

USER'S GUIDE TO MaxTox

Developed under OpenTox – An Open Source Predictive Toxicology Framework

(2008-2011)

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Preface

User's guide to MaxTox is an attempt to list simplified instructions so that an end-user who is unaware of the detailed logic behind MaxTox can also go through few simple steps and learn to use the services offered by MaxTox.

MaxTox documentation is periodically updated and the latest versions are available at the site:

<http://www.opentox.org/tutorials/maxtox>

Any queries, bug-reports and feature-requests should be addressed to indirag@mail.jnu.ac.in or sunil@seascaplearning.com.

MaxTox is a service developed under OpenTox to provide a set of tools to build toxicity models against a specific endpoint using toxicity data. OpenTox is developed to provide an interoperable predictive toxicology framework to build and validate in-silico models and algorithms, and to provide a quality source of structures and toxicity data in order to develop a support of alternative methods to in-vitro assays for toxicity testing.

Note: OpenTox covers all products or services described in this manual. This document is meant for testing of the described services, as they exist on the current date of publication. The services are continuously developing so the manual and features described herein are subject to change without notice.

Acknowledgement: OpenTox - An Open Source Predictive Toxicology Framework, www.opentox.org, is funded under the EU Seventh Framework Program: HEALTH-2007-1.3-3 Promotion, development, validation, acceptance and implementation of QSARs (Quantitative Structure-Activity Relationships) for toxicology, Project Reference Number Health-F5-2008-200787 (2008-2011).

Audience

User's guide to MaxTox is intended for use of researchers, chemists and drug designers who wish to build in-silico models for predicting toxicity. MaxTox web application is available online and users may submit tasks from anywhere, which will run on the MaxTox server, and the links to results are sent to user's email address given at the time of job submission. MaxTox has a user friendly GUI and this manual guides a user how to use it with the help of properly illustrated screenshots. The manual also describes how to use MaxTox through command line calls.

Organization of the manual

The **User's guide to MaxTox** is organized as follows

Introduction: Gives the introduction about the MaxTox.

Algorithms: Description of the algorithms used.

Services: Services provided by the MaxTox.

Glossary: Description of terms used in MaxTox.

Introduction to MaxTox

MaxTox is a suite of tools to make models to predict toxicity of novel compounds based on their structural similarity to compounds with known toxicities. Compounds forming a model have the same Endpoint Toxicity.

For a training set of compounds, substructures occurring (in more than 1 compound and which consist of more than 2 atoms) are extracted and dictionaries built. New compounds are compared to this dictionary and a fingerprint denoting the presence/absence (of dictionary fragments in the test molecule) is generated. These fingerprints are binary i.e. they are represented using 0/1 for denoting absence/presence of a substructure in the compound. The fingerprints are then used to pass through a statistical Random Forest Model or SVM model to generate a predictive model. This predictive model is then used to predict the toxicity of the unknown set against the particular endpoint.

MaxTox is delivered as an open source application. It uses open source packages like CDK, Restlet, Jena & R to generate models and predict toxicities. It is part of the OpenTox initiative to create freely accessible resources to predict toxicity.

SVM used in MaxTox is SVMlight which is an implementation of Support Vector Machines (SVMs) in C (<http://svmlight.joachims.org>).

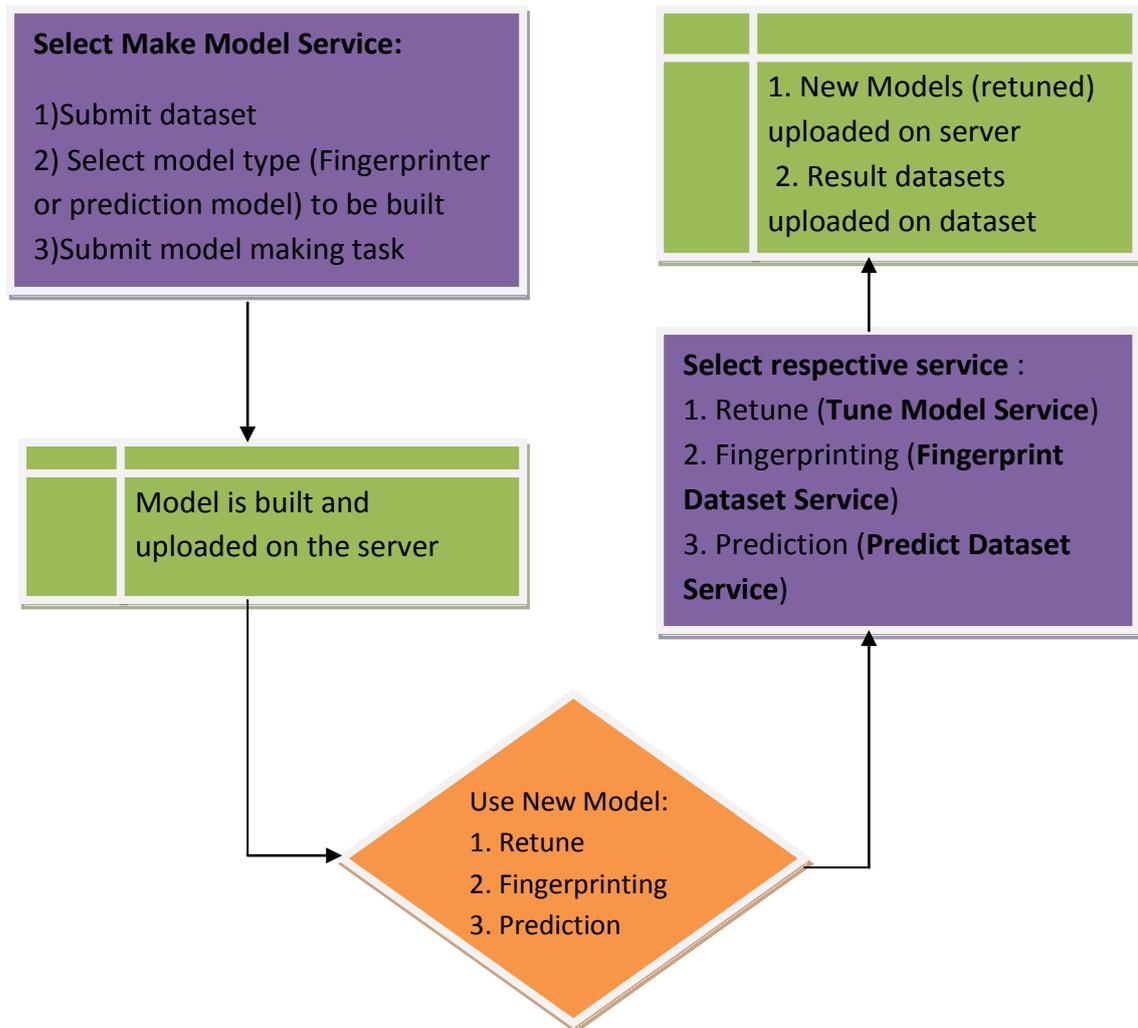
MaxTox can consume and respond in RDF datatypes and works with the OpenTox API specification. The MaxTox application can be used as a component of other prediction use-cases hosted from other servers, as long as the data transactions are performed according to the OpenTox API.

The link to MaxTox web application is <http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS>.

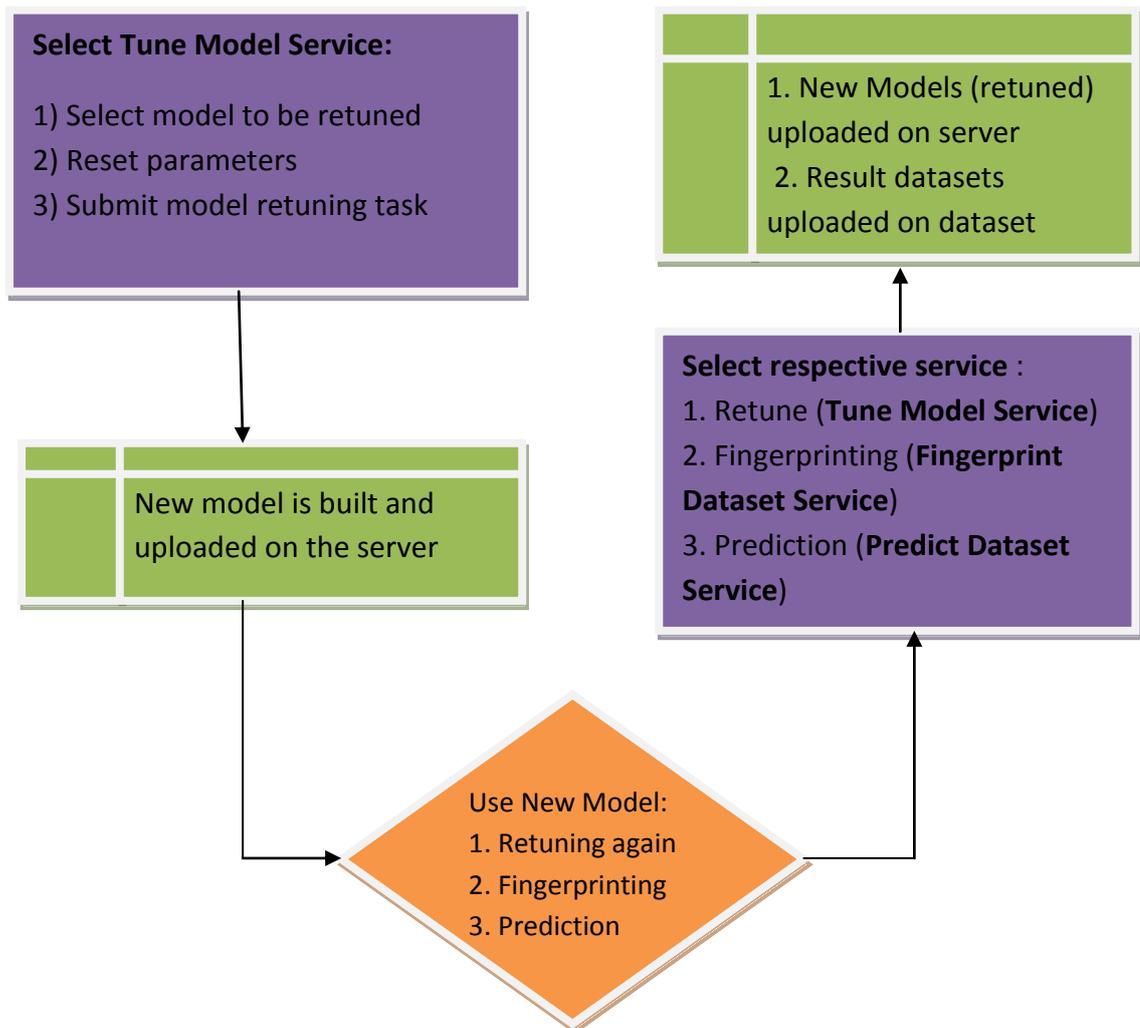
Use Cases

MaxTox offers a number of services, but mainly its utility can be summarised under following use cases. Following flowcharts explain how to use MaxTox for various use cases. Click on the respective services to go onto details.

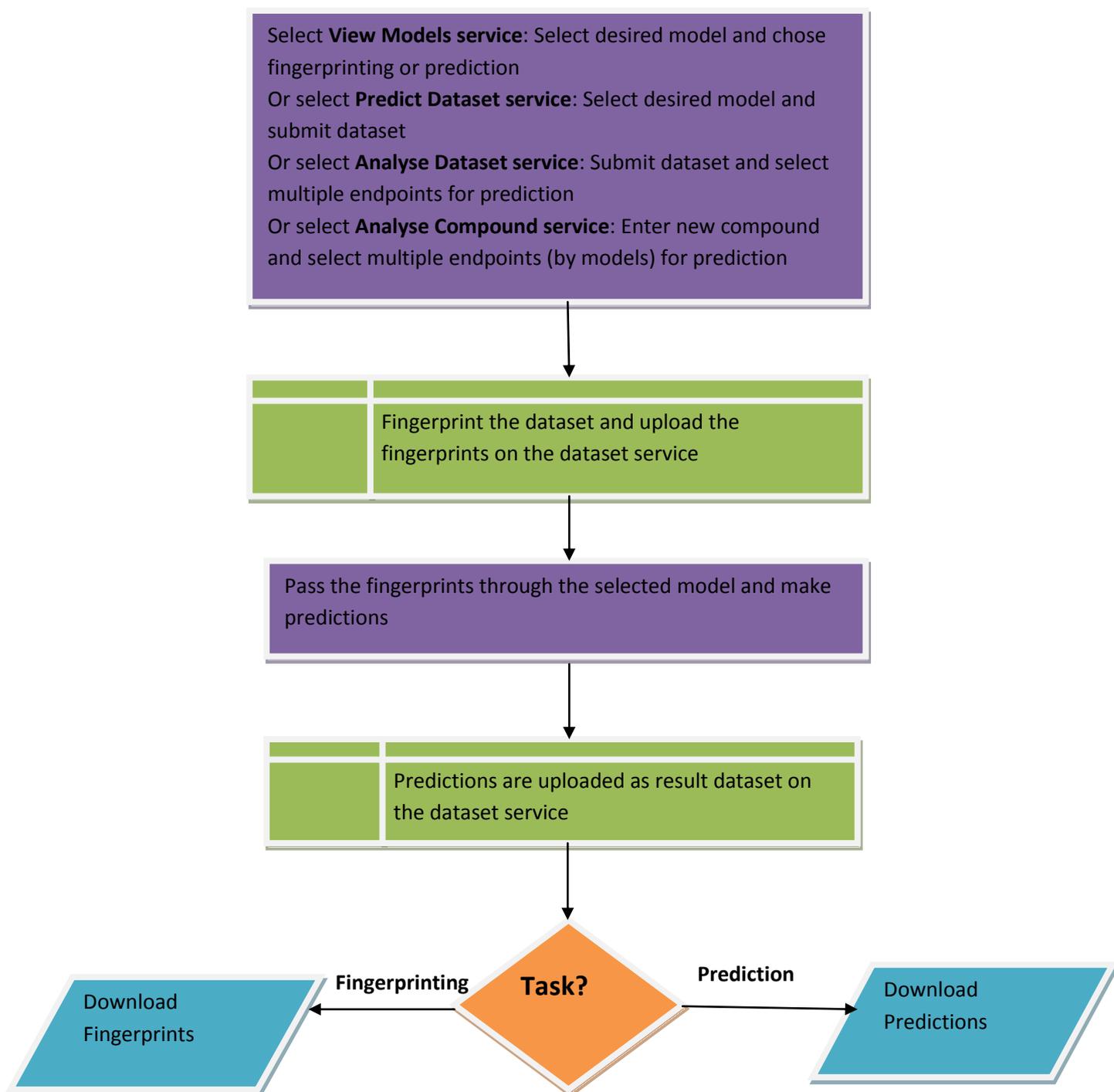
Making new model



Retuning existing model



Prediction/Fingerprinting using an existing model



Algorithms and Services developed under MaxTox

ALGORITHMS

Algorithms developed under MaxTox are listed below and are available at the address:

curl <http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/algorithm>

- **MCSSFinder:** Extracts Substructures from dataset and removes redundants to create a dictionary. Fingerprints the dataset and optionally creates an SVM model. Details of the algorithm are available at address :

<http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/algorithm/MCSSFinder>

- **SVMRemodeller:** Remodels an existing SVM model using new parameters. Details of the algorithm are available at address :

<http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/algorithm/SVMRemodeller>

- **MultiModelAnalyser:** An algorithm to use multiple models for predictions.

<http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/algorithm/MultiModelAnalyser>

SERVICES

MaxTox offers a number of services for building models and generating fingerprints based on three basic algorithms developed under MaxTox, which are mentioned above. The services offered by MaxTox are:

- View Models
- Make Model
- Tune Model
- Fingerprint dataset
- Predict dataset
- Analyse dataset
- Analyse compound

The above-mentioned services are detailed in the later sections of the manual along with suitable examples to understand.

MaxTox GUI

MaxTox homepage shows the various services offered by MaxTox as shown in the following figure.

developed by JNU in collaboration with SL as a part of the OpenTox project.

OpenTox **MaxTox** MCSS

NAVIGATION

- Home
- View Models
- Make Model
- Tune Model
- Fingerprint Dataset
- Predict Dataset
- Analyse Dataset
- Analyse Compound
- Credits

SERVER STATS

- View Tasks

Maxtox is a suite of tools to make models of training sets (of compounds) with data on toxicity against a particular endpoint. These models can then be used to predict the toxicity of novel compounds based on their structural similarity to compounds in the training set. The Maxtox application is built around the Opentox API 1.2. The various resources can be accessed through this web/html interface, or programmatically using the RDF interface. To access the RDF interface use the "curl" command line tool.

RELATED LINKS

- OpenTox
- ToxCreat
- ToxPredict

OPENSOURCE

- Restlets
- Jena
- CDK
- R (statistics)
- Rserve

Make Models

Tune Models

Fingerprint Dataset

Predict Dataset

Analyse Dataset

Analyse Compound

Steps behind making Maxtox models :

- All Compounds in training set are compared pairwise to obtain the largest overlaps (Including the MCSS).
- The overlaps (which are fragments) are filtered to remove duplicates. The resulting set of fragments is used for fingerprinting
- The fingerprints of the training set compound are then passed through an SVM model, to make predictive model.
- Optionally the fingerprints of the training set compound are then passed through a RandomForest model in R, to improve the model.
- The predictive model is then used to predict the training set. A cross validated accuracy is obtained.
- The predictive models are then used to predict new and un-known compounds.

Fig 1 Home page

View Models

Address for the View Models service:

<http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/model>

Step 1: Click on the View Models link to navigate to the page displaying the list of all the models available at MaxTox.

NAVIGATION

- Home
- View Models
- Make Model
- Tune Model
- Fingerprint Dataset
- Predict Dataset
- Analyse Dataset
- Analyse Compound
- Credits

SERVER STATS

- View Tasks

List of all models ...

Model_2bbd0400_4fa4_45cb_b7c7_0925bfe3f741	
Description	A Maxtox Basic Model (Fingerprinter) : The MCSS (MAnimum Common Substructures) have been extracted from the dataset using a series of pairwise comparisons. The structures are then filtered for duplicates to yield a set of unique substructures. This set can be used to build a predictive model by fingerprinting the source dataset molecules, and then using the fingerprint to to create a prediction model for the feature to be predicted (from the source dataset).
SVM Model ?	No
RandomForest Model?	No
Source Dataset URI	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=20

Model_e8342231_e3a0_4f20_b624_415a3a5673e0	
Description	A Maxtox Basic Model (Fingerprinter) : The MCSS (MAnimum Common Substructures) have been extracted from the dataset using a series of pairwise comparisons. The structures are then filtered for duplicates to yield a set of unique substructures. This set can be used to build a predictive model by fingerprinting the source dataset molecules, and then using the fingerprint to to create a prediction model for the feature to be predicted (from the source dataset).
SVM Model ?	No
RandomForest Model?	No
Source Dataset URI	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=20

Model_729e7130_4491_4ab2_b87a_998e7bdb1e50	
Description	A Maxtox SVM Predictor Model (Fingerprinter + Predictor) : The MCSS (MAnimum Common Substructures) have been extracted from the dataset using a series of pairwise comparisons. The structures are then filtered for duplicates to yield a set of unique substructures. This set can be used to build a predictive model by fingerprinting the source dataset molecules, and then using the fingerprint to to create a prediction model for the feature to be predicted (from the source dataset). An SVM Model is also available for predicitions. This is a classifier type model.
SVM Model ?	Yes
RandomForest Model?	No
Source Dataset URI	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=20

RELATED LINKS

- OpenTox
- ToxCreate
- ToxPredict

OPENSOURCE

- Restlets
- Jena
- CDK
- R (statistics)
- Rserve

Fig 2: List of all models

Step 2: Click on model id to view the details of a particular model, for example, when you click on model id Model_729e7130_4491_4ab2_b87a_998e7bdb1e50, it takes you to the details about that model (Fig 3).

developed by JNU in collaboration with SL as a part of the OpenTox project.





NAVIGATION

- Home
- View Models
- Make Model
- Tune Model
- Fingerprint Dataset
- Predict Dataset
- Analyse Dataset
- Analyse Compound
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SERVER STATS

- View Tasks

Model Number :
Model_729e7130_4491_4ab2_b87a_998e7bdb1e50

Unique ID	Model_729e7130_4491_4ab2_b87a_998e7bdb1e50
Title	Model with Predictions for Ames test categorisation
Description	A Maxtox SVM Predictor Model (Fingerprinter + Predictor) : The MCSS (MAximum Common Substructures) have been extracted from the dataset using a series of pairwise comparisons. The structures are then filtered for duplicates to yield a set of unique substructures. This set can be used to build a predictive model by fingerprinting the source dataset molecules, and then using the fingerprint to to create a prediction model for the feature to be predicted (from the source dataset). An SVM Model is also available for predicitions. This is a classifier type model.
Creator	Maxtox User.
SVM Model ?	Yes
SVM Predicted Training Dataset URI	http://apps.ideaconsult.net:8080/ambit2/dataset/601421
RandomForest Model?	No
Source Dataset URI	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=20
Fragment Set	Fragments
Created By	Task_f4f22a1d_225b_4b4a_bd6f_18af1b4d5ccd
Algorithm	http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/algorithm/MCSSFinder/Algorithm_74a198b0_817c_4f8f_8fd7_6821f2fec420

Model details and actions ...

SVM PARAMETERS

Refer to <http://svmlight.joachims.org>

Parameter	Value
Cross Validation	
-v [3,5...]	5
Learning	
-z {c,r,p}	c
-c float	20
-w [0..]	0.1
-i float	1

PERFORMANCE

True Positives : 14
 True Negatives : 6
 False Positives : 0
 False Negatives : 0
 Total Positives : 14
 Total Negatives : 6
 Sensitivity : 1.0
 Specificity : 1.0
 Recall Rate: 1.0
 Cross Validated Recall Rate : 0.7
 Cross Validation Folds : 5

RELATED LINKS

- OpenTox
- ToxCreate
- ToxPredict

OPENSOURCE

- Restlets
- Jena
- CDK
- R (statistics)
- Rserve

Fig 3a : Details of the model available at MaxTox

Algorithm /algorithm/MCSSFinder
/Algorithm_74a198b0_817c_4f8f_8fd7_6821f2fec420

Model details and actions ...

SVM PARAMETERS
Refer to <http://svmlight.joachims.org>

Parameter	Value
Cross Validation	
-v [3,5...]	5
Learning	
-z {c,r,p}	c
-c float	20
-w [0..]	0.1
-j float	1
-b [0,1]	1
-i [0,1]	0
Performance	
-x [0,1]	0
-o [0..2]	1
-k [0..100]	0
Transduction	
-p [0..1]	
Kernel	
-t int	0
-d int	
-g float	
-s float	
-r float	
Optimization	
-q [2..]	10
-n [2..q]	10
-m [5..]	40
-e float	0.001
-h [5..]	100
-f [0,1]	1
-# int	100000

PERFORMANCE

True Positives : 14
True Negatives : 6
False Positives : 0
False Negatives : 0
Total Positives : 14
Total Negatives : 6
Sensitivity : 1.0
Specificity : 1.0
Recall Rate : 1.0
Cross Validated Recall Rate : 0.7
Cross Validation Folds : 5
Matthews Correlation Coefficient : 1.0

ACTIONS

Remodel SVM

Fingerprint Dataset

Predict Dataset

running on Tomcat 6.0 bug-reports/feature-requests : support@maxtox.org

OpenTox - An Open Source Predictive Toxicology Framework, www.opentox.org, is funded under the EU Seventh Framework Program: HEALTH-2007-1.3-3 Promotion, development, validation, acceptance and implementation of QSARs (Quantitative Structure-Activity Relationships) for toxicology, Project Reference Number Health-F5-2008-200787 (2008-2011)

Fig 3b : Details of the model available at MaxTox

Now you can use this model to

Step 2a: Remodel SVM- If you wish to change the parameters used for SVM model building, click on the option Remodel SVM. This will take you to the Tune Model service of MaxTox. For details go to section **Tune Model**.

Step 2b: Fingerprint Dataset- If you wish to use this model to generate fingerprints using MaxTox algorithm, click on the option Fingerprint Dataset. This will take you to the Fingerprint Dataset service of MaxTox. For details go to section **Fingerprint Dataset**.

Step 2c: Predict Dataset- If you wish to use this model to predict a dataset, click on the option Predict Dataset. This will take you to the Predict Dataset service of MaxTox. For details go to section **Predict Dataset**.

User's Discussion :

The following main features are described for each enlisted model:

Description : It states that whether the model built is only a Fingerprinter model or a (Fingerprinter + predictor) model. A Fingerprinter only creates a dictionary of unique substructures, extracted from the dataset using MaxTox MCSSFinder algorithm. This dictionary can then be used for fingerprinting the source dataset compounds and the fingerprints can be used to create a prediction model either using the SVM, a machine-learning algorithm available at MaxTox or some other model building service compliant with OpenTox API version. While a (Fingerprinter + Predictor) is a classifier type model where the dictionary of MCSS is built, fingerprints are generated, the prediction model for the feature (like active-inactive, mutagen-nonmutagen etc) is built using SVM algorithm and the training dataset is predicted at one go.

SVM Model /RandomForest Model : This feature is valid for (Fingerprinter + Predictor) model. It says 'Yes' against SVM Model if the prediction model is built using SVM algorithm. Note: Currently RF model building option is not provided by MaxTox web application.

Source dataset URI: This gives the address of the source dataset used for making MCSS dictionary or the prediction models. If you want to look at the structure of compounds used for building the model, click on this link.

Fragments: Fragments link you to the page where all the substructure fragments are listed in detail along with their SMILES, structures and their occurrences in the dataset. These unique substructures are extracted by pairwise comparison of compounds of training set.

developed by JNU in collaboration with SL as a part of the OpenTox project.





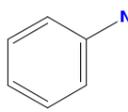
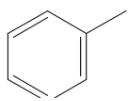
NAVIGATION

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- Tune Model
- Fingerprint Dataset
- Predict Dataset
- Analyse Dataset
- Analyse Compound
- Credits

SERVER STATS

- View Tasks

Dataset :
Fragments_of_Model_729e7130_4491_4ab2_b87a_99

SlNo	Smile	Occurences	Atomcontainer
1	<chem>C1=CC=CC=C1</chem>	44	
2	<chem>CC</chem>	27	
3	<chem>C[N+]</chem>	22	
4	<chem>[N+]C1=CC=CC=C1</chem>	16	
5	<chem>CC1=CC=CC=C1</chem>	13	

RELATED LINKS

- OpenTox
- ToxCreate
- ToxPredict

OPENSOURCE

- Restlets
- Jena
- CDK
- R (statistics)
- Rserve

Fig 4: Fragments

SVM Predicted Training dataset URI : This is the address for the training set after being predicted using this model and contains original class of compound(as in source dataset), the predicted class of compound (using MaxTox model) an fragments present or absent in each compound. These datasets are uploaded on an external dataset service like ambit, for example in Fig 3, the predicted training dataset URI is <http://apps.ideaconsult.net:8080/ambit2/dataset/601421>.

Make Model

Address for the Make Model service:

<http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/makeMaxtoxModel>

MaxTox can be used to generate Fingerprinter model or Prediction (or Fingerprinter + Predictor) model depending upon the user's requirements. (See user's discussion in View Models section for details)

If you wish to build a new model for your own dataset rather than using one of the existing models, Make Models service at MaxTox enables you to do so by following few simple steps.

The screenshot shows the MaxTox MCSS web interface. At the top, it says 'developed by JNU in collaboration with SL as a part of the OpenTox project.' The main header includes the 'OpenTox' logo and 'MaxTox MCSS'. On the left, there is a 'NAVIGATION' menu with links: Home, View Models, Make Model, Tune Model, Fingerprint Dataset, Predict Dataset, Analyse Dataset, Analyse Compound, and Credits. Below this is a 'SERVER STATS' section with a 'View Tasks' link. The main content area is titled 'Make Maxtox Fingerprinters and Models' and includes instructions: 'Use this service to' followed by two bullet points: 'Find MCSS and large common fragments between compounds in a dataset. The fragments will form the basis of a fingerprinter.' and 'Optionally make a prediction model to predict a feature. The input dataset in this case should have the target feature embedded inside.' Below this is a 'FINGERPRINTER BASICS' section with a 'Submit a dataset uri' heading. It provides an example URI: <http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=10> and a note: 'Maxtox uses datasets which have already been uploaded to a dataset service. The following box is not for a local file. To test this service you can cut and paste the above link to the box below. To see what is contained in the above dataset click on the link (it will open the dataset in a new window so be sure to allow the same for your browser). To use your own dataset you have to upload it first to a dataset service. Go to the default dataset service.' There is a text input box below. The next section is 'Submit a dataset service uri for uploading of results' with a default service URI: <http://apps.ideaconsult.net:8080/ambit2/dataset> and a note: 'If you plan to use the default service you can leave the following field blank. If however you have a custom dataset service [compatible with OpenTox Dataset API] then paste the link to that dataset below.' There is another text input box. The final section is 'Submit an email address for notifications.' with a note: 'An email will be sent to this address when the task completes. Some of these tasks take pretty long [depending on the no of compounds in the input dataset] and it is advisable to mention an email address here to free you from the onerous job of repeatedly refreshing the task page to find if it has been completed.' There is a third text input box. On the right side, there are 'RELATED LINKS' (OpenTox, ToxCreate, ToxPredict) and 'OPENSOURCE' (Restlets, Jena, CDK, R (statistics), Rserve) sections.

Fig 5: Making MaxTox Fingerprinter and Prediction models.

Step 1: Uploading datasets

First, you have to upload your datasets to a dataset service. Since MaxTox works on the lines of OpenTox API framework, a dataset service is mandatory to upload source dataset and where the result dataset will be uploaded once MaxTox completes the task. The default dataset service that we are using for example use case is <http://apps.ideaconsult.net:8080/ambit2/dataset>.

The example dataset that we are using is <http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=10>. Here dataset id is 272. max=10 simply means that we are selecting first ten compounds from an otherwise large dataset for example use case because fingerprint generation and model building may take very long for a large number of compounds. For example, full prediction run with existing models for fifteen compounds of Bursi mutagenicity dataset (<http://apps.ideaconsult.net:8080/ambit2/dataset/272>) took whole 1 minute and

15 seconds to complete.

Step 2: Submit a dataset URI

Enter the example dataset in this field. This will be the source dataset that is used to make the model.

Step 3: Submit a dataset URI for uploading of results

Enter a dataset service address that is OpenTox Dataset API compatible or if you want to use the default dataset service that is, AMBIT dataset service, leave this field blank.

Step 4: Submit an email address for notifications

The notification about successful task completion or any unexpected failure caused during the job processing will be sent to the email submitted. Users are requested to give a valid email in this field to free them from repeatedly checking for the completion of the tedious task of model building.

Step 5: Submit a Fingerprinter maker task

If you intend to make only a Fingerprinter model that is, only MCSS dictionary is to be generated, click on the button 'Submit a Fingerprinter-Model maker task'. However if you also want a prediction model to be built, proceed to next step.

Step 6: Submit a Prediction-Model maker task

If you want to create a Prediction Model using SVM algorithm, select radio button for 'Yes' against the text **'Would you like to predict features using SVM?'** This would unveil a set of modelling parameters. Each field describes clearly, what that parameter means (see Fig 6). Fill up these fields and then click on the button **'Submit a Fingerprinter-Model maker task'** to submit the task.

Submit a Fingerprinter-Model maker task

MODELING FOR PREDICTION

Would you like to predict features using SVM ? Yes No

Note : If you chose to make a prediction model then you will get a fingerprint and a prediction from the created model. If you chose not to make a prediction model (default condition) then the resulting model will only give fingerprints. However making a prediction model is significantly resource intensive and the task may take much longer to complete !

MODELING PARAMETERS

Submit a URI of feature to be predicted .

Example : <http://apps.ideaconsult.net:8080/ambit2/feature/26221>

Note : This feature has to be available within the input dataset mentioned in the first field. For testing you can cut and paste this feature link - provided you are using the example dataset in step one. If you are using your own dataset then you will have to find out the features contained within that dataset and use one of them as the target of the prediction.

What is the feature type ? Integer Float String

Note : Features with values like "mutagen" or "carcinogen" etc qualify for being string features. Features with values like "4.5" or "0.5" etc qualify for being a float feature. Features with values like "1" or "3" etc are integer features.

If String feature then what are the two classes ?

Note : If its an integer/float feature you can leave these blank. The algorithm will automatically generate a label like : "Value is less than cutoff" ... etc. Class 1 is considered to be the "active" class , which means all specificity and sensitivity measurements are done w.r.t Class 1

Class 1 (active) :

Class 2 (inactive):

If Integer or Float Feature what is the cutoff ?

Note : If you have a FLOAT feature with values like "3.5", "4.5" etc OR an INTEGER feature with values like "1" . "2" etc ... then the cutoff is the value around which the dataset will be classified. By default any

Fig 6: Modelling parameters to make SVM prediction model

Step 7: Submission of task

When the task is submitted, it will provide you with a unique task id, for example, for our example use case, we have **Task_dbe8b6e5_9ef8_4f37_a1ff_848bcc8ff2d2**.

developed by JNU in collaboration with SL as a part of the OpenTox project.




NAVIGATION

- Home
- View Models
- Make Model
- Tune Model
- Fingerprint Dataset
- Predict Dataset
- Analyse Dataset
- Analyse Compound
- Credits

SERVER STATS

- View Tasks

Task name :
Task_dbe8b6e5_9ef8_4f37_a1ff_848bcc8ff2d2

taskName	Task_dbe8b6e5_9ef8_4f37_a1ff_848bcc8ff2d2
type	1
title	MCSSFinder and Modeller Run
description	A workflow to get MCSS and other common fragments between two compounds and then model it using SVM.
status	Running
percentageCompleted	10
dateStarted	15-Jul-2011 02:23:42
dateEnded	n/a
requestingIP	180.149.62.227
result_uri	n/a
source	http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/algorithm/MCSSFinder/Algorithm_045bf38f_c844_4e4c_9dcd_55692e9c1a1f

[Get the Task Logs](#)

RELATED LINKS

- OpenTox
- ToxCreat
- ToxPredict

OPENSOURCE

- Restlets
- Jena
- CDK
- R (statistics)
- Rserve

running on Tomcat 6.0 bug-reports/feature-requests : support@maxtox.org

OpenTox - An Open Source Predictive Toxicology Framework, www.opentox.org, is funded under the EU Seventh Framework Program: HEALTH-2007-1.3-3 Promotion, development, validation, acceptance and implementation of QSARs (Quantitative Structure-Activity Relationships) for toxicology, Project Reference Number Health-F5-2008-200787 (2008-2011)

Fig 7: Task details

The details of the task like description, start time, end time, percentage completion etc is given at the address http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/task/Task_dbe8b6e5_9ef8_4f37_a1ff_848bcc8ff2d2. The model building may take time, so when the task is completed an email notification is sent to you.

Step 8: See the results

Refresh the task details page. If the task is completed, percentage completed is shown 100 and a result URI is provided which navigates to the detailed page for model built using the submitted dataset (same as Fig 3). Model details include SVM parameters used for model building and model performance measures like sensitivity, specificity, cross validation accuracy, correlation coefficient etc. To proceed from here refer to step 2 of View Models section.

User's Discussion:

When a source dataset is submitted for model building, first the MCSS substructures are extracted using pairwise comparisons of compounds done to obtain the largest overlaps. The fragments or MCSS dictionary is prepared for the training dataset by removing the duplicates. This MCSS dictionary is then used to generate fingerprints. These fingerprints are then used as input for SVM algorithm and a classifier type prediction model is built using the SVM parameters submitted by the user at the time of task submission. N fold cross validation during SVM modeling, gives a cross validation accuracy (n may be equal to 5 or 10, default is 5). In addition, sensitivity and specificity of the model give an idea about the model performance. This model can be further used for making predictions on unknown compounds against the same end-point.

View Tasks: MaxTox has a feature that enables a user to see the list of task histories submitted at MaxTox server and their status at the address: <http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/task>. Click on the task id, whose details you want to see.

OpenTox **MaxTox** MCSS JNU

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Task List

TaskName	DateStarted	Title	Status
Task_31859c1e_f415_49ea_b8c1_cb91282da5f4	04-Jun-2011 07:57:36	MCSSFinder Run	Completed
Task_a12aed08_00c7_414e_ba49_23d67d4d7d01	04-Jun-2011 08:35:47	MCSSFinder Run	Completed
Task_f4f22a1d_225b_4b4a_bd6f_18af1b4d5ccd	04-Jun-2011 08:55:44	MCSSFinder and Modeller Run	Completed
Task_4c5eb805_c67c_4eb4_aaef_0576b4b1127b	04-Jun-2011 08:58:14	SVM ReModeller Run	Completed
Task_673f2629_755b_4a85_be50_cd785605e5e4	04-Jun-2011 09:01:52	Fingerprinting Task.	Completed
Task_ce3652c7_ad97_4994_858e_dc4b0ac093c0	05-Jun-2011 10:47:46	Full Prediction Run with existing models	Completed
Task_dad10442_4b49_414e_8e65_1111a5932e1b	05-Jun-2011 10:53:51	Fingerprinting Task.	Completed
Task_28c66cdc_1ac9_4f16_9789_4f6869c4e3b2	06-Jun-2011 09:46:38	Fingerprinting Task.	Completed
Task_174d96ec_2f47_4228_ab21_ca4927801e14	06-Jun-2011 09:55:29	Fingerprinting Task.	Completed
Task_c3083449_ed2f_483d_b927_272ffc71e2c8	06-Jun-2011 09:57:35	Full Prediction Run with existing models	Completed
Task_aca2de88_a4d2_425b_845b_99eb60fcaaff	06-Jun-2011 10:08:11	Full Prediction Run with multiple models	Completed
Task_2444953f_cc8d_49cc_a02d_73c42ed874be	06-Jun-2011 10:20:28	Full Prediction Run with multiple models	Completed
Task_a7d12b95_4bfd_4fed_9c02_9f723cc8a6f2	06-Jun-2011 10:32:08	MCSSFinder Run	Completed
Task_0d33ef5d_cc3c_4395_8376_83eb5d5b6fff	06-Jun-2011 11:38:42	MCSSFinder and Modeller Run	Completed
Task_99212929_d40f_49b1_98aa_0ba5bf5898de	06-Jun-2011 11:51:44	Fingerprinting Task.	Completed
Task_8e616ca3_957f_48b9_b7b1_7d260d884be0	06-Jun-2011 12:06:51	Full Prediction Run with existing models	Completed
Task_4f5c50f5_f1ca_4044_8b3e_e8332a9f0c3c	06-Jun-2011 12:10:42	Full Prediction Run with multiple models	Completed

RELATED LINKS

- OpenTox
- ToxCreate
- ToxPredict

OPENSOURCE

- Restlets
- Jena
- CDK
- R (statistics)
- Rserve

Fig 8: Task history

Get Task Logs: Also, you can get the step-by-step log of your task specially if there is some unexpected error during the task processing. This helps the user as well as the developer in debugging.

Tune Model

Address for the Tune Model service:

<http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/remakeModel>

Suppose you want to use an already existing model. The source dataset, the feature, and models everything is desirable but you are not satisfied with the model performance and you want to play around with the parameters used in SVM model building. Here the Tune Model service (Fig 9) comes in handy.

developed by JNU in collaboration with SL as a part of the OpenTox project.

OpenTox **MaxTox** MCSS 

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Submit a Model re-tuning Task - Step 1

Select a model to use ...

Available models

	Model 729e7130_4491_4ab2_b87a_998e7bdb1e50
Description	A Maxtox SVM Predictor Model (Fingerprinter + Predictor) : The MCSS (MMaximum Common Substructures) have been extracted from the dataset using a series of pairwise comparisons. The structures are then filtered for duplicates to yield a set of unique substructures. This set can be used to build a predictive model by fingerprinting the source dataset molecules, and then using the fingerprint to to create a prediction model for the feature to be predicted (from the source dataset). An SVM Model is also available for predicitions. This is a classifier type model.
SVM Model ?	Yes
RandomForest Model?	No
Source Dataset URI	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=20

	Model 7e0ef05c_050d_41dd_afbb_cc0900dfac95
Description	A Maxtox SVM Predictor Model (Fingerprinter + Predictor) : The MCSS (MMaximum Common Substructures) have been extracted from the dataset using a series of pairwise comparisons. The structures are then filtered for duplicates to yield a set of unique substructures. This set can be used to build a predictive model by fingerprinting the source dataset molecules, and then using the fingerprint to to create a prediction model for the feature to be predicted (from the source dataset). An SVM Model is also available for predicitions. This is a classifier type model.
SVM Model ?	Yes
RandomForest Model?	No
Source Dataset URI	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=20

	Model 2d79f457_3b8d_43b4_bbde_87df1d47151a
Description	A Maxtox SVM Predictor Model (Fingerprinter + Predictor) : The MCSS (MMaximum Common Substructures) have been extracted from the dataset using a series of pairwise comparisons. The structures are then filtered for duplicates to yield a set of unique substructures. This set can be used to build a predictive model by fingerprinting the source dataset molecules, and then using the fingerprint to to create a prediction model for the feature to be predicted (from the source dataset). An SVM Model is also available for predicitions. This is a classifier type model.

RELATED LINKS

- OpenTox
- ToxCreat
- ToxPredict

OPENSOURCE

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Fig 9: Submit a model for retuning

Step 1: Select the model

First, select the model whose parameters you want to tune and then click on the button **'Submit selected model for re-tuning'**. This will navigate you to a page where you can set new parameters for SVM model building (see Fig 10) like different kernel function or different number of folds of cross-validation.

Make Model

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SVM OPTIONS

What are the new SVM options ?
Refer to <http://svmlight.joachims.org>

Parameter	Description	New Value	Existing Value
Cross Validation options for checking accuracy :			
-v [3,5...]	No. of folds of cross-validation (default 5)	<input type="text" value="5"/>	5
Learning options:			
-z {c,r,p}	select between classification (c), regression (r), and preference ranking (p) (see [Joachims, 2002c]) (default classification)	<input type="text" value="c"/>	c
-c float	C: trade-off between training error and margin (default [avg. x*x] ⁻¹)	<input type="text" value="20"/>	20
-w [0..]	epsilon width of tube for regression (default 0.1)	<input type="text" value="0.1"/>	0.1
-j float	Cost: cost-factor, by which training errors on positive examples outweigh errors on negative examples (default 1) (see [Morik et al., 1999])	<input type="text" value="1"/>	1
-b [0,1]	use biased hyperplane (i.e. x*w+b0) instead of unbiased hyperplane (i.e. x*w0) (default 1)	<input type="text" value="1"/>	1
-i [0,1]	remove inconsistent training examples and retrain (default 0)	<input type="text" value="0"/>	0
Performance estimation options:			
-x [0,1]	compute leave-one-out estimates (default 0)	<input type="text" value="0"/>	0
-o [0..2]	value of rho for XiAlpha-estimator and for pruning leave-one-out computation (default 1.0) see [Joachims, 2002a])	<input type="text" value="1"/>	1
-k [0..100]	search depth for extended XiAlpha-estimator (default 0)	<input type="text" value="0"/>	0
Transduction options (see [Joachims, 1999c], [Joachims, 2002a]):			
-p [0..1]	fraction of unlabeled examples to be classified into the positive class (default is the ratio of positive and negative examples in the training data)	<input type="text"/>	
Kernel options:			
-t int	type of kernel function: <ul style="list-style-type: none"> • 0: linear (default) • 1: polynomial (s a*b+c)^d • 2: radial basis function exp(-gamma a-b ²) • 3: sigmoid tanh(s a*b + c) 	<input type="text" value="0"/>	0
-d int	parameter d in polynomial kernel	<input type="text"/>	

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Fig 10: Tuning parameters of an existing SVM model

Step 2: Retune the parameters

After submitting the new SVM parameters, click on the button '**Submit model for re-tuning**' and submit the task. This will return a task id leading you to a page showing task details like the percentage completed, start time, end time etc. This may take a while.

Step 3: Check for re-tuned model

When you refresh the task page, the percentage completed is 100 and a result URI is provided which leads you to the re-tuned model that you desired. Now you can use your new model for future predictions.

developed by JNU in collaboration with SL as a part of the OpenTox project.





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Task name :
Task_f8ffea84_d023_48f2_862b_361059a907ad

taskName	Task_f8ffea84_d023_48f2_862b_361059a907ad
type	4
title	SVM ReModeller Run
description	A workflow to remodel the SVM part of a previous model with new paramerters
status	Completed
percentageCompleted	100
dateStarted	15-Jul-2011 03:17:28
dateEnded	15-Jul-2011 03:18:17
requestingIP	180.149.62.227
result_uri	http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/model/Model_24e8e611_c9eb_4aa2_8b74_0311e972ab29
source	/algorithm/SVMRemodeller

[Get the Task Logs](#)

RELATED LINKS

- OpenTox
- ToxCreat
- ToxPredict

OPENSOURCE

- Restlets
- Jena
- CDK
- R (statistics)
- Rserve

running on Tomcat 6.0 bug-reports/feature-requests : support@maxtox.org

OpenTox - An Open Source Predictive Toxicology Framework, www.opentox.org, is funded under the EU Seventh Framework Program: HEALTH-2007-1.3-3 Promotion, development, validation, acceptance and implementation of QSARs (Quantitative Structure-Activity Relationships) for toxicology, Project Reference Number Health-F5-2008-200787 (2008-2011)

Fig 11: Getting a retuned model

User's Discussion:

SVM models performance that is, sensitivity and specificity can be improved by optimising the SVM parameters. Therefore, Tune Model service here provides user an option to improve model's performance. The algorithm used behind this service is SVMRemodeller instead of the MCSSFinder algorithm that was operating behind the Make Model service.

Fingerprint Dataset

Address for the Fingerprint Dataset service:

<http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/fingerprint>

Step 1: Select a model for fingerprinting

To fingerprint a dataset using the models available at MaxTox, first select a model as shown in Fig 12 and then click on the button '**Submit selected model to use for fingerprinting**'. This will take you to the next page (see Fig 13).

developed by JNU in collaboration with SL as a part of the OpenTox project.

OpenTox **MaxTox** MCSS JNU

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Submit a Fingerprinting Task - Step 1

Select a model to use ...

Available models

Model_2bbd0400_4fa4_45cb_b7c7_0925bfe3f741	
Description	A Maxtox Basic Model (Fingerprinter) : The MCSS (MAximum Common Substructures) have been extracted from the dataset using a series of pairwise comparisons. The structures are then filtered for duplicates to yield a set of unique substructures. This set can be used to build a predictive model by fingerprinting the source dataset molecules, and then using the fingerprint to to create a prediction model for the feature to be predicted (from the source dataset).
SVM Model ?	No
RandomForest Model?	No
Source Dataset URI	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=20

Model_e8342231_e3a0_4f20_b624_415a3a5673e0	
Description	A Maxtox Basic Model (Fingerprinter) : The MCSS (MAximum Common Substructures) have been extracted from the dataset using a series of pairwise comparisons. The structures are then filtered for duplicates to yield a set of unique substructures. This set can be used to build a predictive model by fingerprinting the source dataset molecules, and then using the fingerprint to to create a prediction model for the feature to be predicted (from the source dataset).
SVM Model ?	No
RandomForest Model?	No
Source Dataset URI	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=20

Model_729e7130_4491_4ab2_b87a_998e7bdb1e50	
Description	A Maxtox SVM Predictor Model (Fingerprinter + Predictor) : The MCSS (MAximum Common Substructures) have been extracted from the dataset using a series of pairwise comparisons. The structures are then filtered for duplicates to yield a set of unique substructures. This set can be used to build a predictive model by fingerprinting the source dataset molecules, and then using the fingerprint to to create a prediction model for the feature to be predicted (from the source dataset). An SVM Model is also available for predicitions. This is a classifier type model.
SVM Model ?	Yes

RELATED LINKS

- OpenTox
- ToxCreate
- ToxPredict

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Fig 12: Submit a fingerprinting task

Step 2: Submit a dataset for fingerprinting

Now first enter the address of the dataset whose fingerprints has to be generated using the model that was selected in step 1, for example, <http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=10> . Then enter a dataset service URI for uploading of results or leave the field blank (see Fig 13) to use the default dataset service at AMBIT.

Fig 13: Submit a dataset for fingerprinting

After entering the respective fields, click on the button ‘**Submit dataset for fingerprinting**’. This will return a unique id for the task you have submitted and you will see a page showing task details like percentage completed. Completion of task may take a while.

Step 3: Task completion and obtaining the results

You will get an email notification on completion of the task. Refresh the page, the percentage completed will be 100 and the result URI will be provided which will eventually point at the dataset uploaded at the dataset service.

User’s Discussion:

When a model is used for fingerprinting an unknown dataset, each of the fragments from the MCSS dictionary of the model is checked for its presence in each compound of the dataset. The absence/presence of these fragments is denoted by 0/1, thus generating the binary fingerprints for each compound that are uploaded at the result URI at the dataset service. These fingerprints can be downloaded from the result URI in a desired format (csv, text, pdf etc).

Predict Dataset

Address for the Predict Dataset service:

<http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/predict>

Step 1: Select a model to use for prediction task

After selecting the desired model, click on the submit button provided on the bottom of the

page.

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Submit a Fingerprinting/Prediction Task - Step 1

Select a model to use ...

Available models

Model ID	Description
<input checked="" type="radio"/> Model_729e7130_4491_4ab2_b87a_998e7bdb1e50	A Maxtox SVM Predictor Model (Fingerprinter + Predictor) : The MCSS (Maximum Common Substructures) have been extracted from the dataset using a series of pairwise comparisons. The structures are then filtered for duplicates to yield a set of unique substructures. This set can be used to build a predictive model by fingerprinting the source dataset molecules, and then using the fingerprint to create a prediction model for the feature to be predicted (from the source dataset). An SVM Model is also available for predictions. This is a classifier type model.
<input type="radio"/> Model_7e0ef05c_050d_41dd_afbb_cc0900dfac95	A Maxtox SVM Predictor Model (Fingerprinter + Predictor) : The MCSS (Maximum Common Substructures) have been extracted from the dataset using a series of pairwise comparisons. The structures are then filtered for duplicates to yield a set of unique substructures. This set can be used to build a predictive model by fingerprinting the source dataset molecules, and then using the fingerprint to create a prediction model for the feature to be predicted (from the source dataset). An SVM Model is also available for predictions. This is a classifier type model.
<input type="radio"/> Model_2d79f457_3b8d_43b4_bbde_87df1d47151a	

RELATED LINKS

- OpenTox
- ToxCreat
- ToxPredict

OPENSOURCE

- Restlets
- Jena
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- R (statistics)
- Rserve

Fig 14: Select a model for prediction task

Step 2: Submit dataset for predictions

Step 1 will lead you to the next page (see Fig 15) showing a set of fields to enter the dataset for prediction. Enter appropriate values in all the required fields and click on the submit button provided on the bottom of the page '**Submit dataset for fingerprinting/predictions**' and you will be directed to the task detail page showing the percentage completion of the task.

OpenTox MaxTox MCSS

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Submit a dataset for predictions

Submit a dataset uri
Example : <http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=10>
Note : Maxtox uses datasets which have already been uploaded to a dataset service. The following box is not for a local file. To test this service you can cut and paste the above link to the box below. To see what is contained in the above dataset click on the link (it will open the dataset in a new window so be sure to allow the same for your browser). To use your own dataset you have to upload it first to a dataset service. Go to the default dataset service.

Submit a dataset service uri for uploading of results
Default Service : <http://apps.ideaconsult.net:8080/ambit2/dataset>
Note : If you plan to use the default service you can leave the following field blank. If however you have a custom dataset service [compatible with OpenTox Dataset API] then paste the link to that dataset below.

Do you want to include original dataset features in the result dataset ? Yes No
Note : Once a prediction model is made a result dataset will be created and uploaded to the dataset service mentioned above. This result dataset will have all the compounds of the training set along with their fingerprints w.r.t. to the model and a prediction feature to show the predicted values of the training set compounds. This dataset can optionally contain the original features as well. This may be useful if the fingerprint or the predicted feature needs to be used in another model, in conjunction with the original features.

Submit an email address for notifications.
Note : An email will be sent to this address when the task completes. Some of these tasks take pretty long [depending on the no of compounds in the input dataset] and it is advisable to mention an email address here to free you from the onerous job of repeatedly refreshing the task page to find if it has been completed.

RELATED LINKS

- OpenTox
- ToxCreat
- ToxPredict

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Fig 15: Submit dataset for predictions

Step 3: Task completion and prediction results

Once you are notified about the task completion by email, refresh the page and check for 100 percent completion of the task. Click on the result URI that is uploaded on the dataset service to see the predictions made by the model selected in the step 1.

User's Discussion:

When a model is selected for predicting an unknown dataset, one important thing to consider is that a model built for a dataset having aquatic toxicity, as the endpoint should not be used to predict the mutagenicity of a dataset.

Prediction task involves fingerprinting of the unknown dataset using the MCSS dictionary of the model and then using these fingerprints to pass through the prediction model (classifier type) to decide whether a particular compound belongs to one class or the other. The prediction results can always be downloaded from the dataset service using the result URI provided on task completion.

Note that MaxTox models presently work only for binary endpoint data, that is, dataset having two classes.

Analyse Dataset

Address for the Analyse Dataset service:

<http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/predictDataset>

Step 1: Submit a dataset for multi endpoint analysis

Enter the dataset URI which has to be analysed using more than one endpoint in the field given at the above address and click on the submit button '**Submit dataset for analysis**' given at the bottom of the page.

Step 2: Select endpoints to predict

Select as many endpoints or models as you want to analyse your dataset for as shown in Fig 16, and then click on the submit button on the bottom of the page to submit the task.

The screenshot shows the OpenTox Dataset REST API interface. On the left, there are buttons for 'Credits', 'SERVER STATS', and 'View Tasks'. On the right, there are buttons for 'R (statistics)' and 'Rserve'. The main area displays a list of model endpoints for prediction. Each model entry includes a checkbox, a model ID, and a table of details:

Model ID	End Point	SVM Model?	RandomForest Model?	Source Dataset URI
Model_7e0ef05c_050d_41dd_afbb_cc0900dfac95	Ames test categorisation	Yes	No	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=20
Model_2d79f457_3b8d_43b4_bbde_87df1d47151a	Ames test categorisation	Yes	No	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=20
Model_2c3c816d_8480_4130_8a9e_8af5565229cd	SAL	Yes	No	http://apps.ideaconsult.net:8080/ambit2/dataset/429390?max=20
Model_6cc0a560_b5ee_4209_a207_e567f93a33ff	Ames test categorisation	Yes	No	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=10

Fig 16: Select endpoints to predict

Step 3: Task completion and analysis results

When you refresh the task detail page on completion, it will provide you a result URI. Click on the result URI to see the multi-endpoint analysis results for the given dataset (see Fig 17).

The screenshot shows the OpenTox Dataset REST API interface with search results. The search bar contains 'ambit' and the search results are displayed in a table. The table columns are 'Compound', 'Default pr', and three prediction columns for different models. The results show 'nonmutagen' and 'mutagen' predictions for three compounds.

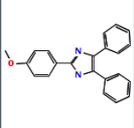
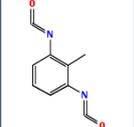
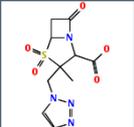
#	Compound	Default pr	http://ope	http://ope	http://ope
1		1728-95-6	nonmutagen	mutagen	mutagen
2		91-08-7	nonmutagen	mutagen	mutagen
3		89786-04-9	nonmutagen	nonmutagen	nonmutagen

Fig 17: Multi-endpoint analysis results uploaded on the dataset service

User's Discussion:

In the multi endpoint analysis of a dataset using MaxTox Analyse Dataset service, you can predict a dataset using more than one model (and endpoints). The MaxTox algorithm running

behind this service is the MultiModelAnalyser. It enables you to predict your dataset for multiple endpoints, for example, Salmonella mutagenicity, Aquatic toxicity or carcinogenicity simultaneously by selecting the respective endpoint models at the same time.

Analyse Compound

Address for the Analyse Compound service:

<http://opentox2.informatik.uni-freiburg.de:8080/MaxtoxMCSS/enterNewCompound>

If a user wants to use MaxTox services for a private compound instead of the whole dataset, he can use Analyse Compound utility of MaxTox as follows.

Step 1: Enter a new compound

You can draw your compound or submit SMILES directly and then submit the compound for analysis by clicking on the submit button at the bottom of the page. For example, we have submitted benzene for testing.

Fig 18: Enter a new compound for analysis

Step 2: Make new compound or select an existing one

When you submit a compound for analysis, first it is searched through the already available database. If the compound is already available in the database, select your compound and if not, there is a **Make new compound** option at the bottom of the page (see Fig 19).

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NAVIGATION

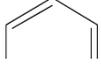
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Input SMILE of compound to be analysed is : C1=CC=CC=C1

Select compound from list of existing compounds.

Http://apps.ideaconsult.net:8080/ambit2/compound/119711/conformer/206258
<div style="display: flex; align-items: center;">  <div> <p style="font-size: 0.8em; margin: 0;">30.11.2010 UHOVQNZJYSORNB-UHFFFAOYSA-N InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H Naphtha white spirit 617-047-3 8030-31-7</p> </div> </div>
Http://apps.ideaconsult.net:8080/ambit2/compound/29530/conformer/213754
<div style="display: flex; align-items: center;">  <div> <p style="font-size: 0.8em; margin: 0;">30.11.2010 UHOVQNZJYSORNB-UHFFFAOYSA-N InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H Asphalt 232-490-9 8052-42-4</p> </div> </div>
Http://apps.ideaconsult.net:8080/ambit2/compound/29529/conformer/213753
<div style="display: flex; align-items: center;">  <div> <p style="font-size: 0.8em; margin: 0;">30.11.2010 UHOVQNZJYSORNB-UHFFFAOYSA-N InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H</p> </div> </div>

RELATED LINKS

- OpenTox
- ToxCreat
- ToxPredict

OPENSOURCE

- Restlets
- Jena
- CDK
- R (statistics)
- Rserve

Fig 19a: Make new compound or select an existing one

	<p style="font-size: 0.8em; margin: 0;">30.11.2010 UHOVQNZJYSORNB-UHFFFAOYSA-N InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H Petroleum PETROLEUM OIL 232-298-5 8002-05-9</p>
Http://apps.ideaconsult.net:8080/ambit2/compound/684/conformer/144514	
<div style="display: flex; align-items: center;">  <div> <p style="font-size: 0.8em; margin: 0;">c1ccccc1 C1=CC=CC=C1 c(cccc1)c1 71-43-2 NOCAS benzene UHOVQNZJYSORNB-UHFFFAOYSA-N benzene (6)annulene; benzine; Benzol; Benzolene; bicarburet of hydrogen; carbon oil; Coal naphtha; cyclohexatriene; mineral naphtha; motor benzol; nitration benzene; Phene; Phenyl hydride; pyrobenzol. Benzene BENZENE C6H6 mol_1 Benzene; 71-43-2; mol_1 Benzene; 71-43-2; -0.12 c1ccccc1 Benzene; Transgenic model evaluation II (Benzene) Benzene + aniline combo Benzene + aniline 30.11.2010 InChI=1S:C6H6/c1-2-4-6-5-3-1/h1-6H 200-753-7</p> </div> </div>	OR
<p>Make new compound ?</p> <p> <input type="radio"/> Yes <input checked="" type="radio"/> No </p>	
<p style="background-color: #4CAF50; color: white; padding: 5px 15px; border-radius: 5px; display: inline-block;">Submit compound for analysis</p>	
<p style="background-color: #4CAF50; color: white; padding: 2px 5px; border-radius: 5px; display: inline-block; font-size: 0.8em;">I Love CURL !</p>	

Fig 19b: Make new compound or select an existing one

Click on the submit button on the bottom either to select an existing compound or create a new compound and upload it on the dataset service.

Step 3: Select endpoints of models to predict

When you create a new compound, a new compound URI is obtained. For example, despite existence of benzene we opted for **Make new compound** option, and a new compound is formed at the URI:

<http://apps.ideaconsult.net:8080/ambit2/compound/23575/conformer/709842>

Now select the endpoints (or Models) for which you want to analyse your compound (see Fig 20) just like in case of multi-endpoint analysis of the dataset described in section **Analyse Dataset**.

The screenshot shows a web application interface for selecting endpoints to predict. The main content area contains the following information:

Select endpoints (of Models) to predict ...

Input SMILE of compound to be analysed is : C1=CC=CC=C1

URI of compound to be analysed is : <http://apps.ideaconsult.net:8080/ambit2/compound/23575/conformer/709842>

Select a model to use ...

Available models

<input type="checkbox"/>	Model_729e7130_4491_4ab2_b87a_998e7bdb1e50
End Point	Ames test categorisation
SVM Model ?	Yes
RandomForest Model?	No
Source Dataset URI	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=20

<input type="checkbox"/>	Model_7e0ef05c_050d_41dd_afbb_cc0900dfac95
End Point	Ames test categorisation
SVM Model ?	Yes
RandomForest Model?	No
Source Dataset URI	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=20

<input type="checkbox"/>	Model_2d79f457_3b8d_43b4_bbde_87df1d47151a
End Point	Ames test categorisation
SVM Model ?	Yes
RandomForest Model?	No
Source Dataset URI	http://apps.ideaconsult.net:8080/ambit2/dataset/272?max=20

<input type="checkbox"/>	Model_2c3c816d_8480_4130_8a9e_8af5565229cd
End Point	SAL

Fig 20: Select endpoints to predict

After selecting, click on the submit button to submit the task.

Step 4: Task completion and compound analysis results

Refresh the task detail page on completion and click on the result URI to see the analysis result for the compound you entered against the multiple endpoints.

User's Discussion:

Analysis Compound service is same as the Analyse Dataset service except the fact that in compound analysis you can provide a single compound instead of the whole dataset. Even for a single compound analysis, first, it has to be uploaded on the dataset service, only then it can be used by a MaxTox service. **Make new compound** option thus uploads the compound on the dataset service and provides the user with the compound URI.

Prediction results can be downloaded from the dataset service using the result URI for predictions where the given compound is predicted against the multiple endpoints selected in step 3.

Note: For using command line calls, one can click on the "I Love CURL" button provided at the bottom of each page and use the cURL command displayed to perform the same task as the respective GUI will do.

Glossary

End-point: End-point for toxicity denotes the result of the study conducted to determine how toxic or harmful a substance is. For example, Carcinogen/Noncarcinogen, Mutagen/Nonmutagen etc

Fingerprints: Fingerprint is a binary descriptor for a molecule denoting the absence/presence of a substructure fragment as 0/1.

MCSS: Maximum Common Substructure Search (MCSS) is an approach where Maximum Common Substructure (MCS) is the largest substructure that appears in structures of both compounds. MCS can be used as a measure of chemical similarity to compute chemical descriptors, which can be further used for activity predictions.

QSAR: Quantitative Structure Activity Relationship is the process by which the chemical structure of a compound is quantitatively correlated with biological or chemical activity of that compound.

SVM: Support Vector Machines is a machine-learning algorithm that is based on supervised learning mechanism and is used for classification and regression analysis of data. When a training set of data belonging to one of the two classes is given as input, SVM builds a prediction model that can classify new data entries to either of the two input classes.

RF: Random Forest is an ensemble classifier that makes its decision based on outputs from multiple decision trees so that the final class predicted is mode of the class's output by individual trees.

URI: Uniform Resource Identifier represents the name or address of a resource on the internet. URIs are of two types: URN (Uniform Resource Name) and URL (Uniform Resource Locator).

SMILES: Simplified Molecular Input Line Entry Specification is a chemical language to represent chemicals and reactions using ASCII characters.

Dataset service: Dataset service refers to a service, which contains data in the format specified by OpenTox API guidelines and where a service like MaxTox can upload more datasets and retrieve the existing ones from the service.

References

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