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DETERMINING EXTRAPOLATED DIFFERENTIAL CROSS SECTIONS FROM DATA SETS IN BEAMDB USING MACHINE LEARNING ALGORITHMS

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Abstract. Here we exploit a large data set maintained in the Belgrade electron-atom/ molecule database (BEAMDB) to explore the possibilities how to determine extrapolated differential cross sections (DCS) obtained in experimental investigations by using machine learning algorithms. DCSs for different atomic and molecular species are represented by squared weighted sum of Legendre polynomials

1. INTRODUCTION

The importance of electron collisions with atomic particles (atoms, molecules, ions, radicals) is evident in the fields of plasma processes (Petrović et al. 2014), astrophysical plasmas (Jevremović et al. 2020), radiation damage (Mason 2008), etc. In low-temperature non-equilibrium molecular plasmas electron interactions are responsible for vibrational non-equilibrium and electron-driven ionization and dissociation that produces reactive species. The strength of electron interaction with atomic species is usually characterized by cross sections which can be state specific and angle and energy resolved. In classical experiments with electron spectrometers that are not equipped with the magnetic-angle-changing device (Cho et al. 2006) determination of electron differential cross sections, DCS(θ), is performed in the limited range of scattering angles. In order to obtain integral cross

sections, σ_i (1), or momentum transfer, σ_{mt} (2), one needs to extrapolate experimental data to zero and 180^o angles and then to carry out the integrations:

$$\sigma_i(\theta) = 2\pi \int_0^{\pi} DCS(\theta) \sin\theta \, d\theta \tag{1}$$

$$\sigma_{mt}(\theta) = 2\pi \int_0^{\pi} DCS(\theta) \left[1 - \left(1 - \frac{\Delta E}{E_o}\right)^{1/2} \cos\theta\right] \sin\theta \, d\theta \tag{2}$$

The question that arises is how to conduct the extrapolation procedure, either to use calculated values obtained by some theoretical approximation (see e.g. Bartschat et al. 2017) or to perform complex phaseshift analysis (Brunger et al. 1992). In this contribution we explore the possibility to use a large set of DCS(θ) data curated within BEAMDB database (http://servo.aob.rs/emol) to determine extrapolated values using machine learning techniques.

2. BELGRADE ELECTRON-ATOM/MOLECULE (BEAM) DATABASE

Belgrade Electron –Atom/Molecule (BEAM) database (Marinković et al. 2017) is a node of a common portal "Virtual Atomic and Molecular Data Centre", VAMDC, (https://portal.vamdc.eu/vamdc_portal/home.seam) and it collects and maintains a series of data on electron interaction with atomic particles. It holds electron differential and integral cross sections for elastic scattering, electronic excitations and ionization as well as electron energy loss-spectra and threshold photoelectron spectra. Numerous atomic species (Ag, Ar, Bi, Ca, Cd, He, Hg, Kr, Mg, Na, Ne, Pb, Rb, Sb, Xe, Yb) are accompanied by 18 other molecular species. Differential cross sections are organized as four raw data (E_o, θ, DCS, error) where E_o is impact energy, θ is scattering angle, DCS is the value of differential cross section for E_o and at scattering angle θ, error is the value of the absolute uncertainty of DCS values. These data sets represent a pool for implementing machine learning technique.

3. MACHINE LEARNING ALGORTIMS

Machine learning (ML) techniques nowadays are becoming a "New tool in the box" for physics researchers (Zdeborová, 2017). ML is a new paradigm of performing research, like taking experiment, providing theoretical approximation or execute numerical simulation (ibid.). Mapping the relation and structure of scientific knowledge in physical disciplines could be efficiently obtained and then visualized by a ML approach (Chinazzi et al. 2019). Since early and classical textbook of Michel (1997), the learning to classify new astronomical structures has been recognized as one of the examples of usefulness of ML concepts. Recently, Stokes et al. (2019) utilized a deep neural networks for the solution of the inverse swarm problem of deriving cross sections from swarm transport data.

