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Janez Demsar and Blaz Zupan

From Experimental Machine Learning to Interactive Data Mining

Orange is a comprehensive, component-based framework for both experienced data mining and machine learning users and developers, and for those just entering the field that can interface Orange through short Python scripts or visually design data mining applications using Orange Canvas and widgets.

Quite a few years ago, we were (each!) writing our own code for attribute scoring, decision tree induction, ten-fold cross validation and alike (not to mention routines for loading the data and pretty-printing). We got bored. Knowing that coding of the basic set of tools from the ground up was within the job description of just about any researcher in machine learning did not help. At the time quite a few machine learning programs like C4.5 and CN2 were available, but they were coded separately, used different data file formats, and were incompatible in every other respect. There were very few machine learning suites available, which did not offer much in terms of easy prototyping and flexibility in experimenting.

Then, thanks to Donald Michie, in 1997 came a meeting called WebLab. Taking place at a romantic site (Lake Bled), it called for at a time rather rule-breaking initiative to build a flexible experimental benchmark where one could easily add his own algorithms, record the experiments through scripts, and do all sorts of data analysis and machine learning. The benchmark would support both scripting and graphical user's interface. WebLab meeting generated a number of good ideas, but never took on a project it was aiming for. Nevertheless, though, it inspired us, and in that year we have started to work on Orange, a machine learning and data mining suite that had occupied us ever since.

Orange, the Data Mining Framework

Orange is a library of C++ core objects and routines that includes a large variety of standard and not-so-standard machine learning and data mining algorithms, plus routines for data input and manipulation. Orange is also a scriptable environment for fast prototyping of new algorithms and testing schemes. It is a collection of Python-based modules that sit over the core library and implement some functionality for which execution time is not crucial and which is easier done in Python than in C++. This includes a variety of tasks such as pretty-print of decision trees, attribute subset, bagging and boosting, and alike. Orange is also a set of graphical widgets that use methods from core library and Orange modules and provide a nice user's interface. Widgets support signal-based communication and can be assembled together into an application by a visual programming tool called Orange Canvas.

All these together make an Orange, a comprehensive, component-based framework for machine learning and data mining. Orange is intended for both experienced users and researchers in machine learning who want to develop and test their own algorithms while reusing as much of the code as possible, and for those just entering the field who can either write short Python scripts for data analysis or enjoy a powerful while easy-to-use visual programming environment.

Data Mining, Fruitful and Fun

Orange provides a versatile environment for developers, researchers and data mining practitioners. Thanks to Python, a new generation scripting language and programming environment, your data mining scripts may be simple but powerful. To further allow for fast prototyping, Orange employs a component-based approach: you can implement your analysis method just like putting together the LEGO bricks, or even use an existing algorithm and replace some of its standard components with your own ones. What are Orange components to scripting are Orange widgets to visual programming. Widgets employ a specially designed communication mechanism for passing objects like data sets, attribute lists, learners, classifiers, regressors and alike, allowing to easily build rather complex data mining schemes that use state-of-the-art approaches and techniques.

Orange core objects and Python modules support various data mining tasks that span from data preprocessing to modeling and evaluation. Among other are techniques for:

* Data input, providing the support for various popular data formats,
* Data manipulation and preprocessing, like sampling, filtering, scaling, discretization, construction of new attributes, and alike,
* Methods for development of classification models, including classification trees, naïve Bayesian classifier, instance-based approaches, logistic regression and support vector machines,
* Regression methods, including linear regression, regression trees, and instance-based approaches,
* Various wrappers, like those for calibration of probability predictions of classification models,
* Ensemble approaches, like boosting and bagging,
* Various state-of-the-art constructive induction methods, including function

decomposition,
* Association rules and data clustering methods,
* Evaluation methods, different hold-out schemes and range of scoring methods for prediction models including classification accuracy, AUC, Brier score, and alike. Various hypothesis testing approaches are also supported,
* Methods to export predictive models to PMML.

