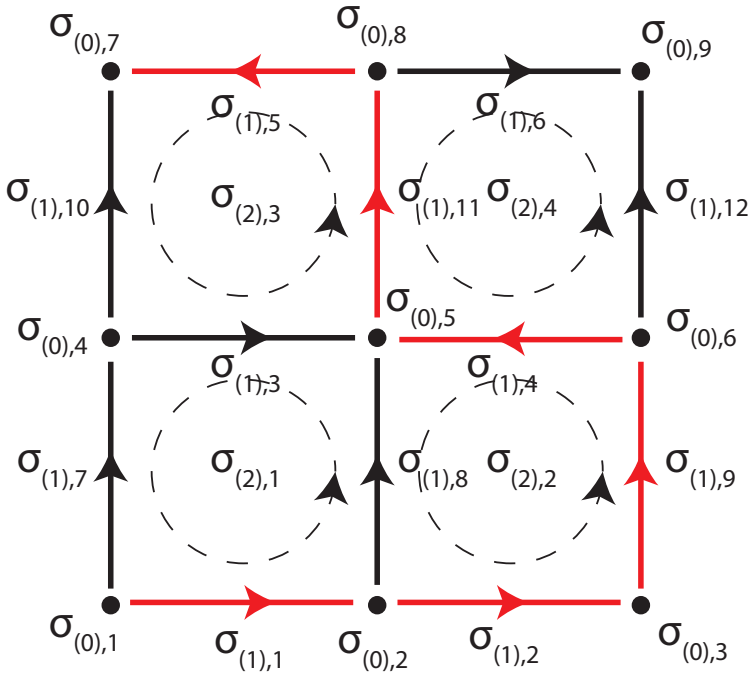
$$\begin{aligned}\mathbf{c}_{(1)} &= \sigma_{(1),1} + \sigma_{(1),2} \\ &\quad + \sigma_{(1),9} - \sigma_{(1),4} \\ &\quad + \sigma_{(1),11} - \sigma_{(1),5}\end{aligned}$$



k-chains

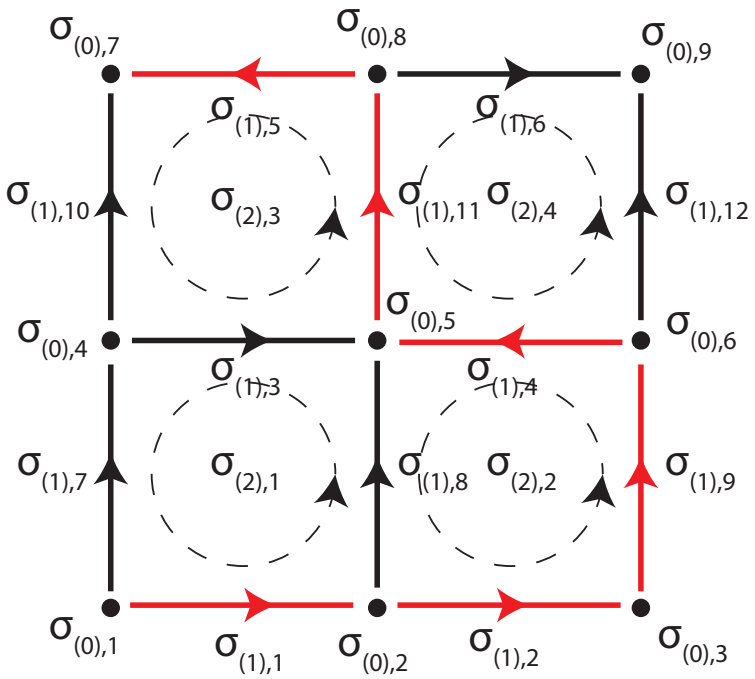
And we can write the 2-chain as a collection of 2-cells. If the coefficient is negative, we change the orientation from counter clock-wise to clockwise.

