# onnx_float32_and_64

April 5, 2022

## 1 ONNX graph, single or double floats

The notebook shows discrepencies obtained by using double floats instead of single float in two cases. The second one involves GaussianProcessRegressor.

[1]:
```
from jyquickhelper import add_notebook_menu
add_notebook_menu()
```

[1]:
```
<IPython.core.display.HTML object>
```

### 1.1 Simple case of a linear regression

A linear regression is simply a matrix multiplication followed by an addition: $Y = AX + B$. Let's train one with scikit-learn.

[2]:
```
from sklearn.linear_model import LinearRegression
from sklearn.datasets import load_boston
from sklearn.model_selection import train_test_split
data = load_boston()
X, y = data.data, data.target
X_train, X_test, y_train, y_test = train_test_split(X, y)
clr = LinearRegression()
clr.fit(X_train, y_train)
```

[2]:
```
LinearRegression()
```

[3]:
```
clr.score(X_test, y_test)
```

[3]:
```
0.7305965839248935
```

[4]:
```
clr.coef_
```

[4]:
```
array([-1.15896254e-01,  3.85174778e-02,  1.59315996e-02,  3.22074735e+00,
       -1.85418374e+01,  3.21813935e+00,  1.12610939e-02, -1.32043742e+00,
        3.67002299e-01, -1.41101521e-02, -1.10152072e+00,  6.17018918e-03,
       -5.71549389e-01])
```

[5]:
```
clr.intercept_
```

[5]:
```
43.97633987084284
```

Let's predict with *scikit-learn* and *python*.

[6]:
```
ypred = clr.predict(X_test)
ypred[:5]
```

[6]:
```
array([17.72795971, 18.69312745, 21.13760633, 16.65607505, 22.47115623])
```

[7]:
```
py_pred = X_test @ clr.coef_ + clr.intercept_
py_pred[:5]
```

[7]:
```
array([17.72795971, 18.69312745, 21.13760633, 16.65607505, 22.47115623])
```

[8]:
```
clr.coef_.dtype, clr.intercept_.dtype
```

[8]:
```
(dtype('float64'), dtype('float64'))
```

## 1.2 With ONNX

With *ONNX*, we would write this operation as follows… We still need to convert everything into single floats = float32.

[9]:
```
%load_ext mlprodict
```

[10]:
```
from skl2onnx.algebra.onnx_ops import OnnxMatMul, OnnxAdd
import numpy

onnx_fct = OnnxAdd(OnnxMatMul('X', clr.coef_.astype(numpy.float32), op_version=12),
                   numpy.array([clr.intercept_], dtype=numpy.float32),
                   output_names=['Y'], op_version=12)
onnx_model32 = onnx_fct.to_onnx({'X': X_test.astype(numpy.float32)})

# add -l 1 if nothing shows up
%onnxview onnx_model32
```

[10]:
```
<jyquickhelper.jspy.render_nb_js_dot.RenderJsDot at 0x2572a083da0>
```

The next line uses a python runtime to compute the prediction.

[11]:
```
from mlprodict.onnxrt import OnnxInference
oinf = OnnxInference(onnx_model32, inplace=False)
ort_pred = oinf.run({'X': X_test.astype(numpy.float32)})['Y']
ort_pred[:5]
```

[11]:
```
array([17.727959, 18.693125, 21.137608, 16.656076, 22.471157],
      dtype=float32)
```

And here is the same with onnxruntime…

[12]:
```
from mlprodict.tools.asv_options_helper import get_ir_version_from_onnx
# line needed when onnx is more recent than onnxruntime
onnx_model32.ir_version = get_ir_version_from_onnx()
oinf = OnnxInference(onnx_model32, runtime="onnxruntime1")
ort_pred = oinf.run({'X': X_test.astype(numpy.float32)})['Y']
ort_pred[:5]
```

[12]:
```
array([17.727959, 18.693125, 21.137608, 16.656076, 22.471157],
      dtype=float32)
```

## 1.3 With double instead of single float

ONNX was originally designed for deep learning which usually uses floats but it does not mean cannot be used. Every number is converted into double floats.

[13]:
```
onnx_fct = OnnxAdd(OnnxMatMul('X', clr.coef_.astype(numpy.float64), op_version=12),
                   numpy.array([clr.intercept_], dtype=numpy.float64),
                   output_names=['Y'], op_version=12)
onnx_model64 = onnx_fct.to_onnx({'X': X_test.astype(numpy.float64)})
```

And now the *python* runtime...

[14]:
```
oinf = OnnxInference(onnx_model64)
ort_pred = oinf.run({'X': X_test})['Y']
ort_pred[:5]
```

[14]:
```
array([17.72795971, 18.69312745, 21.13760633, 16.65607505, 22.47115623])
```

And the *onnxruntime* version of it.

[15]:
```
oinf = OnnxInference(onnx_model64, runtime="onnxruntime1")
ort_pred = oinf.run({'X': X_test.astype(numpy.float64)})['Y']
ort_pred[:5]
```

[15]:
```
array([17.72795971, 18.69312745, 21.13760633, 16.65607505, 22.47115623])
```

## 1.4 And now the GaussianProcessRegressor

This shows a case

[16]:
```
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import DotProduct
gau = GaussianProcessRegressor(alpha=10, kernel=DotProduct())
gau.fit(X_train, y_train)
```

[16]:
```
GaussianProcessRegressor(alpha=10, kernel=DotProduct(sigma_0=1))
```

[17]:
```
from mlprodict.onnx_conv import to_onnx
onnxgau32 = to_onnx(gau, X_train.astype(numpy.float32))
oinf32 = OnnxInference(onnxgau32, runtime="python", inplace=False)
ort_pred32 = oinf32.run({'X': X_test.astype(numpy.float32)})['GPmean']
numpy.squeeze(ort_pred32)[:25]
```

[17]:
```
array([17.25    , 19.59375 , 21.34375 , 17.625   , 21.953125, 30.      ,
       18.875   , 19.625   ,  9.9375  , 20.5     , -0.53125 , 16.375   ,
       16.8125  , 20.6875  , 27.65625 , 16.375   , 39.0625  , 36.0625  ,
       40.71875 , 21.53125 , 29.875   , 30.34375 , 23.53125 , 15.25    ,
       35.5     ], dtype=float32)
```

[18]:
```
onnxgau64 = to_onnx(gau, X_train.astype(numpy.float64))
oinf64 = OnnxInference(onnxgau64, runtime="python", inplace=False)
ort_pred64 = oinf64.run({'X': X_test.astype(numpy.float64)})['GPmean']
numpy.squeeze(ort_pred64)[:25]
```

[18]:
```
array([17.22940605, 19.07756253, 21.000277  , 17.33514034, 22.37701168,
       30.10867125, 18.72937468, 19.2220674 ,  9.74660609, 20.3440565 ,
```

```
-0.1354653 , 16.47852265, 17.12332707, 21.04137646, 27.21477015,
16.2668399 , 39.31065954, 35.99032274, 40.53761676, 21.51909954,
29.49016665, 30.22944875, 23.58969906, 14.56499415, 35.28957228])
```

The differences between the predictions for single floats and double floats…

[19]:
```
numpy.sort(numpy.sort(numpy.squeeze(ort_pred32 - ort_pred64)))[-5:]
```

[19]:
```
array([0.51618747, 0.54317928, 0.61256575, 0.63292898, 0.68500585])
```

Who's right or wrong… The differences between the predictions with the original model…

[20]:
```
pred = gau.predict(X_test.astype(numpy.float64))
```

[21]:
```
numpy.sort(numpy.sort(numpy.squeeze(ort_pred32 - pred)))[-5:]
```

[21]:
```
array([0.51618747, 0.54317928, 0.61256575, 0.63292898, 0.68500585])
```

[22]:
```
numpy.sort(numpy.sort(numpy.squeeze(ort_pred64 - pred)))[-5:]
```

[22]:
```
array([0., 0., 0., 0., 0.])
```

Double predictions clearly wins.

[23]:
```
# add -l 1 if nothing shows up
%onnxview onnxgau64
```

[23]:
```
<jyquickhelper.jspy.render_nb_js_dot.RenderJsDot at 0x257281fd2e8>
```

### 1.5 Saves…

Let's keep track of it.

[24]:
```
with open("gpr_dot_product_boston_32.onnx", "wb") as f:
    f.write(onnxgau32.SerializePartialToString())
from IPython.display import FileLink
FileLink('gpr_dot_product_boston_32.onnx')
```

[24]:
```
C:\xavierdupre\__home_\GitHub\mlprodict\_doc\notebooks\gpr_dot_product_boston_32
.onnx
```

[25]:
```
with open("gpr_dot_product_boston_64.onnx", "wb") as f:
    f.write(onnxgau64.SerializePartialToString())
FileLink('gpr_dot_product_boston_64.onnx')
```

[25]:
```
C:\xavierdupre\__home_\GitHub\mlprodict\_doc\notebooks\gpr_dot_product_boston_64
.onnx
```

### 1.6 Side by side

We may wonder where the discrepencies start. But for that, we need to do a side by side.

[26]:
```
from mlprodict.onnxrt.validate.side_by_side import side_by_side_by_values
sbs = side_by_side_by_values([(oinf32, {'X': X_test.astype(numpy.float32)}),
                              (oinf64, {'X': X_test.astype(numpy.float64)})])
```

```python
from pandas import DataFrame
df = DataFrame(sbs)
# dfd = df.drop(['value[0]', 'value[1]', 'value[2]'], axis=1).copy()
df
```

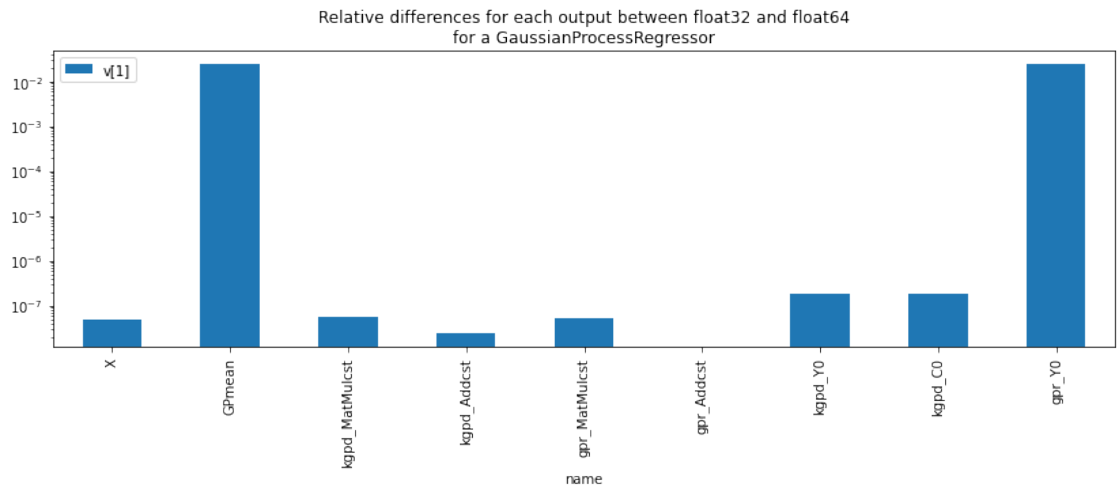
[26]:

```
        metric  step  v[0]          v[1]    cmp            name  \
0   nb_results    -1     9  9.000000e+00     OK             NaN
1     abs-diff     0     0  4.902064e-08     OK               X
2     abs-diff     1     0  2.402577e-02  e<0.1          GPmean
3     abs-diff     2     0  5.553783e-08     OK  kgpd_MatMulcst
4     abs-diff     3     0  2.421959e-08     OK     kgpd_Addcst
5     abs-diff     4     0  5.206948e-08     OK   gpr_MatMulcst
6     abs-diff     5     0  0.000000e+00     OK      gpr_Addcst
7     abs-diff     6     0  1.856291e-07     OK         kgpd_Y0
8     abs-diff     7     0  1.856291e-07     OK         kgpd_C0
9     abs-diff     8     0  2.402577e-02  e<0.1          gpr_Y0

                                            value[0]    shape[0]  \
0                                                NaN         NaN
1  [[0.21977, 0.0, 6.91, 0.0, 0.448, 5.602, 62.0,…   (127, 13)
2  [[17.25, 19.59375, 21.34375, 17.625, 21.953125…    (1, 127)
3  [[16.8118, 0.26169, 7.67202, 0.57529, 1.13081,…   (13, 379)
4                                         [1117.718]        (1,)
5  [-0.040681414, -0.37079695, -0.7959402, 0.4380…      (379,)
6                                            [[0.0]]      (1, 1)
7  [[321007.53, 235496.9, 319374.4, 230849.73, 22…  (127, 379)
8  [[321007.53, 235496.9, 319374.4, 230849.73, 22…  (127, 379)
9  [17.25, 19.59375, 21.34375, 17.625, 21.953125,…      (127,)

                                            value[1]    shape[1]
0                                                NaN         NaN
1  [[0.21977, 0.0, 6.91, 0.0, 0.448, 5.602, 62.0,…   (127, 13)
2  [[17.229406048412784, 19.077562531849253, 21.0…    (1, 127)
3  [[16.8118, 0.26169, 7.67202, 0.57529, 1.13081,…   (13, 379)
4                                [1117.718044648797]        (1,)
5  [-0.04068141268069173, -0.37079693473728526, -…      (379,)
6                                            [[0.0]]      (1, 1)
7  [[321007.55279690475, 235496.9156560601, 31937…  (127, 379)
8  [[321007.55279690475, 235496.9156560601, 31937…  (127, 379)
9  [17.229406048412784, 19.077562531849253, 21.00…      (127,)
```

The differences really starts for output `'O0'` after the matrix multiplication. This matrix melts different number with very different order of magnitudes and that alone explains the discrepencies with doubles and floats on that particular model.

[27]:

```python
%matplotlib inline
ax = df[['name', 'v[1]']].iloc[1:].set_index('name').plot(kind='bar', figsize=(14,4),␣
 ↪logy=True)
ax.set_title("Relative differences for each output between float32 and "
             "float64\nfor a GaussianProcessRegressor");
```




Before going further, let's check how sensitive the trained model is about converting double into floats.

[28]:
```
pg1 = gau.predict(X_test)
pg2 = gau.predict(X_test.astype(numpy.float32).astype(numpy.float64))
numpy.sort(numpy.sort(numpy.squeeze(pg1 - pg2)))[-5:]
```

[28]:
```
array([1.53295696e-06, 1.60621130e-06, 1.65373785e-06, 1.66549580e-06,
       2.36724736e-06])
```

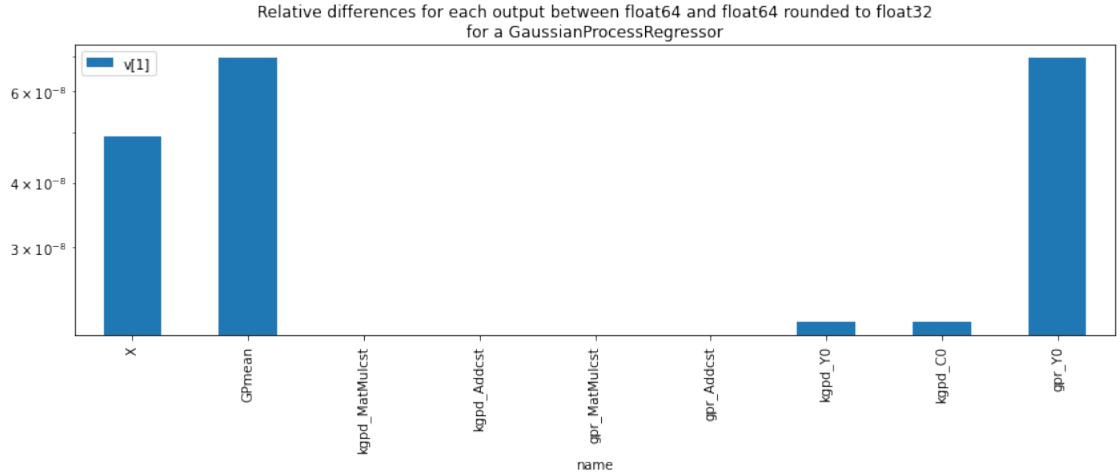
Having float or double inputs should not matter. We confirm that with the model converted into ONNX.

[29]:
```
p1 = oinf64.run({'X': X_test})['GPmean']
p2 = oinf64.run({'X': X_test.astype(numpy.float32).astype(numpy.float64)})['GPmean']
numpy.sort(numpy.sort(numpy.squeeze(p1 - p2)))[-5:]
```

[29]:
```
array([1.53295696e-06, 1.60621130e-06, 1.65373785e-06, 1.66549580e-06,
       2.36724736e-06])
```

Last verification.

[30]:
```
sbs = side_by_side_by_values([(oinf64, {'X': X_test.astype(numpy.float32).astype(numpy.
 ↪float64)}),
                              (oinf64, {'X': X_test.astype(numpy.float64)})])
df = DataFrame(sbs)
ax = df[['name', 'v[1]']].iloc[1:].set_index('name').plot(kind='bar', figsize=(14,4),␣
 ↪logy=True)
ax.set_title("Relative differences for each output between float64 and float64 rounded␣
 ↪to float32"
             "\nfor a GaussianProcessRegressor");
```


Relative differences for each output between float64 and float64 rounded to float32
for a GaussianProcessRegressor
v[1]
$6 \times 10^{-8}$
$4 \times 10^{-8}$
$3 \times 10^{-8}$
X
GPmean
kgpd_MatMulcst
kgpd_Addcst
gpr_MatMulcst
gpr_Addcst
kgpd_Y0
kgpd_C0
gpr_Y0
name

[31]: