optimization

March 21, 2022

1 Example of optimizing lowess fit and max and redundant set selection

[1]:
```
import os,errno
import dRFEtools
import numpy as np
import pandas as pd
from sklearn.model_selection import KFold
from sklearn.datasets import make_regression
from sklearn.datasets import make_classification
from sklearn.model_selection import StratifiedKFold
from sklearn.model_selection import train_test_split
```

[2]:
```
def mkdir_p(directory):
    try:
        os.makedirs(directory)
    except OSError as e:
        if e.errno != errno.EEXIST:
            raise
```

1.1 Optimize classification

[3]:
```
outdir = 'classification/'
mkdir_p(outdir)
```

[4]:
```
# Create a dataset with only 10 informative features
X, y = make_classification(
    n_samples=500, n_features=20000, n_informative=100, n_redundant=300,
    n_repeated=0, n_classes=2, n_clusters_per_class=1, random_state=13
)

cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=13)
#cla = dRFEtools.LogisticRegression(max_iter=1000, n_jobs=-1)
cla = dRFEtools.RandomForestClassifier(n_estimators=100, n_jobs=-1,
                                       oob_score=True, random_state=13)
```

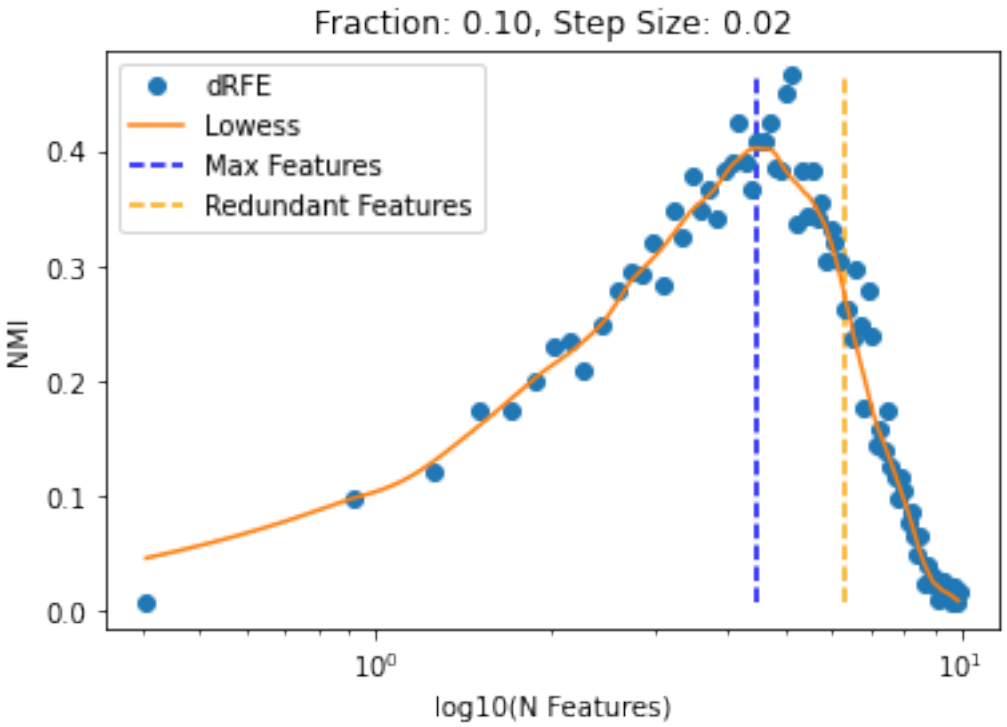
[5]:
```
fold = 1
for train_index, test_index in cv.split(X, y):
    X_train, X_test = X[train_index], X[test_index]
    y_train, y_test = y[train_index], y[test_index]
    fold += 1
fold -= 1

features = ["feature_%d" % x for x in range(X_train.shape[1])]
d, pfirst = dRFEtools.rf_rfe(cla, X_train, y_train, np.array(features),
                             fold, outdir, elimination_rate=0.1, RANK=False)
```

1.1.1 Optimize lowess fit: fraction of data to use when estimating y-values

[6]:
```
## Single Fold examination
for frac in [0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4]:
    dRFEtools.optimize_lowess_plot(d, fold, outdir, frac=frac, step_size=0.02,
                                   classify=True, save_plot=True)
```

```
<Figure size 432x288 with 0 Axes>
```




```
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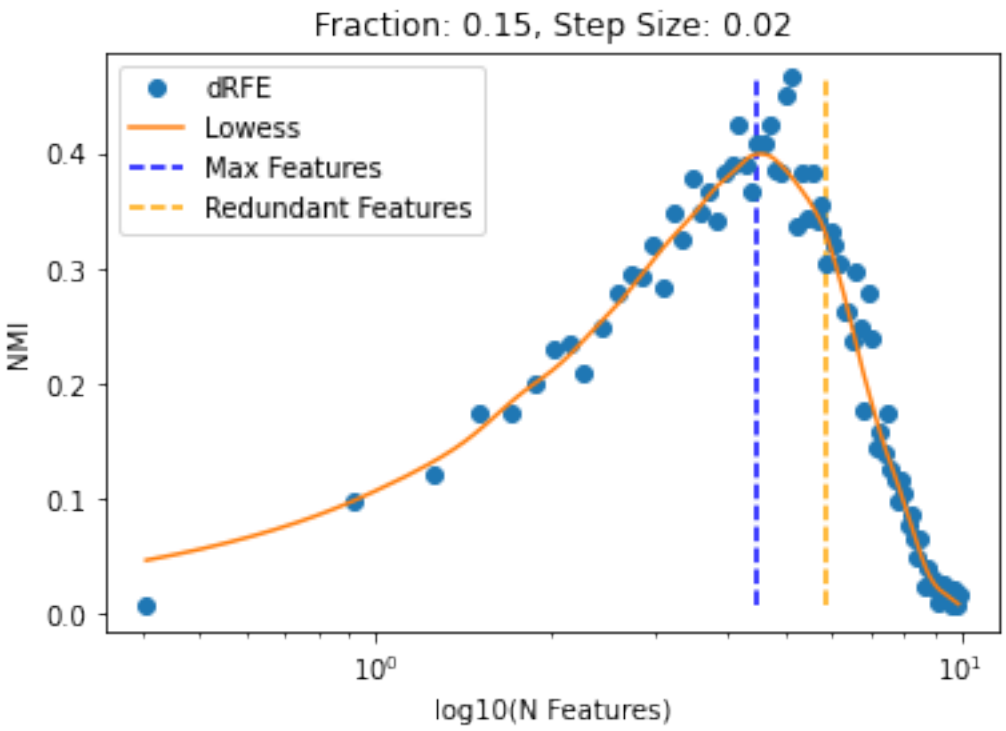
```




```
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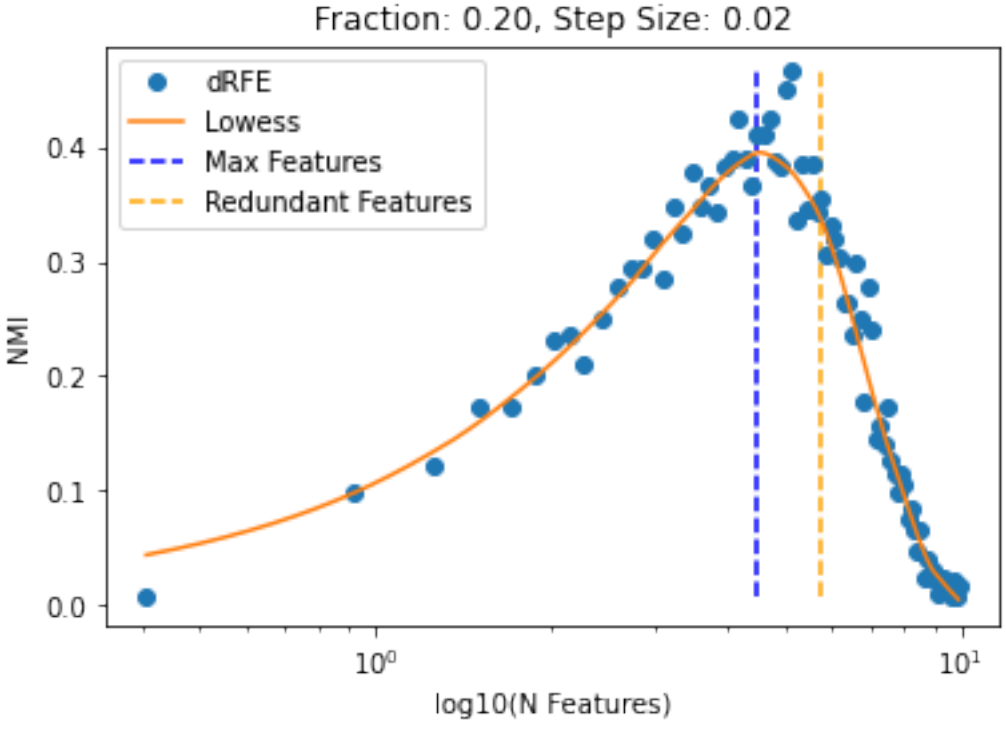
```



```
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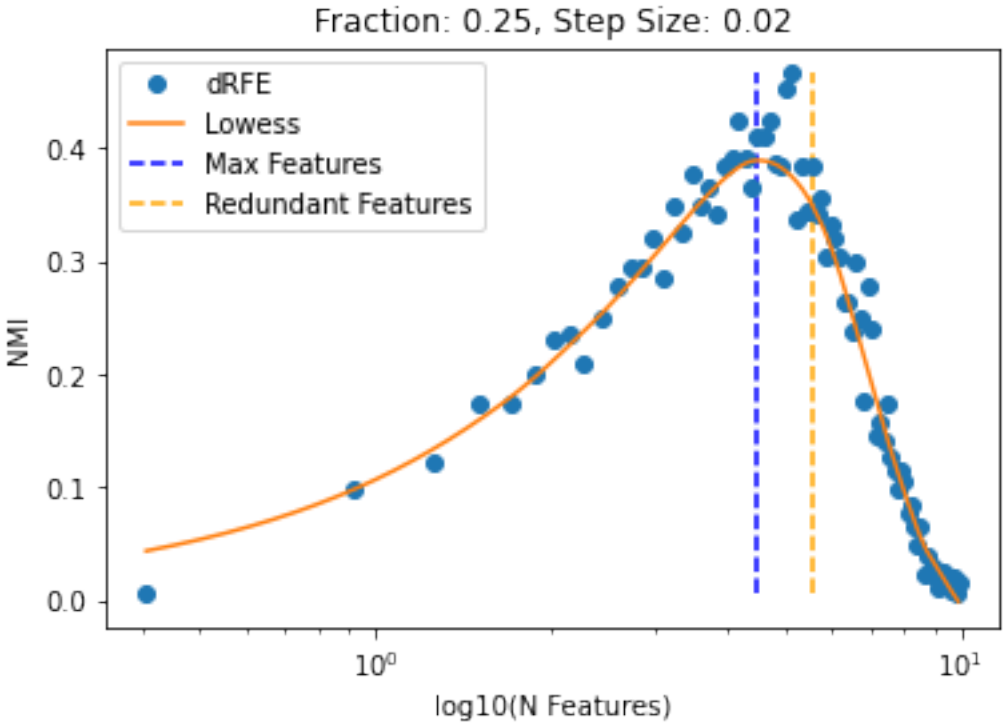
```




```
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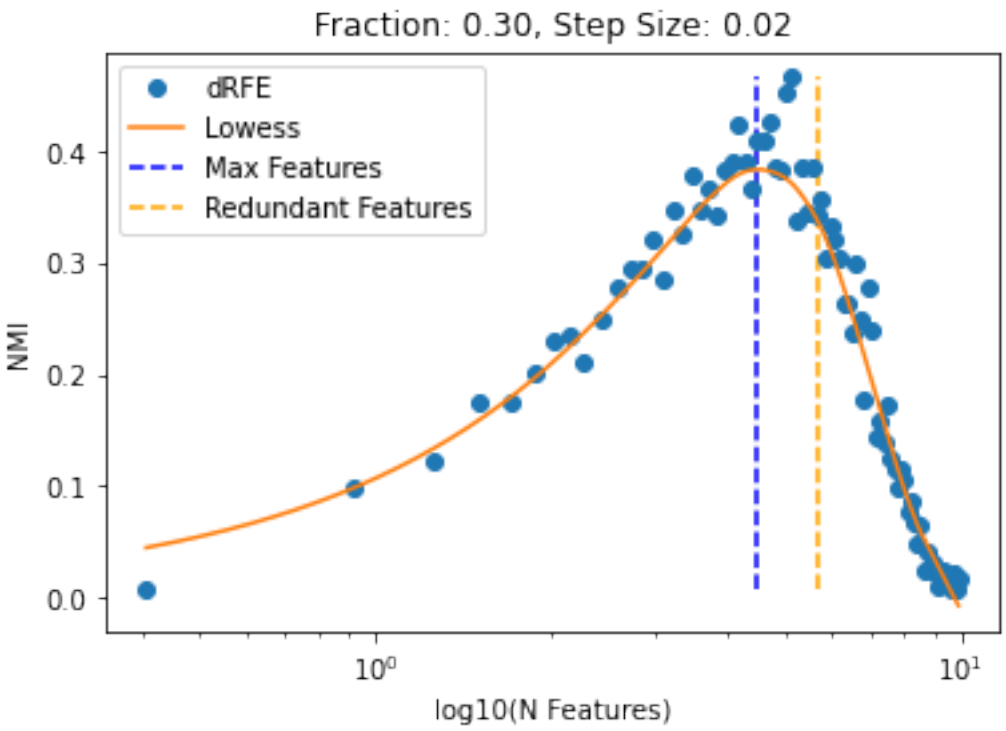
```




```
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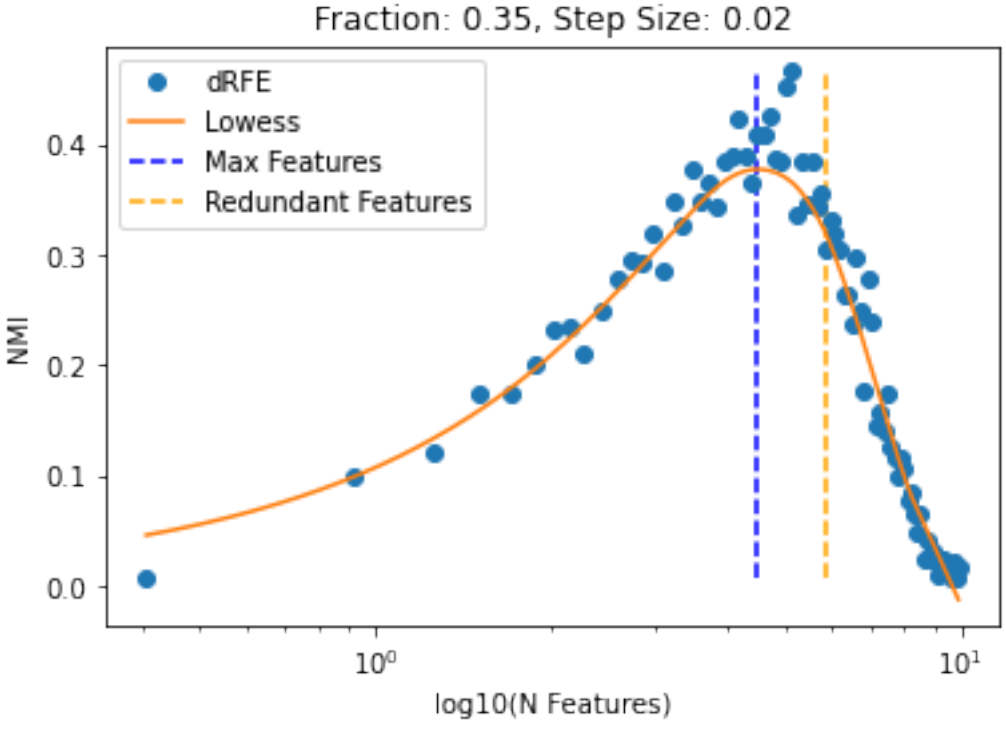
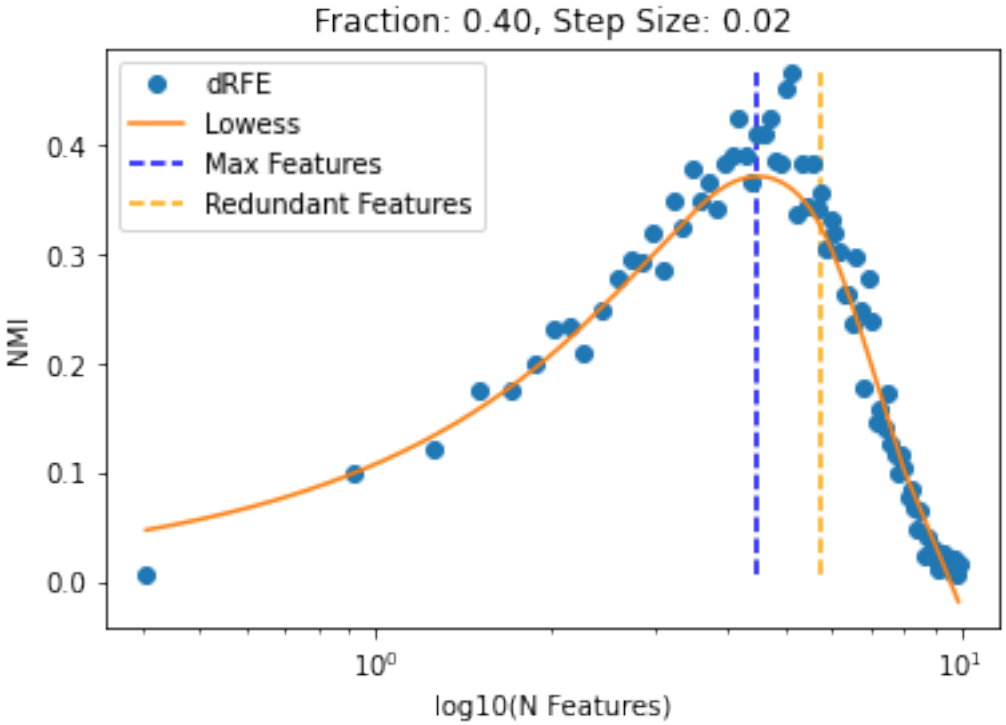


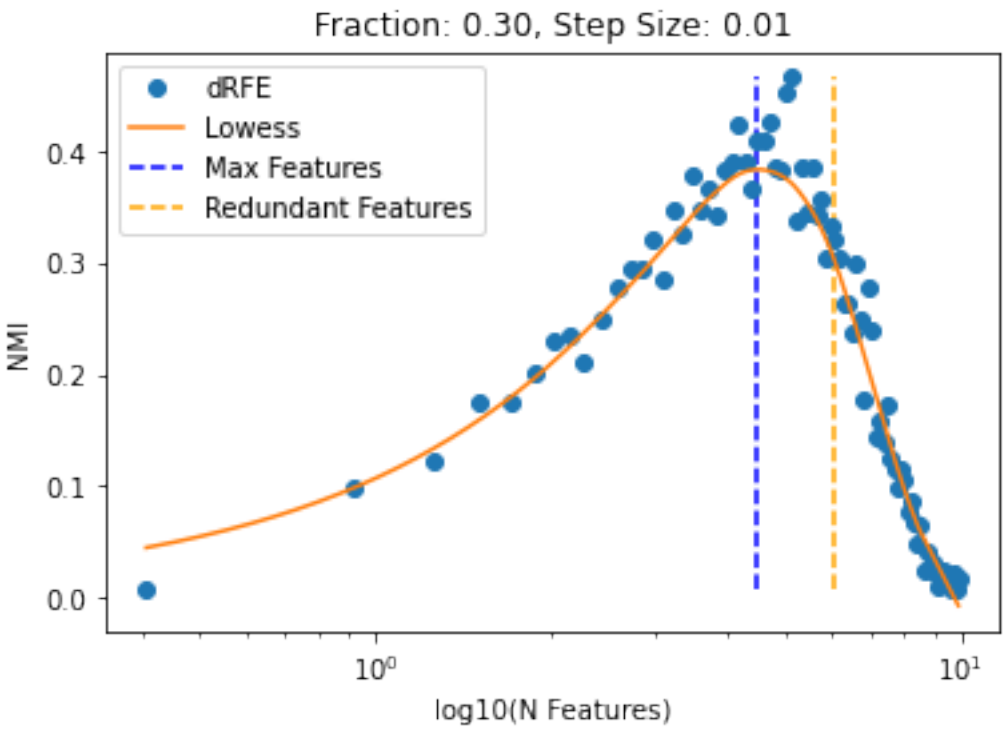
<Figure size 432x288 with 0 Axes>



1.1.2 Optimize redundant selection: examine rate change

[7]:
```
for step_size in [0.01, 0.02, 0.03, 0.04, 0.05, 0.1]:
    dRFEtools.optimize_lowess_plot(d, fold, outdir, frac=0.3,␣
 ↪step_size=step_size,
                                   classify=True, save_plot=True)
```

<Figure size 432x288 with 0 Axes>