Usually, we only take the weights 0 (not in the chain), 1 (in the chain with default orientation) and -1 (in the chain with orientation opposite to default orientation)



k-chains

Note that the boundary of a k-cell is in fact a $(k-1)$-chain.



How are we doing sofar?

We set out to have a discrete description of differential forms and the exterior derivative

- We have a discrete representation of space: cell-complex, k-chains
- We have a discrete representation of the boundary operator: Incidence matrices

If we can develop discrete differential forms and define discrete integration, we can use the generalized Stokes Theorem to define the discrete exterior derivative.

k-cochains I

The dual space of k-chains, $C_k(D)$, is the space of k-cochains, $C^k(D)$, defined as the set of homomorphisms

$$\mathbf{c}^{(k)} \; : \; C_k(D) \to \mathbb{R}$$

So a k-cochains assigns a real number to a k-chain

$$\left\langle \mathbf{c}^{(k)}, \mathbf{c}_{(k)} \right\rangle := \mathbf{c}^{(k)}(\mathbf{c}_{(k)})$$

Since it is a homomorphism, the action of $\mathbf{c}^{(k)}$ is completely determined by its action on the k-cells.

k-cochains II

Introduce the elementary k-cochains $\sigma^{(k),i}$ which have the property that

$$\left\langle \sigma^{(k),i}, \sigma_{(k),j} \right\rangle = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{elsewhere} \end{cases}$$

This cochain assigns the number 1 to k-cell i and the number 0 to all other k-cells.

Any k-cochain can then be written as

$$\mathbf{c}^{(k)} = \sum_{i=1}^{\#k} \alpha_i \sigma^{(k),i}$$

k-cochains III

If we apply the k-cochain

$$\mathbf{c}^{(k)} = \sum_{i=1}^{\#k} \alpha_i \sigma^{(k),i}$$

to a k-cell $\sigma_{(k),j}$, we obtain

$$\begin{aligned} \left\langle \mathbf{c}^{(k)}, \sigma_{(k),j} \right\rangle &= \left\langle \sum_{i=1}^{\#k} \alpha_i \sigma^{(k),i}, \sigma_{(k),j} \right\rangle \\ &= \sum_{i=1}^{\#k} \alpha_i \left\langle \sigma^{(k),i}, \sigma_{(k),j} \right\rangle \\ &= \alpha_j \end{aligned}$$

so the k-cochain assigns the value α_j to k-cell $\sigma^{(k),i}$.

k-cochains IV

Note that we wrote the k-chain as a row vector of k-cells multiplied by a column vector of coefficients

$$\mathbf{c}_{(k)} = \begin{pmatrix} \sigma_{(k),1} & \dots & \sigma_{(k)_{\#k}} \end{pmatrix} \begin{pmatrix} w^1 \\ \vdots \\ w^{\#k} \end{pmatrix}$$

We will write the k-cochain as a row vector of coefficients multiplied by a column vector of basis cochains

$$\mathbf{c}^{(k)} = \begin{pmatrix} \alpha_1 & \dots & \alpha_{\#k} \end{pmatrix} \begin{pmatrix} \sigma^{(k),1} \\ \vdots \\ \sigma^{(k)_{\#k}} \end{pmatrix}$$

k-cochains IV

Then duality pairing between k-cochain and k-chain gives

$$\left\langle \mathbf{c}^{(k)}, \mathbf{c}_{(k)} \right\rangle = \alpha_i w^i$$

Discrete differential forms and integration

Now we have the two missing ingredients in our discrete model:

- Discrete k-forms $\rightarrow$ k-cochains
- Integration of k-forms $\rightarrow$ Duality pairing of cochains with chain.

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Coboundary operator I

Let $\mathbf{c}^{(k)}$ be a k-cochain and let $\mathbf{c}_{(k+1)}$ be an arbitrary $(k+1)$-chain. Then $\partial\mathbf{c}_{(k+1)}$ is a k-chain. So it makes sense to evaluate

$$\left\langle \mathbf{c}^{(k)}, \partial\mathbf{c}_{(k+1)} \right\rangle$$

Then there exists a unique $(k+1)$-cochain $\mathbf{b}^{(k+1)}$ such that

$$\left\langle \mathbf{b}^{(k+1)}, \mathbf{c}_{(k+1)} \right\rangle = \left\langle \mathbf{c}^{(k)}, \partial\mathbf{c}_{(k+1)} \right\rangle \quad \forall \mathbf{c}_{(k+1)}$$

We will call $\mathbf{b}^{(k+1)}$ the coboundary of $\mathbf{c}^{(k)}$

$$\mathbf{b}^{(k+1)} = \delta\mathbf{c}^{(k)}$$

Coboundary operator II

So with the coboundary operator

$$\mathbf{b}^{(k+1)} = \delta \mathbf{c}^{(k)}$$

we have

$$\left\langle \delta \mathbf{c}^{(k)}, \mathbf{c}_{(k+1)} \right\rangle = \left\langle \mathbf{c}^{(k)}, \partial \mathbf{c}_{(k+1)} \right\rangle \quad \forall \mathbf{c}_{(k+1)}$$

Compare this with

$$\left\langle \mathrm{d}\boldsymbol{\alpha}^{(k)}, \Omega_{k+1} \right\rangle = \left\langle \boldsymbol{\alpha}^{(k)}, \partial \Omega_{k+1} \right\rangle$$

The coboundary is the discrete exterior derivative!

Coboundary operator II

So with the coboundary operator

$$\mathbf{b}^{(k+1)} = \delta \mathbf{c}^{(k)}$$

we have

$$\left\langle \delta \mathbf{c}^{(k)}, \mathbf{c}_{(k+1)} \right\rangle = \left\langle \mathbf{c}^{(k)}, \partial \mathbf{c}_{(k+1)} \right\rangle \quad \forall \mathbf{c}_{(k+1)}$$

Compare this with

$$\left\langle \mathrm{d}\boldsymbol{\alpha}^{(k)}, \Omega_{k+1} \right\rangle = \left\langle \boldsymbol{\alpha}^{(k)}, \partial \Omega_{k+1} \right\rangle$$

The coboundary is the discrete exterior derivative!

Coboundary operator III

The exterior derivative maps k-forms into $(k+1)$-forms, the coboundary operator maps k-cochains to $(k+1)$-cochains.

Applying the exterior derivative twice always yields zero (vector identities), application of the coboundary operator twice also gives zero (discrete vector identities)

Coboundary operator III

The exterior derivative maps k-forms into $(k+1)$-forms, the coboundary operator maps k-cochains to $(k+1)$-cochains.

Applying the exterior derivative twice always yields zero (vector identities), application of the coboundary operator twice also gives zero (discrete vector identities)

Coboundary operator IV

Since we have a matrix representation for the boundary operator – the incidence matrix – we also have a matrix representation for the coboundary operator.

If the k-cochain is represented by

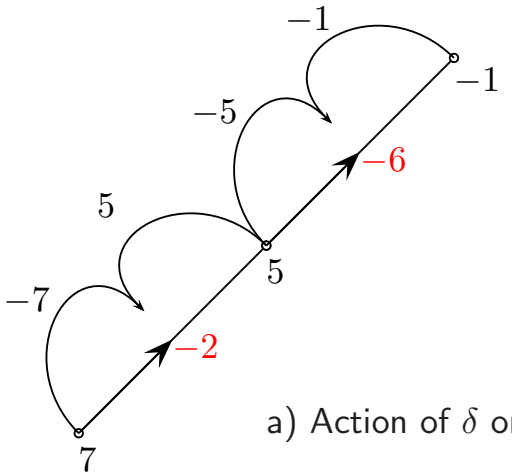
$$\mathbf{c}^{(k)} = \begin{pmatrix} \alpha_1 & \dots & \alpha_{\#k} \end{pmatrix} \begin{pmatrix} \sigma^{(k),1} \\ \vdots \\ \sigma^{(k)}{}_{\#k} \end{pmatrix}$$

