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Mathematical Models of Oversaturated Protein Spots

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Introduction

In proteomics two-dimensional gel electrophoresis (2DE) is used for protein separation according to their isoelectric point (p*I*) and molecular mass (MM). The result of 2DE process is then scanned with high sensitivity scanner for the further image analysis. *Detection* and *quantification* of protein spots in scanned 2DE image are bottlenecks in the proteomics initial workflow.

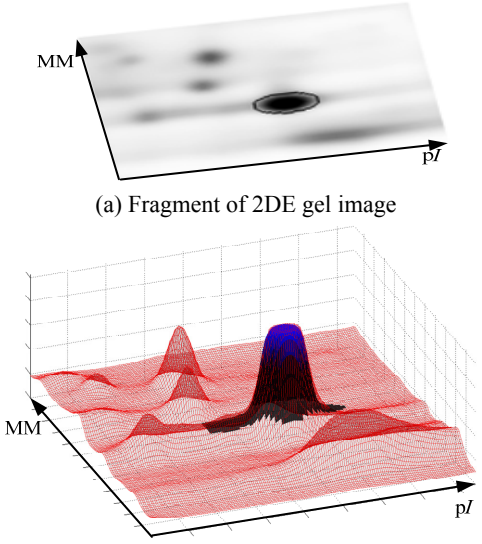
Protein spots in 2DE gel images (see Fig. 1.a) can be detected by numerous ways that in general can be classified as nonparametric or parametric spot detection methods. Melanie II software package, for example, uses nonparametric procedures based on Laplacian of the pixel intensities to decide whether pixel belongs to the protein spot or not [1]. Another popular nonparametric method is based on watershed transformation. It and its modifications preventing over-segmentation are used to segment 2DE gel images, too. [2, 3].

Parametric protein spot detection methods for data fitting require mathematical model of the spot shape (intensity distribution). Such protein spot shape models found in literature are: Gaussian [4], Flat-Top [5], Irregular [6], extension of Gaussians with Hermite functions [7], conjunction of two or three Gaussians with different parameters [8].

Images of 2DE gels vary in resolution, their geometry and can be affected by oversaturation. These artefacts prohibits from correct image segmentation and spot quantification sometimes forcing to use the blue toning after silver staining or even to repeat the 2DE.

In order to increase the visibility (separateness) of individual proteins that are distributed in a gel several specific staining methods are used. Silver staining is one of the most sensitive methods used for protein staining after 2DE fractionation. If staining reagent is overdosed or development time is prolonged, then truncated spots with saturation effects in gel images can appear.

The shape model used for parametric protein spot detection must cope with most of the artefacts appearing in images. That is why models (see Fig. 1.b) to be presented assume the influence of diffusion, oversaturation and artefacts when intensities are highest near the edge of the spot and smaller near the spot centre.



(a) Fragment of 2DE gel image

(b) 3D view of protein spot and its reconstruction

Fig. 1. Protein oversaturated spot and its shape modeling

In the following we overview all available in the literature protein spot shape models, including those used in processing data from microarrays, introduce to three original – 4 Gaussian, Bell and 4 Splines – oversaturated protein spot shape models and present experimental results on comparison of different shape models success to represent oversaturated protein spots.

Spot Shape Models for 2DE Gel Images

The most commonly used [4] for parametric protein spot detection in 2DE gel images is the *Anisotropic Gaussian Shape Model*:

$$S_{\mathrm{AG}}(x,y) = B + I \cdot \mathrm{e}^{-\left(\frac{(x-x_0)^2}{2\sigma_{\mathrm{x}}^2}+\frac{(y-y_0)^2}{2\sigma_{\mathrm{y}}^2}\right)}. \qquad (1)$$

Here B – background intensity; I – spot intensity; x_0 and y_0 are coordinates of control spot location; σ_{x} and σ_{y} – spread of the Gaussian distribution in x (isoelectric point) and y (molecular mass) directions, respectively.