```
<Figure size 432x288 with 0 Axes>
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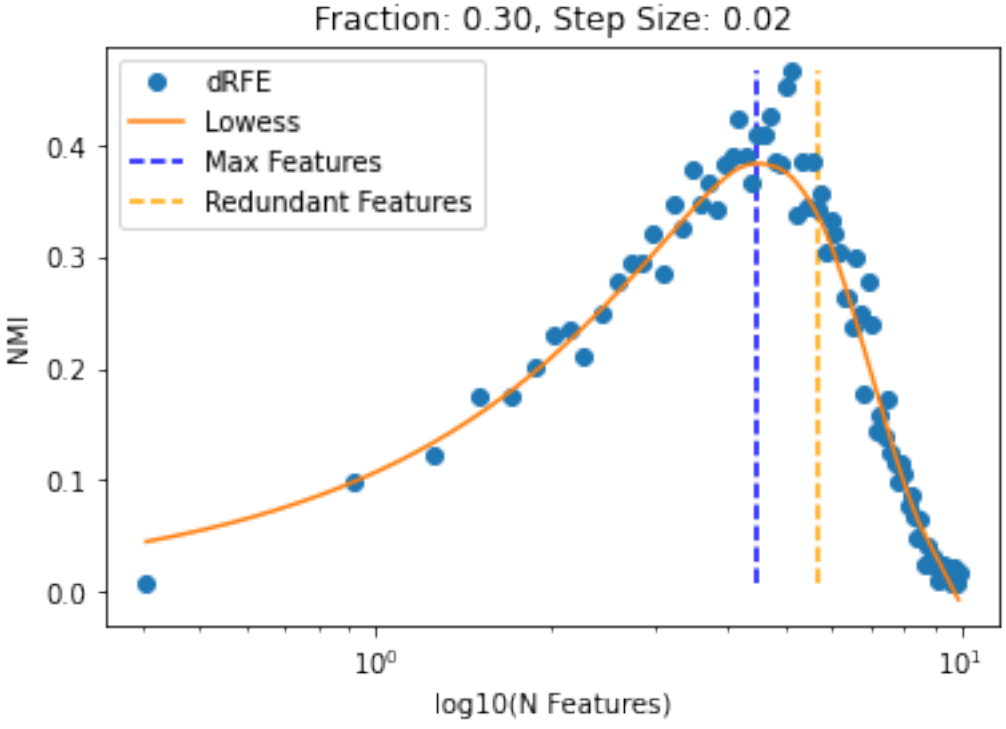
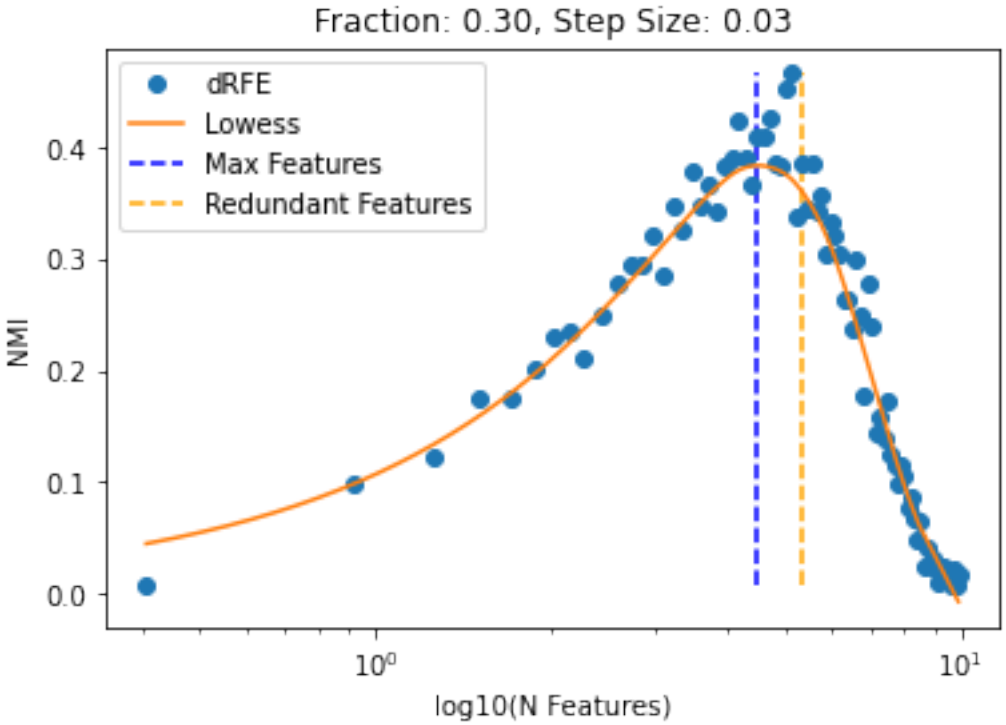
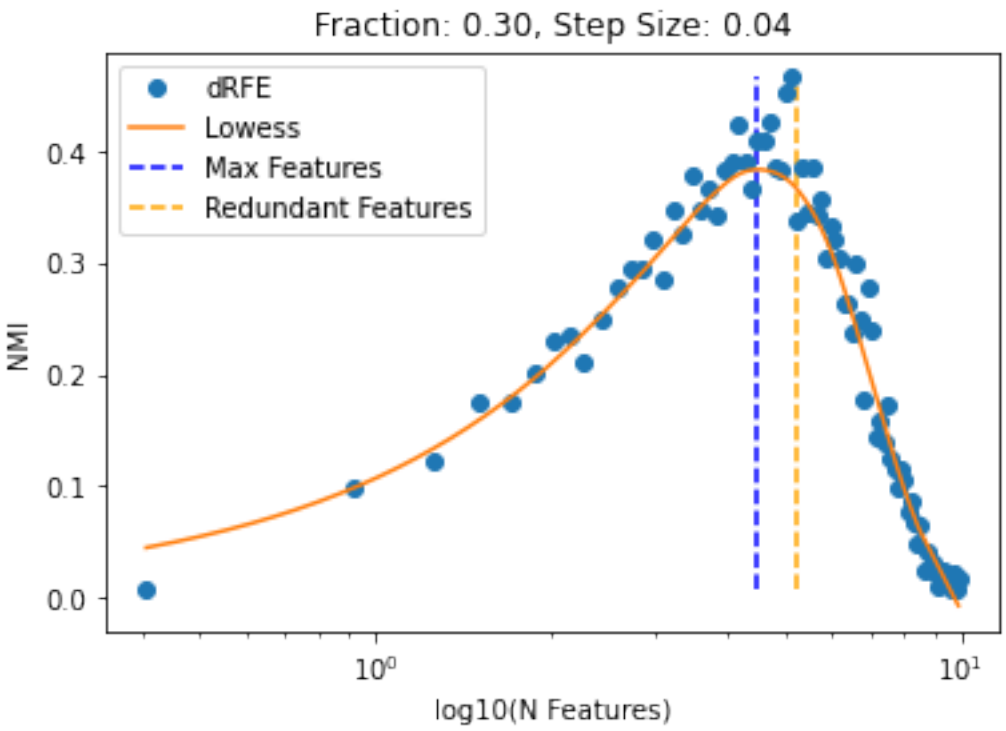