then the coboundary of $\mathbf{c}^{(k)}$ is represented by

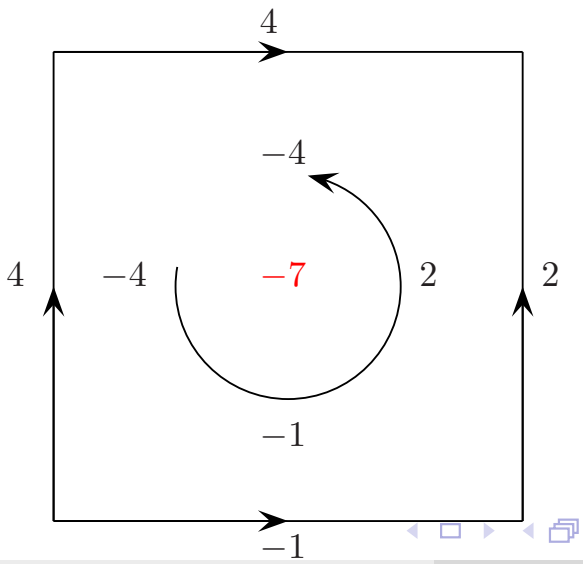
$$\delta\mathbf{c}^{(k)} = \underbrace{\begin{pmatrix} \alpha_1 & \dots & \alpha_{\#k} \end{pmatrix}\mathbb{E}_{k,k+1}}_{\text{newcoeff.}} \begin{pmatrix} \sigma^{(k+1),1} \\ \vdots \\ \sigma^{(k+1)}{}_{\#(k+1)} \end{pmatrix}$$