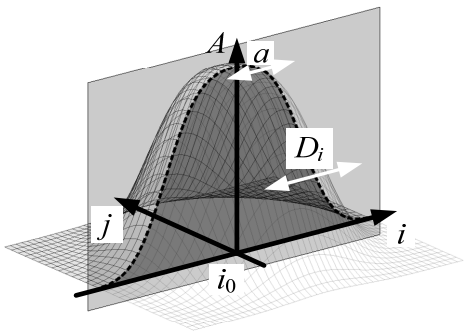


Fig. 2. Cross-section of Flat-Top shape model

Though this shape model is unsophisticated and gives opportunity to assume the spread of intensities in both x and y directions, model fits properly only for symmetric protein spots without saturation.

In case of over saturation, *Flat-Top Shape Model* [5] represents protein spot more adequately:

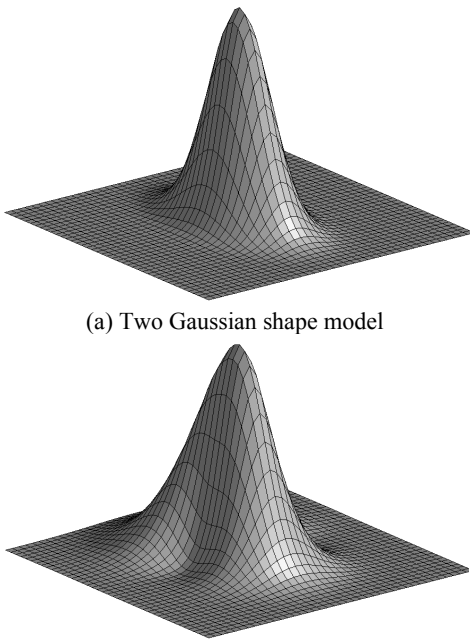
$$S_{\mathrm{FT}}(x,y) = B + \frac{C_0}{2}\left[\operatorname{erf}\left(\frac{a'+r'}{2}\right) + \operatorname{erf}\left(\frac{a'-r'}{2}\right)\right] + \frac{C_0}{r'\sqrt{\pi}} \cdot \mathrm{e}^{-\left[\left(\frac{a'+r'}{2}\right)^2 + \left(\frac{a'-r'}{2}\right)^2\right]}. \quad (2)$$

Here B – background intensity; C_0 – initial protein concentration; $r' = \sqrt{(x-x_0)^2 / D'_{\mathrm{x}} + (y-y_0)^2 / D'_{\mathrm{y}}}$; D'_{x} and D'_{y} are constants, related to diffusion in respective directions; x_0 and y_0 are coordinates of control spot location; a' – radius of circular protein substance diffusion area. This model (see Fig. 2) assumes the flatted top of the oversaturated protein spot and fits more adequately than Anisotropic Gaussian Shape Model [5].

Both presented protein spot shape models can represent regular and symmetric spots, however in 2DE gel images irregular spot shape variation frequently appears. Such protein spots can be represented with model, proposed by Mike Rogers et al. [6]. *Irregular Spot Shape Model* is constructed with two-dimensional convolution of protein spot shape and Gaussian distribution. The shape of the protein spot is obtained with use of Point Distribution Model, for representing variation of protein spot shape observed in a training set.

The Irregular Spot Shape Model fits protein spot more adequately than other two mentioned above, still it does not represent the oversaturated spot. Parametric protein spot detection methods based on this model are more suitable for 2DE gels with fluorescent staining and give major residual error in silver stained 2DE gels, where oversaturation and spots overlapping appear frequently [6]. In silver stained 2DE gels with protein overdosing, protein spots with loss off central quantity may appear. None of presented three shape models counts for this type of artifacts.

Conjunction of two or three Gaussians with different set of parameters opens possibilities to fit protein spots that are symmetric but have different radiuses in x and y axes



(a) Two Gaussian shape model

(b) Three Gaussian shape model

Fig. 3. Modified Gaussian shape models

directions (see Fig. 3a), or have tips that are shifted in a particular direction (see Fig. 3.b).

Let us in brief discuss how modified Gaussian shape models are constructed (for detailed treatment of this issue consult [8]). The *Two Gaussian Shape Model* construction algorithm works as follows.

Step 1 – *Protein Spot Contour Extraction*: gel image inversion; watershed transformation in order to segment area; detection of the anchor point maximum of local minima; morphological filling started at anchor point; morphological erosion followed by dilation; formation of the contour.

Step 2 – *Detection of a Centre of Protein Spot*. It is done fitting an ellipse to extracted contour using least square fitting procedure. The aim of selected conic fitting procedure is to minimize the sum of squared algebraic distances. Found centre of the ellipse is afterwards treated as the centre of protein spot to be reconstructed.

Step 3 – *Selection of Estimation Data.* It is used for following spot construction.

Step 4 – *Calculation of Parameters of Two Gaussian Models*. The peak value of reconstructed spot intensity is calculated based on all estimation data. The shape of protein spot in x and y directions is determined based on mean values of estimation data taken from both sides with respect to the centre of protein spot.

Step 5 - *Synthesis of Gaussian Distributions*. It also involves mixture of different distributions with the original protein spot data.

Because of irregularity of oversaturated spots, the reconstruction based on symmetric Gaussian distributions can give inaccurate results for protein quantification. Distributions of protein spot intensity in directions parallel to vertical axis are often different. This can be justified by the nature of proteins movement in the gel. Thus *Three Gaussian Shape Model* assumes the symmetry of protein spot intensity only in isoelectric point axis.

Spot Shape Models for Microarray Images

DNA-array technology is frequently used for the generation of genome-wide gene expression profiles. The scanned arrays are analyzed with specialized image analysis software to identify and quantify spots, which yields information about differentially expressed or coregulated genes [9].

Spots in microarrays are different due to array preparation procedure for experiment, array type, nature of the DNA material. Spot models for microarrays are created predicating on experimental evidence. According to empirical observations three spot shape properties are given for the microarrays:

1) the distribution of intensity is isotropic;

2) protein spot intensities are often highest near the edge of the spot and smaller near the centre (such features of the protein spot shape can be observed in 2DE gels for oversaturated spots);

3) pixels close together and with the same distance from the protein spot centre should be more correlated than pixels further apart.

Several spot shape distribution models [9, 10] are used for processing:

1) *Normalized Cylindrical shape model*

$$S_{\mathrm{NC}}(r)=\begin{cases}\dfrac{1}{\pi d^2}, & \text{if } r\le d;\\ 0, & \text{otherwise.}\end{cases} \tag{3}$$

Here r – Euclidean distance to the centre of the spot; d – the radius of the spot;

2) *Normalized 2D Gaussian shape model*

$$S_{\mathrm{NG}}(r)=\frac{1}{2\pi\sigma^2}\cdot \mathrm{e}^{-\frac{(r-r_0)^2}{2\sigma^2}}. \tag{4}$$

Here r_0 – the centre of the spot; σ – standard deviation;

3) *Two Subtracted Normalized 2D Gaussian shape model*

$$S_{\mathrm{SNG}}(r)=\frac{1}{1-s}\left[\frac{1}{2\pi\sigma_1^2}\cdot \mathrm{e}^{-\frac{(r-r_0)^2}{2\sigma_1^2}}-\frac{s}{2\pi\sigma_2^2}\cdot \mathrm{e}^{-\frac{(r-r_0)^2}{2\sigma_2^2}}\right]. \tag{5}$$

Here s – scaling-factor ($s=0.1$); σ_1 and σ_2 are standard deviations for the initial and subtracted Gaussians respectively.

