avant

Release 0.0.1

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 ${\tt avant} \ is \ a \ python \ package \ to \ extract \ values \ from \ {\tt refl_database} \ to \ create \ informed \ or \ uniform \ priors \ to \ be \ used \ in \ reflectometry \ analysis.$

The aim of avant is to improve reflectometry analysis by applying Bayesian Statistics and creating 'informed priors' which take into account literature values in the prior probability distributions of the parameters. The priors are created in a way where they can be directly implemented into refnx to perform reflectometry analysis. Plus, the package has plotting functionalities so you can see what the prior probability distributions look like.

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INSTALLATION

avant can be installed from the PyPi package manager with pip

pip install avant

The package can also be found on Github along with installation instructions.

TWO

FEATURES

Currently, avant only contains priors for the following five parameters for DMPC: head volume, tail volume, head thickness, tail thickness and roughness. It can create an informed prior, *Gauss*, with the following methods:

- pdf: probability distribution function
- logpdf: natural log of the probability distribution function
- cdf: cumulative distribution function
- **ppf**: percentile point function (also known as quantile function or inverse cdf)
- rvs: random variate sampling

It can also create a uniform prior which is an upper and lower bound for the prior range.

The following plotting functionalities are available:

- plotGauss(name): Plot an informed *Gauss* prior probability distribution.
- plotUniform(name): Plot a uniform prior probability distribution.

THREE

EXAMPLES

For example, to plot the informed prior for the head volume for DMPC:

For example, to plot the uniform prior for the head volume for DMPC:

Here is an example of setting the value of the parameter to that of the Gauss object - this is a class containing statistical information about the prior and can be fed straight into Refnx.

For example, to set a parameter for the head volume of DMPC:

Here is an example of setting the value of the parameter to a tuple containing the lower and upper bound of the uniform range of values for the parameter. This can be fed straight into Refnx.

For example, to set a parameter for the head volume of DMPC:

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FREQUENTLY ASKED QUESTIONS

• Where can I find the database where the values are stored?

The refl-database can be found on GitHub .

FIVE

API REFERENCE

5.1 avant - Creating informed priors for reflectometry analysis in Python

5.1.1 Modules

avant.parameter

- genindex
- modindex