DOI: 10.61782/fa.2025.0539

FORUM ACUSTICUM EURONOISE 2025

# MACHINE LEARNING FOR MODELLING BAND STRUCTURE PROPERTIES

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## ABSTRACT

Although there are various analytical approaches and numerical methods for solving sonic crystal problems, analytical expressions for modelling the band structure properties are limited to a few special cases. The access to a numerical model offers a solid foundation for data-driven discovery. In our approach, we employed the Webster equation for the unit cell and Floquet-Bloch theory for periodic structures, with the waveguide parametrized by cubic splines. To extract analytical formulae linking the waveguide geometry to the corresponding dispersion relation, we applied methods of physics-informed machine learning, such as coordinate transformation and symbolic regression. These results provide a deeper understanding of the underlying principles and serve as an efficient alternative to computationally demanding numerical optimization. Moving toward a Schrödinger-like equation and parametrization by Gaussian curvature allows for a more multiphysical approach, yet it also presents challenges related to the feasibility limits of the geometry.


**Keywords:** *locally periodic structures, symbolic regression, data-driven discovery*

## 1. INTRODUCTION

This research aims to analytically model acoustic transmission and band structure properties in sonic crystals. So far, the transmission was solved mainly numerically. To propose an optimized design for a desired band gap width, one has to opt for numerical optimization repeatedly going back and forth from geometry to the dispersion relation. Since this approach is computationally demanding, we proposed a method how to discover analytical formulae for design of one-dimensional sonic crystals with smooth geometry [1]. Our goal is to explore further possibilities of this approach and transform our problem to a Schrödinger-like equation, which is a common ground for various problems of propagation through inhomogeneous structures. If the data-driven discovery shows to be feasible also for this transformed problem, the applications of this follow-up would have potential to be multiphysical.

This short paper focuses on the discovery of the first bandgap width and is organized as follows: first, the governing equations are introduced. Next, the methods from [1] are revisited and applied to our newly defined problem. Finally, the discovered equations are presented and the conclusions are drawn.

## 2. GOVERNING EQUATIONS

Throughout this paper, we consider an axis-symmetric waveguide with cross-sectional area function $A(x) = \pi R(x)^2$ and we assume the time-harmonic behavior (with the sign convention $e^{-\mathrm{i}\omega t)}$). The Webster wave equation holds for the propagation of quasi-plane waves:

$$p'' + \frac{2R'}{R}p' + \kappa^2 p = 0\,, \tag{1}$$

where $x$, $p = p(x,\kappa)$, $R = R(x)$ and $\kappa = \omega\ell/c_0$ denote the axial coordinate, complex amplitude of the acoustic pressure, local radius and wavenumber, respectively, with $\ell$ being the axial characteristic length. All of the variables are non-dimensional, except for $\ell$.

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Introducing a transformation $\psi = pR$, we can map Eq. (1) to a Schrödinger-like equation:

$$\psi'' + (\kappa^2 + G)\psi = 0 \,, \tag{2}$$

where the condition on transformation is

$$G = -\frac{R''}{R} \,. \tag{3}$$

Compare Eq. (3) with the formula for Gaussian curvature of a smooth surface in three-dimensional space:

$$K = k_1 k_2 = \frac{1}{R}\frac{R''}{(1+R'^2)^{3/2}} \approx \frac{R''}{R} \,, \tag{4}$$

where $k_1$, $k_2$ are the principal curvatures of the waveguide (see Fig. 1).

From this comparison, we can conclude, that the transformation condition $G(x)$ can be geometrically interpreted as a Gaussian curvature (or, to be precise, negative Gaussian curvature).

Note, that this specific interpretation is possible only for transformation condition from the Webster equation to Schrödinger-like eq. by a coincidence. When mapping different equations to Schrödinger-like eq., the transformation condition $G(x)$ might have different physical meanings or no physical meaning at all.

The caveat of parametrizing the unit cell geometry by Gaussian curvature $G(x)$ and not the radius function $R(x)$ is the following: for a given $G(x)$, the $R(x)$ is not always realizable. Furthermore, the realizability differs from one application to another and therefore, needs to be checked based on the field of physics one wants to apply this method to.

### 3. METHODS

The first step of the previously established approach was preparing the dataset, which consisted of the four parameters controlling the geometry and the bandgap widths. Then, the bandgap widths were related to geometry control parameters by employing symbolic regression, implemented in an open-source library PySR [2].

Following this approach, it is needed to choose a parametrization of the waveguide geometry. The requirements for the parametrization stem from the governing equations of transmission in locally periodic structures. Due to combined prerequisites of the Webster equation validity and the Floquet-Bloch theory, a smooth, slowly varying radius function $R(x)$ is needed, and the unit cells

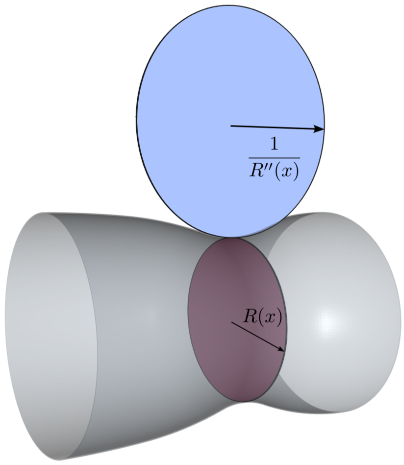


**Figure 1**. Illustration of Gaussian curvature $G(x)$ on a unit cell.

have to be connected periodically and continuously to form a waveguide.

Considering this, it was decided to begin with a piecewise constant Gaussian curvature which allows feasible control that $R(x)$ exists. Previously, when dealing with geometries defined by $R(x)$, we parametrized them by cubic splines with four control parameters [1]. Hence, we decided to choose for four parameters again: the values $g_1, \ldots g_4$ parametrize the problem. This number of parameters allows the geometry to be sufficiently variable, while the equation discovery algorithm is transparent enough. Example of such geometry is shown in Fig. 2.

To prevent the symbolic regression from focusing on too small values of $w_1$, we decided to regularize the relative error by one-tenth of the mean band gap width, and take its third quartile:

$$\mathcal{L} = Q_3\left(\frac{|\hat{w}_1 - w_1|}{w_1 + 0.1\bar{w}_1}\right) \,, \tag{5}$$

where $w_1$, $\bar{w}_1$, $\hat{w}_1$ stand for the dataset value for first bandgap width, the mean $w_1$, and the predicted value, respectively.

### 4. RESULTS & DISCUSSION

The discovered formula for first bandgap width $w_1$ reads

$$w_1 = 0.085\sqrt{\left|g_2^2 + g_3^2 - \frac{2}{3}(g_1 g_3 + g_2 g_4)\right|} + 0.006(g_2 + g_3) \,. \tag{6}$$

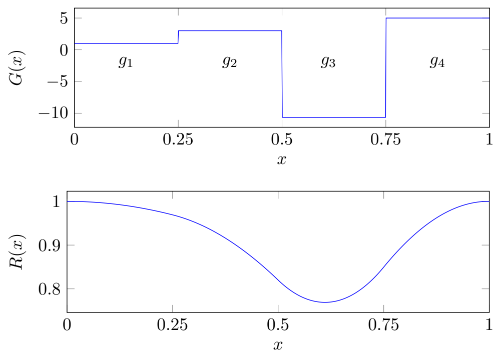


**Figure 2**. Top: Gaussian curvature $G(x)$, bottom: corresponding radius function $R(x)$.

To confirm that Eq. (6) is physically interpretable, consider a narrow waveguide. Such waveguide has all geometry control parameters equal to zero: $g_1 = g_2 = g_3 = g_4 = 0$ and hence, $w_1$ equals to zero as expected. Moreover, the formula respects that the locally periodic structures are in this case independent of the mirror symmetry of the unit cell, i.e. the system description is independent of swapping $g_1 \leftrightarrow g_4$ simultaneously with $g_2 \leftrightarrow g_2$.

For comparison, we show formula from [1], that is written in terms of

$$w_1 = 2.61\left[\max(r_m, r_d) - \min(0, r_m)\right]. \quad (7)$$

The relative error of the newly discovered formula and the formula published in [1] is shown in Fig. 3. Note that this is a comparison done on different datasets to obtain at least some error estimation of the new follow-up. The mean relative error is comparable: previously, it was achieved 7.32 % and now 5.41 %. These results show, that eventhough when we are relating the bandgap width to parameters controlling the Gaussian curvature, it is possible to achieve results of similar precision as before in [1].

## 5. CONCLUSION

We have confirmed that the previously established approach can be applied to the transformed problem, allowing us to fit a formula using symbolic regression to link the first bandgap width with geometry control parameters, now redefined in terms of Gaussian curvature. Although the influence of each control parameter on the radius function is not as easily visible as before, having the problem defined through the Schrödinger-like equation offers wider range of application possibilities not only in acoustics, but also, e.g., in optics. Therefore, future work will focus on finding formulae for the second and third bandgap width and improving their accuracy, while maintaining the interpretability.

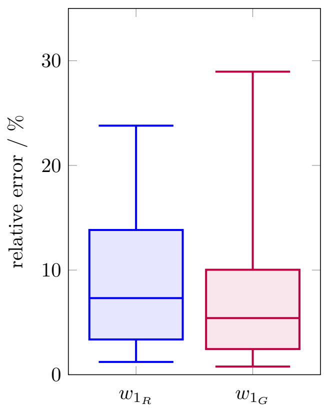


**Figure 3**. Relative error for bandgap width prediction. The box is indicating the median and the interquartile range, the whiskers 8th and 92th percentile of error. The subscripts $R$ and $G$ denote the way, how the geometry is defined: by radius function $R(x)$ and by Gauss curvature $G(x)$, respectively.

## 6. ACKNOWLEDGMENTS

This work was supported by the Grant Agency of the Czech Technical University in Prague, grant No. SGS25/136/OHK3/3T/13.

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