<Figure size 432x288 with 0 Axes>



<Figure size 432x288 with 0 Axes>




```
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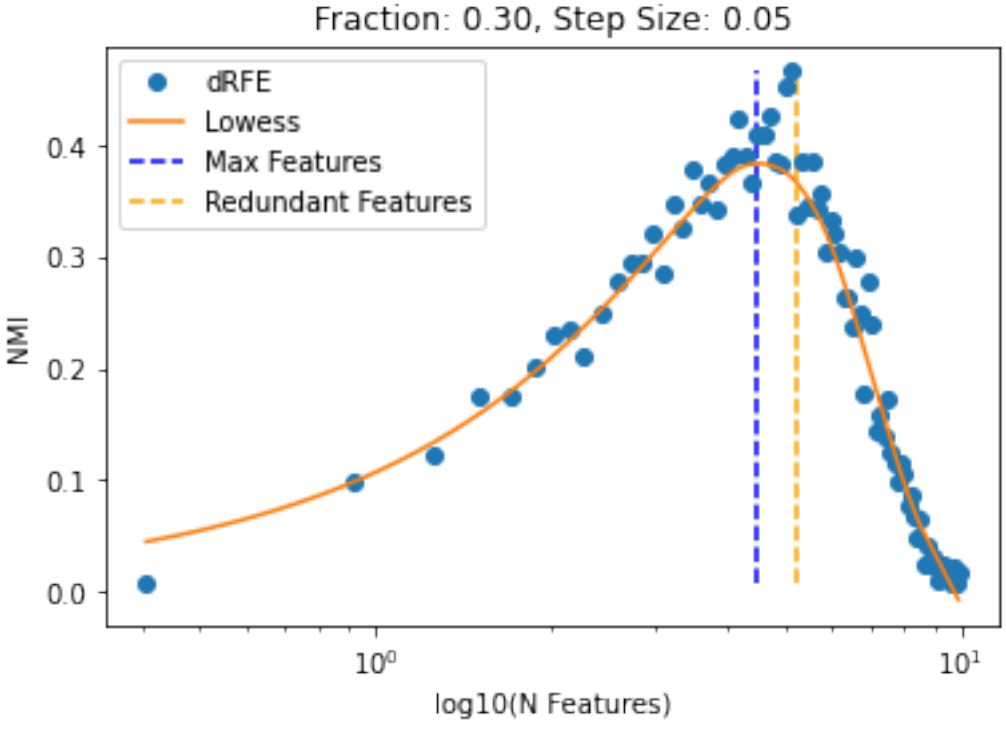

```
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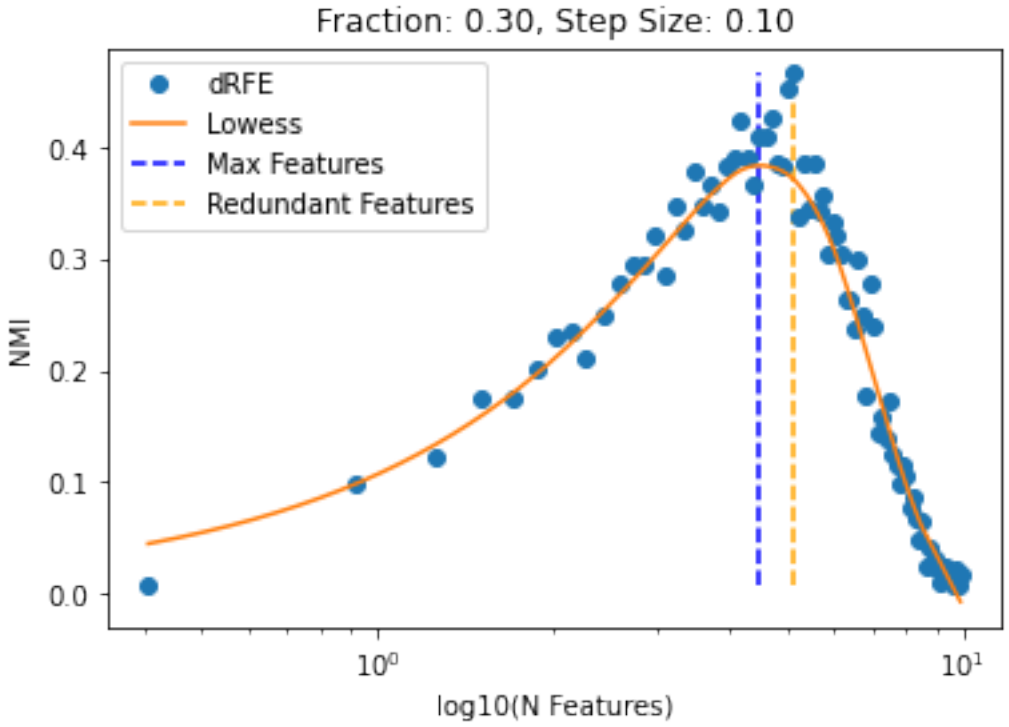


[8]:
```
## Highest value (without smoothing)
max(d, key=lambda x: d[x][1])
```

[8]:
```
170
```

[9]:
```
print(dRFEtools.extract_max_lowess(d, frac=0.30))
## Using a conservative step size
dRFEtools.extract_redundant_lowess(d, frac=0.30, step_size=0.02)
```

```
(89, 4.4942386252808095)
```

[9]:
```
(291, 5.675040005790547)
```

1.2 Optimize regression

[10]:
```
outdir = 'regression/'
mkdir_p(outdir)
```

[11]:
```
# Create a dataset with only 10 informative features
X, y = make_regression(
    n_samples=500, n_features=20000, n_informative=200, bias=0.2,
    n_targets=1, noise=10, random_state=13
)
cv = KFold(n_splits=5, shuffle=True, random_state=13)
regr = dRFEtools.RandomForestRegressor(n_estimators=100, oob_score=True,
                                       n_jobs=-1, random_state=13)
```

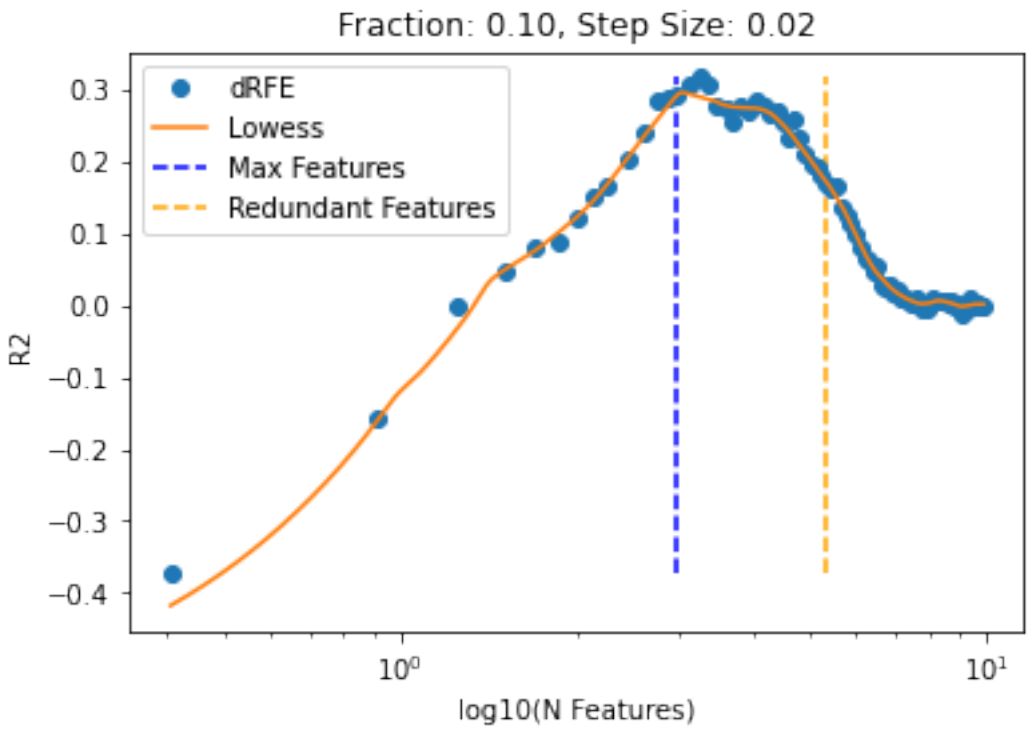
[12]:
```
fold = 1
for train_index, test_index in cv.split(X, y):
    X_train, X_test = X[train_index], X[test_index]
    y_train, y_test = y[train_index], y[test_index]
    fold += 1
fold -= 1

features = ["feature_%d" % x for x in range(X_train.shape[1])]
d, pfirst = dRFEtools.rf_rfe(regr, X_train, y_train, np.array(features),
                             fold, outdir, elimination_rate=0.1, RANK=False)
```