The guiding principle in Orange is not to cover just about any method and aspect in machine learning and data mining (although through years of development quite a few have been build up), but to cover those that are implemented deeply and thoroughly, building them from reusable components that expert users can change or replace with the newly prototyped ones. For instance, Orange's top-down induction of decision trees is a method build of various components of which any can be prototyped in Python and used in place of the original one. Orange widgets are not just graphical objects that provide a graphical interface for a particular method in Orange – they also include versatile signaling mechanism that is for communication and exchange of objects like data sets, learners, classification models, objects that store the results of the evaluation, … All these concepts are important, and together distinguish Orange from other data mining frameworks.

Orange framework was carefully designed to balance between speed of execution and speed of development: time-critical components are implemented in C++, while the code that glues them together is in Python.

Orange Scripting

You can access Orange objects, write your own components, and design your test schemes and machine learning applications through scripting. Orange interfaces to Python, a modern easy-to-use scripting language with clear but powerful syntax and extensive set of additional libraries. Just like any scripting language, Python can be used to test some ideas interactively, on-the-fly, or to develop more elaborate scripts and programs.

To give you a taste of how easy it is to use Python and Orange, here is a set of examples. We start with a simple script that reads the data set and prints the number of attributes used and instances defined. We will use a classification data set called "voting" from UCI Machine Learning Repository that records sixteen key votes of each of the U.S. House of Representatives Congressmen and labels each instance (congressman) with a party membership:

```
import orange
data = orange.ExampleTable('voting.tab')
print 'Instances:', len(data)
print 'Attributes:', len(data.domain.attributes)
```

Notice that the script first loads in the Orange library, reads the data file and prints out what we were interested in. If we store this script in script.py, and run it by a shell command "python script.py" – making sure that the data file is in the same directory – we get:

```
Instances: 435
Attributes: 16
```

Let us continue with our script (that is, use the same data), build a naïve Bayesian classifier and print the classification of the first five instances:

```
model = orange.BayesLearner(data)
for i in range(5):
    print model(data[i])
```

This is simple! To induce the classification model, we have just called Orange's object called BayesLearner and gave it the data set: it returned another object (naïve Bayesian classifier), that when given an instance returns the label of most probable class. Here is the output of this part of the script:

```
republican
republican
republican
democrat
democrat
```

To find out what the right classifications were, we can print the original labels of our five instances:

```
for i in range(5):
    print model(data[i]), 'originally', data[i].getclass()
```

What we find out is that naïve Bayesian classifier has misclassified the third instance:

```
republican originally republican
republican originally republican
republican originally democrat
democrat originally democrat
```

```
democrat originally democrat
```

All classifiers implemented in Orange are probabilistic, e.g. they estimate the class probabilities. So is the naïve Bayesian classifier, and we may be interested in how much we have missed in the third case:

```
p = model(data[2], orange.GetProbabilities)
print data.domain.classVar.values[0], ':', p[0]
```

Notice that Python's indices start with 0 and that classification model returns a probability vector when a classifier is called with argument `orange.GetProbabilities`. Well, our model was unjustly overconfident here, estimating a very high probability for a republican:

```
republican : 0.995421469212
```

Now, we could go on like this, but we won't. For some more illustrative examples check the three somewhat more complex scripts in the sidebars. There are many more examples available in Orange's distribution and at Orange's web pages and described in accompanying tutorials and documentation.

Evaluation and Comparison of Classifiers

Here is a simple script that uses 10-fold cross validation to test a naïve Bayesian classifier and k-nearest neighbors algorithm on a voting data set.

```
import orange, orngTest, orngStat

# set up the learners
bayes = orange.BayesLearner(name='naive bayes')
knn = orange.kNNLearner(name='knn')
learners = [bayes, knn]

# compute accuracies on data
data = orange.ExampleTable("voting")
results = orngTest.crossValidation(learners, data, folds=10)
cdt = orngStat.computeCDT(results) # req. for AUC

# output the results
print "Learner  CA     IS     Brier    AUC"
for i in range(len(learners)):
    print "%-8s %5.3f  %5.3f  %5.3f  %5.3f" %
        (learners[i].name,
```

```
        orngStat.CA(results)[i],
        orngStat.IS(results)[i],
        orngStat.BrierScore(results)[i],
        orngStat.AROCFromCDT(cdt[i])[7])
```

Scores reported in this script are classification accuracy, information score, brier score, and area under ROC. Running the script, we get the following report:

```
Learner      CA     IS     Brier  AUC
naive bayes  0.903  0.759  0.175  0.973
knn          0.933  0.824  0.134  0.934
```

Study of Sensitivity of Decision Tree Induction Parameter

Following is a script that tests how a parameter that defines the minimum number of examples in the internal nodes of classification tree influences the size of the tree and accuracy on the test set.

```
import orange, orngTest, orngStat, orngTree

# set up the learners
learners = []
me_set = [0, 1, 5, 10, 100]
for me in me_set:
    learners.append(orngTree.TreeLearner(minExamples=me))

# load data, split it to train and test data set
data = orange.ExampleTable("voting")
selection = orange.MakeRandomIndices2(data, 0.7)
train_data = data.select(selection, 0)
test_data = data.select(selection, 1)

# obtain and report on results
results = orngTest.learnAndTestOnTestData(learners,
            train_data, test_data, storeClassifiers = 1)
CA = orngStat.CA(results)
IS = orngStat.IS(results)
print " Ex Size  CA     IS"
for i in range(len(learners)):
    print "%3d %4d  %5.3f  %5.3f" %
        (me_set[i],
         results.classifiers[i].treesize(),
         CA[i], IS[i])
```

For testing, the script splits the voting data set to train (70%) and test set (30% of all instances). To report on the sizes of the resulting classification trees, evaluation method has to store all the classifiers induced. The output of the script is:

```
 Ex Size  CA     IS
  0  615  0.802  0.561
  1  465  0.840  0.638
  5  151  0.931  0.800
 10   85  0.939  0.826
100   25  0.954  0.796
```

Working with Components

Machine learning algorithms often rely on common procedures, such as conditional probability estimation, scoring of attributes, data filtering and selection, random sampling, and others. Orange embeds these procedures in components, and develops its methods by assembling components into algorithms. But the real power comes with designing new components: one can prototype them in Python, use them in place of the default components in some of Orange's algorithms or use them together with an existing set of components to develop a completely new algorithm.

Not to be driven astray with too abstract descriptions, here is a simple example. We'll take Orange's algorithm for induction of decision trees which is itself assembled from components like those for attribute ranking, condition-based data splitting and a component that implements the evaluation for a stopping criterion. The induction procedure for classification trees uses some heuristics to pick the best attribute on which to split the data set, so what if instead we simply randomly choose the attribute? Here is a script that designs the new learner by replacing the split component of a standard classification tree learner with a newly constructed one that randomly selects the attribute. To see if that makes a difference, we build a standard classification tree and a tree with a random choice of attributes in nodes and measure their size (number of tree nodes):

```
import orange, random
def randomChoice(instances, *args):
    attr = random.choice(instances.domain.attributes)
    cl = orange.ClassifierFromVar(whichVar=attr, classVar=attr)
    return cl, attr.values, None, 1
```

```
data = orange.ExampleTable('voting.tab')
treeLearner = orange.TreeLearner()
rndLearner = orange.TreeLearner()
rndLearner.split = randomChoice

tree = treeLearner(data)
rndtree = rndLearner(data)
print tree.treesize(), 'vs.', rndtree.treesize()
```

A function randomChoice does the whole trick: in the first line it randomly selects an attribute from the list, and in the second returns what a split component for decision tree would need to return. The rest of the script is trivial, and if you run it, you will find out that the random tree is substantially bigger (as was expected).

Data Models in Orange are Structured Objects

And so is virtually everything else returned by any Orange object or function. But just like Orange methods which are modular and component based, so are the objects. The advantage? Classification trees in Orange are not just trees one can print out, but are structures that, for instance, one can iterate through, count the number of nodes that satisfy some criteria, devise one's own methods for printing them out, or inspect them to find frequently appearing and related attribute pairs. To get a feeling for this, the sidebar example shows how to count how many times each attribute appears in the constructed classification tree. And just like classification trees, association rules are something that one can dissect to any detail: in Python, they are a regular list of tuples that can be accessed in dissected to any desired detail. This helps if, for instance, one wants to implement his own scoring functions, or some particular rule filter, or even some nice graphical presentation of the rules. For an illustration, in a sidebar we give an example of counting the rules that include a specific attribute rule's condition.

Attribute Frequency in Classification Trees

Here is a script which shows why we really like Python. We intend to count the number of times each attribute appears in the node of the classification tree. For this we need the dictionary which stores the frequencies of the attributes (initialized to 0). We also need a function which recursively traverses the tree and for each node adds 1 to the corresponding attribute's count in the dic-

tionary. Once you get used to it, programming with dictionaries and lists in Python is really fun.

```
import orange

data = orange.ExampleTable("voting")
classifier = orange.TreeLearner(data)

# a dictionary to store attribute frequencies
freq = dict([(a,0) for a in data.domain.attributes])

# tree traversal
def count(node):
    if node.branches:
        freq[node.branchSelector.classVar] += 1
        for branch in node.branches:
            if branch: # make sure not a null leaf
                count(branch)

# count frequencies starting from root, and print out results
count(classifier.tree)
for a in data.domain.attributes[:3]:
    print freq[a], 'x', a.name
```

This script reports on the frequencies of the first three attributes in the data domain:

```
14 x handicapped-infants
16 x water-project-cost-sharing
4 x adoption-of-the-budget-resolution
```

Induction and Filtering of Association Rules

The following script builds a list of association rules from imports-85 data set (attribute-based descriptions of cars imported to US in 1985). We discretize the continuously-valued attributes and use only first ten attributes in analysis.

```
import orange, orngAssoc

# read and preprocess data
data = orange.ExampleTable("imports-85")
data = orange.Preprocessor_discretize(data, \
  method=orange.EquiNDiscretization(numberOfIntervals=3))
data = data.select(data.domain.attributes[:10])
```

```
# build a list of association rules with required support
minSupport = 0.4
rules = orngAssoc.build(data, minSupport)
print "%i rules found (support >= %3.1f)" % (len(rules), minSupport)

# choose first five rules, print them out
subset = rules[0:5]
subset.printMeasures(['support','confidence'])
```

The script reports on the number of rules and prints out the first five rules together with information on their support and confidence:

```
87 rules found (support >= 0.4)
supp  conf  rule
0.888 0.984      fuel-type=gas -> engine-location=front
0.888 0.901      engine-location=front -> fuel-type=gas
0.805 0.982      aspiration=std -> engine-location=front
0.805 0.817      engine-location=front -> aspiration=std
0.785 0.958      aspiration=std -> fuel-type=gas
```

We can now count how many of the 87 rules include attribute on fuel type in their condition:

```
att = "fuel-type"
subset = filter(lambda x: x.left[att]<>"~", rules)
print "%i rules with %s in conditional part" % (len(subset), att)

And here is what we find out:
31 rules with fuel-type in conditional part
```

Programming with other data models and objects in Orange is as easy as working with classification trees and association rules. The guiding principle in designing Orange was to make most of the data structures used in C++ routines available to scripts in Python.

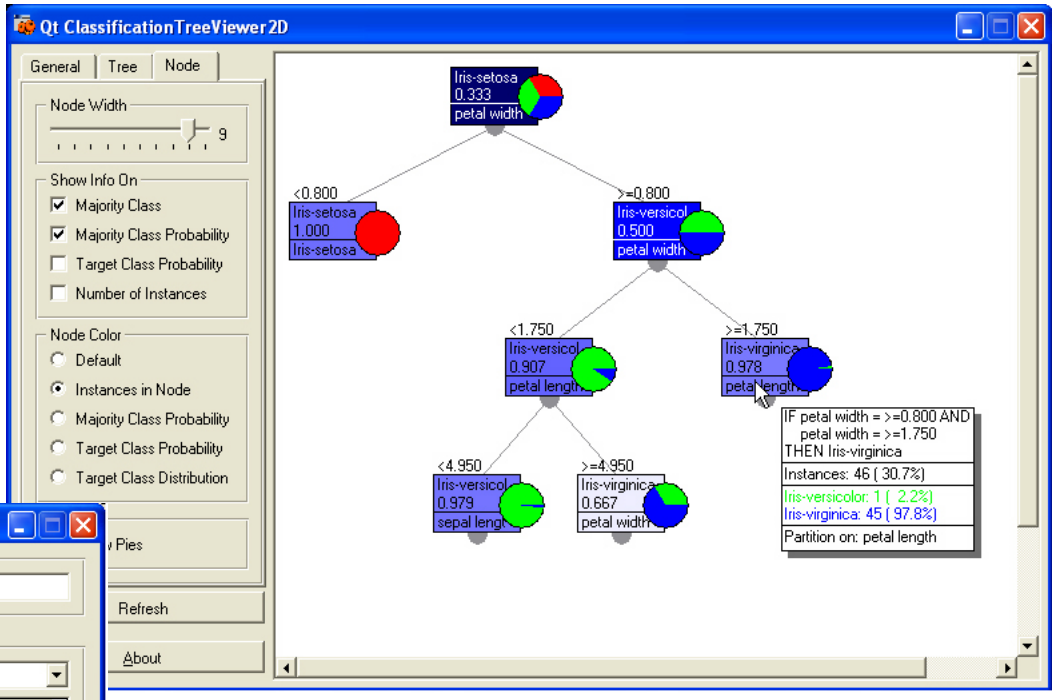
Orange Widgets

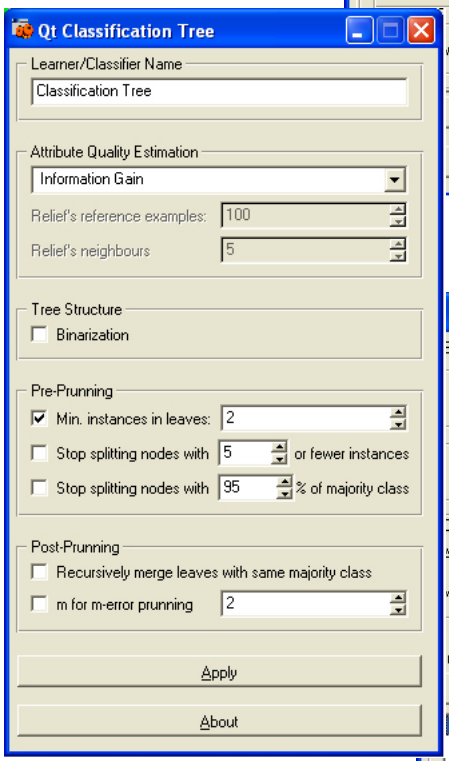
Orange widgets provide a graphical user's interface to Orange's data mining and machine learning methods. They include widgets for data entry and preprocessing, data visualization, classification, regression, association rules and clustering, a set of widgets for model evaluation and visualization of evaluation results, and widgets for exporting the models into PMML or Decisions@Hand model files.

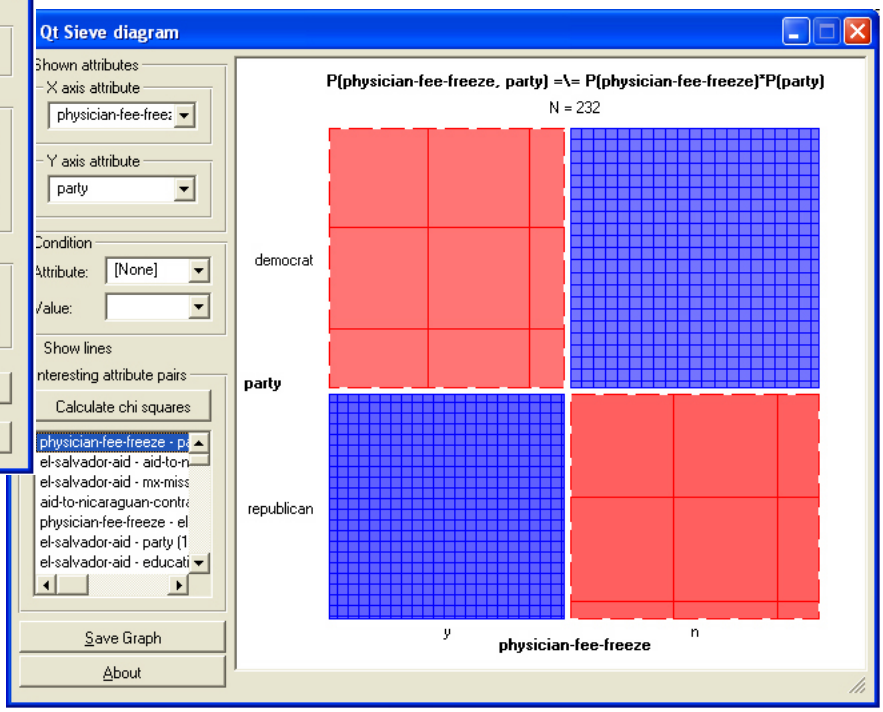
Widgets communicate by tokens that are passed from the sender to receiver widget. For example, a file widget outputs the data object, which can be received by a widget classification tree learner widget, which builds a classification model that can then be sent to a widget that graphically shows the tree. Or, an evaluation widget may receive a data set from the file widget and objects that learn the classification models (say, from logistic regression and naïve Bayesian learner widgets). It can then cross-validate the learners, presenting the results in the table while at the same time passing the object that stores the results to a widget for interactive visualization of ROC graphs.

Widgets usually support a number of standardized signals, and can be creatively combined to build a desired application. While being inspired by some popular data flow visual programming environments (admittedly, SGI's Data Explorer influenced us most), the innovative part of Orange Widgets is that on interactivity and signals. For instance, clicking on a classification tree node will make that widget output a data set which is associated with the node, and as this signal can be fed to any data processing widget like those for data visualization, one can interactively walk through the tree in one widget and have the visualization of a particular data set at the other widget.

Orange widgets for classification tree visualization (top), classification tree learner (middle) and sieve diagram (bottom).



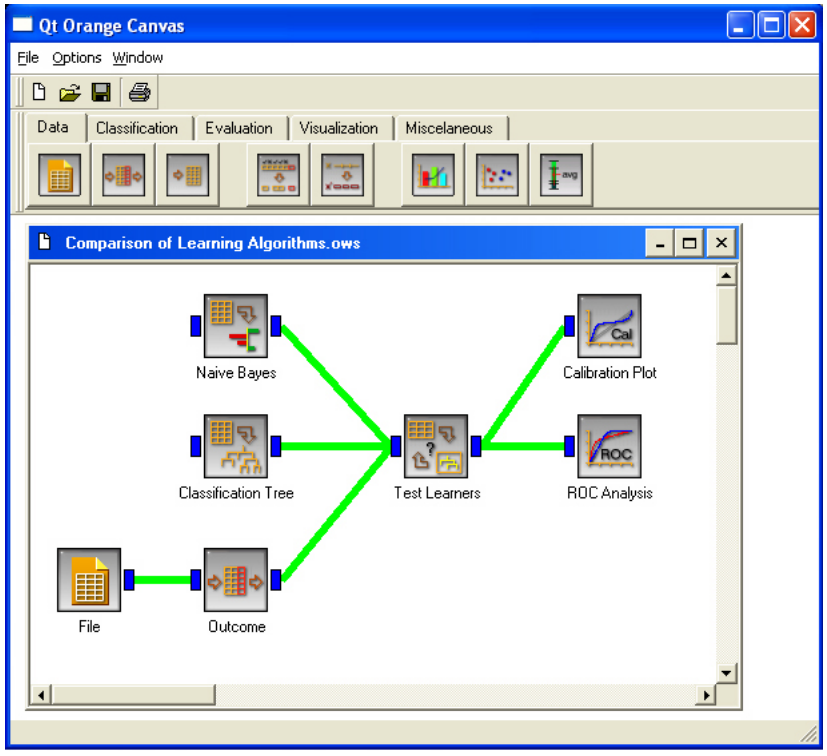




Data Mining by Visual Programming

Applications that include widgets are therefore a data flow schemes, where widgets process the information and provide for the user's interface. One can script such applications by hand, or use Orange Canvas, our visual programming environment, to interactively design the scheme. Like any visual programming environment, Orange Canvas is simple and fun to use.

Orange widgets and Orange Canvas are all written in pure Python, using Qt graphical user's interface library. This allows Orange to run on various platforms, including MS Windows and Linux.



Orange Canvas, with a schema that compares two different learners (classification tree learner and naïve Bayesian classifier) on a selected data set. Evaluation results are also studied through calibration and ROC plots.

Starting With Orange

If you use Orange or any of its components for research and publish the results, please cite the following whitepaper:

Demsar J, Zupan B: Orange: From Experimental Machine Learning to Interactive Data Mining, White Paper (www.ailab.si/orange), Faculty of Computer and Information Science, University of Ljubljana, 2004.

Also, your applications may use additional Orange modules made available by other researchers, so other citations may be in place as well.

Orange is available at http://magix.fri.uni-lj.si/orange. The site includes orange distribution for Windows, Linux and Macintosh OS X, the documentation, the extensive set of more that one hundred examples of Orange scripts, and a browsable repository of data sets.

To start with Orange scripting, we suggest downloading and unpacking Orange, and then going through Orange for Beginners, a tutorial that teaches the basics of Orange and Python programming. If you have done any programming previously, this may be almost enough to start writing your own scripts. If Python will look like something worth investigating further, there is a wealth of resources and documentation available at http://www.python.org.

Orange is released under General Programming License (GPL) and as such is free if you use it under these terms. We do, however, oblige the users to cite the following white paper together with any other work that accompanied Orange any time you use Orange in your publications:

> Demsar J, Zupan B (2004) Orange: From Experimental Machine Learning to Interactive Data Mining, White Paper (www.ailab.si/orange), Faculty of Computer and Information Science, University of Ljubljana.

And if you will become an Orange user, we won't mind getting a postcard from you. Please use the following address:

> Orange, AI Lab, Faculty of Computer and Informations Science, University of Ljubljana, Trzaska 25, SI-1000 Ljubljana, Slovenia.

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If you use Orange, you can send us a postcard with any comments and wishes for further development. Please use the following address:

Orange, AI Lab, Faculty of Computer and Information Science, Trzaska 25, SI-1000 Slovenia.

Acknowledgements

We are thankful for comments, encouragements and contributions of our colleagues and friends. We would first like to thank members of our AI Laboratory in Ljubljana for all the help and support in the development of the framework. Particular thanks go to Gregor Leban, Tomaz Curk, Aleks Jakulin, Martin Mozina, Peter Juvan, and Ivan Bratko. Marko Kavcic developed the first prototype of widget communication mechanism and tested it on first few widgets. Some of association rules algorithms were implemented by Matjaz Jursic. Martin Znidarsic helped us in development of several very useful methods and in beta testing. Jure Zabkar programmed several modules in Python. Matjaz Kukar was involved in early conversations about Orange and, most importantly, introduced us to Python. Chad Shaw helped us with discussions on kernel-based probability estimators continuous attributes and classification. Gaj Vidmar was always available to help us answering questions on various problems we had with statistics. Martin Znidarsic and Daniel Vladusic used Orange even in times of its greatest instability and thus contributed their share by annoying us with bug reports. In porting Orange to various platforms we are in particular thankful to Ljupco Todorovski and Mark E. Fenner (Linux), Daniel Rubin (Solaris) and Larry Bugbee (Mac OS X).

Orange exists thanks to a number of open source projects. Python is used as a scripting language that connects the core components coded in C++. Qt saved us from having to prepare and maintain separate graphical interfaces for MS Windows, Linux and Mac OS X. Python to Qt interface is taken care by PyQt. Additional packets used are Qwt (a set of Qt widgets for technical applications) among with PyQwt that allows us to use it from Python, and Numeric Python (a linear algebra module).

A number of Orange components were built as an implementation of methods that stem from our research. This was generously supported by Slovene Ministry of Education, Science and Sport (the Program Grant on Artificial Intelligence), Slovene Ministry of Information Society (two smaller grants on development of open source programs), American Cancer Society (in collaboration with Baylor College of Medicine, grant on predictive models for outcomes of prostate cancer treatments), and USA's National Institute of Health (in collaboration with Baylor College of Medicine, program grant on functional genomics of *D. discoideum*).

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