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Approximation of spectroradiometric data by fractional model

***Abstract**. In the paper results of approximation of spectroradiometric data by fractional model are presented. Investigations of fractional parameters show that they depend on the interval of lambda. By fractional model approximation we illustrate the theoretical basement for a model of an emission intensity. For the development we use the fractional series model that comes from the similar model for energy.*

Streszczenie.** W pracy została dokonana analiza aproksymacji modelem potęgowym, z potęgą niecałkowitą, danych pochodzących z pomiaru spektroradiometrycznego. Model opisu z potęgą niecałkowitego rzędu wykazuje zbieżność z teoretycznym opisem zjawiska. Użyto modelu szeregu potęg niecałkowitego rzędu, który pochodzi z podobnego modelu dla zależności od energii. (**Aproksymacja modelem potęgowym ułamkowego rzędu rozkładu egzytancjii widmowej mierzonego promieniowania świetlnego)

Keywords: approximation, fractional model, spectroradiometric data.
Słowa kluczowe: aproksymacja, model potęgowy, pomiary spektroradiometryczne.

Introduction

In the paper we analyze the possibility of describing the spectroradiometric measured data. The question is what an approximation method and what type of a mathematical model we can use. We discuss some privileged models. As a shape of line seems to be Gaussian we checked the goodness of fitting by that type of models. Moreover we take under consideration also the nature of optical properties of the emission intensity for an ideal LED, [1]. After analysis of the theoretical description we propose the exact fractional power model that coincides with the theoretical assumptions.

We use the approximation, not interpolation [2]. Methods of interpolation or approximation is widely discussed in the literature, e.g. see [3]. However one can find the discussion of sensitivity analysis of regression.

All calculations are done in MATLAB 7.5.0 (R2007b). As the main criterion we take the minimum of the sum of squares of errors – SSE and the same time the maximization of the determination coefficient *R-square*. Such parameters we obtain directly working with *Curve Fitting Toolbox* in MATLAB program. We also point the important case like confidence intervals for parameters. They are given by 95% realization of confidence intervals. We do not make any revision of approximation general methods. Additionally one can find the description of methods and guide of used commands in Matlab in description of *Spline Toolbox 3* or *in Curve Fitting User's Guide*. Moreover some basic commands are explored in the text. For Polish readers we refer also [4,5,6].

Theoretical emission spectrum of an LED [1]

The physical mechanism by which semiconductor LEDs emit light is spontaneous recombination of electron-hole pairs and simultaneous emission of photons. The properties of spontaneous emission in LEDs are discussed in [1]. In our paper we only shortly describe the situation following this book. The emission intensity as a function of energy is proportional to the product of the joint density of states $\rho(E)$ and the distribution of carriers in the allowed bands. Moreover, according to [1], we have that

(1) $$\rho(\mathrm{E}) = \frac{1}{2\pi^2}\left(\frac{2m_r^*}{(h/2\pi)^2}\right)^{3/2}\sqrt{E-E_g},$$

where *h* is Planck's constant,

(2) $$m_r^* = \frac{1}{m_e^*} + \frac{1}{m_h^*}$$

is the reduced mass for m_e^* and m_h^* being the electron and hole effective masses, E_g is the bandgap energy.

The distribution of carriers in the allowed bands is given by the Boltzman distribution, i.e.

(3) $$\mathrm{f_B}(E) \propto \exp\left(-\frac{E}{kT}\right).$$

Then the emission intensity is written accordingly to multiplication in Eqs. (1) and (3).

(4) $$I(E) \propto \sqrt{E-E_g}\,\exp\left(-\frac{E}{kT}\right).$$

In that case we easily see that $I(E)$ is the multiplication of power function of $E-E_g$ and exponential function for E. Then theoretical emission intensity of an LED as the function of E is presented in Fig. 1.

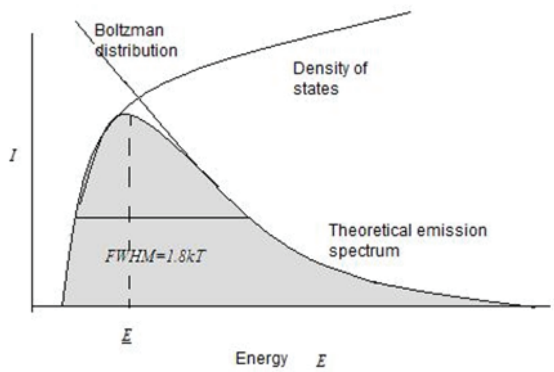

Fig. 1. Theoretical emission spectrum of an LED. The full width at half maximum (FWHM) of the emission line is 1.8kT [1] .

The full width at half of the maximum of the emission is:

(5) $$\Delta E = FWHM = 1.8kT.$$

Let us notice that as $E = \frac{hc}{\lambda}$, where c is the light velocity and λ is wavelength then the relation given by Eqs. (3) can be interpreted as the function of the inverse $\frac{1}{\lambda}$. It can be analytically proved that the relation remains to be the power type function of λ. Then we claim that the emission intensity given by Eqs. (4) we can rewrite as

$$(6) \qquad I(\lambda) \propto \sqrt{\lambda}\sqrt{hc - \lambda E_g}\,\exp\left(-\frac{hc}{\lambda kT}\right).$$

The formula in Eqs. (6) is very sensitive in using it in nonlinear approximation and it is dependent on E_g. However it can be investigated by using series expansion to two one-sided infinite series of the following type

$$(7) \qquad \sum_{-\infty}^{+\infty} a_k (E_g - \lambda)^{\frac{k}{2}} \text{ and } \sum_{-\infty}^{+\infty} a_k (\lambda - E_g)^{\frac{k}{2}}.$$

But from another side we can also think about two-sided approximation: one type of function up to the point of maximum and the next function on the right of maximum. In our investigations we can use a class of approximated function as comes from the model of the emission intensity given by formula in Eqs. (4).

Approximation for measurement LED data type

For a chosen measurement vector data type for LEDs firstly we consider general Gaussian model. And applying the curve fitting tool we get the following results for the model its goodness.

General model Gauss2:

*fittedmodel1(x) = a1*exp(-((x-b1)/c1)^2) + a2*exp(-((x-b2)/c2)^2)*

Coefficients (with 95% confidence bounds):

a1 = 0.4571 (0.4537, 0.4605)
b1 = 379.8 (379.7, 379.8)
c1 = 10.07 (9.98, 10.15)
a2 = 0.001245 (-0.001518, 0.004008)
b2 = 506.9 (479.2, 534.6)
c2 = 15.27 (-23.87, 54.41)

Goodness of fit:

SSE: 0.01614; R-square: 0.9937

The plot of fitting curve is presented at the Fig. 2. (red line: fitting curve, blue points: measurement points). From the values of SSE and R-squared we see that the model is very well fitted to the data. What it is only with doubt are some points on the top excluded from the fitted curve.

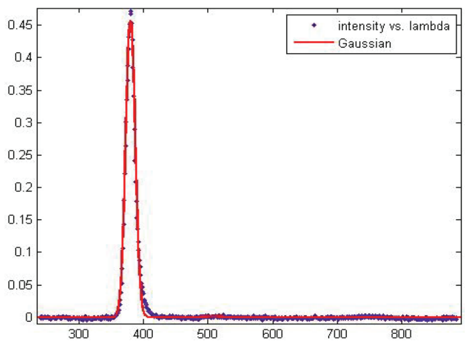

Fig.2. Gaussian approximation function for LEDs data type.

As the next step we reconsider the half right part of the data and the left part of data.

General model Power1:

*f(x) = a*x^b*

Coefficients (with 95% confidence bounds):

a = 3.68e+131 (-2.311e+132, 3.047e+132)
b = -51.09 (-52.31, -49.86)

Goodness of fit:

SSE: 0.008155; R-square: 0.9925

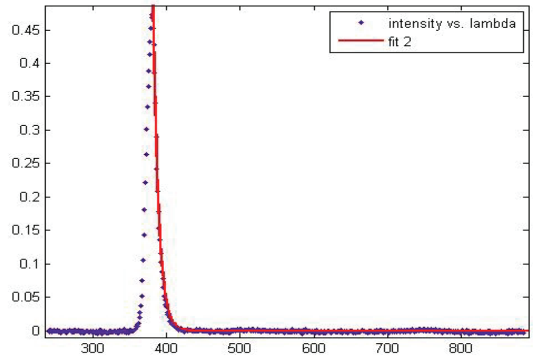

Fig. 3. Right part approximation function for LEDs data type for lambda>380 *nm.*

General model:

f(x) = a(385-x)^c*

Coefficients (with 95% confidence bounds):

a = 1.761e+004 (8614, 2.66e+004)
c = -4.294 (-4.486, -4.102)

Goodness of fit:

SSE: 0.003924; R-square: 0.979

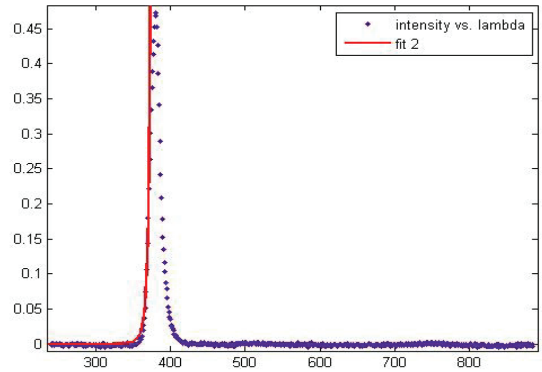

Fig.4. Left part approximation function for LEDs data type for lambda<380 nm.

We also show by the example that considered model is with agreement with measured data. For those purpose we produce two vectors by excluding procedure in Matlab. One for data with wavelengths longer than 380 nm and the second with wavelengths not longer than 380 nm. And we use the following models with calculated coefficients.

I) For wavelength greater than 380 nm we use the following model:

General model:

f(x) =a+b(x-380)^(0.5)+c*(x-380)^(-0.5)+d*(x-380) +e*(x-380)^(3/2)+f*(x-380)^(-3/2)*

Coefficients (with 95% confidence bounds):

a = -0.7023 (-0.7502, -0.6544)
b = 0.08275 (0.0741, 0.09141)
c = 2.078 (1.991, 2.166)
d = -0.004044 (-0.004656, -0.003432)
e = 7.012e-005 (5.561e-005, 8.463e-005)
f = -1.004 (-1.059, -0.9479)

Goodness of fit:

SSE: 0.01205
R-square: 0.9889

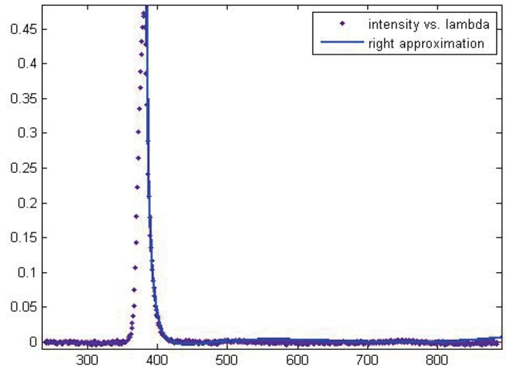

Fig.5. Right approximation by the sum of power functions: *f(x)=a+b*(x-380)^(0.5)+c*(x-380)^(-0.5)+d*(x-380)+e*(x-380)^(3/2)+f*(x-380)^(-3/2)* for lambda>380 nm.

II) For wavelength less than 380 nm we use the following model

General model:

f(x)=a+b(380-x)^(0.5)+c*(380-x)^(-0.5)*
+d(380-x)+e*(380-x)^(3/2)+f*(380-x)^(-3/2)*

Coefficients (with 95% confidence bounds):

a = -0.7667 (-1.529, -0.004206)
b = 0.2014 (0.06283, 0.34)
c = 0.3815 (-1.295, 2.058)
d = -0.01943 (-0.03078, -0.008083)
e = 0.0006445 (0.000298, 0.0009911)
f = 10.97 (7.721, 14.22)

Goodness of fit:
SSE: 0.001904
R-square: 0.9898

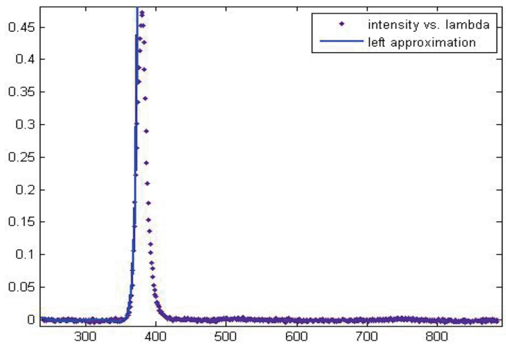

Fig.6. Left approximation by the sum of power functions:

Conclusions

In all presented models we got very high value of criterions. Considered data can be approximated by fractional power model by one-sided function because of its behavior. Series given by Equations (7) are used by extracting few terms and then checking if the goodness of fit is high enough. It is worthy to notice that also the confidence intervals for coefficients are short. Our goal was to confirm if from the model for energy we can introduce also a model for the wavelength and if using measurement data there exists an approximating function close to the theoretical model.

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