Bioinformatika III

Trimačių struktūrų analizė ir spėjimas

Paskaita 4 – koordinačių sistemos

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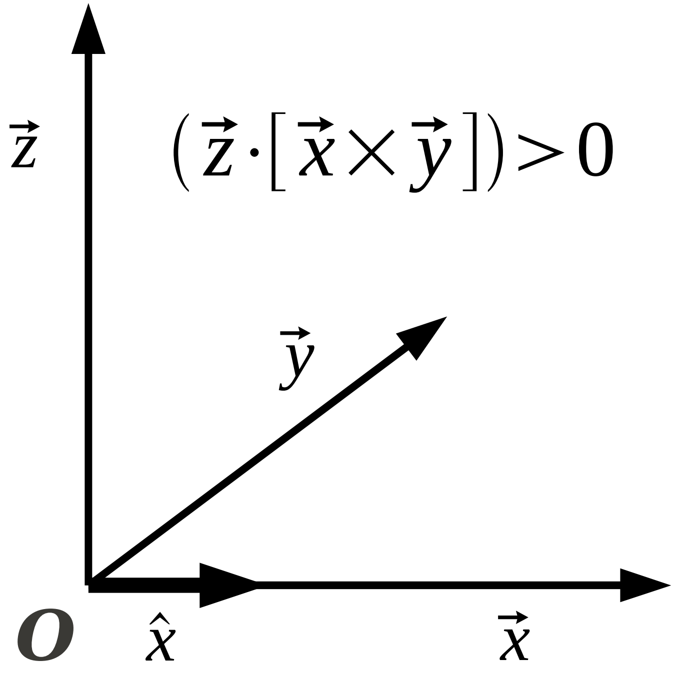
Koordinačių sistemos

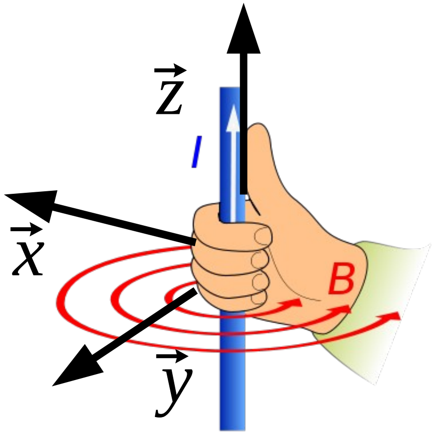
- Kas reikalinga koordinačių sistemai apibrėžti
  - koordinačių pradžia
  - koordinačių ašys
- Kokių tipų būna koordinačių sistemos
  - Kreivinės (pvz. polinės, cilindrines, sferinės)
  - Tiesinės
    - **afininės (nestačiakampės)**
      - **ortogonaliosios (stačiakampės, Dekarto)**
      - **ortonormuotos (su ortonormuota baze)**

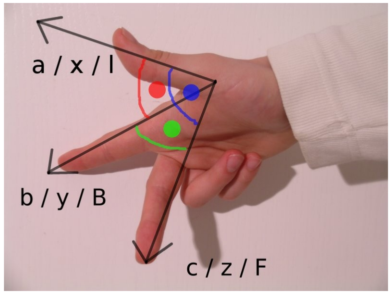
Vektorinės algebros priminimas:
http://saulius-grazulis.lt/~saulius/paskaitos/VU/bioinformatika-III/medžiaga-studentams/vektorių-algebros-faktai.pdf

Koordinačių sistemos komponentai

- Koordinačių pradžia (origin)
- Koordinačių ašys (axes, sg. axis)
- Matavimo vienetai, skalė (units, scale)
- „Ranka“ („hand“, handedness)