Coboundary operator V

The action of the coboundary operator in pictures

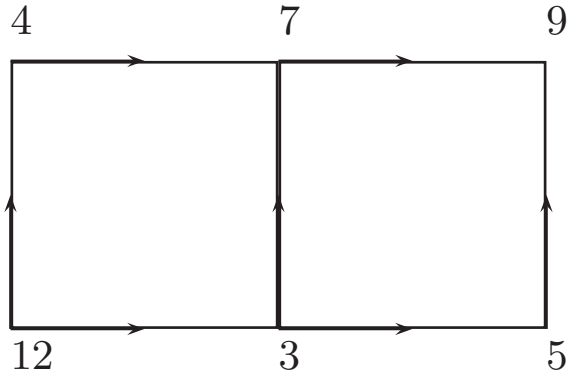


a) Action of δ on 0-chain



Coboundary operator V

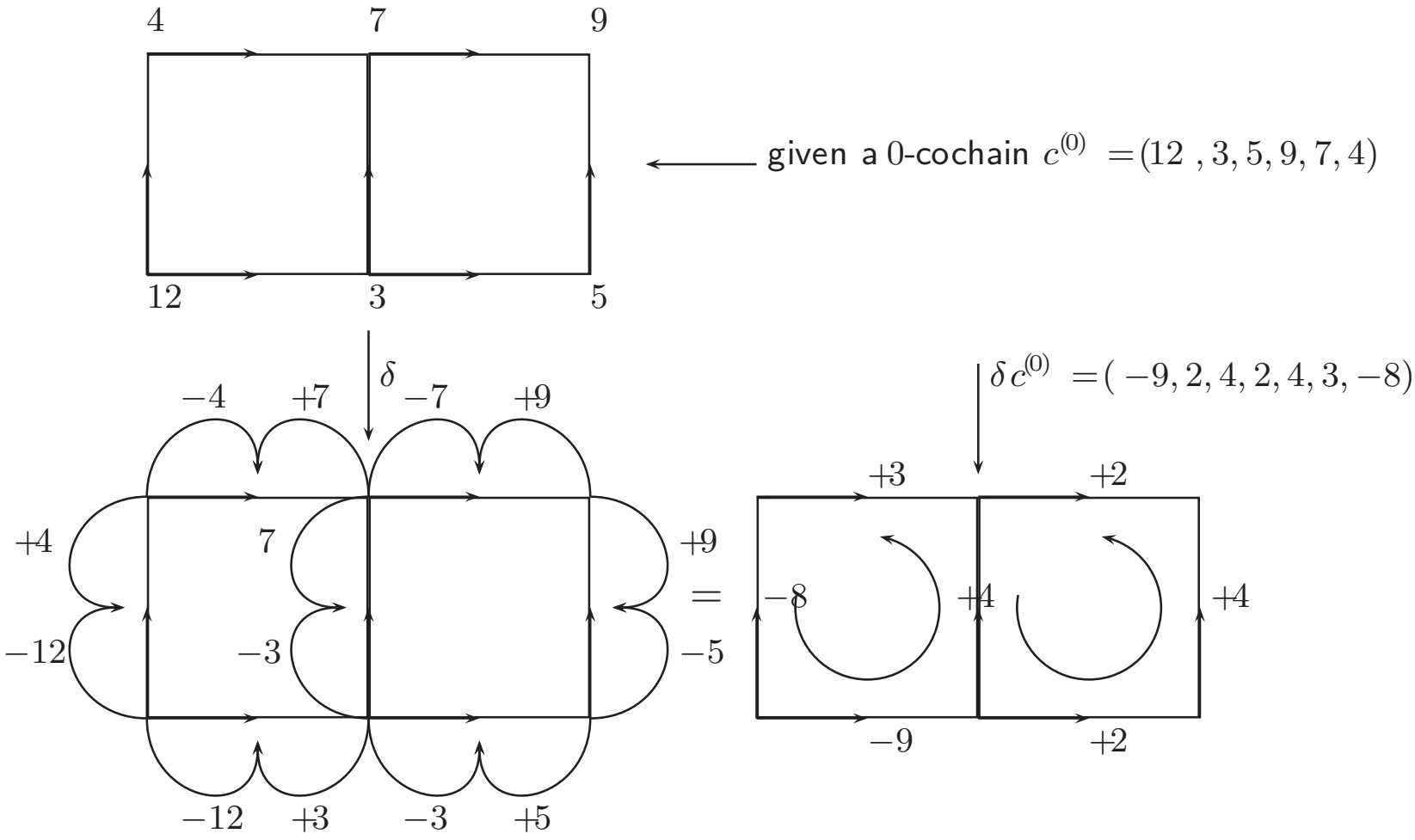
Example illustrating the property $\delta\,\delta\,c^{(0)} = 0^{(2)}$



given a 0-cochain $c^{(0)} = (12\ , 3, 5, 9, 7, 4)$

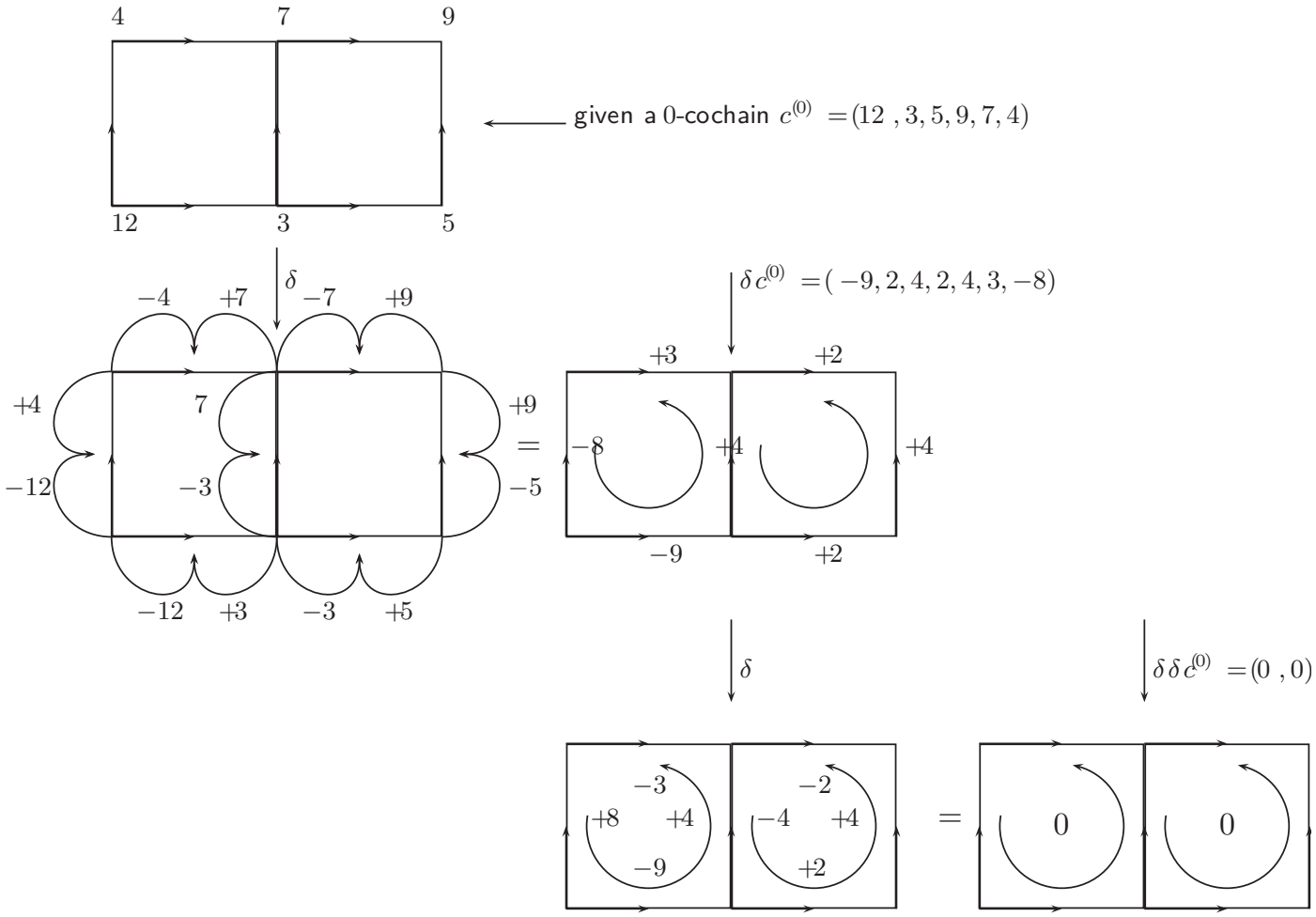
Coboundary operator V

Example illustrating the property $\delta\,\delta\,c^{(0)} = 0^{(2)}$



Coboundary operator V

Example illustrating the property $\delta\,\delta\,c^{(0)} = 0^{(2)}$



Useful??

We saw that the action of the exterior derivative d resembles the grad, curl and div in differential geometry.

The action of the coboundary operator δ represents the grad, curl and div in a discrete setting. In a sense this is an exact representation (see tomorrow).

The incidence matrices $\mathbb{E}_{k,k+1}$ explicitly show up in finite volume, finite element and spectral element methods.

Remember that $\mathbb{E}_{k,k+1}$ was obtained from the topology of the mesh. See Maxwell!

The next step

We have now differential geometry at the continuous level and algebraic topology at the discrete level.

Both description are very similar, but not the same

Tomorrow we will look how to convert operations at the continuous level to the discrete level and from the discrete level to the continuous level.