chem-bla-ics

Weka Decision Trees to Java Conversion

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Java, Cheminf, Cdk

Abstract
Some time ago I wrote a small Perl script to convert a decision tree created with Weka in the ARFF format to Java source code, for use in the ionization potential prediction in CDK. The advantage is that Weka is no longer used are runtime, and that there is no model that needs to be loaded and interpreted. Instead, it is simple Java code that does the work, much faster.

Some time ago I wrote a small Perl script to convert a decision tree created with Weka in the ARFF format to Java source code, for use in the ionization potential prediction in CDK. The advantage is that Weka is no longer used are runtime, and that there is no model that needs to be loaded and interpreted. Instead, it is simple Java code that does the work, much faster.

This is the code:

```
#!/usr/bin/perl
#
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use diagnostics;
use strict;

my $filename = $ARGV[0];

print "double result = 0.0;\n";
open(INPUT, "<$filename");
my $level = 0;
my $prevLevel = -1;
while (my $line = <INPUT>) {
  $line =~ s/\n//g;
  $level = 0;
  while ($line =~ /^\|\s*(.*)/) {
    $level++;
    $line = $1;
  }
  my $else = "";
  if ($prevLevel == $level) {
    $else = "else ";
  } elsif ($prevLevel < $level) {
    # we increase one level at a time
    for (my $i=0; $i<($level-1); $i++) { print "  "; };
    print "{\n";
    $prevLevel = $level;
  } else {
    # this is a bit more tricky: we possibly need more than
    # one end bracket
    my $diff = $prevLevel - $level;
    for (my $closes=0; $closes<$diff; $closes++) {
      for (my $i=0; $i<($prevLevel-$closes-1); $i++) { print "  "; };
      print "}\n";
    }
```

```
    $prevLevel = $level;
  }
  if ($line =~ /:/) {
    my ($if, $then) = split(":",$line);
    for (my $i=0; $i<$level; $i++) { print "  "; };
    # FIXME: java-fy $then
    if ($then =~ /([\d|_]*)\s*\(([^\)]*)\)/) {
      my $result = $1;
      my $stats = $2;
      $result =~ s/_/\./g;
      print $else . "if ($if) { result = $result; // $stats }\n";
    } else {
      print $else . "if ($if) { result = $then; }\n";
    }
  } else {
    for (my $i=0; $i<$level; $i++) { print "  "; };
    print $else . "if ($line)\n";
  }
}

# OK, now add the rest of the closing brackets
for (my $closes=$prevLevel; $closes>0; $closes--) {
  for (my $i=0; $i<($closes-1); $i++) { print "  "; };
  print "}\n";
}
```