3.1. TASK, PERFORMANCE MEASURE, EXPERIENCE

We define a task for our ML algorithm as determining the extrapolated differential cross sections from a given data of experimentally measured values at a limited range of scattering angles. The performance measure would be the value of $\chi 2$ defined as a goodness of fit by Pearson's chi-squared test. Training experience is provided as a database of calculated DCS(θ) values existing in the BEAMDB under all available theoretical approximations (distorted wave, optical potential, convergent close-coupling, B-spline R-matrix semi-relativistic or fully relativistic calculations). Additionally, the performance is measured in comparison of integrated cross sections (integral and momentum transfer) obtained with combination of experimental data and extrapolated data that resulted in such ML process with those already contained within the BEAM database or if existing, recommended set of data.

3.2. LEARNING ALGORITHMS

We performed inductive learning algorithm which at best guarantee that the output hypothesis fits the target concept over the training data (Mitchell, 1997). Our inductive bias assumption is that extrapolated DCS(θ) values can be represented by the scattering amplitudes $f(\theta,k)$, k being wave vector. Scattering amplitude consists of the sum of the phaseshifts δ_l and Legendre polynomials P_l (cos θ) as defined in (3).

$$\mathrm{DCS}(\boldsymbol{\theta}) = |\boldsymbol{f}(\boldsymbol{\theta},\boldsymbol{k})|^2 = \frac{\mathbf{1}}{\boldsymbol{k}^2}\left|\sum_{\boldsymbol{l}=\mathbf{0}}^{\infty}(\mathbf{2}\boldsymbol{l}+\mathbf{1})\boldsymbol{e}^{\boldsymbol{i}\boldsymbol{\delta}_l}\,\mathbf{sin}\,\boldsymbol{\delta}_l\,\boldsymbol{P}_l(\mathbf{cos}\,\boldsymbol{\theta})\right|^2 \qquad (3)$$

All data are divided in three subsets, validation, training and test sets (Maček, 2019). Validation set accounts for less than one third of all data and is used to resolve overfitting problem while test set is used to provide an estimate of accuracy over new data sets.

4. DISSCUSSION

The first results of squared weighted sum of Legendre polynomials up to 60^o are given in Fig.1. Although data sets in BEAMDB seemed to be large, it turns out that it is a limited number examples that could be used in ML process. This fact urges data curators to enlarge the coverage of data entries. Also, provided software within Service of VAMDC portal, like XSAMS Convertor or graphical tool used for data visualization (http://www.vamdc.org/activities/research/software/) need to be implemented within BEAMDB in its further developments.

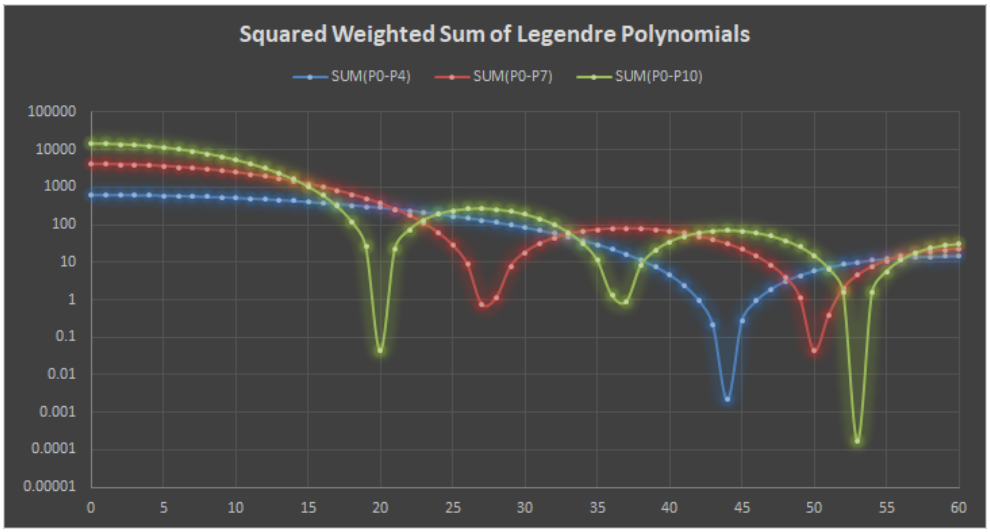

Figure 1: Squared weighted sum of 4, 7 and 10 first Legendre polynomials.

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