1.2.1 Optimize lowess fit: fraction of data to use when estimating y-values

[13]:
```
## Single Fold examination
for frac in [0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4]:
    dRFEtools.optimize_lowess_plot(d, fold, outdir, frac=frac, step_size=0.02,
                                   classify=False, save_plot=True)
```

```
<Figure size 432x288 with 0 Axes>
```




```
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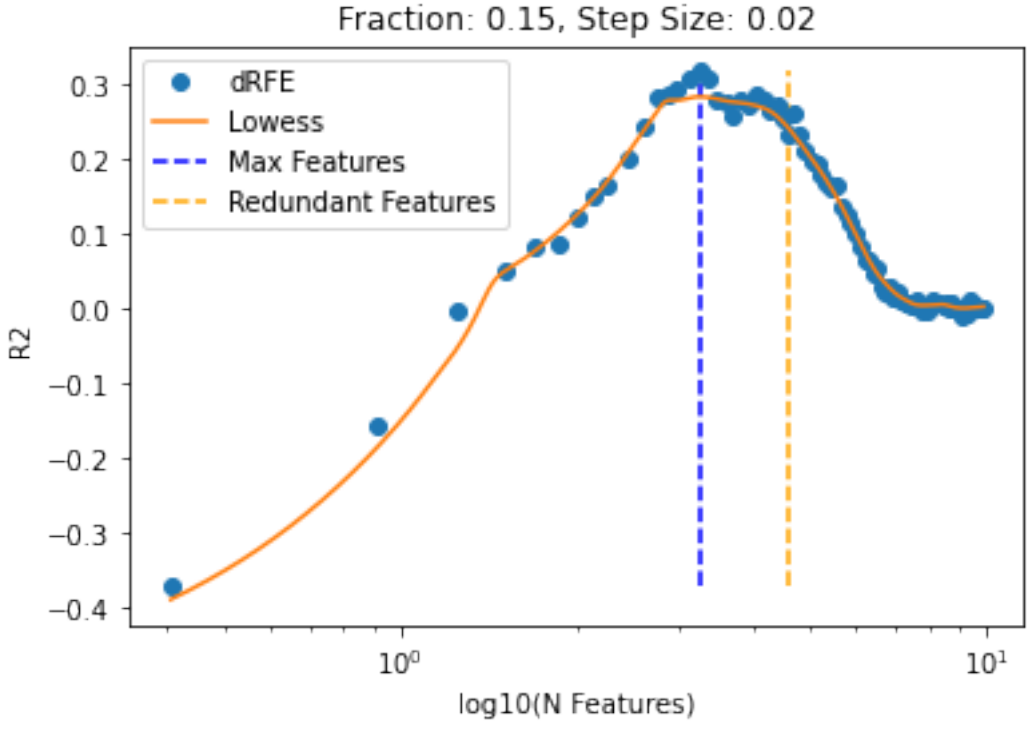

```
<Figure size 432x288 with 0 Axes>
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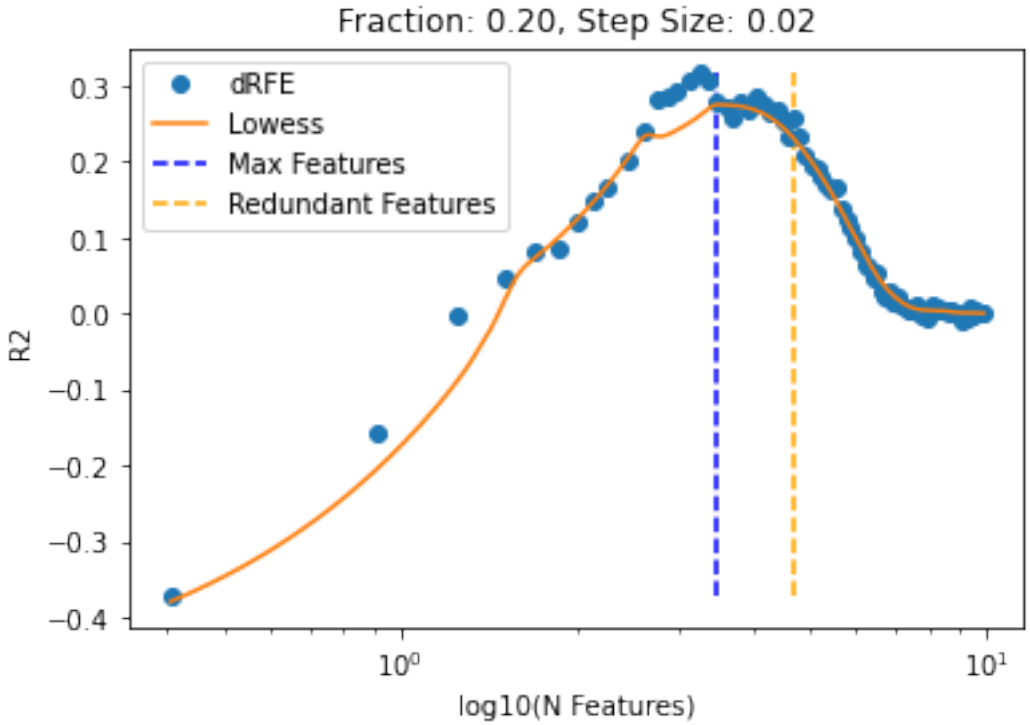


```
<Figure size 432x288 with 0 Axes>
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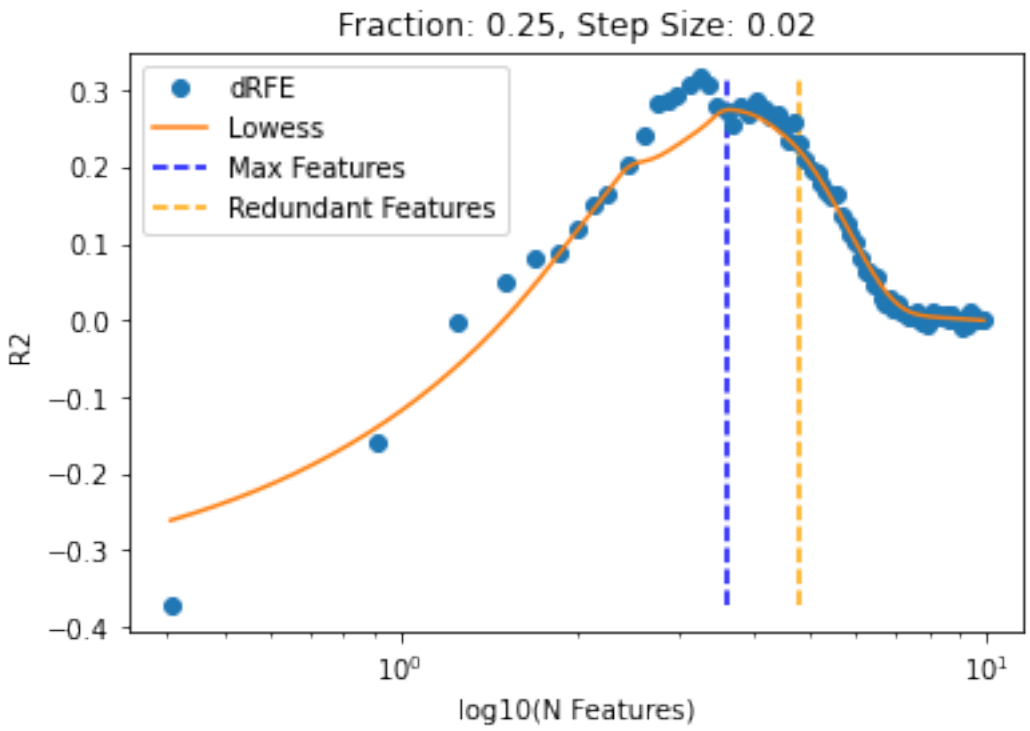


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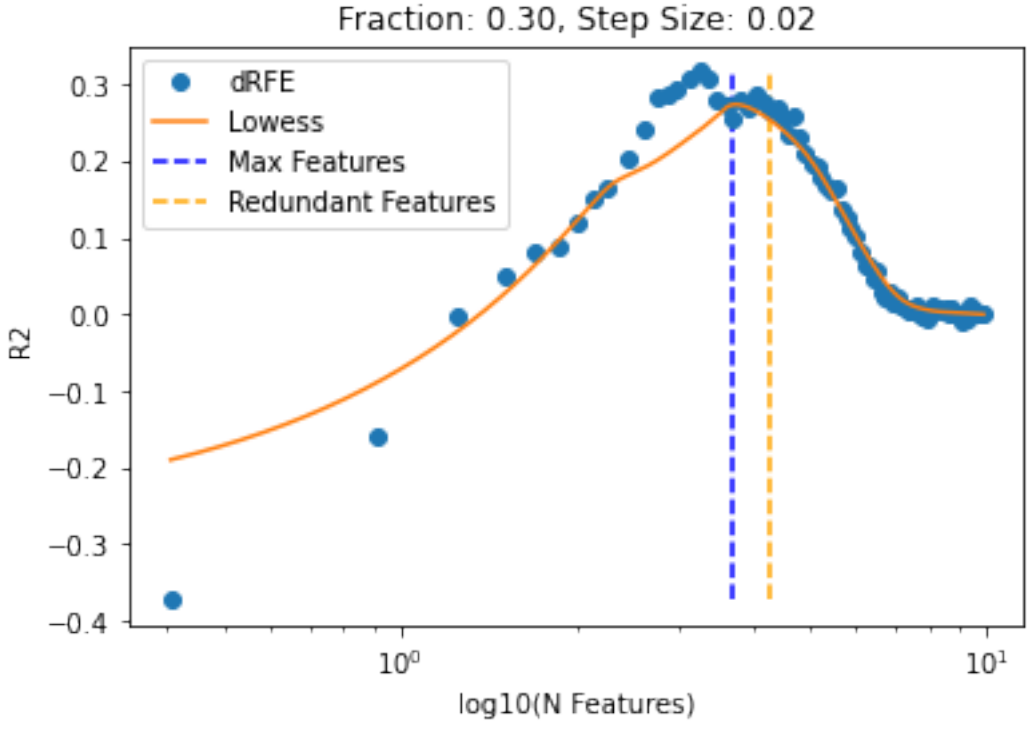

```
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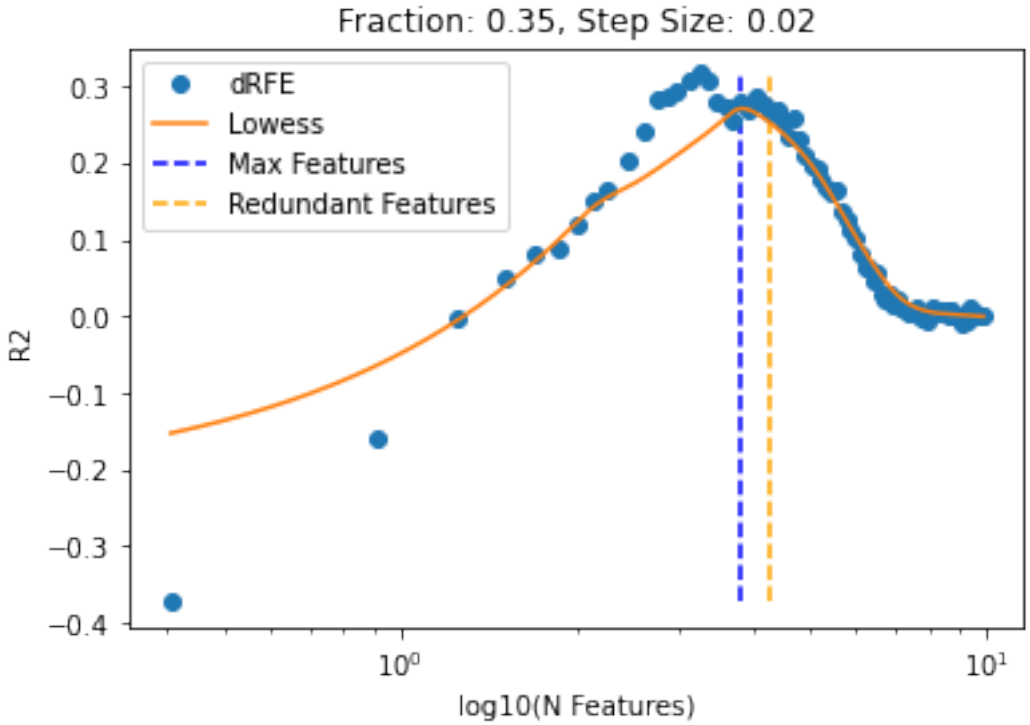


```
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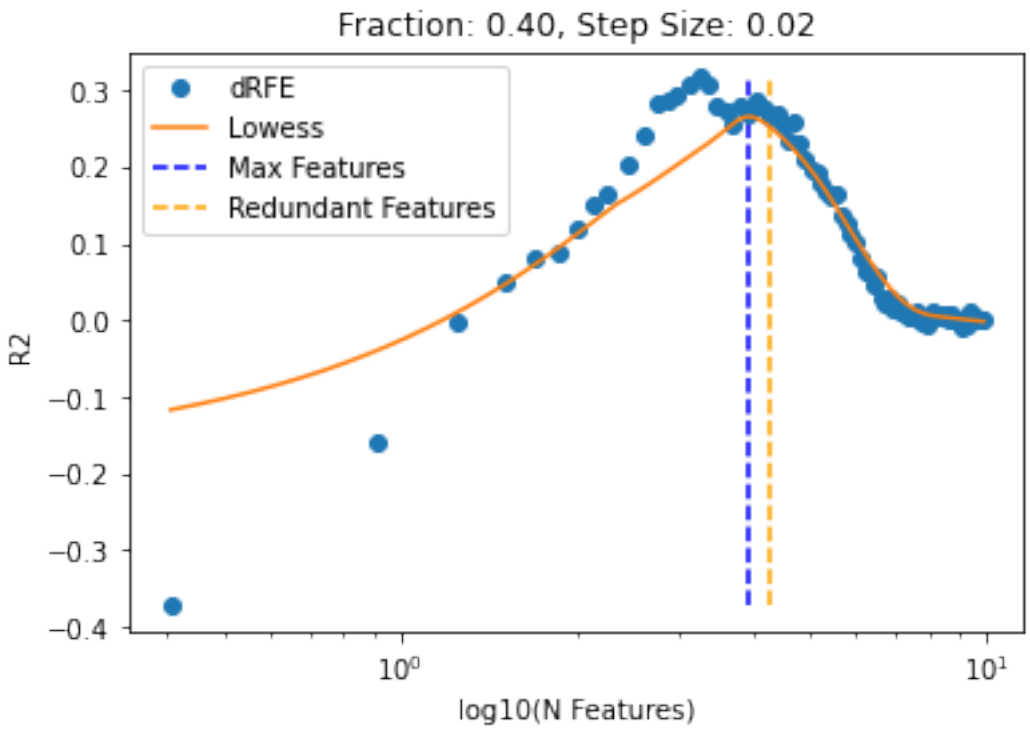
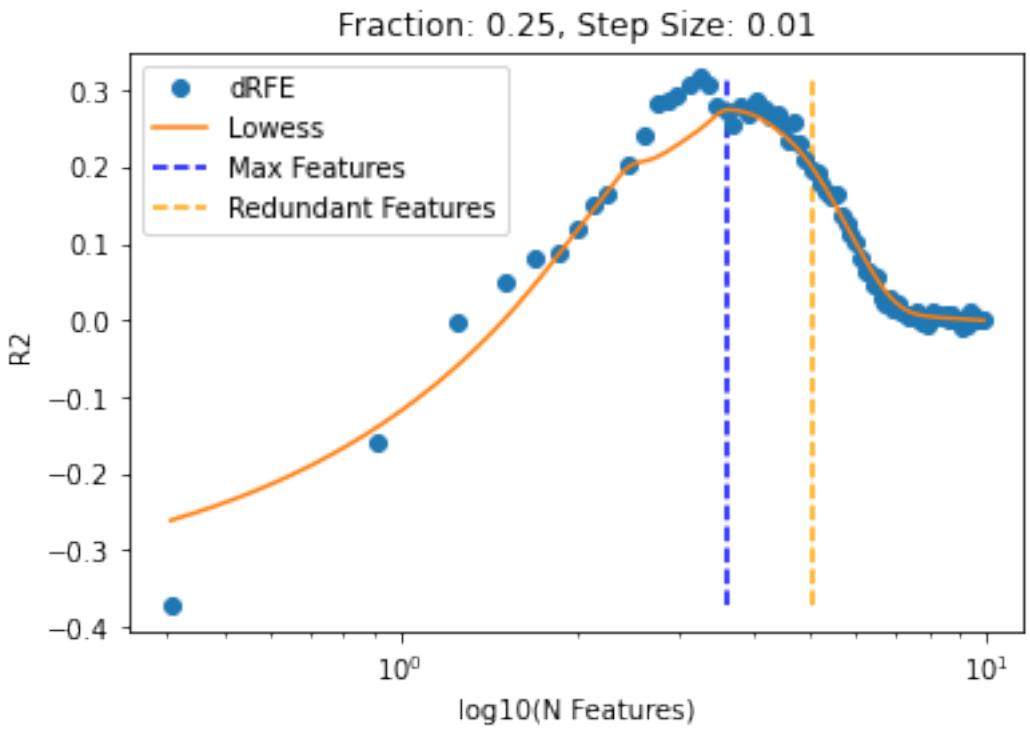
```