4) *Polynomial-Hyperbolic shape model*

$$S_{\mathrm{PH}}(r)=\begin{cases}\dfrac{K}{d^2}\cdot \mathrm{e}^{g(r/d)}, & \text{if } 0\le r<\gamma d;\\ 0, & \text{otherwise.}\end{cases} \tag{6}$$

Here K – a constant function of the parameters $b_1,\ldots,b_I$, a, and γ such that:

$$\int_0^{\infty}\int_0^{2\pi} S(r)\,r\,dr\,d\theta=1. \tag{7}$$

Parameters a and γ determine the steepness of the spot edge, while g is the function of r:

$$g(r)=\sum_{i=1}^{I} b_i r^i-\frac{a}{\gamma-r}, \quad \text{where } 0\le r<\gamma \ . \tag{8}$$

All of the shown spot models are adapted to microarray images. However, comparing spots in microarrays with protein spots in 2DE gels some general statements about spots in microarrays can be made:

1) the diffusion in only one direction manifests;

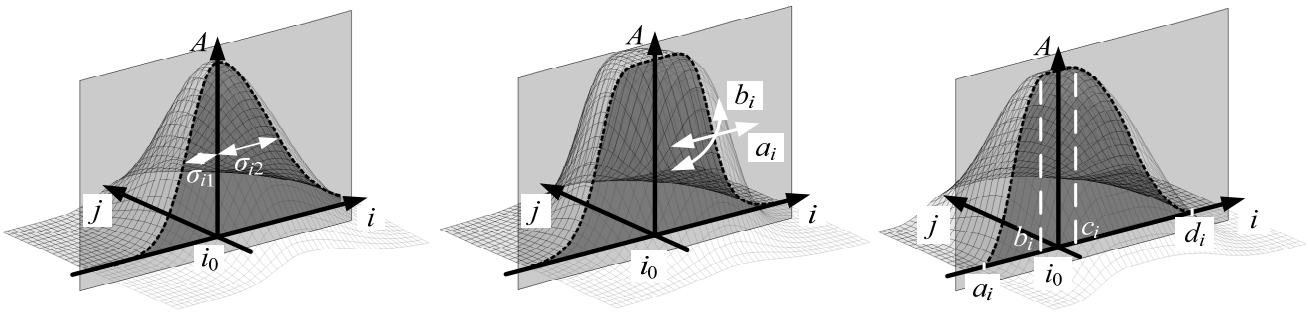
2) the spot saturation similar to protein spots in 2DE gels appears.

Consequently, shape models used for spots in microarrays could be adjusted to suit protein spots in 2DE gel images by incorporation of additional variables that should describe the protein diffusion in two directions.

New Oversaturated Protein Spot Shape Models

Given the natural need to use small as possible number of model parameters, shape model flexibility is a major concern in the oversaturated protein spot modelling. The more flexible spot shape model is used for protein spot detection, the more accurate matching can be expected for differently distorted spot shapes.

Frequently in 2DE gels various diffusion effects appear, when protein in the spot dilates in all four different directions with individual dispersion. Anisotropic Gaussian Spot Shape Model can only partially fit such spots.



(a) Four Gaussian shape model (b) Bell shape model (c) Four Splines shape model

Fig. 4. Cross-sections of three protein spot shape models

One solution can be to use generalized *Four Gaussian Spot shape model* with four different dispersion coefficients in each direction (see Fig. 4.a):

$$S_{4G}(x,y) = I + B\left[\delta_x \cdot e^{-\frac{(x-x_0)^2}{2\sigma_{x1}^2}} + \overline{\delta_x} \cdot e^{-\frac{(x-x_0)^2}{2\sigma_{x2}^2}}\right] \times \left[\delta_y \cdot e^{-\frac{(y-y_0)^2}{2\sigma_{y1}^2}} + \overline{\delta_y} \cdot e^{-\frac{(y-y_0)^2}{2\sigma_{y2}^2}}\right], \quad (9)$$

here

$$\delta_x = \begin{cases} 1, & \text{if } x \le x_0; \\ 0, & \text{otherwise;} \end{cases} \quad (10a)$$

$$\delta_y = \begin{cases} 1, & \text{if } y \le y_0; \\ 0, & \text{otherwise.} \end{cases} \quad (10b)$$

The presented shape model fits protein spot more adequately but still does not solve the saturated protein spot case. This shape model likewise anisotropic model uses Gaussian distributions for constructing spot shape. In case of oversaturated protein spot, Gaussian based model gives relatively high inaccuracy of spot shape fitting. However the flat top of the protein spot shape, for the saturated spot may be obtained by defining different centre point for each Gaussian distribution used in shape model.

Other solution for oversaturated protein spot shape modelling is to replace Gaussian with flat-top shape. The generalized Bell Function gives flat-top shape and depends on only three parameters:

$$S_{BF}(x,y) = \frac{1}{1+\left|\frac{x-c_x}{a_x}\right|^{2b_x}} \cdot \frac{1}{1+\left|\frac{y-c_y}{a_y}\right|^{2b_y}}. \quad (11)$$

Here a – distance to the spot centre; b - slope steepness; c – centre of the shape. *Bell Function Spot shape model* assesses the flat-top saturated spot feature, though it is symmetrical in vertical and horizontal axes (see Fig. 4.b).

Finally, using spline-based curve, *Four Splines Protein Spot shape model* can be created (see Fig. 4.c). This shape model consist of four parameters a, b, c and d and could be expressed by:

$$S_{4S}(x,y) = S_E \cdot S_W \cdot S_N \cdot S_S, \quad (12)$$

here

$$S_E = \begin{cases} 0, & \text{if } x \le a; \\ \frac{2(x-a)^2}{(x_0-b-a)^2}, & \text{if } a < x \le \frac{a+x_0-b}{2}; \\ 1-\frac{2(x_0-b-x)^2}{(x_0-b-a)^2}, & \text{if } \frac{a+x_0-b}{2} < x \le x_0-b; \\ 1, & \text{if } x > x_0-b; \end{cases} \quad (13.a)$$

$$S_W = \begin{cases} 1, & \text{if } x \le d; \\ 1-\frac{2(x_0+c-x)^2}{(x_0+c-d)^2}, & \text{if } d < x \le \frac{d+x_0+c}{2}; \\ \frac{2(x-d)^2}{(x_0+c-d)^2}, & \text{if } \frac{d+x_0+c}{2} < x \le x_0+c; \\ 0, & \text{if } x > x_0+c; \end{cases} \quad (13.b)$$

$$S_N = \begin{cases} 0, & \text{if } y \le a; \\ \frac{2(y-a)^2}{(y_0-b-a)^2}, & \text{if } a < y \le \frac{a+y_0-b}{2}; \\ 1-\frac{2(y_0-b-y)^2}{(y_0-b-a)^2}, & \text{if } \frac{a+y_0-b}{2} < y \le y_0-b; \\ 1, & \text{if } y > y_0-b; \end{cases} \quad (13.c)$$

$$S_S = \begin{cases} 1, & \text{if } y \le d; \\ 1-\frac{2(y_0+c-y)^2}{(y_0+c-d)^2}, & \text{if } d < y \le \frac{d+y_0+c}{2}; \\ \frac{2(y-d)^2}{(y_0+c-d)^2}, & \text{if } \frac{d+y_0+c}{2} < y \le y_0+c; \\ 0, & \text{if } y > y_0+c. \end{cases} \quad (13.d)$$

Presented saturated spot shape model may assess different dilation in four directions and should give relatively lower inaccuracy for saturated spot to compare to spot shape model, constructed using four Gaussian distributions.

Experimental Comparative Study of Oversaturated Protein Spot Shape Models

Comparison of the oversaturated spot shape models was done by fitting models to original protein spot data with large-scale nonlinear optimization algorithm based on interior-reflective Newton method [11]. The algorithm determines best model parameters minimizing following residual:

$$E_r = \sum_{x,y \in R} \frac{\left[S(x,y \mid \vec{p}) - I(x,y)\right]^2}{n_R\left(I_R^{max} - I_R^{min}\right)}. \quad (14)$$

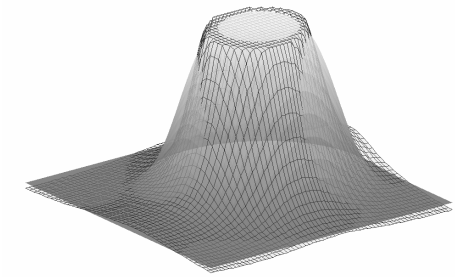
Here R – the region of the image over which fitting takes place; x and y – coordinates of the pixels within the fitting region; $I(x,y)$ – intensity of image in the region; $S(x,y \mid \vec{p})$ – model values given the parameter vectors; I_R^{max} and I_R^{min} are the maximum and minimum image intensity values within the region; n_R – number of pixels within the region.

Table 1 Results of residual error, *r*

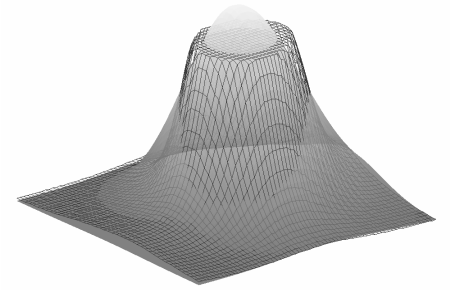
PROTEIN SPOT	SHAPE MODEL							
	Flat-Top		Four Gaussian		Four Splines		Bell	
	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Std. Dev.
Oversaturated	2,300	1,850	2,270	1,960	2,730	1,970	2,030	1,740
Big size	1,170	1,270	0,811	0,839	1,440	1,020	1,050	1,190
Small size	1,160	1,020	0,824	0,753	1,530	0,922	0,992	0,829

Table 2 Results of relative processing time

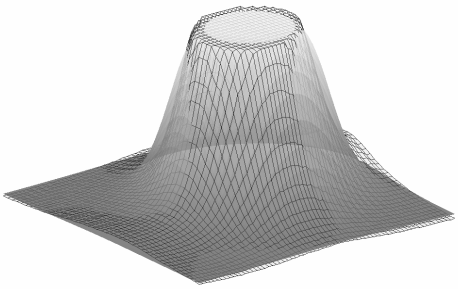
PROTEIN SPOT	SHAPE MODEL							
	Flat-Top		Four Gaussian		Four Splines		Bell	
	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Std. Dev.
Oversaturated	1,000	0,000	0,111	0,073	0,351	0,280	0,169	0,103
Big size	1,000	0,000	0,068	0,038	0,170	0,130	0,118	0,069
Small size	1,000	0,000	0,057	0,024	0,175	0,111	0,126	0,149



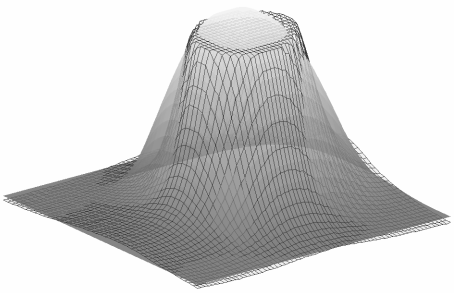
(a) Flat-Top shape model



(b) Four Gaussian shape model



(c) Bell shape model



(d) Four Splines shape model

Fig. 5. Results of four different protein shape models fitted on the same natural oversaturated protein spot

We compare Flat-Top, Four Gaussian, Bell and Four Splines protein spot shape models. In Fig. 5 3D views of the results of these protein shape models fitted on the same natural oversaturated protein spot are presented. It follows, that Four Gaussian shape model clearly overshoots top of oversaturated protein spot data and thus its use in this case does not show promising. On the other hand, Bell shape model seems to better fit top of oversaturated protein spot than Flat-Top shape model. Finally, Four Splines shape model seems to fit lower part of protein spot area more closely than other shape models.

Let us test our statements on 84 various natural protein spot data. In order to discriminate between different shapes, we divide spots into three categories: oversaturated, big and small.

Results of achieved residual errors (14) for shape models under investigation are summarized in Table 1. Minimal mean values for each spot category are emphasized by gray background.

Another important issue in any modeling is a processing time needed to carry out all necessary computations. Thus computation time was measured also and the summary of the results is presented in the Table 2. Again, minimal mean values for each spot category are emphasized by gray background.

Conclusions

The overview of available in the literature protein spot shape models for 2DE gel and microarray images showed the lack of flexible model for oversaturated spot.

Three original oversaturated protein spot shape models – Four Gaussian, Bell and Four Splines – were developed and presented. Experimental comparative study of these models to Flat-Top model showed, that:

a) Bell shape model fits best to oversaturated protein spots with about 1.8 times increase of computational time;

b) Four Gaussian shape model fits best to non-saturated spots and requires smallest computational time.

References

1. **Appel R. D., Palagi P. M., Walther D., Vargas J. R., Sanchez J.-C., Ravier F., Pasquali C., Hochstrasser D. F.** Melanie II – a Third-Generation Software Package for Analysis of Two-Dimensional Electrophoresis Images // Electrophoresis. – 1997. – No.15(18). – P. 2724 – 2734.

2. **Matuzevičius D., Navakauskas D.** Investigation of Segmentation Methods for Proteomics // Electronics and Electrical Engineering. – 2005. – No.7(63). – P. 74 – 78.
3. **Alt H., Hoffmann F., Kriegel K., Wenk C., Pleissner K.-P., Wegner S., Sahlströhm A., Oswald H., Fleck E.** New Algorithmic Approaches to Protein Spot Detection and Pattern Matching in Two Dimensional Electrophoresis Gel Databases // Electrphoresis.– 1999. – No. 20. – P. 755 – 765.
4. **Garrels J. I.** The QUEST System for Quantative Analysis of Two-Dimensional Gels // Journal of Biological Chemistry. – 1989. – No.264(9). – P. 5269 – 5282.
5. **Bettens E., Scheuders P., Van Dyck D., Moens L., Van Osta P.** Computer Analysis of Two-Dimensional Electrophoresis Gels: A New Segmentation and Modelling Algorithm // Electrophoresis.– 1997.– No.18.– P. 792 – 798.
6. **Rogers M., Graham J., Tonge R. P.** Automatic Construction of Statistical Shape Models for Protein Spot Analysis in Electrophoresis Gels // British Machine Vision Conference. – September, 2003.
7. **Wilson R.** Modelling of 2d Gel Electrophoresis Images for Proteomics Databases // 16th International Conference on Pattern Recognition (ICPR'02). – 2002. – Vol. 1. – P. 767 – 770.
8. **Serackis A., Matuzevičius D., Navakauskas D.** Reconstruction of Protein Spots Using DSP Modules // International Conference on Fundamentals of Electronics and Circuit Theory XXIX IC-SPETO. – May 24-27, 2006. – Vol. 2. – P. 573 – 576.
9. **Wierling C., Steinfath M., Elge T., Schulze-Kremer S., Aanstad P., Clark M., Lehrach H., Herwig R.** Simulation of DNA Array Hybridization Experiments and Evaluation of Critical Parameters During Subsequent Image and Data Analysis // BMC Bioinformatics. – 2002. – No.1(3). – P. 29.
10. **Ekstrøm C. T., Bak S., Kristensen C., Rudemo M.** Spot Shape Modelling and Data Transformations for Microarrays // Bioinformatics, 2004. – No.14(20). – P. 2270 – 2278.
11. **Coleman T. F., Y. Li** An Interior, Trust Region Approach for Nonlinear Minimization Subject to Bounds // SIAM Journal on Optimization. – 1996. – Vol. 6. – P. 418 – 445.

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Two-dimensional electrophoresis is used for protein separation in a special gel according isoelectric point and molecular mass, and remains one of most progressive technologies for protein analysis. As a result, gels are digitized and their images are process with software. The dynamic diapason of intensities of protein spots is very wide, thus software tools become too sensitive to various artefacts inevitable present in gel images. Often matching with reference or modelling of protein spot intensity distribution is done willing to get better protein spot estimates. Nevertheless that many protein spot models exist, they take into account only particular spot shape artefact. In the article modern protein spot models applicable in two-dimensional electrophoresis and DNR arrays are analysed. It is shown that symmetry is preserved only for protein spots in DNR arrays. Three new protein spots shape models – 4G, 4S and Bell shape – are presented in order to cope with shape distortion and asymmetry. Results of experimentation with 84 distorted protein spots applying three developed shape models and one of most popular – Flat-Top shape model are presented. It is shown that Bell shape model fits best to oversaturated protein spots while 4G shape model fits best to non-saturated spots and requires smallest computational time. Ill. 5, bibl. 11 (in English; summaries in English, Russian and Lithuanian).

Д. Матузявичус, А. Серацкис, Д. Навакаускас. Математическая модель искажённых пятен двухмерного электрофореза белков // Электроника и электротехника. – Каунас: Технология, 2006. – № 1(73). – С. 63–68.

Двумерный электрофорез является одной из лучших технологий выделения белков, позволяющая в специальном геле разделить белки по их молекулярной массе и изоэлектронной точке. Большой динамический диапазон яркостей, присущий пятнам белков, делает современное программное обеспечение очень чувствительным к неизбежным искажениям изображений гелей. Для повышения точности оценки искаженных пятен белков производится моделирование двумерного распределения интенсивности пятен белков. Чаще всего модели пятен белков предназначены для оценки только одного типа искажений формы. В настоящей статье рассматриваются современные модели пятен белков, используемые в двумерном электрофорезе и для анализа изображений цепочек ДНК. Представлены три новые модели – 4G, 4S и колоколообразной формы – учитывающие искажения формы и асимметрию пятен белков. Представлены результаты экспериментального моделирования 84 искаженных в различной степени пятен белков с использованием трех предлагаемых моделей и одной из популярнейшей в настоящее время модели пятен белков – формы «плоской шляпы». Установлено, что: а) наименьшая усредненная погрешность для пятен белков с ограниченной вершиной получается при использовании колоколообразной модели пятна; б) модель пятна 4G формы подстраивается быстрее других и получается наименьшая погрешность, если вершины пятен белков не ограничены. Ил. 5, библ. 11 (на английском языке; рефераты на английском, русском и литовском яз.).

D. Matuzevičius, A. Serackis, D. Navakauskas. Persisotinusiųjų baltymų dėmių matematiniai modeliai // Elektronika ir elektrotechnika. – Kaunas: Technologija, 2006. – Nr. 1(73). – P. 63–68.

Dvimatė elektroforezė yra viena pažangiausių baltymų išskyrimo technologijų, leidžianti specialiame gelyje suskirstyti baltymus pagal jų molekulinę masę ir izoelektrinį tašką. Šio proceso metu gautų gelių vaizdai yra skaitmeninami ir toliau apdorojami naudojant programinę įrangą. Didelis baltymų dėmių skaisčio dinaminis diapazonas daro šiuolaikines programas jautrias neišvengiamiems gelių vaizdų iškraipymams. Norint tiksliau įvertinti iškraipytas baltymų dėmes, dažniausiai lyginama su etalonu arba modeliuojamas baltymų dėmių intensyvumo dvimatis pasiskirstymas. Nors šiuo metu turima daug baltymų dėmių modelių, tačiau dažniausiai jie skirti tik vienos rūšies formos iškraipymams įvertinti. Straipsnyje apžvelgiami šiuolaikiniai baltymų dėmių modeliai, naudojami dvimatės elektroforezės ir DNR rinkinių vaizdams analizuoti. Parodoma, kad tik DNR rinkiniuose esančioms baltymų dėmėms būdinga dvikryptė simetrija. Pristatomi trys nauji baltymų dėmių modeliai – 4G, 4S ir varpo formos, sudaryti atsižvelgiant į formos iškraipymus ir baltymų dėmių asimetriją. Pateikiami modeliavimo eksperimentų su 84 skirtingomis iškraipytomis baltymų dėmėmis rezultatai, gauti naudojant tris siūlomus ir šiuo metu populiariausią – plokščios skrybėlės formos – baltymų dėmių modelius. Nustatyta, kad: a) mažiausia vidutinė priderinimo klaida viršūnėse apribotoms baltymų dėmėms gaunama naudojant naują varpo formos dėmės modelį; b) 4G dėmės formos modelis greičiausiai priderinimas ir gaunama mažiausia vidutinė priderinimo klaida, jei baltymų dėmių viršūnės nėra apribotos. Il. 5, bibl. 11 (anglų kalba; santraukos anglų, rusų ir lietuvių k.).

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