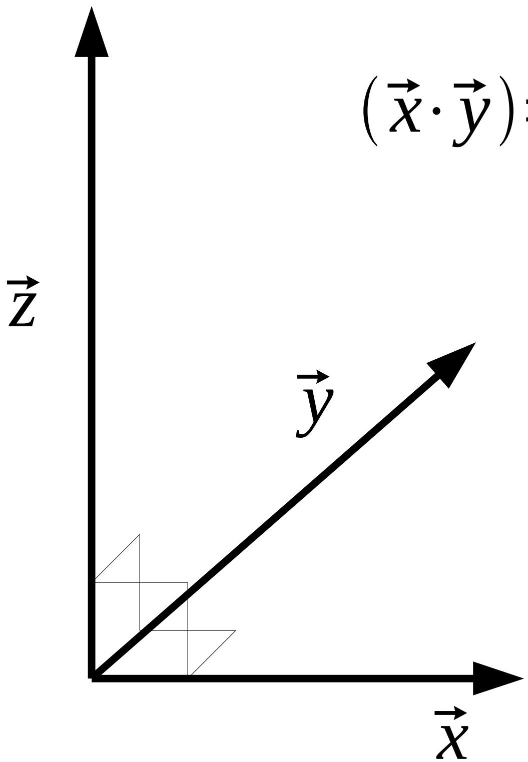


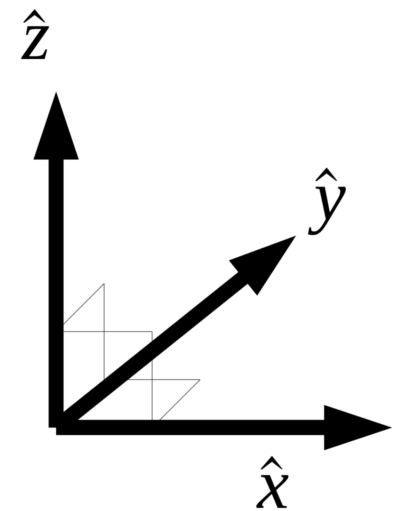




Ortogonaliosios koordinatės

$$(\vec{x}\cdot\vec{y})=(\vec{y}\cdot\vec{z})=(\vec{x}\cdot\vec{z})=0$$





Ortogonaliosios:

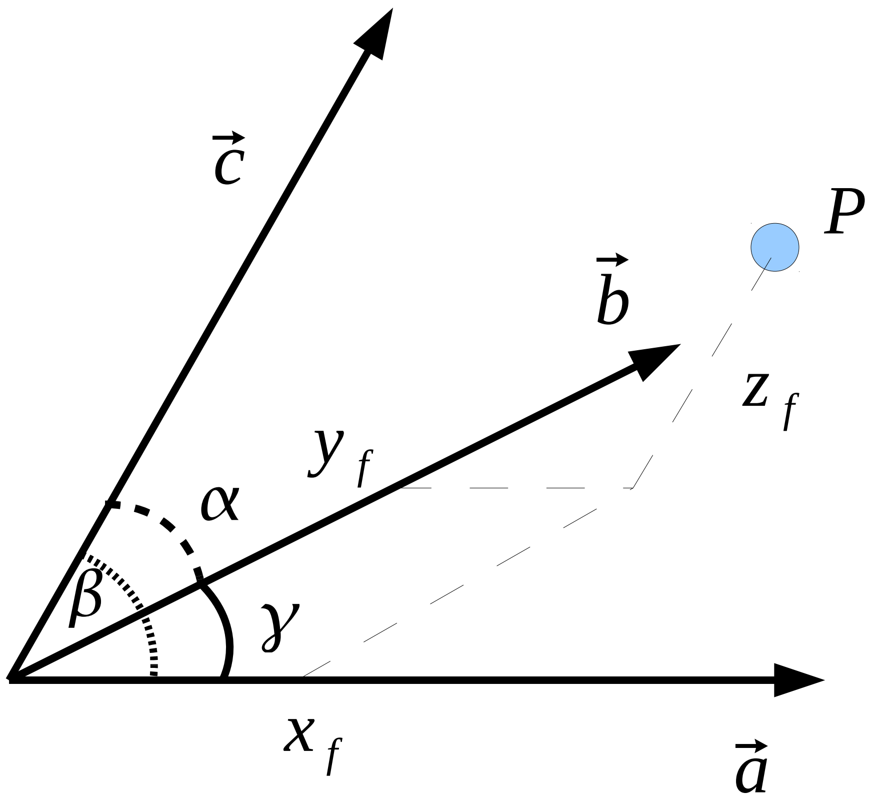
$$(\vec{x}\cdot\vec{x})\neq 0\,;(\vec{y}\cdot\vec{y})\neq 0\,;(\vec{z}\cdot\vec{z})\neq 0$$

Ortonormuotos:

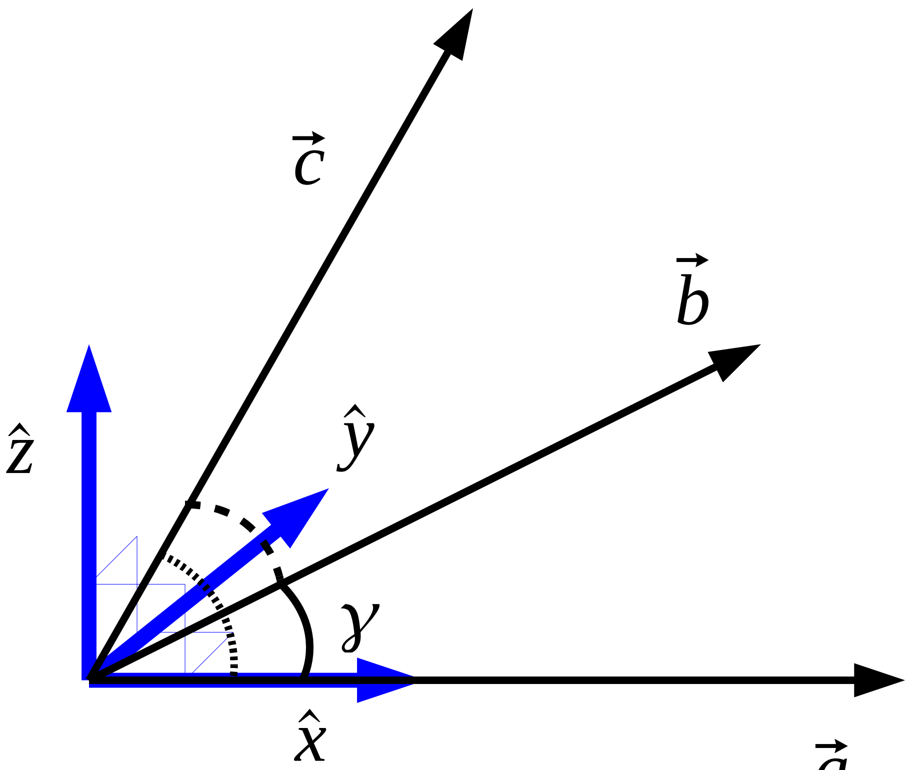
$$(\hat{x}\cdot\hat{x})=(\hat{y}\cdot\hat{y})=(\hat{z}\cdot\hat{z})=1$$

$$\hat{x}=\hat{e}_1\,;\quad \hat{y}=\hat{e}_2\,;\quad \hat{z}=\hat{e}_3\,;\quad \left|(\hat{e}_i\cdot\hat{e}_j)\right|=\delta_{ij}$$

Trupmeninės (afininės) koordinatės



Ortogonalizacija. Gramo-Šmito (Gram–Schmidt) procesas



$$\hat{x}=\vec{a}/\|\vec{a}\|=\vec{a}/a$$

$$\vec{y}=\vec{b}-(\vec{b}\cdot\hat{x})\,\hat{x}$$
$$\hat{y}=\vec{y}/\|\vec{y}\|$$

$$\vec{z}=\vec{c}-(\vec{c}\cdot\hat{x})\,\hat{x}-(\vec{c}\cdot\hat{y})\,\hat{y}$$
$$\hat{z}=\vec{z}/\|\vec{z}\|$$

$$\hat{z}=[\hat{x}\times\hat{y}]$$

PDB ortogonalizacijos susitarimai

If vector a, vector b, vector c describe the crystallographic cell edges, and vector A, vector B, vector C are unit cell vectors in the default orthogonal Angstroms system, then vector A, vector B, vector C and vector a, vector b, vector c have the same origin; vector A is parallel to vector a, vector B is parallel to vector C times vector A, and vector C is parallel to vector a times vector b (i.e., vector c*).

$$\hat{A} = \hat{x} = \vec{a} / \|\vec{a}\| = \vec{a} / a$$

$$\vec{y} = \vec{b} - (\vec{b} \cdot \hat{x})\, \hat{x}$$

$$\hat{y} = \vec{y} / \|\vec{y}\|$$

$$\hat{B} = \vec{B} = [\vec{C} \times \vec{A}]$$

$$\vec{z} = \vec{c} - (\vec{c} \cdot \hat{x})\, \hat{x} - (\vec{c} \cdot \hat{y})\, \hat{y}$$

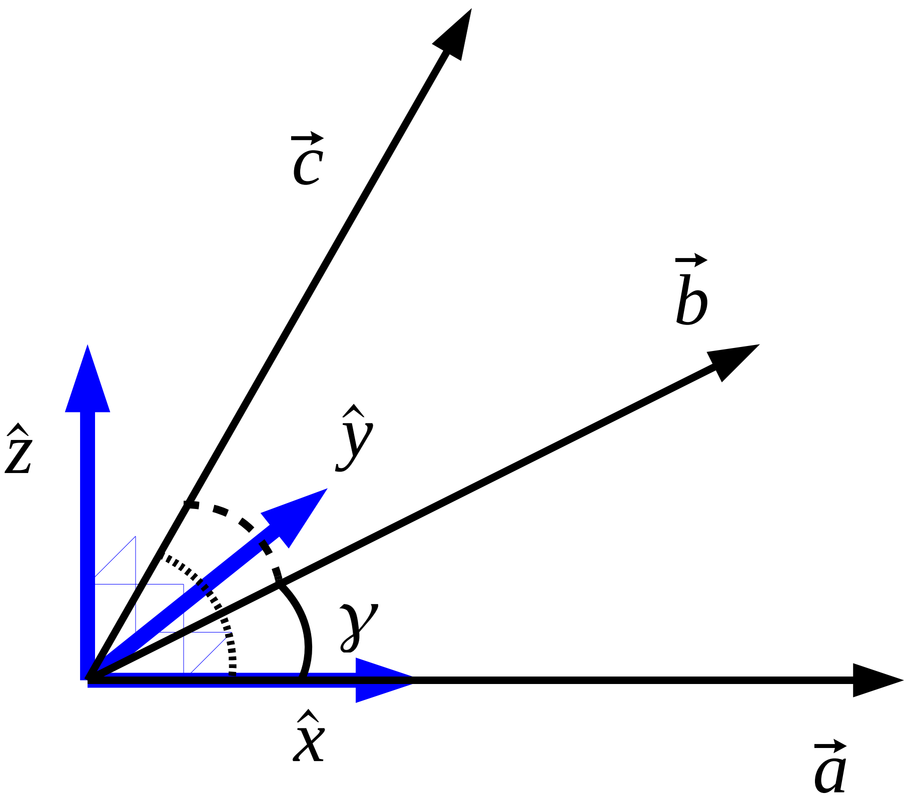
$$\hat{z} = \vec{z} / \|\vec{z}\|$$

$$\vec{C} = \vec{c}^{\,*} = \frac{[\vec{a} \times \vec{b}]}{(\vec{a} \cdot [\vec{b} \times \vec{c}])} ;\ \vec{C} \ \| \ \vec{z}$$

$$\hat{C} = \vec{C} / \|\vec{C}\|$$

http://www.wwpdb.org/documentation/format23/sect8.html

Koordinačių transformacijos



$$\begin{bmatrix} x_f \\ y_f \\ z_f \end{bmatrix} = \begin{bmatrix} x_a & y_a & z_a \\ 0 & y_b & z_b \\ 0 & 0 & z_c \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} a_x & b_x & c_x \\ 0 & b_y & c_y \\ 0 & 0 & c_z \end{bmatrix} \begin{bmatrix} x_f \\ y_f \\ z_f \end{bmatrix}$$

Senosios bazės komponentės naujoje bazėje

PDB failų matricos SCALEn

The SCALEn (n = 1, 2, or 3) records present the transformation from the orthogonal coordinates as contained in the entry to fractional crystallographic coordinates.

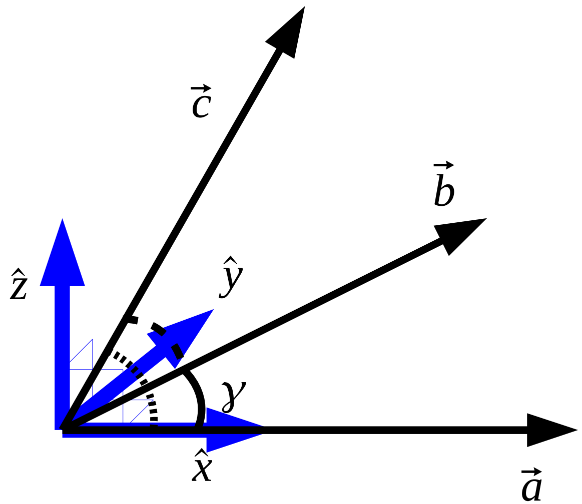
If the orthogonal Angstroms coordinates are X, Y, Z, and the fractional cell coordinates are xfrac, yfrac, zfrac, then:

xfrac = S11X + S12Y + S13Z + U1
yfrac = S21X + S22Y + S23Z + U2
zfrac = S31X + S32Y + S33Z + U3

$$\begin{bmatrix} x_f \\ y_f \\ z_f \end{bmatrix} = \begin{bmatrix} x_a & y_a & z_a \\ 0 & y_b & z_b \\ 0 & 0 & z_c \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

http://www.wwpdb.org/documentation/format23/sect8.html

Skaliarinė sandauga neortogonaliose koordinatėse



$$\begin{bmatrix} x_f \\ y_f \\ z_f \end{bmatrix} = \begin{bmatrix} x_a & y_a & z_a \\ 0 & y_b & z_b \\ 0 & 0 & z_c \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} a_x & b_x & c_x \\ 0 & b_y & c_y \\ 0 & 0 & c_z \end{bmatrix} \begin{bmatrix} x_f \\ y_f \\ z_f \end{bmatrix}$$

Senosios bazės komponentės naujoje bazėje

$$\vec{\mathbf{x}} = \mathbf{E}'\vec{\mathbf{x}}' \qquad \mathbf{E}' = \begin{bmatrix} e_{1x} & e_{2x} & e_{3x} \\ e_{1y} & e_{2y} & e_{3y} \\ e_{1z} & e_{2z} & e_{3z} \end{bmatrix}$$

$$\vec{\mathbf{x}}' = \mathbf{E}\vec{\mathbf{x}}$$

$$\mathbf{E}' = \mathbf{E}^{-1};\ \mathbf{E}\cdot\mathbf{E}' = \mathbf{I}$$

$$(\vec{\mathbf{x}}_1 \cdot \vec{\mathbf{x}}_2) = \vec{x}_1^{\,T}\vec{x}_2 = x_1 x_2 + y_1 y_2 + z_1 z_2 =$$
$$= (\vec{\mathbf{x}}_1' \cdot \vec{\mathbf{x}}_2') =$$
$$= \vec{x}_1'^{T} E'^{T} E' \vec{x}_2'$$

Metrinis tenzorius

$$G = E'^T E'$$

$$G = E'^T E' = \begin{bmatrix} e_{1x} & e_{1y} & e_{1z} \\ e_{2x} & e_{2y} & e_{2z} \\ e_{3x} & e_{3y} & e_{3z} \end{bmatrix} \begin{bmatrix} e_{1x} & e_{2x} & e_{3x} \\ e_{1y} & e_{2y} & e_{3y} \\ e_{1z} & e_{2z} & e_{3z} \end{bmatrix} = \begin{bmatrix} (\vec{\boldsymbol{e}}_1 \cdot \vec{\boldsymbol{e}}_1) & (\vec{\boldsymbol{e}}_1 \cdot \vec{\boldsymbol{e}}_2) & (\vec{\boldsymbol{e}}_1 \cdot \vec{\boldsymbol{e}}_3) \\ (\vec{\boldsymbol{e}}_2 \cdot \vec{\boldsymbol{e}}_1) & (\vec{\boldsymbol{e}}_2 \cdot \vec{\boldsymbol{e}}_2) & (\vec{\boldsymbol{e}}_2 \cdot \vec{\boldsymbol{e}}_3) \\ (\vec{\boldsymbol{e}}_3 \cdot \vec{\boldsymbol{e}}_1) & (\vec{\boldsymbol{e}}_3 \cdot \vec{\boldsymbol{e}}_2) & (\vec{\boldsymbol{e}}_3 \cdot \vec{\boldsymbol{e}}_3) \end{bmatrix}$$

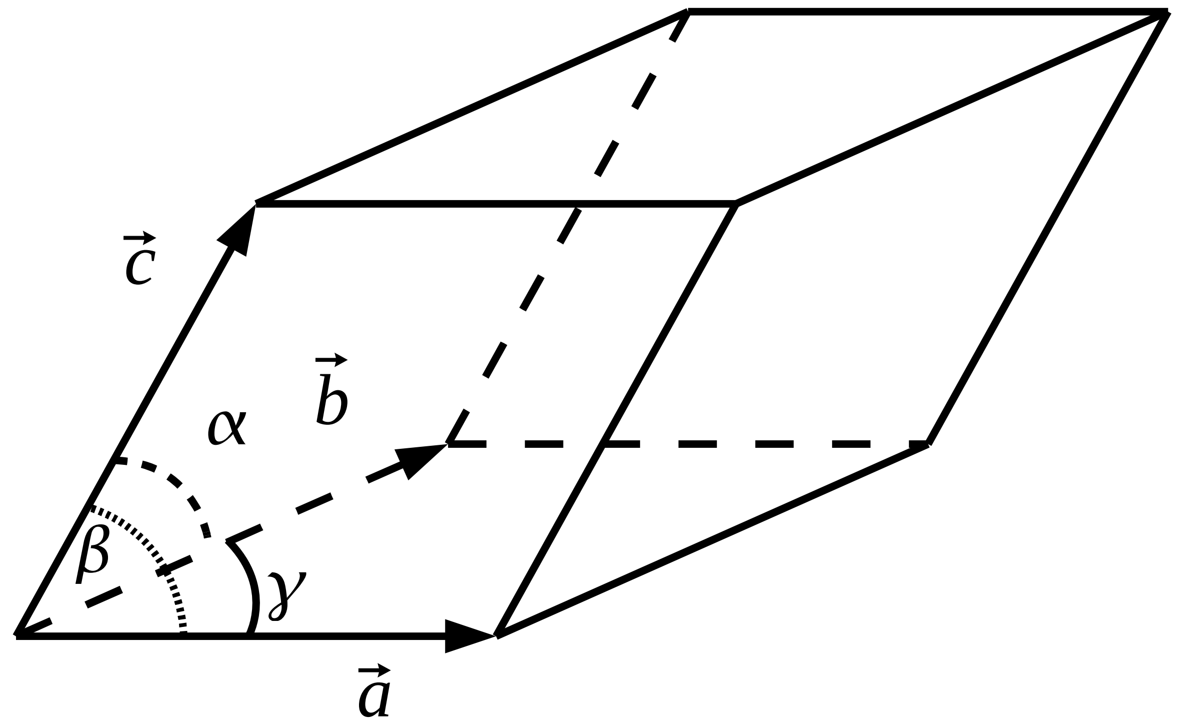
$$G = G^T$$

$$G = \begin{bmatrix} (\vec{\boldsymbol{a}} \cdot \vec{\boldsymbol{a}}) & (\vec{\boldsymbol{a}} \cdot \vec{\boldsymbol{b}}) & (\vec{\boldsymbol{a}} \cdot \vec{\boldsymbol{c}}) \\ (\vec{\boldsymbol{b}} \cdot \vec{\boldsymbol{a}}) & (\vec{\boldsymbol{b}} \cdot \vec{\boldsymbol{b}}) & (\vec{\boldsymbol{b}} \cdot \vec{\boldsymbol{c}}) \\ (\vec{\boldsymbol{c}} \cdot \vec{\boldsymbol{a}}) & (\vec{\boldsymbol{c}} \cdot \vec{\boldsymbol{b}}) & (\vec{\boldsymbol{c}} \cdot \vec{\boldsymbol{c}}) \end{bmatrix}$$

$$(\vec{\boldsymbol{x}}_1 \cdot \vec{\boldsymbol{x}}_2) = \vec{x}_1^{\,T} G \, \vec{x}_2$$

Elementarios gardelės tūris

$$V = (\vec{a} \cdot [\vec{b} \times \vec{c}]) = \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix} = \sqrt{|\det G|}$$



Metrinio tenzoriaus determinantas

$$[\vec{b}\times\vec{c}]=\begin{vmatrix}\hat{\boldsymbol{x}} & \hat{\boldsymbol{y}} & \hat{\boldsymbol{z}}\\ b_x & b_y & b_z\\ c_x & c_y & c_z\end{vmatrix}=\hat{\boldsymbol{x}}(b_y c_z-b_z c_y)+\hat{\boldsymbol{y}}\ldots$$

$$V=(\vec{a}\cdot[\vec{b}\times\vec{c}])=a_x(b_y c_z-b_z c_y)+a_y\ldots=\begin{vmatrix}a_x & a_y & a_z\\ b_x & b_y & b_z\\ c_x & c_y & c_z\end{vmatrix}=$$

$$=\det E'^T=\det E'$$

$$\det G=\det(E'^T E)=\det(E'^T)\det(E')=(\det E')^2$$

$$V=(\vec{a}\cdot[\vec{b}\times\vec{c}])=\det(E')=\sqrt{|\det G|}$$