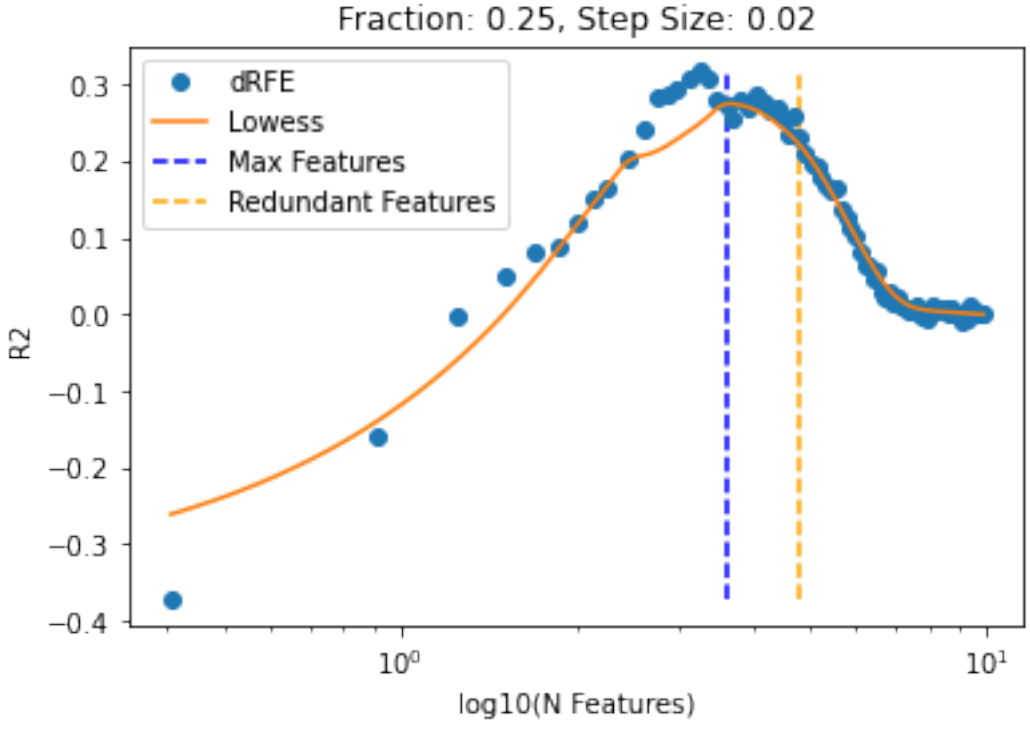
1.2.2 Optimize redundant selection: examine rate change

[14]:
```
for step_size in [0.01, 0.02, 0.03, 0.04, 0.05, 0.1]:
    dRFEtools.optimize_lowess_plot(d, fold, outdir, frac=0.25,␣
 ↪step_size=step_size,
                                   classify=False, save_plot=True)
```

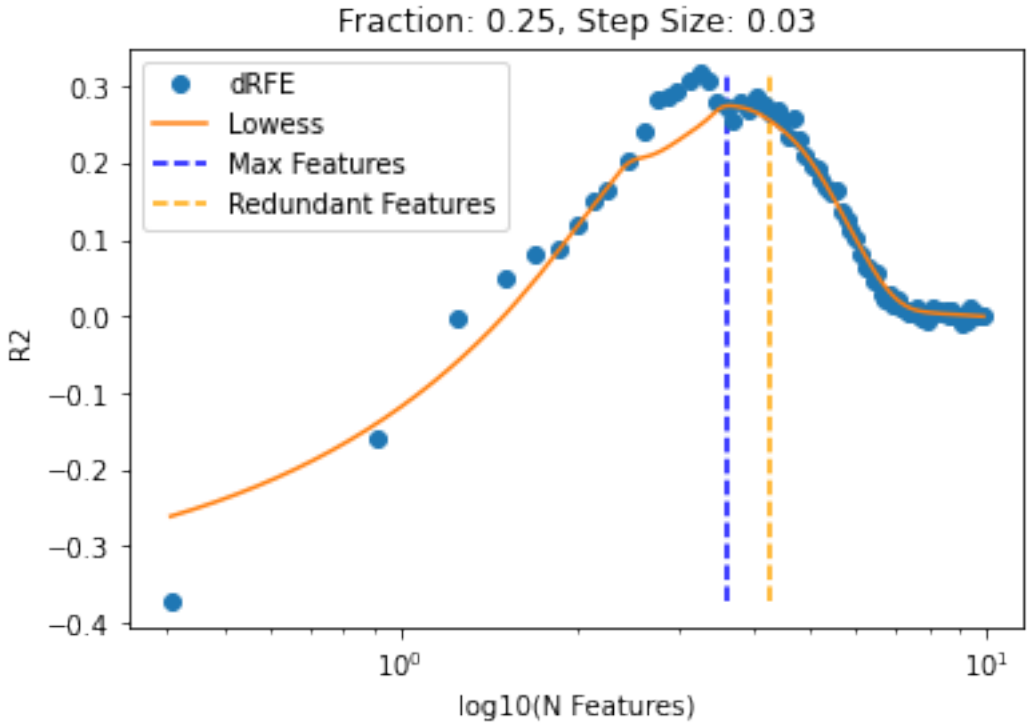
```
<Figure size 432x288 with 0 Axes>
```



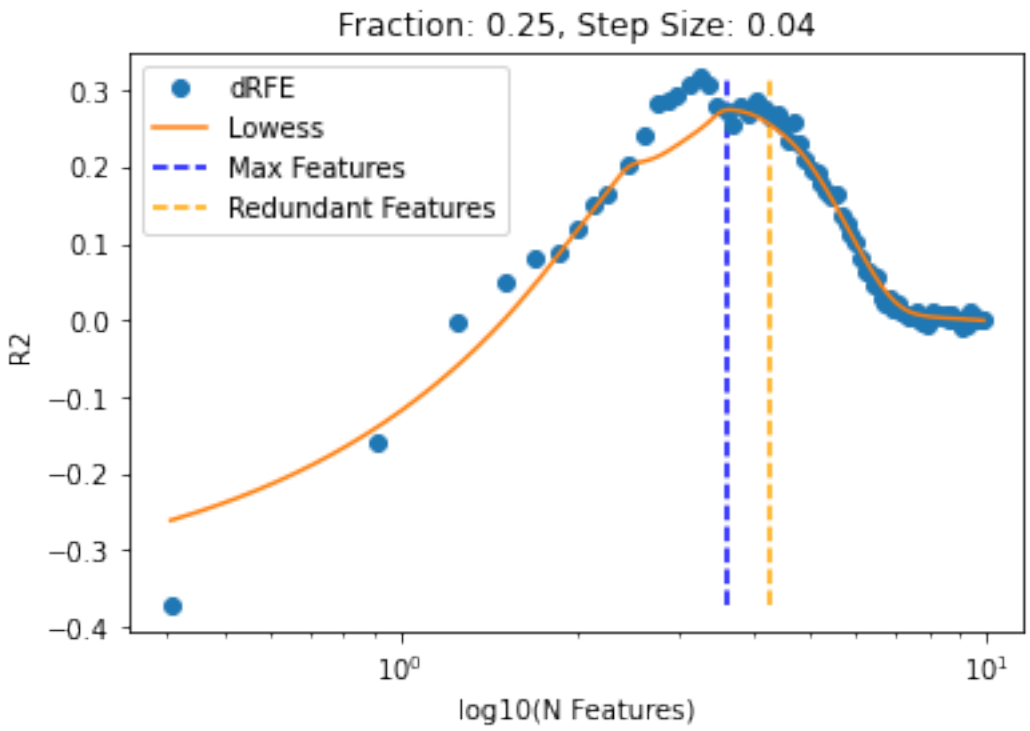

```
<Figure size 432x288 with 0 Axes>
```



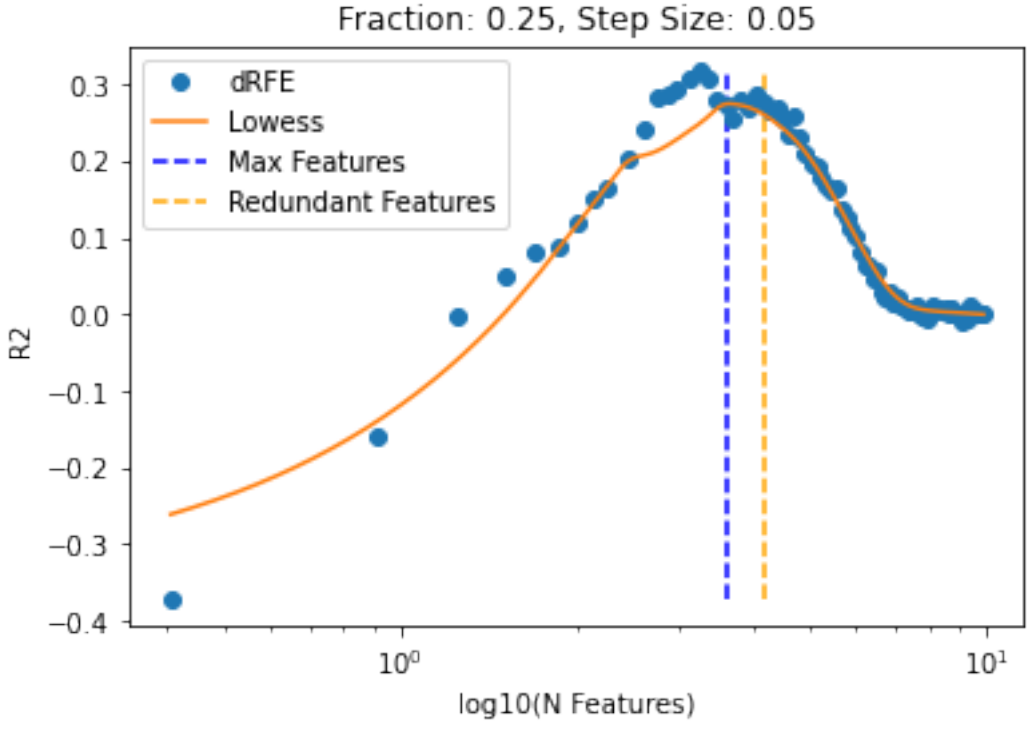
```
<Figure size 432x288 with 0 Axes>
```



