Overview of path homology theory of digraphs II

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1 Spaces of ∂ -invariant paths

1.1 Paths and the boundary operator

Let us fix a finite set V and a field K. For any $p \ge 0$, an *elementary* p-path is any sequence $i_0, ..., i_p$ of p + 1 vertices of V; it will be denoted by $e_{i_0...i_p}$.

A *p*-path is any formal linear combinations of of elementary *p*-paths with coefficients in \mathbb{K} ; that is, any *p*-path *u* has a form

$$u = \sum_{i_0, i_1, \dots, i_p \in V} u^{i_0 i_1 \dots i_p} e_{i_0 i_1 \dots i_p},$$

where $u^{i_0i_1\dots i_p} \in \mathbb{K}$. The set of all *p*-paths is a \mathbb{K} -linear space denoted by $\Lambda_p = \Lambda_p(V, \mathbb{K})$. For example, $\Lambda_0 = \langle e_i : i \in V \rangle$, $\Lambda_1 = \langle e_{ij} : i, j \in V \rangle$, $\Lambda_2 = \langle e_{ijk} : i, j, k \in V \rangle$.

Definition. Define for any $p \ge 1$ a linear boundary operator $\partial : \Lambda_p \to \Lambda_{p-1}$ by

$$\partial e_{i_0...i_p} = \sum_{q=0}^{p} (-1)^q e_{i_0...\hat{i_q}...i_p}, \qquad (1.1)$$

where $\widehat{}$ means omission of the index. For p = 0 set $\partial e_i = 0$ (and, hence, $\Lambda_{-1} = \{0\}$).

For example,

$$\partial e_{ij} = e_j - e_i$$
 and $\partial e_{ijk} = e_{jk} - e_{ik} + e_{ij}$.

It is easy to show that $\partial^2 = 0$. Hence, we obtain a chain complex $\Lambda_*(V)$:

$$0 \leftarrow \Lambda_0 \stackrel{\partial}{\leftarrow} \Lambda_1 \stackrel{\partial}{\leftarrow} \dots \stackrel{\partial}{\leftarrow} \Lambda_{p-1} \stackrel{\partial}{\leftarrow} \Lambda_p \stackrel{\partial}{\leftarrow} \dots$$

An elementary *p*-path $e_{i_0...i_p}$ is called *regular* if $i_k \neq i_{k+1}$ for all k = 0, ..., p-1, and *irregular* otherwise. A *p*-path is called regular (resp. irregular) if it is a linear combination of regular (resp. irregular) elementary paths.

It is easy to show that if u is irregular then ∂u is also irregular. Denote by \mathcal{R}_p the space of all regular p-paths. Then ∂ is well defined on the spaces \mathcal{R}_p if we identify all irregular paths with 0. For example, if $i \neq j$ then $e_{iji} \in \mathcal{R}_2$ and

$$\partial e_{iji} = e_{ji} - e_{ii} + e_{ij} = e_{ji} + e_{ij} \in \mathcal{R}_1,$$

because $e_{ii} = 0$. Hence, we obtain a chain complex

$$0 \leftarrow \mathcal{R}_0 \stackrel{\partial}{\leftarrow} \mathcal{R}_1 \stackrel{\partial}{\leftarrow} \dots \stackrel{\partial}{\leftarrow} \mathcal{R}_{p-1} \stackrel{\partial}{\leftarrow} \mathcal{R}_p \stackrel{\partial}{\leftarrow} \dots$$

1.2 Chain complex on digraphs

A digraph (directed graph) is a pair G = (V, E) of a set V of vertices and $E \subset \{V \times V \setminus \text{diag}\}$ is a set of arrows (directed edges). If $(i, j) \in E$ then we write $i \to j$.

Definition. Let G = (V, E) be a digraph. An elementary *p*-path $e_{i_0...i_p}$ on *V* is called allowed if $i_k \rightarrow i_{k+1}$ for any k = 0, ..., p-1, and non-allowed otherwise. A *p*-path is called allowed if it is a linear combination of allowed elementary *p*-paths.

Let $\mathcal{A}_p = \mathcal{A}_p(G, \mathbb{K})$ be the space of all allowed *p*-paths. Since any allowed path is regular, we have $\mathcal{A}_p \subset \mathcal{R}_p$.

We would like to build a chain complex based on spaces \mathcal{A}_p . However, in general ∂ does not act on the spaces \mathcal{A}_p . For example, in the digraph $\overset{a}{\bullet} \to \overset{b}{\bullet} \to \overset{c}{\bullet}$ we have $e_{abc} \in \mathcal{A}_2$ but $\partial e_{abc} = e_{bc} - e_{ac} + e_{ab} \notin \mathcal{A}_1$ because e_{ac} is not allowed.

Consider the following subspace of \mathcal{A}_p :

$$\Omega_p \equiv \Omega_p \left(G, \mathbb{K} \right) := \left\{ u \in \mathcal{A}_p : \partial u \in \mathcal{A}_{p-1} \right\}.$$

We claim that $\partial \Omega_p \subset \Omega_{p-1}$. Indeed, $u \in \Omega_p$ implies $\partial u \in \mathcal{A}_{p-1}$ and $\partial (\partial u) = 0 \in \mathcal{A}_{p-2}$, whence $\partial u \in \Omega_{p-1}$.

Definition. The elements of Ω_p are called ∂ -invariant p-paths.

Hence, we obtain a chain complex $\Omega_* = \Omega_* (G, \mathbb{K})$:

$$0 \leftarrow \Omega_0 \stackrel{\partial}{\leftarrow} \Omega_1 \stackrel{\partial}{\leftarrow} \dots \stackrel{\partial}{\leftarrow} \Omega_{p-1} \stackrel{\partial}{\leftarrow} \Omega_p \stackrel{\partial}{\leftarrow} \dots$$
(1.2)

that reflects the digraph structure of G. Homology groups of the chain complex (1.2) are called *path homologies* of G and are denoted by $H_p(G)$. By construction we have

$$\Omega_0 = \mathcal{A}_0 = \langle e_i : i \in V \rangle \text{ and } \Omega_1 = \mathcal{A}_1 = \{ e_{ij} : i \to j \}$$

while in general $\Omega_p \subset \mathcal{A}_p$.

1.3 Examples of ∂ -invariant paths

A triangle is a sequence of three distinct vertices a, b, csuch that $a \to b \to c, a \to c$. It determines a 2-path $e_{abc} \in \Omega_2$ because $e_{abc} \in \mathcal{A}_2$ and $\partial e_{abc} = e_{bc} - e_{ac} + e_{ab} \in \mathcal{A}_1$.

The path e_{abc} is also referred to as a triangle.



and among them the following m squares are linearly independent: 7

$$u_{0j} = e_{ab_0c} - e_{ab_jc}, \quad j = 1, ..., m.$$

$$u_{ij} = e_{ab_ic} - e_{ab_jc} \in \Omega_2 \quad \text{for all } i, j = 0, ..., m,$$

Clearly, a square is an 1-square. Any *m*-square with $m \ge 2$ is also called a *multisquare*. The *m*-square determines ∂ -invariant 2-paths (squares) as follows:

An *m*-square is a sequence of
$$m + 3$$

that $a \to b \to c$, $a \to b' \to c$ while $a \not\to c$.

and $\partial u = (e_{bc} - e_{ac} + e_{ab}) - (e_{b'c} - e_{ac} + e_{ab'})$ $= e_{ab} + e_{bc} - e_{ab'} - e_{b'c} \in \mathcal{A}_1.$

The path u is also referred to as a square.

A square is a sequence of four distinct vertices a, b, b', c such

It determines a 2-path $u = e_{abc} - e_{ab'c} \in \Omega_2$ because $u \in \mathcal{A}_2$

$$a, b_0, b_1, \dots, b_m, c$$

such that
$$a \to b_k \to c \quad \forall k = 0, \dots, m$$
,
while $a \not\to c$.

$$b_0$$
 \cdots b_i \cdots b_j \cdots b_m



A 3-*cube* is a sequence of 8 vertices 0, 1, 2, 3, 4, 5, 6, 7, connected by arrows as shown here:

A 3-cube determines a ∂ -invariant 3-path

$$u = e_{0237} - e_{0137} + e_{0157} - e_{0457} + e_{0467} - e_{0267} \in \Omega_3,$$

also called a 3-cube. Indeed, we have $u \in \mathcal{A}_3$ and
 $\partial u = (e_{013} - e_{023}) + (e_{157} - e_{137}) + (e_{237} - e_{267})$
 $- (e_{046} - e_{026}) - (e_{457} - e_{467}) - (e_{015} - e_{045}) \in \mathcal{A}_2$

A trapezohedron of order $m \ge 2$ is a configuration of 2m + 2 vertices: $a, b, i_0, \ldots, i_{m-1}, j_0, \ldots, j_{m-1}$ with 4m arrows: $a \to i_k, j_k \to b, i_k \to j_k, i_k \to j_{k+1},$ $\forall k = 0, \ldots, m-1$, where k + 1 is understood mod m.

It determines the following ∂ -invariant 3-path:





that is called a *trapezohedral* path. Clearly, τ_m is allowed. Let us verify that $\partial \tau_m \in \mathcal{A}_2$. Indeed, we have

$$\partial \tau_m = \sum_{k=0}^{m-1} \partial \left(e_{ai_k j_k b} - e_{ai_k j_{k+1} b} \right)$$

=
$$\sum_{k=0}^{m-1} \left(e_{i_k j_k b} - e_{i_k j_{k+1} b} \right) - \sum_{k=0}^{m-1} \left(e_{ai_k j_k} - e_{ai_k j_{k+1}} \right)$$

-
$$\sum_{k=0}^{m-1} \left(e_{aj_k b} - e_{aj_{k+1} b} \right) + \sum_{k=0}^{m-1} \left(e_{ai_k b} - e_{ai_k b} \right) \in \mathcal{A}_2, \qquad (1.5)$$

because the both sums in (1.4) are allowed, while the both sums in (1.5) vanish.

For example, a trapezohedron of order m = 2 is shown here:

In this case we have

$$\tau_2 = e_{ai_0j_0b} - e_{ai_0j_1b} + e_{ai_1j_1b} - e_{ai_1j_0b}.$$



Trapezohedra of order $m \geq 3$ can be realized as convex polyhedra in \mathbb{R}^3 . For example, trapezohedron of order m = 3 coincides with a 3-cube:

In this case we have

$$\tau_3 = e_{ai_0j_0b} - e_{ai_0j_1b} + e_{ai_1j_1b} - e_{ai_1j_2b} + e_{ai_2j_2b} - e_{ai_2j_0b},$$

and τ_3 coincides (up to a sign) with the aforementioned ∂ -invariant 3-path determined by a 3-cube (see p. 8).

Trapezohedron of order m = 4 can be realized in \mathbb{R}^3 as a *tetragonal trapezohedron:* In this case we have

$$\tau_4 = e_{ai_0j_0b} - e_{ai_0j_1b} + e_{ai_1j_1b} - e_{ai_1j_2b} + e_{ai_2j_2b} - e_{ai_2j_3b} + e_{ai_3j_3b} - e_{ai_3j_0b}.$$





Here are some pictures from Wikipedia of trapezohedra as convex polyhedra:



1.4 Digraph morphisms

Let X and Y be two digraphs. For simplicity of notations, we denote the vertices of X and Y by the same letters X resp. Y.

Definition. A mapping $f : X \to Y$ between the sets of vertices of X and Y called a digraph map (or morphism) if

$$a \to b \text{ on } X \implies f(a) \to f(b) \text{ or } f(a) = f(b) \text{ on } Y.$$

In other words, any arrow of X under the mapping f either goes to an arrow of Y or collapses to a vertex of Y.

We say that a digraph Y is a *subgraph* of a digraph X if the sets of vertices and arrows of Y are subset of the sets of vertices and arrows of X, respectively. In this case we have a natural inclusion $i: Y \to X$ that is clearly a digraph morphism.

To give another example of a morphism, let us split the vertex set of a digraph X into a disjoint union of n subsets $A_1, ..., A_n$, and construct a digraph Y of n vertices $a_1, ..., a_n$ that is obtained from X by merging all the vertices from A_i into a single vertex a_i of Y. More precisely, we have an arrow $a_i \to a_j$ in Y if and only if there are $x \in A_i$ and $y \in A_j$ such that $x \to y$ in X.



An example of a merging map μ

We have a natural merging map $\mu : X \to Y$ such that $\mu(x) = a_i$ for any $x \in A_i$. Clearly, a merging map is a digraph morphism that keeps any arrow $x \to y$ if x and y belong to different sets A_i and collapses an arrow $x \to y$ into a vertex if x, y belong to the same A_i .

Any mapping $f: X \to Y$ induces a mapping $f_*: \Lambda_n(X) \to \Lambda_n(Y)$ as follows: first set

$$f_*(e_{i_0...i_n}) = e_{f(i_0)...f(i_n)},$$

and then extend f_{*} by linearity to all of $\Lambda_{n}(X)$.

Proposition 1.1 Let $f : X \to Y$ be a digraph morphism. Then the induced mapping $f_* : \Lambda_n(X) \to \Lambda_n(Y)$ extends to a chain mapping $f_* : \Omega_n(X) \to \Omega_n(Y)$ and, hence, to homomorphism $f_* : H_n(X) \to H_n(Y)$.

1.5 Structure of Ω_2

As we know, $\Omega_0 = \langle e_i \rangle$ consists of all vertices and $\Omega_1 = \langle e_{ij} : i \to j \rangle$ consists of all arrows.

Definition. Let us call a *semi-arrow* any pairs (x, y) of distinct vertices x, y such that $x \not\rightarrow y$ but $x \rightarrow z \rightarrow y$ for some vertex z. We write in this case $x \rightarrow y$

Theorem 1.2

- (a) We have dim $\Omega_2 = \dim \mathcal{A}_2 s$ where s is the number of semi-arrows.
- (b) Space Ω_2 is spanned by all triangles e_{abc} , squares $e_{abc} e_{ab'c}$ and double arrows e_{aba} :



Observe that all the triangles and double edges are linearly independent whereas the squares can be dependent as the example of multisquare shows.

Proof. (a) Recall that

$$\mathcal{A}_2 = \operatorname{span} \left\{ e_{abc} : a \to b \to c \right\}$$

and

$$\Omega_2 = \{ v \in \mathcal{A}_2 : \partial v \in \mathcal{A}_1 \} = \{ v \in \mathcal{A}_2 : \partial v = 0 \operatorname{mod} \mathcal{A}_1 \}.$$

Since $a \to b$ and $b \to c$, we have

$$\partial e_{abc} = e_{bc} - e_{ac} + e_{ab} = -e_{ac} \operatorname{mod} \mathcal{A}_1.$$

If a = c or $a \to c$ then $e_{ac} = 0 \mod \mathcal{A}_1$. Otherwise we have a semi-arrow $a \rightharpoonup c$, and in this case

$$e_{ac} \neq 0 \mod \mathcal{A}_1$$

For any $v \in \mathcal{A}_2$, we have

$$v = \sum_{\{a \to b \to c\}} v^{abc} e_{abc}$$

whence it follows that

$$\partial v = -\sum_{\{a \to b \to c, a \to c\}} v^{abc} e_{ac} \mod \mathcal{A}_1.$$

The condition $\partial v = 0 \mod \mathcal{A}_1$ is equivalent to

$$\sum_{\{a \to b \to c, a \to c\}} v^{abc} e_{ac} = 0 \mod \mathcal{A}_1.$$
(1.6)

Fixing a semi-arrow $a \rightarrow c$ and summing up in all possible b, we obtain that (1.6) is equivalent to

$$\sum_{\{b:a\to b\to c\}} v^{abc} = 0 \quad \text{for any semi-arrow } a \rightharpoonup c.$$
(1.7)

The number of the equations in (1.7) is exactly s, and they all are linearly independent for different semi-arrows. Hence, Ω_2 is obtained from \mathcal{A}_2 by imposing s linearly independent conditions on v^{abc} , which implies dim $\Omega_2 = \dim \mathcal{A}_2 - s$.

(b) Let us prove that any ∂ -invariant 2-path ω is a linear combination of triangles, squares and double arrows. Since ω is allowed, it is a linear combination of some elementary 2paths e_{abc} with $a \to b \to c$, with non-zero coefficients. If a = c then e_{abc} is a double arrow. If $a \to c$ then e_{abc} is a triangle. Subtracting from ω all double arrows and triangles, we can assume that ω has no such terms any more.

Then, for any term e_{abc} in ω , we have $a \neq c$ and $a \not\rightarrow c$, that is, $a \rightarrow c$. Fix such a, c and consider all vertices b with $a \rightarrow b \rightarrow c$ so that we get a multisquare:



Denote by γ_b the coefficient with which e_{abc} enters ω , and set

$$\omega_{ac} = \sum_{b} \gamma_b e_{abc}.$$
 (1.8)

Clearly, we have $\omega = \sum_{a \to c} \omega_{ac}$. Hence, it suffices to verify that each ω_{ac} is a linear combination of squares. We have

$$\partial \omega_{ac} = \sum_{b} \gamma_{b} e_{ab} - \gamma_{b} e_{ac} + \gamma_{b} e_{bc} = -\sum_{b} \gamma_{b} e_{ac} \operatorname{mod} \mathcal{A}_{1}.$$

Since $\partial \omega$ is allowed but e_{ac} is not allowed, the terms $\gamma_b e_{ac}$ should cancel out that is,

$$\sum_{b} \gamma_b = 0. \tag{1.9}$$

Let us fix one of the vertices b_0 such that $a \to b_0 \to c$. It follows from (1.8) and (1.9) that

$$\omega_{ac} = \sum_{b} \gamma_{b} e_{abc} = \sum_{b} \gamma_{b} \left(e_{abc} - e_{ab_{0}c} \right) = \sum_{b \neq b_{0}} \gamma_{b} \left(e_{abc} - e_{ab_{0}c} \right).$$

Hence, ω_{ac} is a linear combination of the squares $e_{abc} - e_{ab_0c}$, which was to be proved.

Observe that a triangle e_{abc} and a double arrow e_{aba} are images of a square $e_{013} - e_{023}$ under some merging maps (cf. Section 1.4) as shown on these pictures:



a merging map from a square onto a triangle

$$e_{013} - e_{023} \mapsto e_{abc} - e_{acc} = e_{abc}$$



a merging map from a square onto a double arrow

$$e_{013} - e_{023} \mapsto e_{aba} - e_{aaa} = e_{aba}$$

Hence, we can rephrase Theorem 1.2 as follows: Ω_2 is spanned by squares and their morphism images. Or: squares are *basic shapes* of Ω_2 .

2 Trapezohedra and structure of Ω_3

2.1 Spaces Ω_p for trapezohedron

For any integer $m \ge 2$, define a trapezohedron T_m of order m as the following digraph:

 T_m consists of 2m + 2 vertices $a, b, i_0, \dots, i_{m-1}, j_0, j_1, \dots, j_{m-1}$ and 4m arrows $a \to i_k, j_k \to b, i_k \to j_k, i_k \to j_{k+1}$ for all $k = 0, \dots, m-1 \mod m$.

A fragment of T_m is shown here:

It is clear that all allowed paths in T_m have the length ≤ 3 , and, hence, $\Omega_p(T_m) = \{0\} \ \forall p > 3.$



Proposition 2.1 For the trapezohedron T_m we have

 $\dim \Omega_2 = 2m, \quad \dim \Omega_3 = 1,$

and $H_p = \{0\}$ for all $p \ge 1$.

Proof. It is easy to detect all the squares in T_m :

$$e_{ai_{k-1}j_k} - e_{ai_kj_k}$$
 and $e_{i_kj_kb} - e_{i_kj_{k+1}b}$, (2.1)

where k = 0, ..., m-1. Hence, T_m contains 2m squares, and they are linearly independent. Since there are neither triangles no double arrows in T_m , we conclude by Theorem 1.2 that dim $\Omega_2 = 2m$.

All allowed 3-paths in T_m are as follows:

$$e_{ai_k j_k b}$$
 and $e_{ai_k j_{k+1} b}$

for all k = 0, ..., m - 1.



Let us find all linear combinations of these paths that are $\partial\text{-invariant}.$ Consider such a linear combination

$$\omega = \sum_{k=0}^{m-1} \left(\alpha_k e_{ai_k j_k b} + \beta_k e_{ai_k j_{k+1} b} \right)$$

with coefficients α_k, β_k . We have

$$\partial \omega = \sum_{k=0}^{m-1} \partial \left(\alpha_k e_{ai_k j_k b} + \beta_k e_{ai_k j_{k+1} b} \right)$$

= $\sum_{k=0}^{m-1} \left(\alpha_k e_{i_k j_k b} + \beta_k e_{i_k j_{k+1} b} \right) - \sum_{k=0}^{m-1} \left(\alpha_k e_{ai_k j_k} + \beta_k e_{ai_k j_{k+1}} \right)$ (2.2)
 $- \sum_{k=0}^{m-1} \left(\alpha_k e_{aj_k b} + \beta_k e_{aj_{k+1} b} \right) + \sum_{k=0}^{m-1} \left(\alpha_k e_{ai_k b} + \beta_k e_{ai_k b} \right).$ (2.3)

The both sums in (2.2) consist of allowed paths. In the rightmost sum in (2.3), the path e_{ai_kb} is not allowed and, hence, must cancel out, which yields

$$\alpha_k = -\beta_k$$

The leftmost sum in (2.3) is then equal to

$$\sum_{k=0}^{m-1} \left(\alpha_k e_{aj_k b} - \alpha_k e_{aj_{k+1} b} \right) = \sum_{k=0}^{m-1} \left(\alpha_k - \alpha_{k-1} \right) e_{aj_k b}$$

and it must vanish as $e_{aj_k b}$ is not allowed, whence

$$\alpha_k = \alpha_{k-1}$$

Setting $\alpha_k \equiv \alpha$ and, hence, $\beta_k \equiv -\alpha$, we obtain that

$$\omega = \alpha \sum_{k=0}^{m-1} \left(e_{ai_k j_k b} - e_{ai_k j_{k+1} b} \right) = \alpha \tau_m \,,$$

where τ_m is a trapezohedral path that was defined by (1.3). It follows that $\Omega_3 = \langle \tau_m \rangle$ and, hence, dim $\Omega_3 = 1$.

It follows from (2.2)-(2.3) that

$$\partial \tau_m = \sum_{k=0}^{m-1} \left(e_{i_k j_k b} - e_{i_k j_{k+1} b} \right) - \sum_{k=0}^{m-1} \left(e_{a i_k j_k} - e_{a i_k j_{k+1}} \right) \neq 0.$$

Hence, ker $\partial|_{\Omega_3} = 0$ whence $H_3 = \{0\}$. Let us show that $H_2 = \{0\}$. Since dim Im $\partial|_{\Omega_3} = 1$, it suffices to show that

$$\dim \ker \partial|_{\Omega_2} = 1. \tag{2.4}$$

Consider the following general element of Ω_2 :

$$u = \sum_{k=0}^{m-1} \alpha_k \left(e_{ai_{k-1}j_k} - e_{ai_kj_k} \right) + \beta_k \left(e_{i_kj_kb} - e_{i_kj_{k+1}b} \right)$$

with arbitrary coefficients α_k, β_k . We have

$$\begin{aligned} \partial u &= \sum_{k=0}^{m-1} \alpha_k \left(e_{ai_{k-1}} + e_{i_{k-1}j_k} - e_{ai_k} - e_{i_k j_k} \right) + \beta_k \left(e_{j_k b} + e_{i_k j_k} - e_{j_{k+1} b} - e_{i_k j_{k+1}} \right) \\ &= \sum_{k=0}^{m-1} \left(\alpha_{k+1} - \alpha_k \right) e_{ai_k} + \sum_{k=0}^{m-1} \left(\beta_k - \beta_{k-1} \right) e_{j_k b} \\ &+ \sum_{k=0}^{m-1} \left(\beta_k - \alpha_k \right) e_{i_k j_k} + \sum_{k=0}^{m-1} \left(\alpha_{k+1} - \beta_k \right) e_{i_k j_{k+1}}. \end{aligned}$$

The condition $\partial u = 0$ is equivalent to

$$\alpha_{k+1} = \alpha_k = \beta_k = \beta_{k-1}$$
 for all $k = 0, ..., m - 1$

which implies (2.4).

Finally, we determine dim H_1 by means of the Euler characteristic

$$\chi = \dim \Omega_0 - \dim \Omega_1 + \dim \Omega_2 - \dim \Omega_3 = (2m+2) - 4m + 2m - 1 = 1.$$

Hence, we obtain

$$\dim H_0 - \dim H_1 + \dim H_2 - \dim H_3 = 1,$$

which yields dim $H_1 = 0$.

2.2 A cluster basis in Ω_p

We start with the following definition.

Definition. A *p*-path $v = \sum v^{i_0 \dots i_p} e_{i_0 \dots i_p}$ is called an (a, b)-cluster if all the elementary paths $e_{i_0 \dots i_p}$ with non-zero values of $v^{i_0 \dots i_p}$ have $i_0 = a$ and $i_p = b$. A path v is called a cluster if it is an (a, b)-cluster for some a, b.

Lemma 2.2 Any ∂ -invariant p-path is a sum of ∂ -invariant clusters.

Proof. Let $v \in \Omega_p$. For any points $a, b \in V$, denote by $v_{a,b}$ the sum of all terms $v^{i_0 \dots i_p} e_{i_0 \dots i_p}$ with $i_0 = a$ and $i_p = b$.

Then $v_{a,b}$ is a cluster and $v = \sum_{a,b \in V} v_{a,b}$, that is, v is a sum of clusters. Let us prove that each non-zero cluster $v_{a,b}$ is ∂ -invariant.



Since v is allowed, also all non-zero terms $v^{i_0...i_p}e_{i_0...i_p}$ are allowed, whence $v_{a,b}$ is also allowed. Let us prove that $\partial v_{a,b}$ is allowed, which will yield the ∂ -invariance of $v_{a,b}$. The

path $v_{a,b}$ is a linear combination of allowed paths of the form $e_{ai_1...i_{p-1}b}$. We have

$$\partial e_{ai_1\dots i_{p-1}b} = e_{i_1\dots i_{p-1}b} + (-1)^p e_{ai_1\dots i_{p-1}} + \sum_{k=1}^{p-1} (-1)^k e_{ai_1\dots i_k\dots i_{p-1}b}.$$

The terms $e_{i_1...i_{p-1}b}$ and $e_{ai_1...i_{p-1}}$ are clearly allowed, while among the terms $e_{ai_1...i_k...i_{p-1}b}$ there may be non-allowed. In the full expansion of

$$\partial v = \sum_{a,b \in V} \partial v_{a,b}$$

all non-allowed terms must cancel out. Since all the terms $e_{ai_1..\hat{i}_k...i_{p-1}b}$ form a (a, b)-cluster, they cannot cancel with terms containing different values of a or b. Therefore, they have to cancel already within $\partial v_{a,b}$, which implies that $\partial v_{a,b}$ is allowed.

Definition. For any *p*-path $v = \sum v^{i_0 \dots i_p} e_{i_0 \dots i_p}$ define its *width* ||v|| as the number of non-zero coefficients $v^{i_0 \dots i_p}$.

Definition. A ∂ -invariant path ω is called *minimal* if ω cannot be represented as a sum of other ∂ -invariant paths with smaller widths.

Example. A square $\omega = e_{abc} - e_{ab'c}$ has width 2 and is minimal because e_{abc} and $e_{ab'c}$ having width 1 are not ∂ -invariant.

Let $a, \{b_0, b_1, b_2\}, c$ be a 2-square. The following path

$$\omega = e_{ab_1c} + e_{ab_2c} - 2e_{ab_0c}$$

is then ∂ -invariant, has width 3 but is not minimal because it can be represented as a sum of two squares:

$$\omega = (e_{ab_1c} - e_{ab_0c}) + (e_{ab_2c} - e_{ab_0c}),$$

where each square has width 2.

Lemma 2.3 Every ∂ -invariant cluster is a sum of minimal ∂ -invariant clusters.

Proof. Let ω be a ∂ -invariant cluster that is not minimal. Then we have

$$\omega = \sum_{k=1}^{n} \omega^{(k)}, \qquad (2.5)$$

where each $\omega^{(k)}$ is a ∂ -invariant path with $\|\omega^{(k)}\| < \|\omega\|$. By Lemma 2.2, each $\omega^{(k)}$ is a sum of clusters $\omega_{a,b}^{(k)}$, and it is clear from the definition of $\omega_{a,b}^{(k)}$ that

$$\|\omega_{a,b}^{(k)}\| \le \|\omega^{(k)}\|$$

Hence, we can replace in (2.5) each $\omega^{(k)}$ by $\sum_{a,b} \omega^{(k)}_{a,b}$ and, hence, assume without loss of generality that all terms $\omega^{(k)}$ in (2.5) are ∂ -invariant clusters.

If some $\omega^{(k)}$ in this sum is not minimal then we replace it further with sum of ∂ -invariant clusters with smaller widths. Continuing this procedure we obtain in the end a representation ω as a sum of minimal ∂ -invariant clusters.

Proposition 2.4 The space Ω_p has a basis that consists of minimal ∂ -invariant clusters.

Proof. Indeed, let \mathcal{M} denote the set of all minimal ∂ -invariant clusters in Ω_p . By Lemmas 2.2, 2.3, every element of Ω_p is a sum of some elements of \mathcal{M} . Choosing in \mathcal{M} a maximal linearly independent subset, we obtain a basis in Ω_p .

2.3 Structure of Ω_3

We use here the trapezohedra T_m and associated trapezohedral paths τ_m that are ∂ -invariant 3-paths for all $m \geq 2$ (see (1.3) and Section 2.1). We prove here that, under an additional mild hypothesis, $\Omega_3(G)$ has a basis that consists of trapezohedral paths and their morphism images.

We start with some examples of morphism images of τ_m .

Example. Here is a merging map from T_2 onto a 3-snake:



The trapezohedral path τ_2 is given by

$$\tau_2 = e_{0123} - e_{0153} + e_{0453} - e_{0423},$$

and its merging image is the 3-path

$$v = e_{0123} - e_{0133} + e_{0233} - e_{0223} = e_{0123},$$

that is, the ∂ -invariant 3-path e_{0123} associated with a 3-snake.

Example. Here is a merging morphism of T_3 (=a 3-cube) onto a pyramid:



The cubical 3-path is given by

$$\tau_3 = e_{0237} - e_{0137} + e_{0157} - e_{0457} + e_{0467} - e_{0267}$$

and its merging image of τ_3 is the following ∂ -invariant 3-path in a pyramid:

$$v = e_{0234} - e_{0134} + e_{0144} - e_{0444} + e_{0444} - e_{0244}$$
$$= e_{0234} - e_{0134}.$$

Example. Consider another merging morphism of T_3 onto a prism:



The merging image of the cubical 3-path

$$\tau_3 = e_{0237} - e_{0137} + e_{0157} - e_{0457} + e_{0467} - e_{0267}$$

is the following ∂ -invariant 3-path of the prism:

$$u = e_{0233} - e_{0133} + e_{0153} - e_{0453} + e_{0423} - e_{0223}$$
$$= e_{0153} - e_{0453} + e_{0423}.$$

Example. Here is a merging morphism $\mu: T_4 \to G$ where the digraph G is a broken cube:



The path τ_4 in the present notation is given by

$$\tau_4 = e_{0159} - e_{0169} + e_{0269} - e_{0279} + e_{0379} - e_{0389} + e_{0489} - e_{0459},$$

and the merging image of τ_4 is the following ∂ -invariant 3-path on the broken cube:

$$w = e_{0158} - e_{0168} + e_{0268} - e_{0278} + e_{0378} - e_{0388} + e_{0488} - e_{0458}$$
$$= e_{0158} - e_{0168} + e_{0268} - e_{0278} + e_{0378} - e_{0458}.$$

The next theorem describes the structure of $\Omega_3(G)$ for a digraph G under the following hypothesis:

G contains neither multisquares (see p.7) nor double arrows. (N)

Under the hypothesis (N), $\Omega_2(G)$ has a basis that consists of triangles and squares. The condition (N) implies that if $a \to b \to c$ and $a \not\to c$ then there is at most one $b' \neq b$ such that $a \to b' \to c$.

Theorem 2.5 Under the hypothesis (N), there is a basis in $\Omega_3(G)$ that consists of trapezohedral paths τ_m with $m \geq 2$ and their merging images.

In other words, trapezohedra are *basic shapes* for Ω_3 .

Proof. By Proposition 2.4, Ω_3 has a basis that consists of minimal ∂ -invariant clusters.

Let a 3-path ω be a minimal ∂ -invariant (a, b)-cluster. It suffices to prove that ω is a merging image of one of the trapezohedral paths τ_m up to a constant factor.

Denote by Q the set of all elementary terms e_{aijb} of ω .



Clearly, the number |Q| of elements in Q is equal to $||\omega||$. We claim that, for any $e_{aijb} \in Q$, either $a \to j$ or $a \nearrow j$

where the notation $a \nearrow j$ means that a and j form a diagonal of a square.

Indeed, if $a \not\rightarrow j$ then the term e_{ajb} appearing in ∂e_{aijb} is non-allowed and must be cancelled out in $\partial \omega$ by the boundary of another elementary 3-path from Q that can only be of the form $e_{ai'jb}$ with

$$a \to i' \to j.$$

Hence, a and j form diagonal of a square a, i, i', j.



By hypothesis (N), the vertex i' with these properties is unique. Hence, in this case we have

$$\omega = ce_{aijb} - ce_{ai'jb} + \dots \tag{2.6}$$

for some scalar $c \neq 0$. In the same way, we have

either
$$i \to b$$
 or $i \nearrow b$,

and, for some $e_{aij'b} \in Q$ and $c \neq 0$,

$$\omega = c e_{aijb} - c e_{aij'b} + \dots . \tag{2.7}$$

If, for some path $e_{aijb} \in Q$, we have both conditions

 $a \to j \text{ and } i \to b,$

then e_{aijb} is ∂ -invariant and, by the minimality of ω ,

 $\omega = \operatorname{const} e_{aijb}.$

Since e_{aijb} is in this case a 3-snake, the path ω is a merging image of τ_2 (see Example on p. 28).



Next, we can assume that, for any path $e_{aijb} \in Q$, we have $a \not\rightarrow j$ or $i \not\rightarrow b$, that is,

$$a \nearrow j \quad \text{or} \quad i \nearrow b.$$
 (2.8)

Define a graph structure on Q with edges of two types (i) and (ii) as follows: for two

distinct elements e_{aijb} and $e_{ai'j'b}$ of Q set

$$e_{aijb} \stackrel{(i)}{\sim} e_{ai'j'b}$$
 if $a \nearrow j = j'$

and

$$e_{aijb} \stackrel{\text{(ii)}}{\sim} e_{ai'j'b}$$
 if $i' = i \nearrow b$.

Both relations $\stackrel{(i)}{\sim}$ and $\stackrel{(ii)}{\sim}$ are symmetric and, hence, can be considered as edges.



Before continuing the proof, consider some examples of graphs Q.

Example A. Let ω be the trapezohedral path of T_2 , that is,

$$\omega = \tau_2 = e_{0123} - e_{0153} + e_{0453} - e_{0423}.$$

This path is an (a, b)-cluster with a = 0 and b = 3. In this case the graph Q consists of 4 vertices as follows:


Example B. Let ω be the ∂ -invariant 3-path of the broken cube (see Example on p. 31), that is,

 $\omega = e_{0158} - e_{0168} + e_{0268} - e_{0278} + e_{0378} - e_{0458}.$

This path is a (a, b)-cluster with a = 0 and b = 8. The graph Q consists of 6 vertices as follows:



By the hypothesis (N), for any $e_{aijb} \in Q$, there is at most one edge of type (i) and at most one edge of type (ii). In particular, the degree of any vertex of the graph (Q, \sim) is at most 2.

Fix a path $e_{aijb} \in Q$. By (2.8) we have $a \nearrow j$ or $i \nearrow b$.



By the above argument, if $a \nearrow j$ then there exists $e_{ai'jb} \in Q$ such that $e_{aijb} \stackrel{(i)}{\sim} e_{ai'jb}$ and

$$\omega = c e_{aijb} - c e_{ai'jb} + \dots \tag{2.9}$$

(cf. (2.6)). Similarly, if $i \nearrow b$ then there exists $e_{aij'b} \in Q$ such that $e_{aijb} \stackrel{\text{(ii)}}{\sim} e_{aij'b}$ and

$$\omega = ce_{aijb} - ce_{aij'b} + \dots \tag{2.10}$$

(cf. (2.7)). In particular, the degree of any vertex of the graph Q is at least 1. Let us prove that the graph (Q, \sim) is connected. Assume from the contrary that Q is disconnected, then Q is a disjoint union of its connected components $\{Q_k\}_{k=1}^n$ with n > 1. Denote by $\omega^{(k)}$ the sum of all elementary terms of ω lying in Q_k , with the same coefficients as in ω , so that

$$\omega = \sum_{k=1}^{n} \omega^{(k)}.$$
(2.11)

Let us prove that each $\omega^{(k)}$ is ∂ -invariant. Clearly, $\omega^{(k)}$ is allowed, and we need to verify

that $\partial \omega^{(k)}$ is also allowed. Indeed, assume that $\partial \omega^{(k)}$ contains a non-allowed term. Then this term comes from the boundary ∂e_{aijb} of some term e_{aijb} of path $\omega^{(k)}$. The non-allowed term of ∂e_{aijb} is either e_{aib} or e_{ajb} ; let it be e_{aib} , that is, let $i \not\rightarrow b$. Then the term e_{aib} cancels out in



 $\partial \omega$, which can only happen when ω contains another term of the form $e_{aij'b}$. However, then e_{aijb} and $e_{aij'b}$ are connected by an edge in Q:

$$e_{aijb} \stackrel{(\mathrm{ii})}{\sim} e_{aij'b}$$

Therefore, $e_{aij'b}$ and e_{aijb} belong to the same connected component of Q, that is, to Q_k . Hence, $e_{aij'b}$ is also an elementary term of $\omega^{(k)}$, and e_{aib} cancels out also in $\partial \omega^{(k)}$. This proves that $\partial \omega^{(k)}$ is allowed and, hence, $\omega^{(k)}$ is ∂ -invariant. As the number n of components is > 1, we have $|Q_k| < |Q|$, whence $||\omega^{(k)}|| < ||\omega||$. But then (2.11) is impossible by the minimality of ω . Hence, n = 1 and Q is connected. Since each vertex of Q has at most two adjacent edges, there are only two possibilities:

- (A): Q is a simple closed polygon;
- (B): Q is a linear graph.



Consider first the case (A). In this case every vertex of Q has two edges: exactly one edge of each type (i), (ii). Hence, the number of edges is even, let 2m, and Q has necessarily the following form:



$$e_{ai_0j_0b} \stackrel{\text{(ii)}}{\sim} e_{ai_0j_1b} \stackrel{\text{(i)}}{\sim} e_{ai_1j_1b} \stackrel{\text{(ii)}}{\sim} \dots \stackrel{\text{(i)}}{\sim} e_{ai_{m-1}j_{m-1}b} \stackrel{\text{(ii)}}{\sim} e_{ai_{m-1}j_0b} \stackrel{\text{(i)}}{\sim} e_{ai_0j_0b}$$
(2.12)
or some vertices i_0, \dots, i_{m-1} and j_0, \dots, j_{m-1} of G . Note that $m \ge 2$ because if $m = 1$ then
2.12) becomes

$$e_{ai_0j_0b} \stackrel{\text{(ii)}}{\sim} e_{ai_0j_1b} \stackrel{\text{(i)}}{\sim} e_{ai_0j_0b},$$

which is impossible as edges of different types between the same vertices of Q do not exist. Since all the terms in (2.12) enter ω with the same coefficients $\pm c$ (cf. (2.9) and (2.10)), we see that

$$\omega = c(e_{ai_0j_0b} - e_{ai_0j_1b} + e_{ai_1j_1b} - e_{ai_1j_2b} + \dots + e_{ai_{m-1}j_{m-1}b} - e_{ai_{m-1}j_0b}).$$
(2.13)

Suppose that all the vertices $a, i_0, \ldots, i_{m-1}, j_0, \ldots, j_{m-1}, b$ are distinct. It follows from (2.12) that these vertices form a trapezohedron T_m as on the next picture:

By (1.3), the trapezohedral path of T_m is

$$\tau_m = (e_{ai_0j_0b} - e_{ai_0j_1b}) + (e_{ai_1j_1b} - e_{ai_1j_2b})$$
$$\dots + (e_{ai_{m-2}j_{m-2}b} - e_{ai_{m-2}j_{m-1}b})$$
$$+ (e_{ai_{m-1}j_{m-1}b} - e_{ai_{m-1}j_0b}).$$

Comparison with (2.13) shows that $\omega = c\tau_m$.

If some of these vertices coincide then the

configuration (2.12) in G is a merging image of T_m , and ω is a merging image of $c\tau_m$.



Consider now the case (B). In this case the linear graph Q has two end vertices of degree 1, while all other vertices have degree 2. There are two essentially different subcases:

 (B_1) the end edges of Q are of different types:

 (B_2) the end edges of Q are of the same type (ii):

(the case of type (i) is similar).

Consider first the case (B_1) when the graph Q must have the form

$$e_{ai_0j_0b} \stackrel{\text{(ii)}}{\sim} e_{ai_0j_1b} \stackrel{\text{(i)}}{\sim} e_{ai_1j_1b} \stackrel{\text{(ii)}}{\sim} e_{ai_1j_2b} \stackrel{\text{(i)}}{\sim} \dots \stackrel{\text{(ii)}}{\sim} e_{ai_{m-1}j_mb} \stackrel{\text{(i)}}{\sim} e_{ai_mj_mb}.$$
(2.14)

Consequently, we have

$$\omega = c(e_{ai_0j_0b} - e_{ai_0j_1b} + e_{ai_1j_1b} - e_{ai_1j_2b} + \dots - e_{ai_{m-1}j_mb} + e_{ai_mj_mb}).$$
(2.15)

Computation of $\partial \omega$ gives

$$\partial \omega = c \left(-e_{aj_0b} + e_{ai_mb} \right) \mod \mathcal{A}_2.$$



Since $\partial \omega = 0 \mod \mathcal{A}_2$, we must have either $e_{aj_0b} = e_{ai_mb}$ or the both e_{aj_0b} and e_{ai_mb} are allowed, that is,

$$a \to j_0 \text{ and } i_m \to b.$$
 (2.16)

In the case $e_{aj_0b} = e_{ai_mb}$ we have $j_0 = i_m$ whence (2.16) follows again so that (2.16) is satisfied in the both cases.

We claim that in the case (B₁) the configuration (2.14) is a merging image of T_{m+2} . Indeed, denote the vertices of T_{m+2} by

$$a, i_0, \dots, i_m, i_{m+1}, j_0, \dots, j_m, j_{m+1}, b,$$

and map all the vertices of T_{m+2} , except for i_{m+1} , j_{m+1} , to the vertices of G with the same names; then merge: $i_{m+1} \mapsto j_0$ and $j_{m+1} \mapsto b$.

The following arrows in T_{m+2} $a \rightarrow i_{m+1}, i_m \rightarrow j_{m+1}, i_{m+1} \rightarrow j_{m+1}$ are mapped to the arrows in G: $a \rightarrow j_0, \quad i_m \rightarrow b, \quad j_0 \rightarrow b$ (cf. (2.16)), while the arrows $i_{m+1} \rightarrow j_0$ and $j_{m+1} \rightarrow b$ go to vertices.



It follows that this mapping of T_{m+2} into G is a digraph morphism. Since by (1.3)

 $\tau_{m+2} = (e_{ai_0j_0b} - e_{ai_0j_1b}) + (e_{ai_1j_1b} - e_{ai_1j_2b}) + \dots + (e_{ai_mj_mb} - e_{ai_mj_{m+1}b}) + (e_{ai_{m+1}j_{m+1}b} - e_{ai_{m+1}j_0b}),$ the image of τ_{m+2} is the following path, where we replace i_{m+1} by j_0 and j_{m+1} by b:

$$u = (e_{ai_0j_0b} - e_{ai_0j_1b}) + (e_{ai_1j_1b} - e_{ai_1j_2b}) + \dots + (e_{ai_mj_mb} - \underline{e_{ai_mbb}}) + (\underline{e_{aj_0bb}} - \underline{e_{aj_0j_0b}}) \\ = e_{ai_0j_0b} - e_{ai_0j_1b} + e_{ai_1j_1b} - e_{ai_1j_2b} + \dots - e_{ai_{m-1}j_mb} + e_{ai_mj_mb}.$$

Comparison with (2.15) shows that $\omega = cu$, that is, ω is a merging image of $c\tau_{m+2}$. In the case m = 1, this merging morphism of T_3 is shown here (cf. Example on p.30):



Consider now the case (B_2) when the graph Q has the form

$$e_{ai_0j_0b} \stackrel{\text{(ii)}}{\sim} e_{ai_0j_1b} \stackrel{\text{(i)}}{\sim} e_{ai_1j_1b} \stackrel{\text{(ii)}}{\sim} e_{ai_1j_2b} \stackrel{\text{(i)}}{\sim} \dots \stackrel{\text{(i)}}{\sim} e_{ai_{m-1}j_{m-1}b} \stackrel{\text{(ii)}}{\sim} e_{ai_{m-1}j_mb},$$
 (2.17)

so that

$$\omega = c(e_{ai_0j_0b} - e_{ai_0j_1b} + e_{ai_1j_1b} - e_{ai_1j_2b} + \dots + e_{ai_{m-1}j_{m-1}b} - e_{ai_{m-1}j_mb}).$$
(2.18)

Since

$$\partial \omega = c \left(-e_{aj_0b} + e_{aj_mb} \right) \mod \mathcal{A}_2,$$

it follows that either $j_0 = j_m$ or the both paths e_{aj_0b} and e_{aj_mb} are allowed, that is,

$$a \to j_0 \text{ and } a \to j_m.$$
 (2.19)

However, $j_0 = j_m$ is not possible because it would imply that

$$e_{ai_0j_0b} \stackrel{(i)}{\sim} e_{ai_{m-1}j_0b}$$

and the line graph Q would close into a polygon, which gives the case (A). Hence, (2.19) is satisfied. We claim that the configuration (2.17) is then a merging image of T_{m+1} . Indeed, denote the vertices of T_{m+1} by

$$a, i_0, ..., i_m, j_0, ... j_m, b$$

Then we map all the vertices of T_{m+1} , except for i_m , to the vertices of G with the same names; then map $i_m \mapsto a$.

Clearly, the following arrows in T_{m+1}

 $i_m \to j_0$ and $i_m \to j_m$

are mapped to the arrows in G:

 $a \to j_0$ and $a \to j_m$ (cf. (2.19)),

and the arrow $a \to i_m$ goes to a vertex.



Hence, we obtain a merging morphism of T_{m+1} into G. Since by (1.3)

$$\tau_{m+1} = (e_{ai_0j_0b} - e_{ai_0j_1b}) + (e_{ai_1j_1b} - e_{ai_1j_2b}) + \dots + (e_{ai_{m-1}j_{m-1}b} - e_{ai_{m-1}j_mb}) + (e_{ai_mj_mb} - e_{ai_mj_0b}),$$

the image of τ_{m+1} is the following path, where we replace i_m by a :

$$v = (e_{ai_0j_0b} - e_{ai_0j_1b}) + (e_{ai_1j_1b} - e_{ai_1j_2b}) + \dots + (e_{ai_{m-1}j_{m-1}b} - e_{ai_{m-1}j_mb}) + (\underline{e_{aaj_mb}} - \underline{e_{aaj_0b}}) = e_{ai_0j_0b} - e_{ai_0j_1b} + e_{ai_1j_1b} - e_{ai_1j_2b} + \dots + e_{ai_{m-1}j_{m-1}b} - e_{ai_{m-1}j_mb}.$$

Comparison with (2.18) shows that $\omega = cv$ so that ω is a merging image of $c\tau_{m+1}$.

2.4 Examples and problems

For example, in the case m = 2the above morphism gives the following merging image of T_3 : $(T_3=3$ -cube)



In the case m = 3, the above morphism gives the merging image of T_4 as broken cube: (cf. Example on p. 31)



Problem 2.6 Prove Theorem 2.5 in the general case without the hypothesis (N).

Perhaps, one can prove the absence of multisquares *inside* each minimal cluster ω using the minimality of ω . Then the rest of the proof remains unchanged.

Problem 2.7 Devise an algorithm for computing a basis in Ω_3 based on Theorem 2.5.

Denote by \mathcal{Q} the set of all elementary allowed 3-paths. For each $e_{aijb} \in \mathcal{Q}$, we have

$$\partial e_{aijb} = -e_{ajb} + e_{aib} \operatorname{mod} \mathcal{A}_2.$$

We say that e_{ajb} is a *bond* of type (i) if $a \not\rightarrow j$; and e_{aib} is a bond of type (ii), if $i \not\rightarrow b$.

Define edges between elements $q_1, q_2 \in \mathcal{Q}$ as follows:

 $q_1 \stackrel{(i)}{\sim} q_2$ if q_1, q_2 have a common bond of the type (i); $q_1 \stackrel{(ii)}{\sim} q_2$ if q_1, q_2 have a common bond of the type (ii).



Some bonds may be attached to only one vertex of \mathcal{Q} , so that we allow in \mathcal{Q} edges with only one vertex. Then the minimal ∂ -invariant clusters in G are determined by the maximal paths in graph \mathcal{Q} that go along the edges with alternating types.

For example, consider the following digraph: and try to determine Ω_3 . For that first find all elementary allowed 3-paths with all their bonds as shown in the following table:



$\mathcal{Q} \setminus \text{bonds}$	054	034	154	012	123	124
0134		(i)				
0152				(ii)		
0153						
0234		(i)				
0523						
0524	(ii)					
0534	(ii)	(i)				
1523					(i)	
1524			(ii)			(i)
1534			(ii)			
5234						

This table determines a (hyper)graph structure in \mathcal{Q} is as follows:



The maximal alternating paths in this graph are

$$0134 \stackrel{\text{(i)}}{\sim} 0234, \qquad 0134 \stackrel{\text{(i)}}{\sim} 0534 \stackrel{\text{(ii)}}{\sim} 0524, \qquad 0153, \qquad 0523, \qquad 5234$$

which yields five minimal ∂ -invariant clusters

$$e_{0134} - e_{0234}, e_{0134} - e_{0534} + e_{0524}, e_{0153}, e_{0523}, e_{5234},$$

that form a basis in Ω_3 . In particular, dim $\Omega_3 = 5$.

Problem 2.8 State and prove similar results for Ω_4 . Are the basic shapes in Ω_4 given by polyhedra in \mathbb{R}^4 ? Devise an algorithm for computing a basis in Ω_4 . The same questions for Ω_p with p > 4.

3 Combinatorial curvature and products

3.1 Definition

Let G = (V, E) be a finite digraph and $\mathbb{K} = \mathbb{R}$. Definition of curvature depends on the choice of inner product in the spaces \mathcal{R}_p of regular *p*-paths. Let us fix in each \mathcal{R}_p the *natural* inner product \langle, \rangle when all regular elementary paths $e_{i_0...i_p}$ form an orthonormal basis in \mathcal{R}_p . Then, for any path $\omega = \sum \omega^{i_0...i_p} e_{i_0...i_p} \in \mathcal{R}_p$, we have

$$\left\|\omega\right\|^{2} = \sum_{i_{0}\dots i_{p} \in V} \left(\omega^{i_{0}\dots i_{p}}\right)^{2}$$

For any regular elementary path $e_{i_0...i_p}$ and for any vertex x, define

$$[x, e_{i_0...i_p}]$$
 = the number of occurrences of x in $i_0, ..., i_p$.

For example, $[a, e_{abca}] = 2$, $[b, e_{abca}] = 1$, $[d, e_{abca}] = 0$.

For a path $\omega = \sum \omega^{i_0 \dots i_p} e_{i_0 \dots i_p} \in \mathcal{R}_p$ and for any $x \in V$, define the *incidence* of x in ω by

$$[x,\omega] = \sum_{i_0\dots i_p \in V} \left(\omega^{i_0\dots i_p}\right)^2 \left[x, e_{i_0\dots i_p}\right].$$

Recall that Ω_p is a subspace of \mathcal{R}_p that is defined by $\Omega_p = \{\omega \in \mathcal{R}_p : \omega \text{ and } \partial \omega \text{ are allowed} \}$. Fix an orthogonal basis $\{\omega_k\}$ in Ω_p and define the *incidence* of any vertex x in Ω_p by

$$[x, \Omega_p] = \sum_k \frac{[x, \omega_k]}{\|\omega_k\|^2}.$$
(3.1)

It is possible to prove that the sum in (3.1) is independent of the choice of a basis $\{\omega_k\}$.

Definition. For any $N \in \mathbb{N}$ define the *curvature of order* N at a vertex x by

$$K_x^{(N)} := \sum_{p=0}^N \frac{(-1)^p}{p+1} [x, \Omega_p].$$

Recall that the Euler characteristic is defined by $\chi^{(N)} := \sum_{p=0}^{N} (-1)^p \dim \Omega_p$.

Proposition 3.1 (Gauss-Bonnet) For any choice of the inner product in \mathcal{R}_p and for any $N \in \mathbb{N}$, we have

$$K_{total}^{(N)} := \sum_{x \in V} K_x^{(N)} = \chi^{(N)}.$$

If dim $\Omega_p = 0$ for all p > N, then write $K_x^{(N)} \equiv K_x$ and $\chi^{(N)} \equiv \chi$. In this case we have $\chi = \sum_{p=0}^{\infty} (-1)^p \dim H_p$.

3.2 Examples of computation

Using the orthonormal basis $\{e_i\}$ in Ω_0 we obtain, for any $x \in V$,

$$[x, \Omega_0] = \sum_i [x, e_i] = 1.$$

Using the orthonormal basis $\{e_{ij}\}$ with $i \to j$ in Ω_1 , we obtain

$$[x, \Omega_1] = \sum_{i \to j} [x, e_{ij}] = \deg(x).$$

Therefore, for any $N \ge 1$,

$$K_x^{(N)} = 1 - \frac{\deg(x)}{2} + \sum_{p=2}^N \frac{(-1)^p}{p+1} [x, \Omega_p].$$
(3.2)

Example. Let G be a triangle $\{0 \rightarrow 1 \rightarrow 2, 0 \rightarrow 2\}$. Then $\Omega_2 = \langle e_{012} \rangle$ and $\Omega_p = \{0\}$ for p > 2. Since $||e_{012}||^2 = 1$, we obtain, for any $x \in \{0, 1, 2\}$, $[x, \Omega_2] = [x, e_{012}] = 1$,

whence

$$K_x = 1 - \frac{\deg(x)}{2} + \frac{1}{3} [x, \Omega_2] = 1 - \frac{2}{2} + \frac{1}{3} = \frac{1}{3}.$$

2	

Example. Let G be a square $\{0 \to 1, 0 \to 2, 1 \to 3, 2 \to 3\}$. Then $\Omega_2 = \langle e_{013} - e_{023} \rangle$ and $\Omega_p = \{0\}$ for p > 2. Since $||e_{013} - e_{023}||^2 = 2$, we obtain $[0, \Omega_2] = \frac{1}{2} [0, e_{013} - e_{023}] = 1$, $[3, \Omega_2] = 1$ $[1, \Omega_2] = \frac{1}{2} [1, e_{013} - e_{023}] = \frac{1}{2}$, $[2, \Omega_2] = \frac{1}{2}$



It follows that

$$K_3 = K_0 = 1 - \frac{\deg(0)}{2} + \frac{1}{3} = \frac{1}{3}, \quad K_2 = K_1 = 1 - \frac{\deg(1)}{2} + \frac{1}{6} = \frac{1}{6},$$

and $K_{total} = 1$. Note for comparison that

$$\chi = \dim \Omega_0 - \dim \Omega_1 + \dim \Omega_2 = 3 - 3 + 1 = 1.$$

The main purpose of what follows is to compute the curvature of the n-cube. For that we revise first the notions of cross product of paths and Cartesian (box) product of digraphs.

3.3 Cross product of paths

Given two finite sets X, Y, consider their Cartesian product

$$Z = X \times Y = \{(a, b) : a \in X \text{ and } b \in Y\}.$$

Let $z = z_0...z_r$ be a regular elementary r-path on Z; let $z_k = (a_k, b_k)$ with $a_k \in X, b_k \in Y$.

We say that z is *stair-like* if, for any k = 1, ..., r, either $a_{k-1} = a_k$ or $b_{k-1} = b_k$. That is, any pair $z_{k-1}z_k$ of consecutive vertices is

- either vertical (when $a_{k-1} = a_k$)
- or *horizontal* (when $b_{k-1} = b_k$).

Given a stair-like path z on Z, define its projection xonto X as a *regular* elementary path x on X obtained from $a_0...a_r$ by collapsing any subsequence of repeated vertices onto one vertex.

In the same way define the projection y of z onto Y.



The projections $x = x_0...x_p$ and $y = y_0...y_q$ are regular elementary paths, and p + q = r.

Let us map every vertex (x_i, y_j) of the path z to a point (i, j) of \mathbb{Z}^2 , so that the path z is mapped to a *staircase* S(z) in \mathbb{Z}^2 connecting (0, 0) and (p, q). Define the *elevation* L(z) of z as the number of cells in \mathbb{Z}^2_+ below the staircase S(z).



For given elementary regular paths x on X and y on Y, denote by $\Pi_{x,y}$ the set of all stair-like paths z on Z whose projections on X and Y are x and y, respectively.

Definition. Given elementary paths $e_x \in \mathcal{R}_p(X)$ and $e_y \in \mathcal{R}_q(Y)$, define their cross product $e_x \times e_y$ as a path in $\mathcal{R}_{p+q}(Z)$ as follows:

$$e_x \times e_y = \sum_{z \in \Pi_{x,y}} (-1)^{L(z)} e_z.$$
 (3.3)

Then extend the operation \times by linearity to all $u \in \mathcal{R}_p(X)$ and $v \in \mathcal{R}_q(Y)$ so that $u \times v \in \mathcal{R}_{p+q}(Z)$.

Example. Let us denote the vertices on X by letters a, b, c etc and the vertices on Y by integers 1, 2, 3, etc. Then the vertices on Z can be denoted as a1, b2 etc as the fields on a chessboard.

We have then

 $e_a \times e_{12} = e_{a1\,a2}, \quad e_{ab} \times e_1 = e_{a1\,b1}$ $e_{ab} \times e_{12} = e_{a1\,b1\,b2} - e_{a1\,a2\,b2}$ $e_{ab} \times e_{123} = e_{a1\,b1\,b2\,b3} - e_{a1\,a2\,b2\,b3} + e_{a1\,a2\,a3\,b3}$ $e_{abc} \times e_{123} = e_{a1\,b1\,c1\,c2\,c3} - e_{a1\,b1\,b2\,c2\,c3} + e_{a1\,b1\,b2\,b3\,c3}$ $+ e_{a1\,a2\,b2\,c2\,c3} - e_{a1\,a2\,b2\,b3\,c3} + e_{a1\,a2\,a3\,b3\,c3}$



(3.4)

Lemma 3.2 If $u \in \mathcal{R}_p(X)$ and $v \in \mathcal{R}_q(Y)$ where $p, q \ge 0$, then $\partial (u \times v) = \partial u \times v + (-1)^p u \times \partial v.$

3.4 Cartesian product of digraphs

We denote here digraphs and their sets of vertices by the same letters. Given two digraphs X and Y, define their Cartesian product (box product) as a digraph $Z = X \Box Y$ as follows:

• the set of vertices of Z is $X \times Y$, that is, the vertices of Z are pairs (a, b) where $a \in X$ and $b \in Y$;

- \bullet the arrows in Z are of two types:
- vertical arrows $(a, b) \rightarrow (a, b')$ if $b \rightarrow b'$ in Y;
- horizontal arrows $(a, b) \rightarrow (a', b)$ if $a \rightarrow a'$ in X.



It follows that any allowed elementary path in Z is stair-like.

Moreover, any regular elementary path on Z is allowed if and only if it is stair-like and its projections onto X and Y are allowed.

It follows from definition (3.3) of the cross product that

$$u \in \mathcal{A}_{p}(X) \text{ and } v \in \mathcal{A}_{q}(Y) \Rightarrow u \times v \in \mathcal{A}_{p+q}(Z).$$

It follows from the product rule (3.4) that

$$u \in \Omega_p(X) \text{ and } v \in \Omega_q(Y) \Rightarrow u \times v \in \Omega_{p+q}(Z).$$

Theorem 3.3 (Künneth formula for product) For any $r \ge 0$, we have

$$\Omega_r \left(X \Box Y \right) \cong \bigoplus_{\{p,q \ge 0: p+q=r\}} \Omega_p \left(X \right) \otimes \Omega_q \left(Y \right), \tag{3.5}$$

where the isomorphism is given by $u \otimes v \mapsto u \times v$ for $u \in \Omega_p(X)$ and $v \in \Omega_q(Y)$.

Equivalent formulation. For any $n \ge 0$, choose a basis $\mathcal{B}_n(X)$ in $\Omega_n(X)$ and a basis $\mathcal{B}_n(Y)$ in $\Omega_n(Y)$. Then $\Omega_r(X \Box Y)$ has the following basis:

$$\{u \times v : u \in \mathcal{B}_p(X), v \in \mathcal{B}_q(Y), p+q=r, p,q \ge 0\}.$$

3.5 ∂ -invariant paths on *n*-cube

Consider the digraph $I = \{0 \rightarrow 1\}$, and define *n*-cube for any $n \in \mathbb{N}$ as follows:

$$n$$
-cube = $I^{\Box n} = \underbrace{I \Box I \Box \dots \Box I}_{n}$.

Our purpose here is to compute the curvature of *n*-cube. For that, we determine first the structure of the spaces $\Omega_p(n\text{-cube}).$



Each vertex $a \in n$ -cube can be identified with a binary sequence $(a_1, ..., a_n)$. For example, $\mathbf{0}_n = (0, ..., 0)$ and $\mathbf{1}_n = (1, ..., 1)$ are the corners of the *n*-cube.

For two vertices $a, b \in n$ -cube, there is an arrow $a \to b$ if $b_k = a_k + 1$ for exactly one value of k and $b_k = a_k$ for all other values of k. Denote

$$|a| = a_1 + \dots + a_n.$$

We write $a \leq b$ (a precedes b) if there is an allowed path in n-cube from a to b, that is,

$$a \leq b \iff a_k \leq b_k$$
 for all $k = 1, \dots, n_k$

Fix a pair of vertices $a \leq b$ and define an induced subgraph $D_{a,b}$ of the *n*-cube as follows:

the vertices of $D_{a,b}$ are all the vertices $c \in n$ -cube such that

 $a \preceq c \preceq b$

(and an arrow exists between two vertices of $D_{a,b}$ if and only if that arrow exists in *n*-cube). Here are a 4-cube, its subgraph $D_{a,b}$ (in red color) and a vertex $c \in D_{a,b}$.



Fix two vertices $a, b \in n$ -cube such that $a \leq b$ and set p = |b| - |a|. Then $(a_1, ..., a_n)$ and $(b_1, ..., b_n)$ differ exactly at p positions, say $i_1, ..., i_p$; that is, $a_{i_1} = ... = a_{i_p} = 0$ and $b_{i_1} = ... = b_{i_p} = 1$. The mapping

$$D_{a,b} \to p\text{-cube}$$
$$(c_1, ..., c_n) \mapsto (c_{i_1}, ..., c_{i_p})$$

is clearly a digraph isomorphism that sends a and b to the corners $\mathbf{0}_p$ and $\mathbf{1}_p$ of p-cube.

Denote by $P_{a,b}$ the set of all elementary allowed paths in *n*-cube going from *a* to *b*. Each path in $P_{a,b}$ lies in $D_{a,b}$, has the length *p*, and the total number of the paths in $P_{a,b}$ is *p*!.

Lemma 3.4 There is a function $\sigma : P_{a,b} \to \{0,1\}$ such that the following p-path on $I^{\Box n}$ is ∂ -invariant:

$$\omega_{a,b} = \sum_{x \in P_{a,b}} (-1)^{\sigma(x)} e_x \,. \tag{3.6}$$

For example, in a 3-cube as shown here, we have

$$\begin{split} \omega_{0,1} &= e_{01}, \\ \omega_{0,3} &= e_{013} - e_{023}, \\ \omega_{0,7} &= e_{0137} - e_{0237} - e_{0157} + e_{0457} + e_{0267} - e_{0467} \\ \text{(cf. p. 8).} \end{split}$$



Proof. As $D_{a,b} \cong p$ -cube, we can assume without loss of generality, that $D_{a,b} = I^{\Box n}$, that is, $a = \mathbf{0}_n, b = \mathbf{1}_n, p = n$. Proof by induction in n. Induction basis for n = 1 is clear. For the induction step from n to n+1, we use the fact that the cross product of ∂ -invariant paths is ∂ -invariant. Set for simplicity of notation $\mathbf{0} \equiv \mathbf{0}_n, \mathbf{1} \equiv \mathbf{1}_n, \mathbf{0}' \equiv \mathbf{0}_{n+1}, \mathbf{1}' \equiv \mathbf{1}_{n+1}$.

By the induction hypothesis, there is a ∂ -invariant *n*-path on $I^{\Box n}$ of the form

$$\omega_{\mathbf{0},\mathbf{1}} = \sum_{x \in P_{\mathbf{0},\mathbf{1}}} \left(-1\right)^{\sigma(x)} e_x$$

Since e_{01} is ∂ -invariant 1-path in I, taking the cross product of $\omega_{0,1}$ and e_{01} , we obtain the following ∂ -invariant (n + 1)-path on $I^{\Box(n+1)}$:

$$\omega_{0,1} \times e_{01} = \sum_{x \in P_{0,1}} (-1)^{\sigma(x)} e_x \times e_y$$
$$= \sum_{x \in P_{0,1}} \sum_{z \in \Pi_{x,y}} (-1)^{\sigma(x)} (-1)^{L(z)} e_z.$$

where y = 01 and where we have used (3.3).



A path $x \in P_{0,1}$ and $z \in \Pi_{x,y}$

Here z is any stair-like path on $I^{\Box(n+1)}$ that projects onto x and y, respectively, while x is any allowed path on $I^{\Box n}$ from **0** to **1**. Clearly, z runs over all allowed paths in $I^{\Box(n+1)}$ from **0**' to **1**', that is, $z \in P_{\mathbf{0}',\mathbf{1}'}$. Defining the function σ on the paths $z \in P_{\mathbf{0}',\mathbf{1}'}$ by

$$\sigma(z) = \sigma(x) + L(z) \operatorname{mod} 2,$$

we obtain that the following (n+1)-path on $I^{\Box(n+1)}$ is ∂ -invariant:

$$\omega_{\mathbf{0}',\mathbf{1}'} := \sum_{z \in P_{\mathbf{0}',\mathbf{1}'}} (-1)^{\sigma(z)} e_z = \omega_{\mathbf{0},\mathbf{1}} \times e_{01},$$

which concludes the proof. \blacksquare

Proposition 3.5 For any $p \ge 0$, we have

$$\Omega_p(n\text{-cube}) = \langle \omega_{a,b} : a \preceq b \text{ and } |b| - |a| = p \rangle.$$

Moreover, $\{\omega_{a,b}\}$ is a basis of $\Omega_p(n\text{-cube})$.

Proof. The proof is again by induction in n. The induction basis for n = 1 is obvious. For the induction step from n to n+1 we use the Künneth formula (3.5). By this formula, the basis in $\Omega_p(I^{\Box(n+1)})$ consists of the p-paths of the form

$u \times v$,

where u runs over a basis in $\Omega_{p'}(I^{\Box n})$ and v runs over a basis in $\Omega_{p''}(I)$ with p' + p'' = p. Since

$$\Omega_0(I) = \langle e_0, e_1 \rangle, \quad \Omega_1(I) = \langle e_{01} \rangle \text{ and } \Omega_{p''}(I) = \{0\} \text{ for } p'' > 1,$$

we obtain the following basis in $\Omega_p(I^{\Box(n+1)})$:

$$\left\{\omega_{a,b} \times e_i : \omega_{a,b} \in \Omega_p(I^{\square n}), i = 0, 1\right\} \cup \left\{\omega_{a,b} \times e_{01} : \omega_{a,b} \in \Omega_{p-1}(I^{\square n})\right\}.$$

The products $\omega_{a,b} \times e_i$ give us the *p*-paths $\omega_{(a,0),(b,0)}$ and $\omega_{(a,1),(b,1)}$, while the products $\omega_{a,b} \times e_{01}$ give the *p*-paths $\omega_{(a,0),(b,1)}$. Clearly, we obtain in this way all *p*-paths $\omega_{a',b'}$ on (n+1)-cube with $a' \leq b'$, |b'| - |a'| = p, which finishes the proof.

3.6 Curvature of *n*-cube

Theorem 3.6 For any vertex $x \in n$ -cube, the curvature K_x is given by the identity

$$K_x = \frac{1}{\left(n+1\right)\binom{n}{\left|x\right|}}.$$
(3.7)

For example, in a 4-cube that is shown here, for a marked vertex x = (0, 1, 0, 1), we have |x| = 2 and

$$K_x = \frac{1}{5\binom{4}{2}} = \frac{1}{30}.$$



Observe the following interesting consequence of (3.7): for

any integer $l \ge 0$, the number of vertices x with |x| = l is equal to $\binom{n}{l}$, which implies that

$$\sum_{x:|x|=l\}} K_x = \frac{1}{n+1}.$$

Since |x| takes the values 0, ..., n, we obtain $K_{total} = 1 = \chi$. We start the proof with some properties of the binomial coefficients. **Lemma 3.7** We have, for all integers $a \ge m \ge 0$,

$$\sum_{j=0}^{m} (-1)^{j} \binom{a}{j} = (-1)^{m} \binom{a-1}{m}.$$
(3.8)

Proof. Induction in a. Induction basis: for a = m we have

$$\sum_{j=0}^{m} (-1)^{j} \binom{m}{j} = (1-1)^{m} = 0 = (-1)^{m} \binom{m-1}{m}.$$

Induction step from a to a + 1:

$$\sum_{j=0}^{m} (-1)^{j} \binom{a+1}{j} = \sum_{j=0}^{m} (-1)^{j} \left(\binom{a}{j} + \binom{a}{j-1} \right) = (-1)^{m} \binom{a-1}{m} + \sum_{j=1}^{m} (-1)^{j} \binom{a}{j-1}$$
$$= (-1)^{m} \binom{a-1}{m} - \sum_{i=0}^{m-1} (-1)^{i} \binom{a}{i} \quad (i=j-1)$$
$$= (-1)^{m} \binom{a-1}{m} - (-1)^{m-1} \binom{a-1}{m-1} = (-1)^{m} \binom{a}{m}.$$

Lemma 3.8 We have, for all integers $a \ge 0$ and $b \ge 1$,

$$\sum_{l=0}^{a} \binom{a}{l} \frac{(-1)^{l}}{l+b} = \frac{1}{b\binom{a+b}{b}}.$$
(3.9)

For example, for b = 1, we obtain by (3.9)

$$\sum_{l=0}^{a} \binom{a}{l} \frac{(-1)^{l}}{l+1} = \binom{a}{0} - \frac{1}{2} \binom{a}{1} + \frac{1}{3} \binom{a}{2} - \dots + (-1)^{a} \frac{1}{a+1} \binom{a}{a} = \frac{1}{a+1}.$$
 (3.10)

Proof. We start with the binomial identity

$$\sum_{l=0}^{a} \binom{a}{l} \left(-z\right)^{l} = \left(1-z\right)^{a}$$

for all $z \in \mathbb{R}$. Multiplying it by $(-z)^{b-1}$, we obtain

$$\sum_{l=0}^{a} \binom{a}{l} (-z)^{l+b-1} = (-1)^{b-1} (1-z)^{a} z^{b-1}$$

Integrating this identity from 0 to 1 yields

$$-\sum_{l=0}^{a} {\binom{a}{l}} \frac{(-z)^{l+b}}{l+b} \Big|_{0}^{1} = (-1)^{b-1} \int_{0}^{1} (1-z)^{a} z^{b-1} dz$$
$$= (-1)^{b-1} B (a+1,b)$$
$$= (-1)^{b-1} \frac{\Gamma (a+1) \Gamma (b)}{\Gamma (a+b+1)}$$
$$= (-1)^{b-1} \frac{a!b!}{b (a+b)!}$$
$$= \frac{(-1)^{b-1}}{b \binom{a+b}{b}}.$$
(3.11)

On the other hand, the left hand side of the above identity is equal to

$$-\sum_{l=0}^{a} \binom{a}{l} \frac{(-1)^{l+b}}{l+b} = (-1)^{b+1} \sum_{l=0}^{a} \binom{a}{l} \frac{(-1)^{l}}{l+b}.$$
(3.12)

Comparing (3.11) and (3.12), we obtain (3.9).

Lemma 3.9 We have, for all integers $m, l \ge 0$,

$$S_{m,l} := \sum_{k=0}^{m} \binom{m}{k} \frac{(-1)^k}{\binom{k+l}{l}(k+l+1)} = \frac{1}{m+l+1}.$$
(3.13)

For example, for l = 0 we obtain

$$\sum_{k=0}^{m} \binom{m}{k} \frac{(-1)^{k}}{k+1} = \frac{1}{m+1},$$

which coincides with (3.10). For l = 1 we have

$$\sum_{k=0}^{m} \binom{m}{k} \frac{(-1)^{k}}{(k+1)(k+2)} = \frac{1}{m+2}.$$

Proof. We have

$$S_{m,l} = l! \sum_{k=0}^{m} \frac{m (m-1) \dots (m-k+1)}{k!} \frac{(-1)^k}{(k+1) \dots (k+l) (k+l+1)}$$
$$= \frac{l!}{(m+l+1) \dots (m+1)} \sum_{k=0}^{m} \frac{(-1)^k (m+l+1) \dots (m+1) m (m-1) \dots (m-k+1)}{(k+l+1)!}$$

$$= \frac{l!m!}{(m+l+1)!} \sum_{k=0}^{m} (-1)^k \binom{m+l+1}{k+l+1}$$
$$= \frac{l!m!}{(m+l+1)!} \sum_{k=0}^{m} (-1)^k \binom{m+l+1}{m-k}$$
$$= \frac{l!m!}{(m+l+1)!} \sum_{j=0}^{m} (-1)^{m-j} \binom{m+l+1}{j} \qquad (j=m-k).$$

By (3.8) with a = m + l + 1 we obtain

$$\sum_{j=0}^{m} (-1)^{j} \binom{m+l+1}{j} = \sum_{j=0}^{m} (-1)^{j} \binom{a}{j} = (-1)^{m} \binom{a-1}{m} = (-1)^{m} \binom{m+l}{m}.$$

It follows that

$$S_{m,l} = \frac{l!m!}{(m+l+1)!} \binom{m+l}{m} = \frac{l!m!}{(m+l+1)!} \frac{(m+l)!}{l!m!} = \frac{1}{m+l+1},$$

which was to be proved. \blacksquare

Lemma 3.10 We have, for all integers $m, m' \ge 0$,

$$K_m := \sum_{k=0}^{m} \sum_{l=0}^{m'} \binom{m}{k} \binom{m'}{l} \frac{(-1)^{k+l}}{\binom{k+l}{l} (k+l+1)} = \frac{1}{(m+m'+1)\binom{m+m'}{m}}$$

Proof. Using (3.13) and applying (3.9) with a = m' and b = m + 1, we obtain

$$K_{m} = \sum_{l=0}^{m'} {m' \choose l} (-1)^{l} \sum_{k=0}^{m} {m \choose k} \frac{(-1)^{k}}{\binom{k+l}{l}(k+l+1)}$$

$$= \sum_{l=0}^{m'} {m' \choose l} (-1)^{l} S_{m,l}$$

$$= \sum_{l=0}^{m'} {m' \choose l} \frac{(-1)^{l}}{m+l+1} = \sum_{l=0}^{a} {a \choose l} \frac{(-1)^{l}}{l+b} = \frac{1}{b\binom{a+b}{b}} = \frac{1}{(m+1)\binom{m+m'+1}{m+1}}$$

$$= \frac{(m+1)!(m')!}{(m+1)(m+m'+1)!} = \frac{m!(m')!}{(m+m'+1)(m+m')!} = \frac{1}{(m+m'+1)\binom{m+m'}{m}}$$

which finishes the proof. \blacksquare

Proof of Theorem 3.6. Fix a vertex $x \in n$ -cube, some $p \ge 0$ and compute $[x, \Omega_p]$. Let a and b be two vertices of the n-cube such

$$a \leq x \leq b$$
 and $|b| - |a| = p$.

Set

$$k = |x| - |a|, \quad l = |b| - |x|$$

so that k + l = p. We claim that, for the ∂ -invariant p-path $\omega_{a,b}$ between a and b (cf. (3.6)),

$$\|\omega_{a,b}\|^2 = p!$$
 and $[x, \omega_{a,b}] = k!l!.$

Indeed, $\omega_{a,b}$ is an alternating sum of p! elementary allowed paths going from a to b, and the number of the elementary allowed paths from a to b that go through x is equal to k!l!,

because the number of such paths from a to x is equal to k! and the number of such paths from x to bis equal to l!.



Consequently, we obtain

$$\frac{[x, \omega_{a,b}]}{\|\omega_{a,b}\|^2} = \frac{k!l!}{p!} = \frac{1}{\binom{k+l}{k}}.$$
Set m = |x| and observe that the number of vertices a with

$$a \leq x$$
 and $|x| - |a| = k$

is equal to $\binom{m}{k}$. Indeed, in the binary representations $a = (a_1, ..., a_n)$ and $x = (x_1, ..., x_n)$, we have $a_i \leq x_i$ and $\sum_i (x_i - a_i) = k$ which is only possible if $a_i = 0$ at k out of m positions where $x_i = 1$.

Similarly, the number of the vertices b with

$$x \leq b$$
 and $|b| - |x| = l$

is equal to $\binom{n-m}{l}$. Hence, the number of pairs a, b such that

$$a \leq x \leq b$$
, $|x| - |a| = k$, $|b| - |x| = l$,

is equal to

$$\binom{m}{k}\binom{n-m}{l}.$$

By Proposition 3.5, all *p*-paths $\omega_{a,b}$ with $a \leq b$ form an orthogonal basis in Ω_p (*n*-cube). If x does not satisfy the condition $a \leq x \leq b$ then we have

$$[x,\omega_{a,b}] = 0.$$

Hence, we obtain

$$[x, \Omega_p] = \sum_{|b|-|a|=p} \frac{[x, \omega_{a,b}]}{\|\omega_{a,b}\|^2} = \sum_{\substack{a \leq x \leq b \\ |b|-|a|=p}} \frac{[x, \omega_{a,b}]}{\|\omega_{a,b}\|^2}$$
$$= \sum_{k+l=p} \sum_{\substack{a \leq x \leq b \\ |x|-|a|=k \\ |b|-|x|=l}} \frac{[x, \omega_{a,b}]}{\|\omega_{a,b}\|^2} = \sum_{k+l=p} \binom{m}{k} \binom{n-m}{l} \frac{1}{\binom{k+l}{k}}.$$

By Lemma 3.10 with m' = n - m, we obtain that

$$K_{x} = \sum_{p \ge 0} \frac{(-1)^{p}}{p+1} [x, \Omega_{p}]$$

= $\sum_{k=0}^{m} \sum_{l=0}^{n-m} {m \choose k} {n-m \choose l} \frac{(-1)^{k+l}}{{\binom{k+l}{l}(k+l+1)}}$
= $\frac{1}{(m+m'+1) {\binom{m+m'}{m}}} = \frac{1}{(n+1) {\binom{n}{m}}},$

which was to be proved. \blacksquare

Problem 3.11 The above proof of Theorem 3.6 is done by a "brute force" computation. Give a conceptual proof without long computations.

Problem 3.12 How to compute $K_z(X \Box Y)$ for general digraphs X, Y (or at least for some classes of digraphs X, Y)?

It is known that if Y is a cyclic digraph $\{0 \to 1 \to 2 \to \dots \to 0\}$ of at least 3 vertices then $K_z(X \Box Y) \equiv 0$.

Problem 3.13 *How the notion of combinatorial curvature compares to other notions of curvature of graphs?*

3.7 Appendix: proof of the product rule

We prove here Lemma 3.2: if $u \in \mathcal{R}_p(X)$ and $v \in \mathcal{R}_q(Y)$ where $p, q \ge 0$, then

$$\partial (u \times v) = \partial u \times v + (-1)^p u \times \partial v.$$
(3.14)

It suffices to prove (3.14) for the case $u = e_x$ and $v = e_y$ where $x = x_0...x_p$ and $y = y_0...y_q$ are regular elementary *p*-path on *X* and *q*-path on *Y*, respectively. Set r = p + q so that $e_x \times e_y \in \mathcal{R}_r(Z)$.

If p = q = 0 then all the terms in (3.14) vanish. Assume p = 0 and $q \ge 1$ (the case $p \ge 1$ and q = 0 is similar). Then $\prod_{x,y}$ contains the only element $z = z_0...z_q$ where $z_i = (x_0, y_i)$. Since L(z) = 0, we obtain by (3.3) that

$$e_x \times e_y = e_{z_0 \dots z_q}$$

By (1.1) obtain

$$\partial \left(e_x \times e_y \right) = \partial e_{z_0 \dots z_q} = e_x \times \partial e_{y_0 \dots y_q},$$

which is equivalent to (3.14), because $\partial u = 0$.

Consider now the main case $p, q \ge 1$. We have by (3.3) and (1.1)

$$\partial \left(e_x \times e_y \right) = \sum_{z \in \Pi_{x,y}} \left(-1 \right)^{L(z)} \partial e_z = \sum_{z \in \Pi_{x,y}} \sum_{k=0}^r \left(-1 \right)^{L(z)+k} e_{z_{(k)}}, \tag{3.15}$$

where we use a shortcut

$$z_{(k)} = z_0 ... \hat{z_k} ... z_r = z_0 ... z_{k-1} z_{k+1} ... z_r.$$

Switching the order of the sums, rewrite (3.15) in the form

$$\partial \left(e_x \times e_y \right) = \sum_{k=0}^r \sum_{z \in \Pi_{x,y}} \left(-1 \right)^{L(z)+k} e_{z_{(k)}}.$$
 (3.16)

Given an index k = 0, ..., r and a path $z \in \Pi_{x,y}$, consider the following four logically possible cases how horizontal and vertical couples combine around z_k :



Here (H) stands for a horizontal position, (V) for vertical, (R) for right and (L) for left. If k = 0 or k = r then z_{k-1} or z_{k+1} should be ignored, so that one has only two distinct positions (H) and (V).

If $z \in \Pi_{x,y}$ and z_k stands in (R) or (L) then consider a path $z' \in \Pi_{x,y}$ such that $z'_i = z_i$ for all $i \neq k$, whereas z'_k stands in the opposite position (L) or (R), respectively, as on the diagrams:



Clearly, we have $L(z') = L(z) \pm 1$ which implies that the terms $e_{z_{(k)}}$ and $e_{z'_{(k)}}$ in (3.16) cancel out.

Denote by $\Pi_{x,y}^k$ the set of paths $z \in \Pi_{x,y}$ such that z_k stands in position (V) and by $\Pi_{x,y}^{k}$ the set of paths $z \in \Pi_{x,y}$ such that z_k stands in position (H). By the above observation, we can restrict the summation in (3.16) to those pairs k, z where z_k is either in vertical or horizontal position, that is,

$$\partial \left(e_x \times e_y \right) = \sum_{k=0}^r \sum_{z \in \Pi_{x,y}^k \sqcup \Pi_{x,y}^k} \left(-1 \right)^{L(z)+k} e_{z_{(k)}}.$$
 (3.17)

Let us now compute the first term in the right hand side of (3.14):

$$(\partial e_x) \times e_y = \sum_{l=0}^p (-1)^l e_x \times e_y = \sum_{l=0}^p \sum_{w \in \Pi_{x_{(l)}}, y} (-1)^{L(w)+l} e_w.$$
(3.18)

Fix some l = 0, ..., p and $w \in \prod_{x_{(l)}, y}$.

Since the projection of w on X is

$$x_{(l)} = x_0 \dots x_{l-1} x_{l+1} \dots x_p,$$

there exists a unique index k such that w_{k-1} projects onto x_{l-1} and w_k projects onto x_{l+1} .

Then w_{k-1} and w_k have a common projection onto Y, say y_m .



Stair-like paths w and z. The shaded area represents the difference L(z) - L(w).

Define a path $z \in \prod_{x,y}^{k}$ by setting

$$z_{i} = \begin{cases} w_{i} & \text{for } i \leq k-1, \\ (x_{l}, y_{m}) & \text{for } i = k, \\ w_{i-1} & \text{for } i \geq k+1. \end{cases}$$
(3.19)

By construction we have $z_{(k)} = w$. It also follows from the construction that

$$L\left(z\right) = L\left(w\right) + m$$

Since k = l + m, we obtain that

$$L(z) + k = L(w) + l + 2m.$$

We see that each pair l, w where l = 0, ..., p and $w \in \prod_{x_{(l)}, y}$ gives rise to a pair k, z where k = 0, ..., r, $z \in \prod_{x,y}^{k}$, and

$$(-1)^{L(z)+k} e_{z_{(k)}} = (-1)^{L(w)+l} e_w.$$

By reversing this argument, we obtain that each such pair k, z gives back l, w so that this correspondence between k, z and l, w is bijective. Hence, we conclude that

$$(\partial e_x) \times e_y = \sum_{l=0}^p \sum_{w \in \Pi_{x_{(l)}}, y} (-1)^{L(w)+l} e_w = \sum_{k=0}^r \sum_{z \in \Pi_{x, y}} (-1)^{L(z)+k} e_{z_{(k)}}.$$
 (3.20)

The second term in the right hand side of (3.14) is computed similarly:

$$(-1)^{p} e_{x} \times \partial e_{y} = \sum_{m=0}^{q} (-1)^{m+p} e_{x} \times e_{y_{(m)}} = \sum_{m=0}^{q} \sum_{w \in \Pi_{x,y_{(m)}}} (-1)^{L(w)+m+p} e_{w}.$$

Each pair m, w here gives rise to a pair k, z where k = 0, ..., r and $z \in \Pi_{x,y}^k$ in the following way: choose k such that w_{k-1} projects onto y_{m-1} and w_k projects onto y_{m+1} . Then w_{k-1} and w_k have a common projection onto X, say x_l . Define the path $z \in \Pi_{x,y}^k$ as in (3.19).

Then we have $w = z_{(k)}$ and L(z) = L(w) + p - l. Since k = l + m, we obtain L(z) + k = L(w) + p + mand

$$(-1)^{p} e_{x} \times \partial e_{y} = \sum_{m=0}^{q} \sum_{w \in \Pi_{x,y_{(m)}}} (-1)^{L(w)+m+p} e_{w}$$
$$= \sum_{k=0}^{r} \sum_{z \in \Pi_{x,y}^{k}} (-1)^{L(z)+k} e_{z_{(k)}}.$$

Combining this with (3.17) and (3.20), we obtain (3.14).



Paths w and z. The shaded area represents L(z) - L(w).