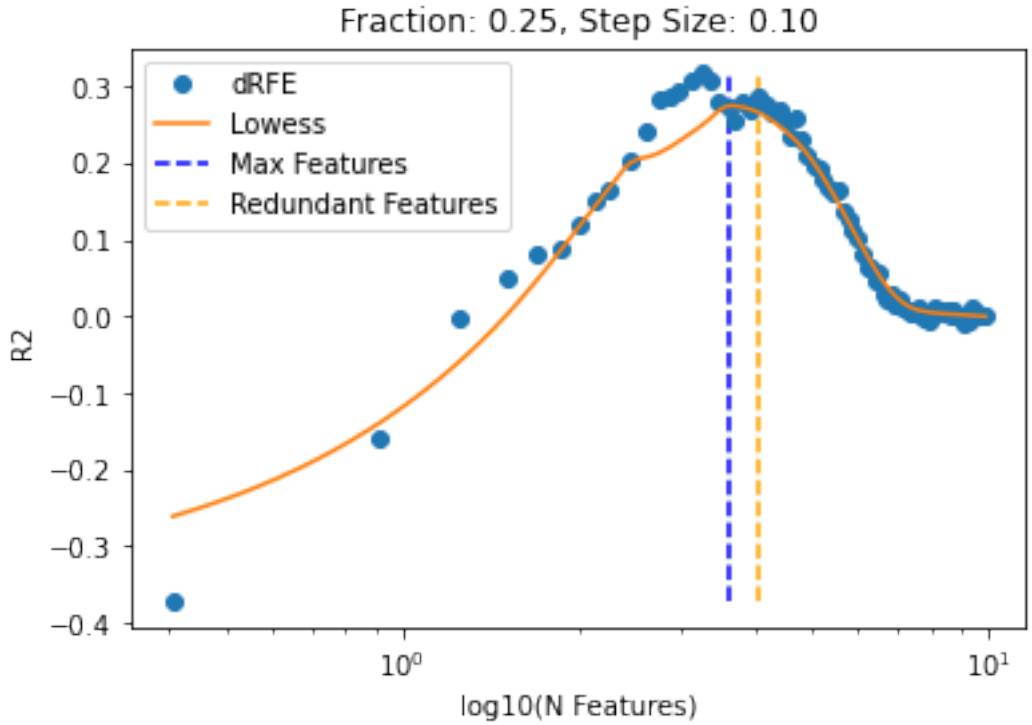

```
<Figure size 432x288 with 0 Axes>
```




```
<Figure size 432x288 with 0 Axes>
```



```
<Figure size 432x288 with 0 Axes>
```



[15]:
```
## Highest values without smoothing
max(d, key=lambda x: d[x][1])
```

[15]: 25

[16]:
```
print(dRFEtools.extract_max_lowess(d, frac=0.25))
dRFEtools.extract_redundant_lowess(d, frac=0.25, step_size=0.02)
```

```
(36, 3.597312260588446)
```

[16]: (123, 4.816241156068032)

1.3 Optimize classification: multi-class

[17]:
```
outdir = 'multiclass/'
mkdir_p(outdir)
```

[18]:
```
# Create a dataset with only 10 informative features
X, y = make_classification(
```

```
    n_samples=500, n_features=20000, n_informative=100, n_redundant=300,
    n_repeated=0, n_classes=4, n_clusters_per_class=1, random_state=13
)

cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=13)
cla = dRFEtools.RandomForestClassifier(n_estimators=100, n_jobs=-1,
                                       oob_score=True, random_state=13)
```

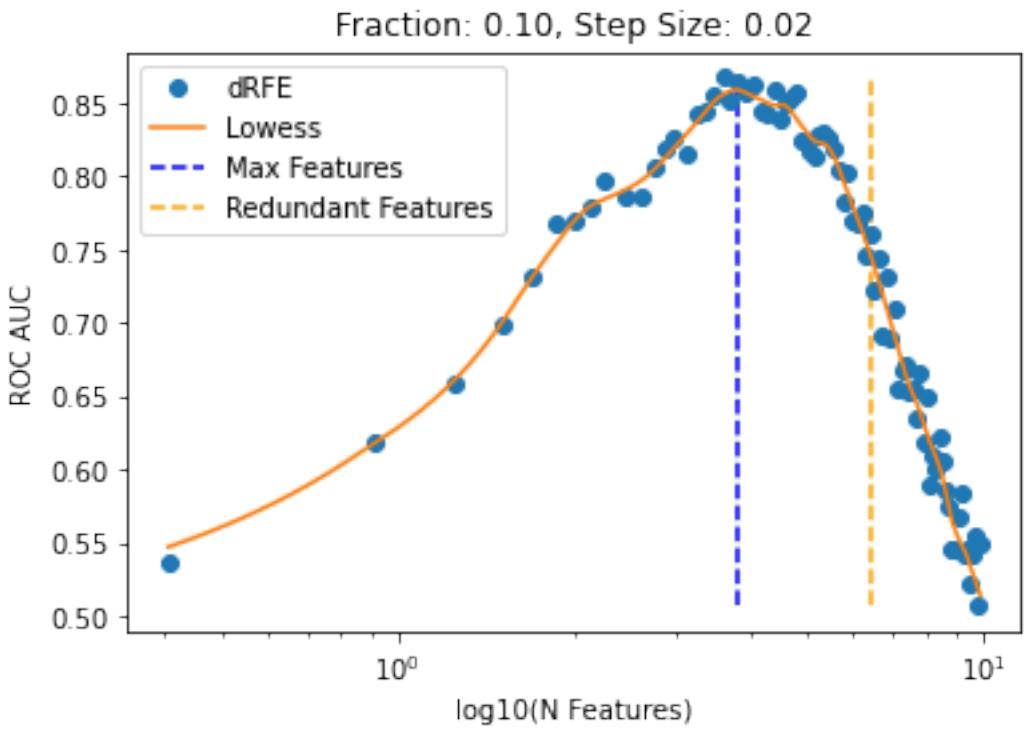
[19]:
```
fold = 1
for train_index, test_index in cv.split(X, y):
    X_train, X_test = X[train_index], X[test_index]
    y_train, y_test = y[train_index], y[test_index]
    fold += 1
fold -= 1

features = ["feature_%d" % x for x in range(X_train.shape[1])]
d, pfirst = dRFEtools.rf_rfe(cla, X_train, y_train, np.array(features),
                             fold, outdir, elimination_rate=0.1, RANK=False)
```

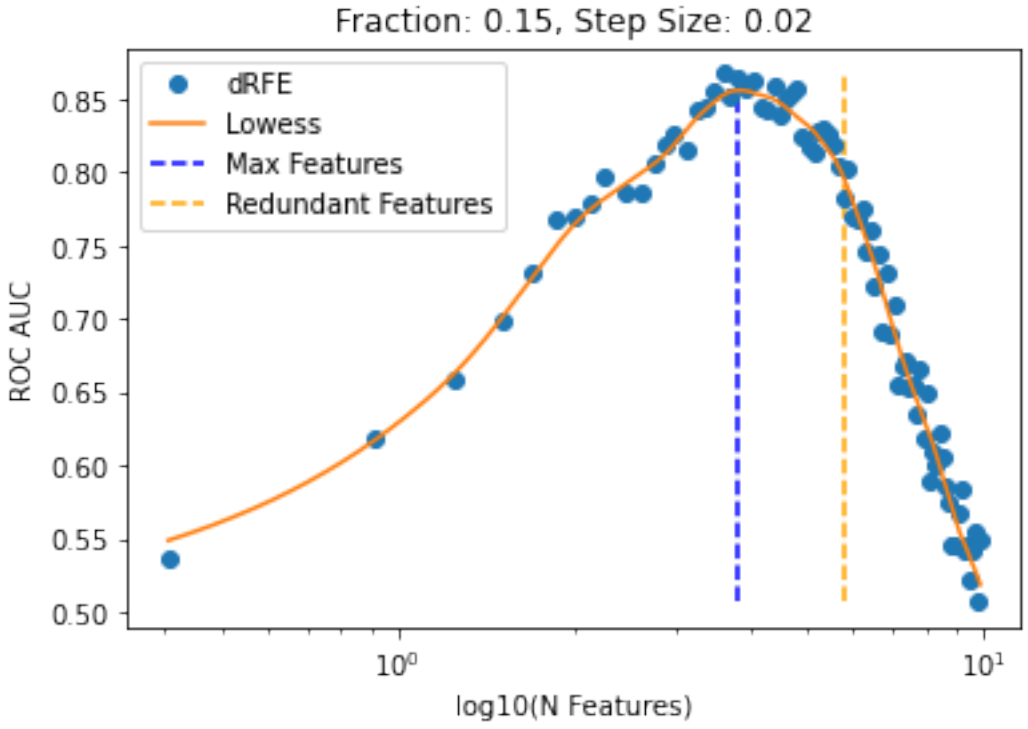
1.3.1 Optimize lowess fit: fraction of data to use when estimating y-values

[20]:
```
## Single Fold examination
for frac in [0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4]:
    dRFEtools.optimize_lowess_plot(d, fold, outdir, frac=frac, step_size=0.02,
                                   classify=True, multi=True, save_plot=True)
```

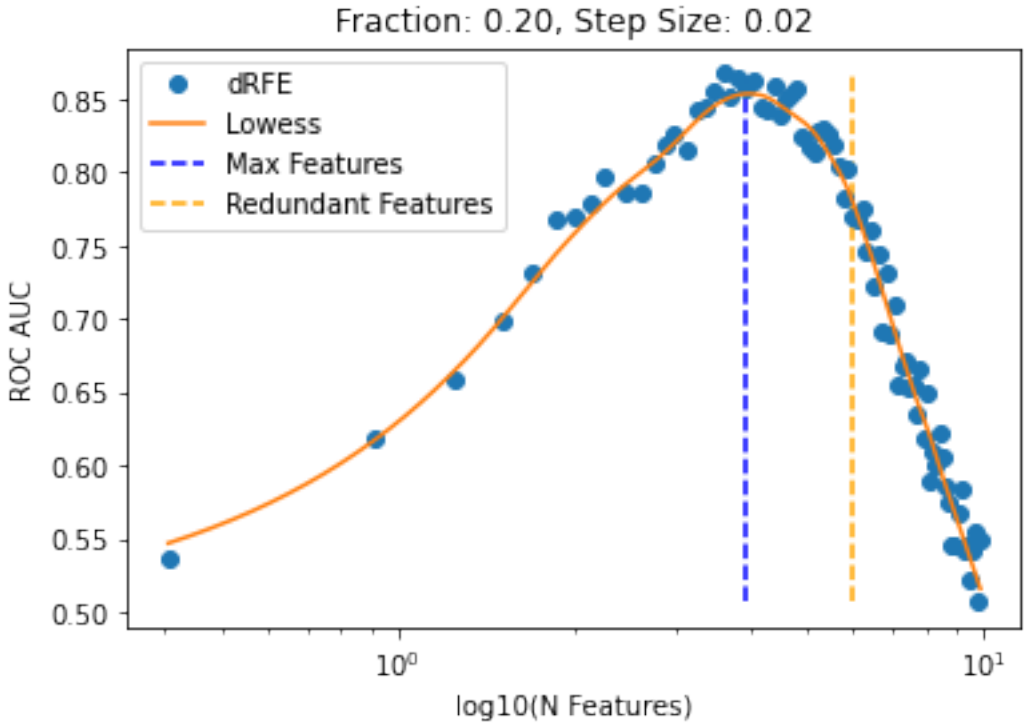
```
<Figure size 432x288 with 0 Axes>
```



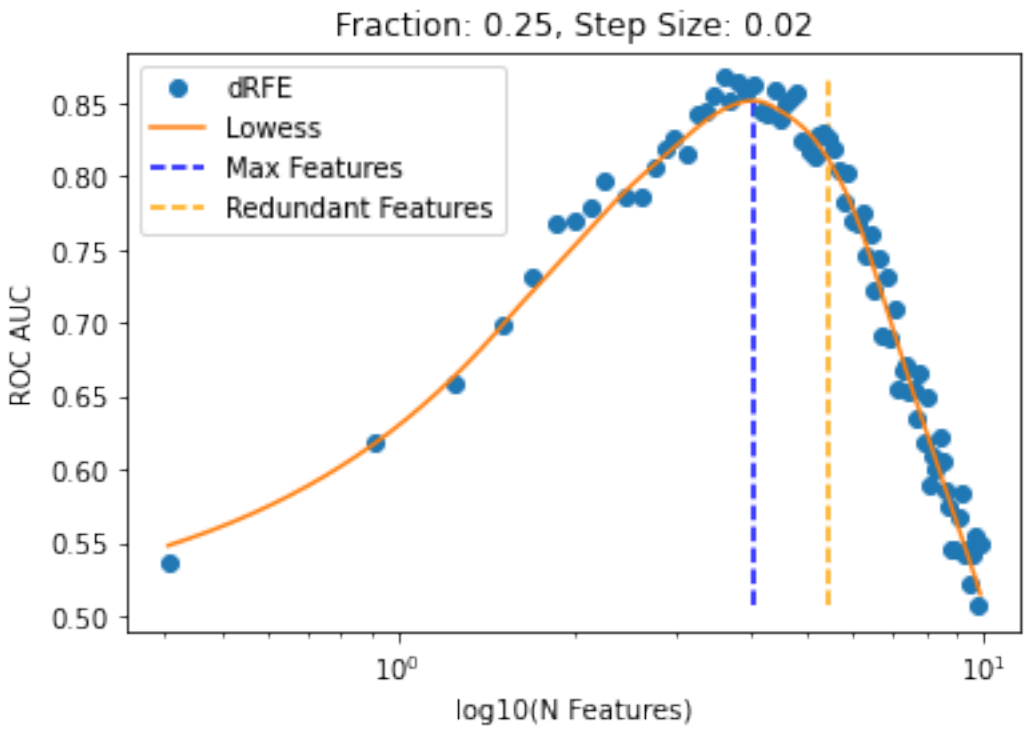
<Figure size 432x288 with 0 Axes>



```
<Figure size 432x288 with 0 Axes>
```




```
<Figure size 432x288 with 0 Axes>
```




```
<Figure size 432x288 with 0 Axes>
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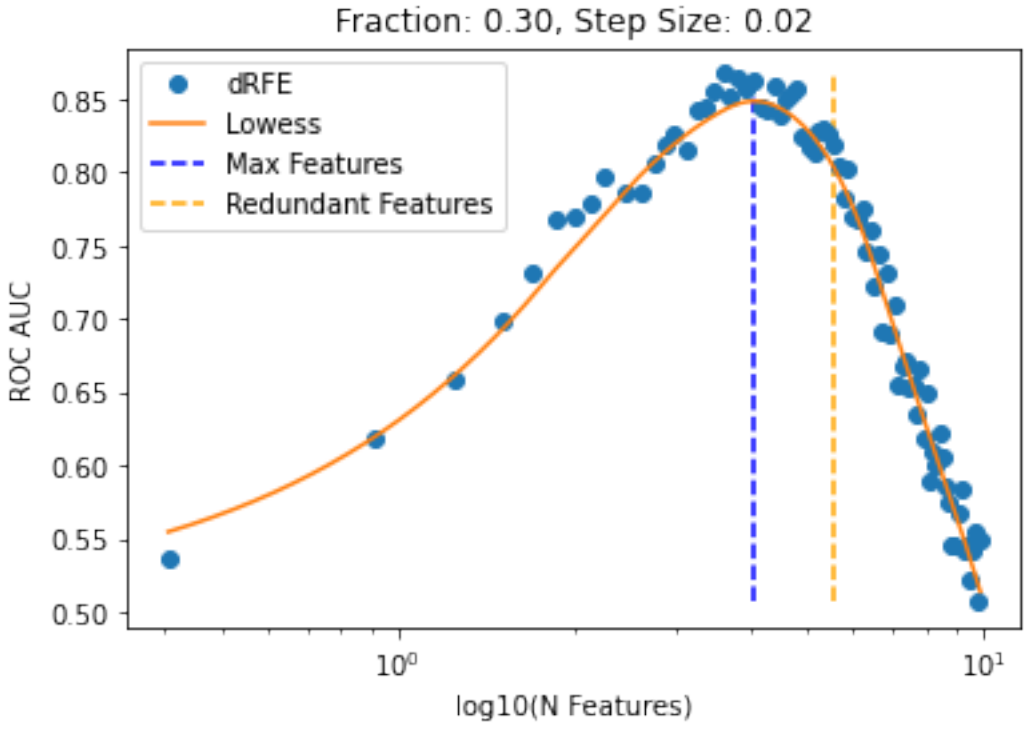
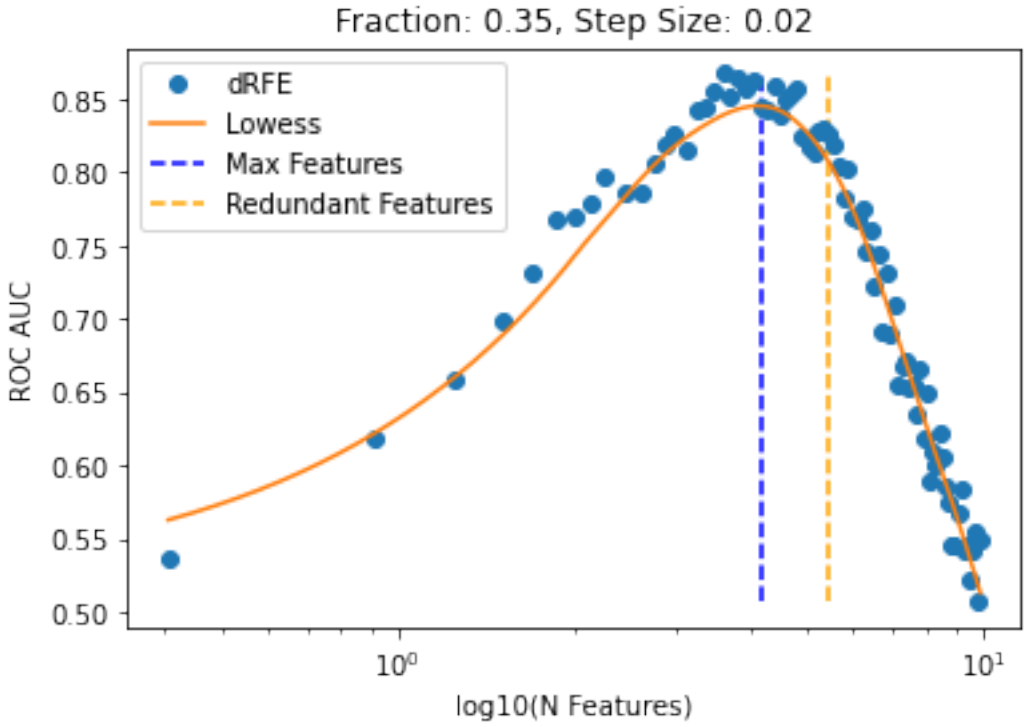
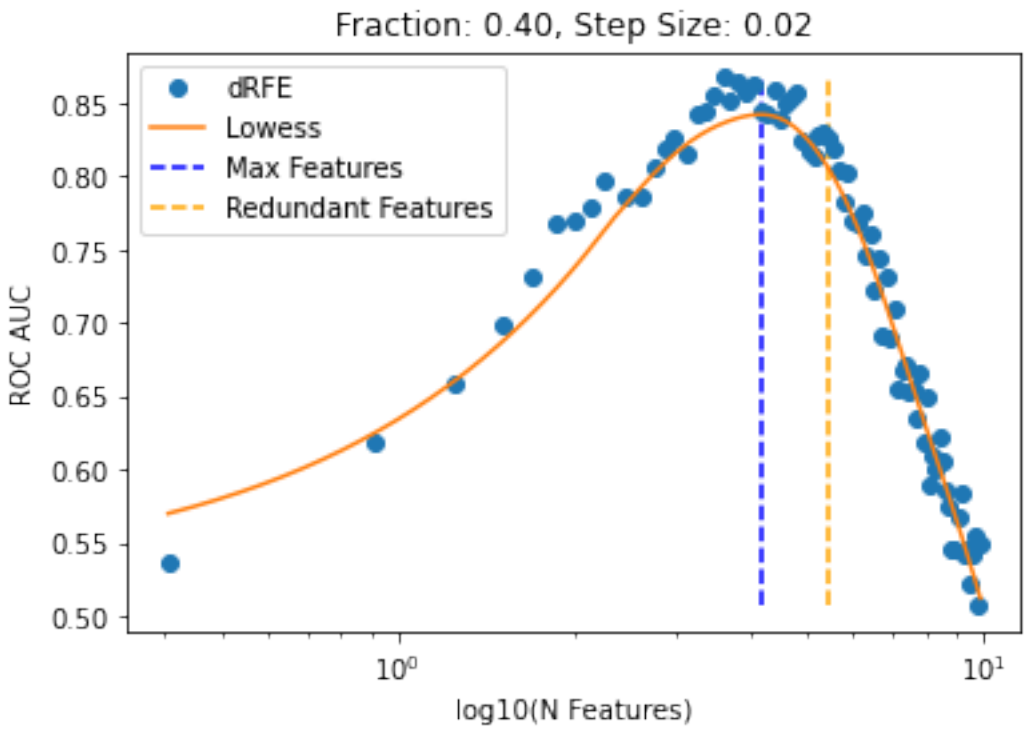


```
<Figure size 432x288 with 0 Axes>
```



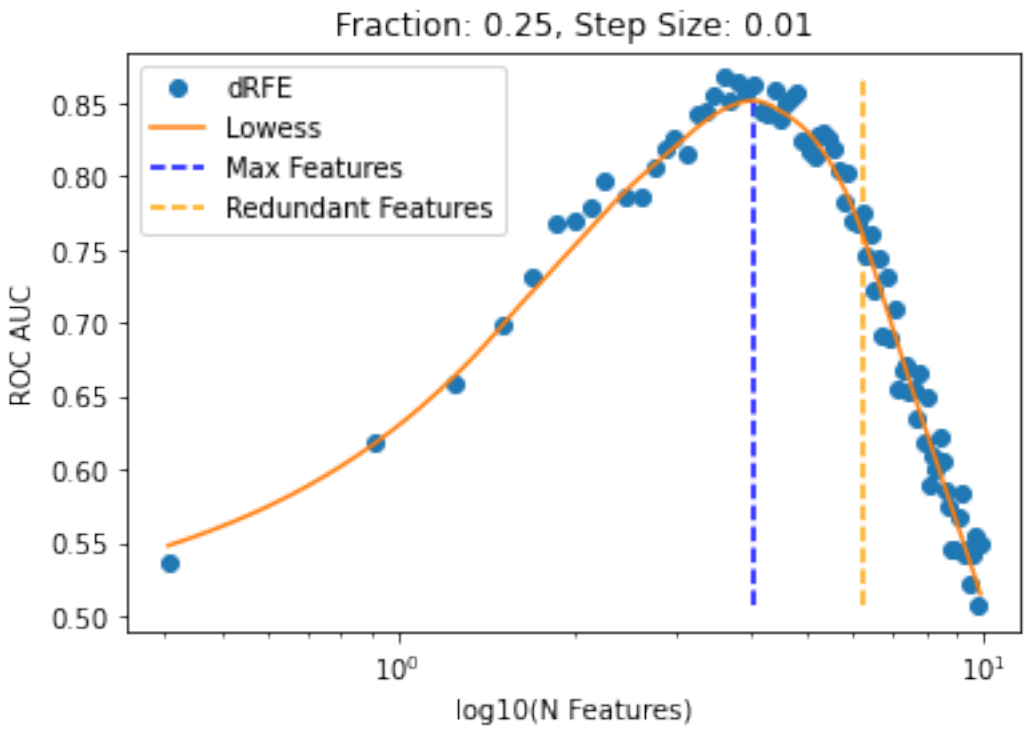

```
<Figure size 432x288 with 0 Axes>
```



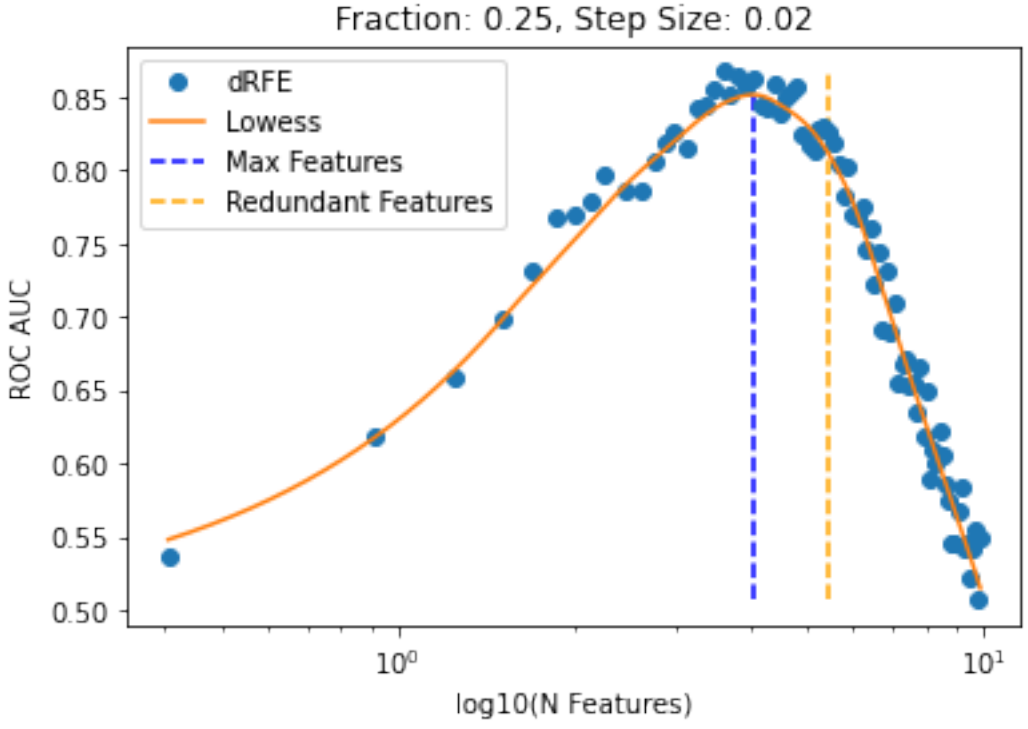
1.3.2 Optimize redundant selection: examine rate change

[21]:
```
for step_size in [0.01, 0.02, 0.03, 0.04, 0.05, 0.1]:
    dRFEtools.optimize_lowess_plot(d, fold, outdir, frac=0.25,␣
 ↪step_size=step_size,
                                   classify=True, multi=True, save_plot=True)
```

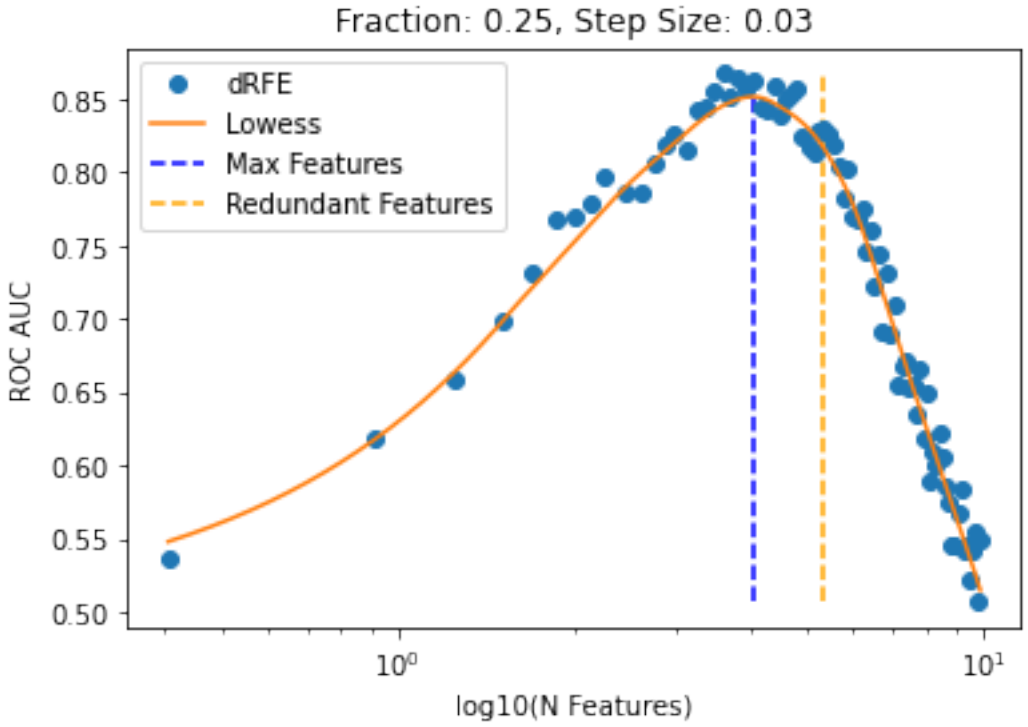
```
<Figure size 432x288 with 0 Axes>
```



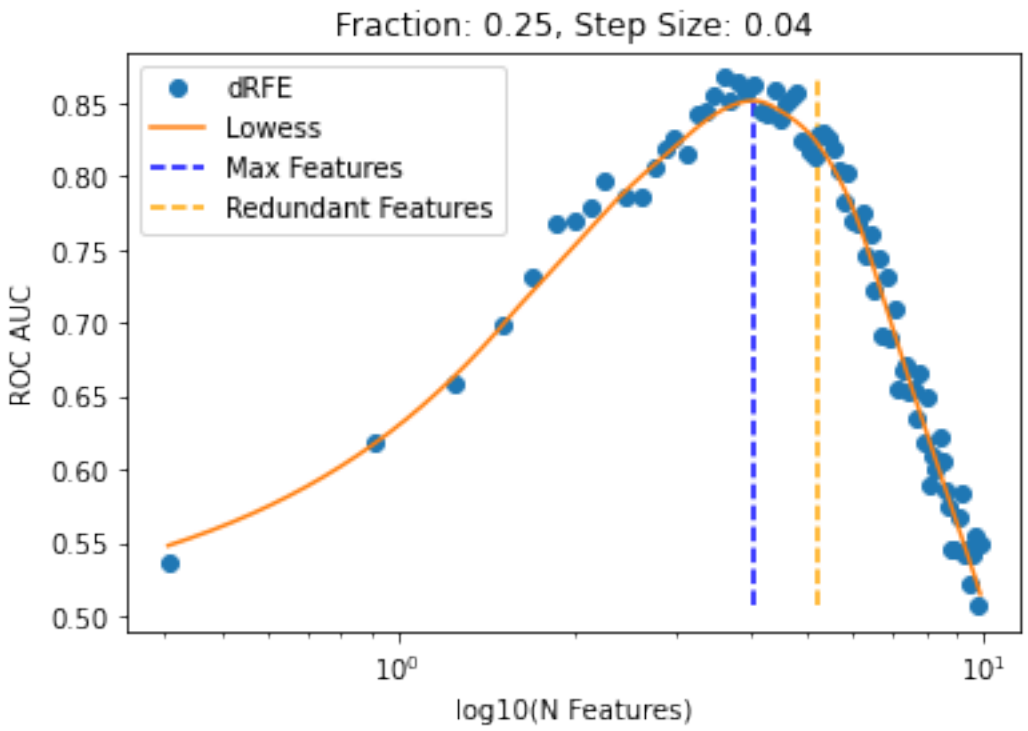

```
<Figure size 432x288 with 0 Axes>
```



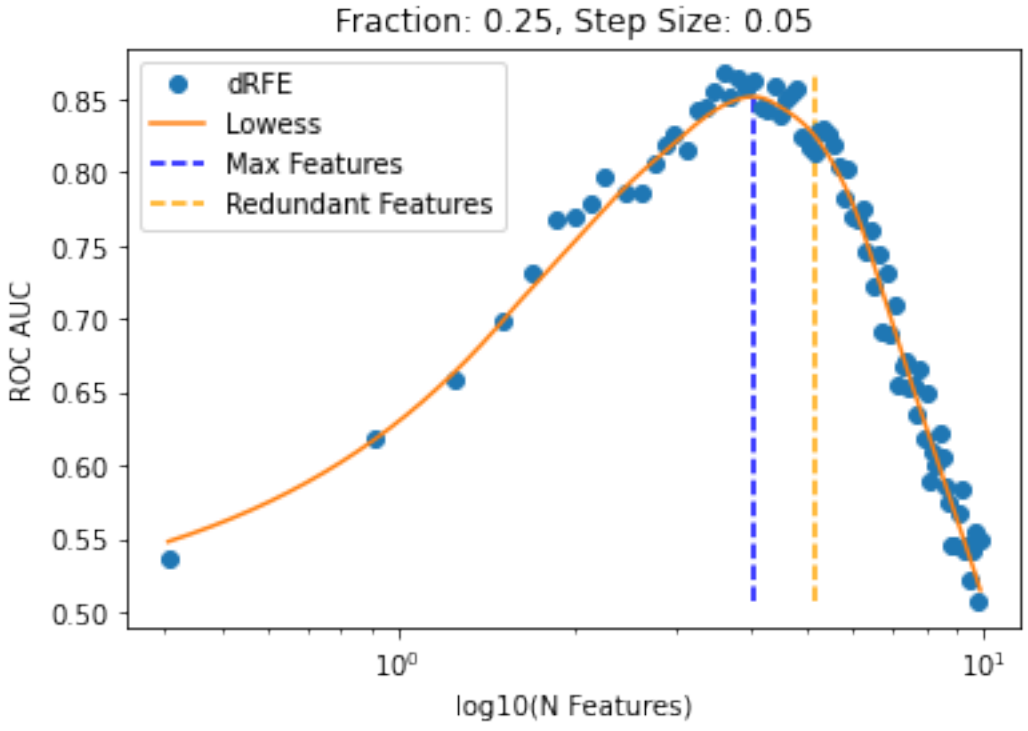
<Figure size 432x288 with 0 Axes>



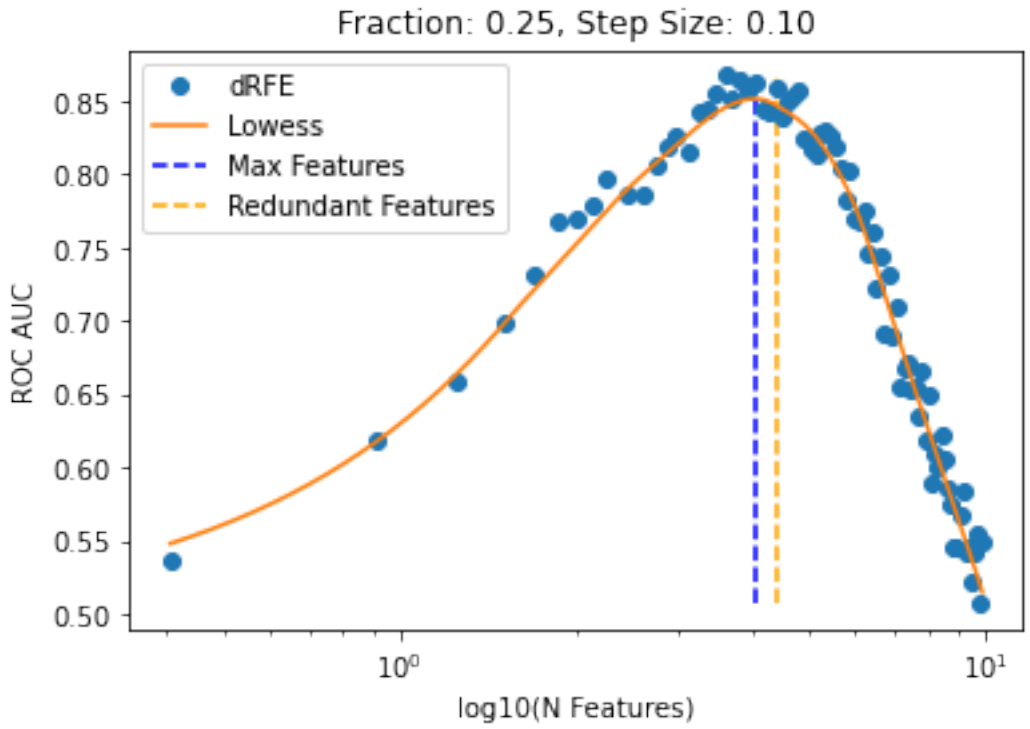
<Figure size 432x288 with 0 Axes>




```
<Figure size 432x288 with 0 Axes>
```



```
<Figure size 432x288 with 0 Axes>
```



[22]:
```
## Highest value (without smoothing)
max(d, key=lambda x: d[x][1])
```

[22]: 28

[23]:
```
print(dRFEtools.extract_max_lowess(d, frac=0.25))
dRFEtools.extract_redundant_lowess(d, frac=0.25, step_size=0.015)
```

```
(25, 3.2386784521643803)
```

[23]: (72, 4.283586561860629)

[ ]: