Unsupervised Learning and Dimensionality Reduction

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1 Unsupervised Learning and Dimensionality Reduction

1.1 Introduction

The goal of the previous analysis was finding the models (function approximations) that map some unseen data to most likely outcome. Supervized algorithms which were applied to the task provided predictive power measarable by ratio of correct answers. However, even the most accurate models revealed little about the structure of the data. Unsupervized algorithms help fill out this gap by providing means of finding subpopulations within the data by estimating distributions of data over different clusters.

```
In [455]: %matplotlib inline
          from algo_evaluation.handle_imports import *
```

1.2 Classification Data Review

Higgs Data quick review:

- given outcomes of particle decays, detect Higgs boson particle (signal);
- most of the **supervised** algorithms gave acceptable accuracy ranging from **0.8 - 0.9** and far outperforming the **backpropagation** algorithm for neural networks (**0.5** which is as good as flip of the coin but a lot more computationaly expensive)
- **learning weights** with Randomized Optimization algorithms improved accuracy of the neural network to **0.7** and higher (genetic algorithm)

Additional Data Wrangling:

- features were **rescaled** as a requirement to feature transformation alogrithms
- previously manually pruned features were put back to allow feature selection algorithms to autotically choose the most informative ones
- dataset was not reduced in size since dimensionality reduction provides speed advantage (the main reason for sampling records in the previous analysis)

```
In [374]: higgs_data = datasets.load_higgs_train(sample_size=None, verbose=True, scale=True,
                                                 prune_features=False)
          all_higgs_features = higgs_data[0].shape[1]
```

```
Size of the dataset: 68114
Number of features: 30
Number of positives (signal): 31894
Number of negatives (background): 36220
```

Converters Data quick review:

- given online users' behavior and preferences predict whether or not ad display will result in conversion;
- in contrast to Higgs dataset, supervized algorithm on this datataseprovided high accuracy >94%
- converters dataset as a result was not subjected to randomized optimization analysis

```
In [392]: bid_data = datasets.load_bidding_train(verbose=True, scale=True)
          all_bid_data_features = bid_data[0].shape[1]
```

```
Size of the dataset: 57970
Number of features: 15
Number of converters: 399
Number of non-converters: 54615
Number of leads: 2956
```

1.3 K-means Clustering

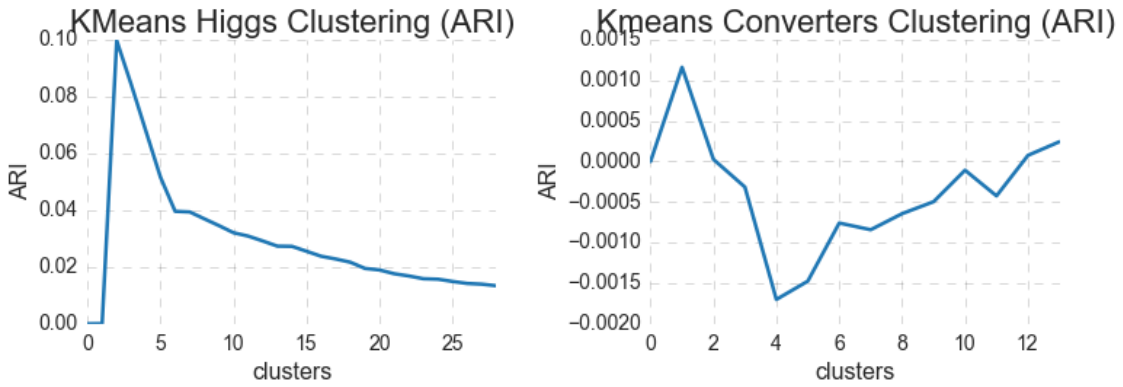
Evaluating cluster performance is different from the techiques used in Supervised Algorithms where accuracy was estimated roughly as a count of wrong answers. For clustering we must imploy similarity metric: did clustering define separations of data similar to ground truth. Here I shall use **Adjusted Rand Index** that measures the similarity of the two assignments, ignoring permutations and with chance normalization.

Model Selection (cluster complexity) Best model is selected by iterating over the number of clusters and measuring the performance of each with ARI score.

```
In [350]: df_kmeans_higgs = kmeans_eval.estimate_clusters(higgs_data)
```

```
In [367]: df_kmeans_converters = kmeans_eval.estimate_clusters(bid_data)
```

```
In [368]: plot_cluster_estimation.plot_kmeans_cluster_score(df_kmeans_higgs, df_kmeans_converters)
```



Choosing K:

Best data separation for **Higgs** data achieved with number of clusters equal **2** which makes sense since there are two classes in the data: signal and background, so the clustering lined up with labels. As number of the clusters grow, similarity measure gradually approaches zero and uniformity of the data withing each group decreases.

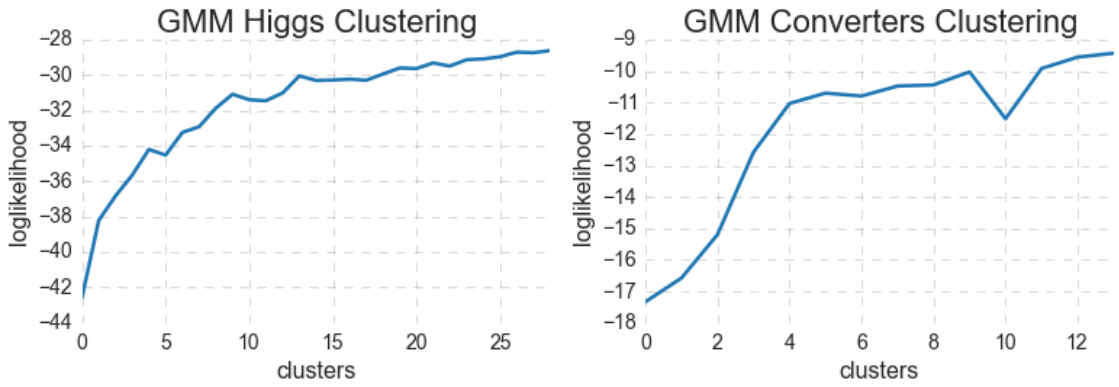
Converters dataset achieves best separation for a single class which is the same as saying that clustering algorithm could not split data into groups. Since a single cluster does not make sense, it is reasonable to analyze next best separation. There is no clear convergence in this case towards a certain number of clusters and moreover, cluster assighment does not line up with labels, so it is ok to choose an arbitrary number (we can stick with **10** and see how well that compares with dimensionality reduction algorithms)

Insight: Neither of the above data separation is considered good (ARI=1.0 is a perfect score). Since scores are close to 0.0, label assignment is rather uniform especially for converters data. This suggests that datasets have more complex structure and are not easily separable into groups.

1.4 Expectation Maximization

As a second approach to clustering we will use the probabilistic model with assumption that all data points are generated from the number of Gaussian distributions. As a measure metric, we can use the scoring method which computes the **log probability** under the model.

```
In [355]: df_gmm_higgs = gmm_eval.estimate_clusters(higgs_data)

In [369]: df_gmm_converters = gmm_eval.estimate_clusters(bid_data)

In [370]: plot_cluster_estimation.plot_gmm_cluster_score(df_gmm_higgs, df_gmm_converters)
```



For **Higgs** dataset, loglikelihood of data is increasing as number of latent variables (here number of gaussian distributions) is increasing which suggests that every single feature came from a gaussian distribution with unique paramters (means and variances).

For **Converters** dataset, loglikelihood is increasing as well, however it is important to note that in the range of clusters from 4 to 9 probability increase is not very significant, so it is ok to make an assumption that data generally comes from 4 distinct distributions.

1.5 Feature Selection and Transformation for Higgs Dataset

In the previous analysis Higgs records were sampled and features were manually pruned due to the slow speed of supervized algorithms. In this analysis, complete dataset is restored to take advantage of automatic feature selection using dimensionality reduction algorithms.

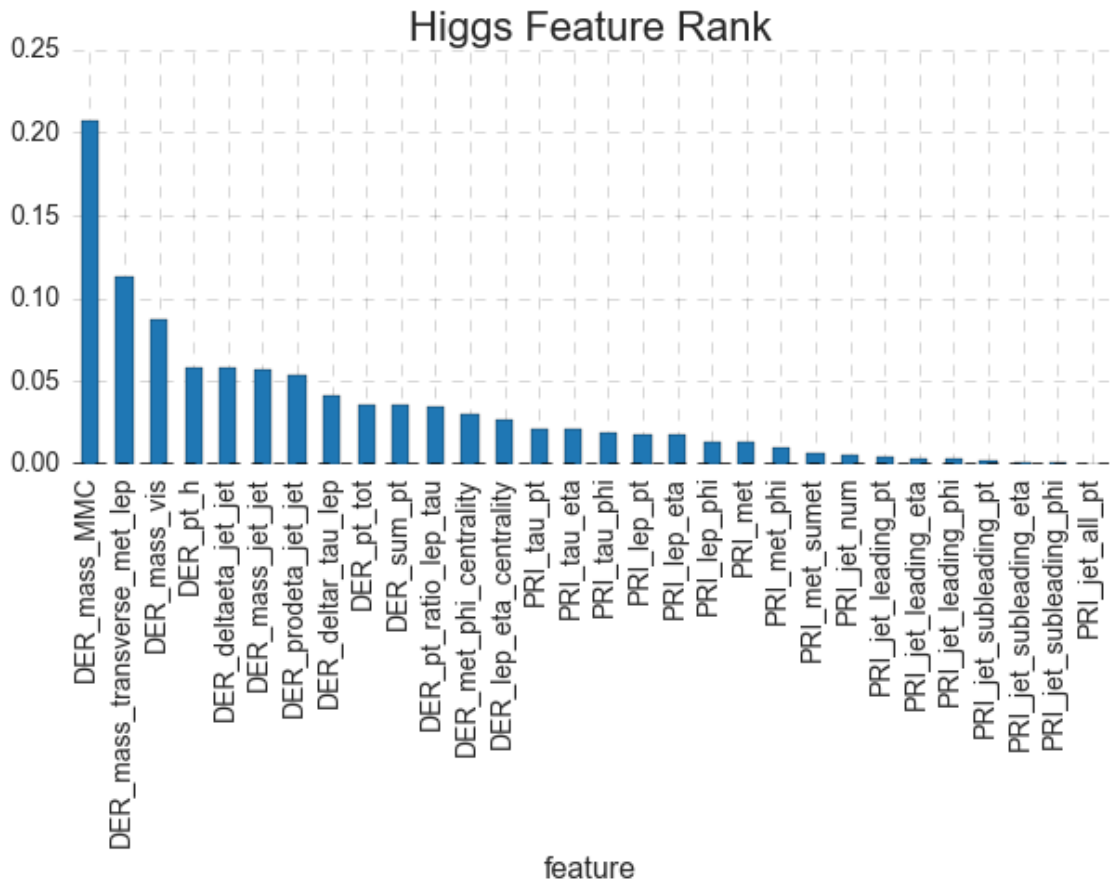
Dimensionality reduction is the task of deriving a set of features that is smaller than the original feature set while retaining most of the variance of the original data. To estimate the best number of components to be used for data transformation, I used **data variance** and **reconstruction error** analysis to choose optimal setting.

1.5.1 Principal Component Analysis (PCA)

```
In [162]: pca_rank = pca_eval.rank_features(higgs_data, n_components=all_higgs_features)
```

PCA estimates percentage of variance explained by each of the components. I extracted those variances (eigen values) for each feature and sorted them from largest to smallest. Visualizing the results made it clear that "Derived" features from Hiigs dataset have larger spread than "Primitives" and thus are more informative for classification. This supports the decision made in the previous analysis where "Primitive" features were pruned based on feature by feature analysis.

```
In [282]: pca_eval.plot_rank(pca_rank, title='Higgs Feature Rank')
```



Reducing features while retaining data variance:

When applying dimensionality reduction, it is important to retain certain threshold of data variance. In addition to visual inspeaction, I selected features which retained **95%** of data variance (dimensionality reduced from 30 to 7). Algorithm ranked features *DER_mass_MMC* the highest which makes sense since this feature estimates mass of the Higgs boson candidate and indeed is the most informative.

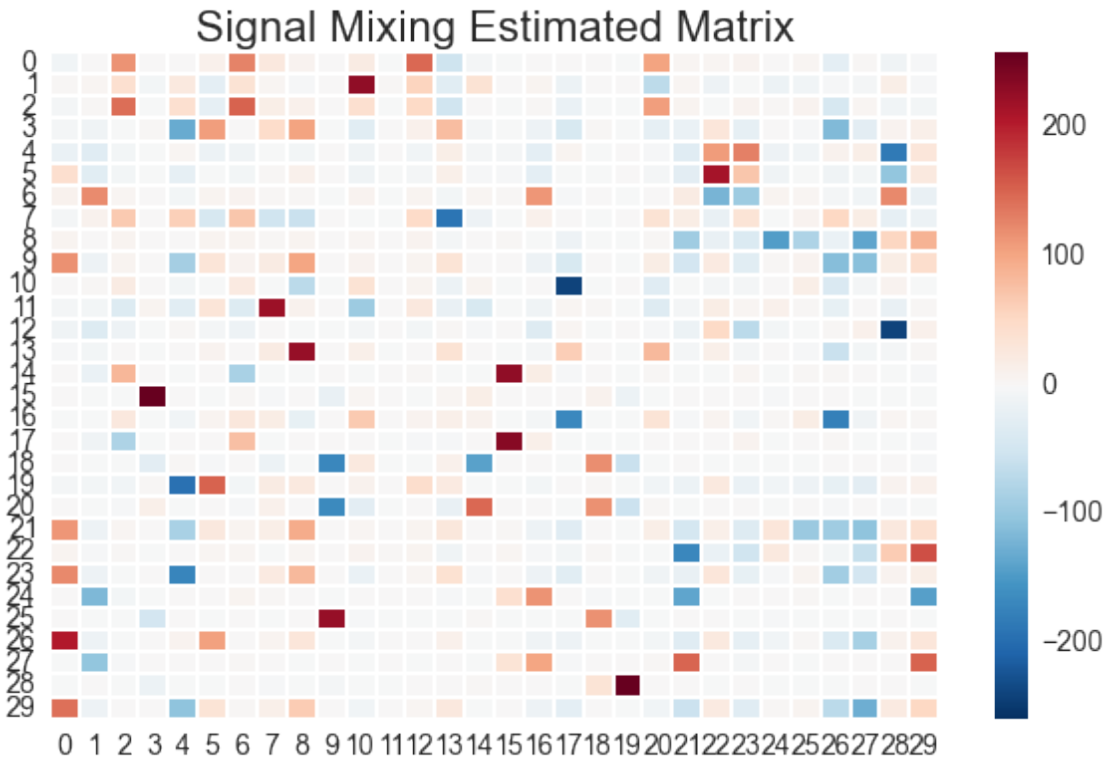
```
In [168]: reduced_features = pca_rank.variance_ratio[pca_rank.variance_ratio > 0.05]
          reduced_features

Out[168]: feature
          DER_mass_MMC                  0.207485
          DER_mass_transverse_met_lep   0.112727
          DER_mass_vis                  0.087133
          DER_pt_h                      0.058547
          DER_deltaeta_jet_jet          0.058122
          DER_mass_jet_jet              0.057542
          DER_prodeta_jet_jet           0.053497
          Name: variance_ratio, dtype: float64
```

1.5.2 Independent Component Analysis (ICA)

By minimizing the Gaussianity of the projection, ICA is designed to recover the underlying physical process which generated the observed data. Using heatmap I plotted the estimated mixing matrix to see how much

each of independent components are mixed in the observable features.

```
In [616]: mm = ica_eval.mixing_matrix(higgs_data, all_higgs_features, display=True)
```

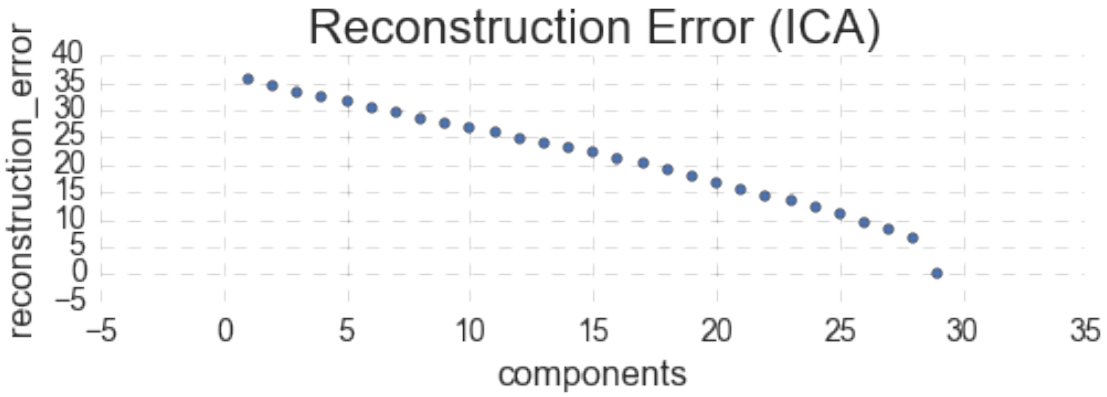


Finding reconstrcution error: Another method for estimating number of components is to analyze reconstruction error and choose dimensionality with acceptable thresholds (in this case 30% error).

Note: all algorithms gave the same reconstruction error so it is sufficient to visualize results for only one of them (in this case, ICA)

```
In [195]: ica_comp = ica_eval.estimate_components(higgs_data)
```

```
In [556]: reconstruction_error = ica_comp.plot(x='components',
                                                y='reconstruction_error',
                                                kind='scatter',
                                                figsize=(8,2), title='Reconstruction Error (ICA)')
```



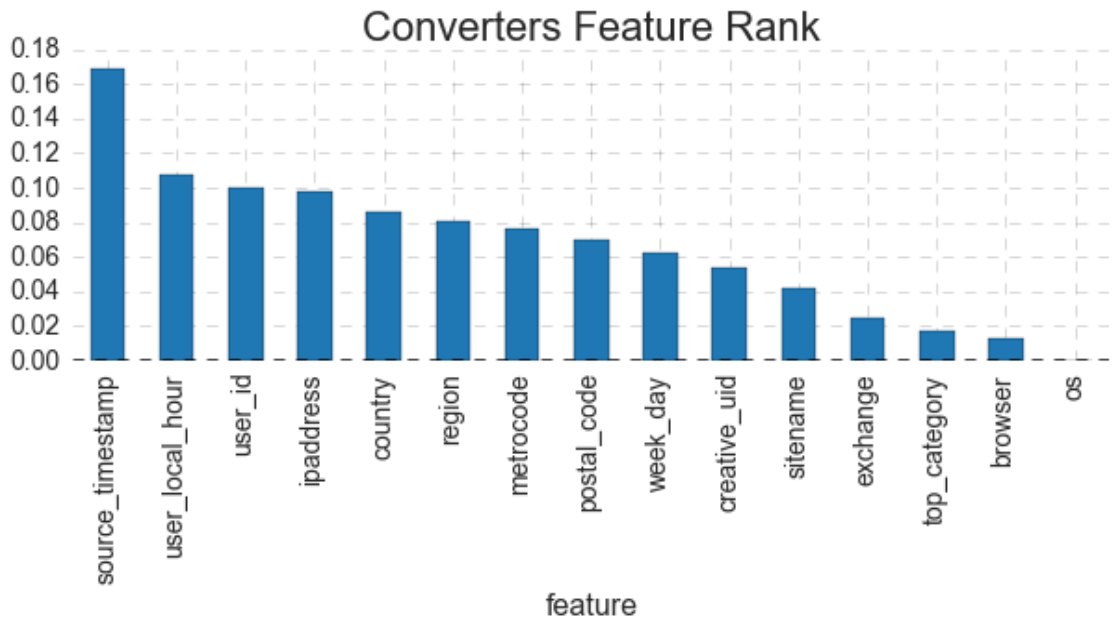
```
In [286]: reduced_higgs_dimension = df[df.reconstruction_error < 30].components.min()
          print 'Estimated number of reduced components for Higgs dataset =', reduced_dimension

Estimated number of reduced components for Higgs dataset = 7
```

With both methods for estimating number of components, 7 seems to be the optimal and thus shall be considered for dimensionality reduction for further analysis of the Higgs data.

1.6 Feature Selection and Transformation for Converters Dataset

Same principles and technique were applied to select features for converters dataset (retaining data variance of 95%)

```
In [251]: pca_rank_bid = pca_eval.rank_features(bid_data, n_components=all_bid_data_features)

In [284]: pca_eval.plot_rank(pca_rank_bid, title='Converters Feature Rank', figsize=(10,3))
```




```
In [593]: red_conv_feat = pca_rank_bid.variance_ratio[pca_rank_bid.variance_ratio > 0.05]
          reduced_conv_dimension = len(red_conv_feat)
          print 'Estimated number of reduced components =', reduced_conv_dimension
          print red_conv_feat

Estimated number of reduced components = 10
feature
source_timestamp    0.168507
user_local_hour     0.107505
user_id             0.100265
ipaddress           0.097562
country             0.085957
```

```
region              0.080283
metrocode           0.076695
postal_code         0.069630
week_day            0.062470
creative_uid        0.054318
Name: variance_ratio, dtype: float64
```

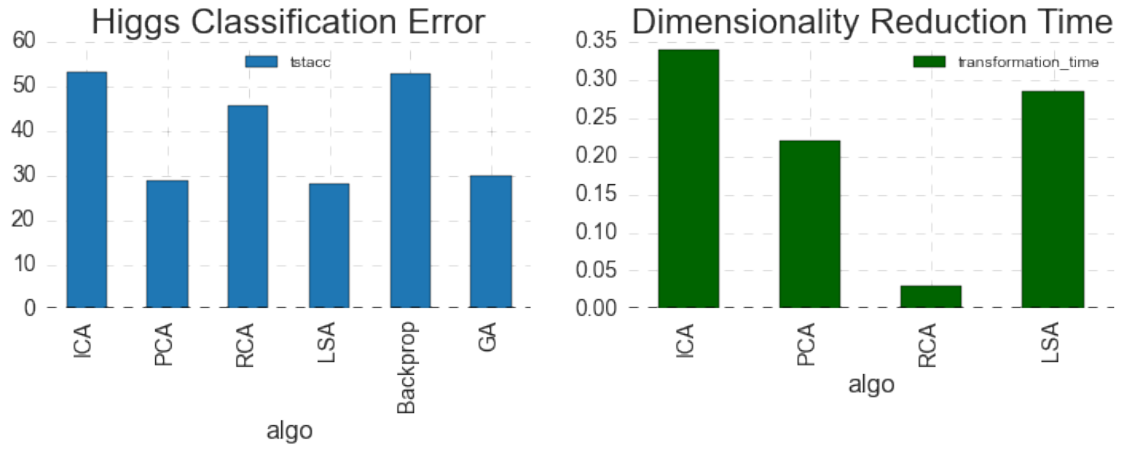
Insight: Some of features (like sitename) were pruned by not contributing to data spread (small eigen value); this suggests that the local user time is more important differentiator as to whether or not ad will result in conversion.

1.7 Neural Networks on Higgs dataset post Dimensionality Reduction

In the following experiment setup Higgs data set is reduced using four algorithms: PCA, ICA, RCA and LSA. Same error measure is applied as in the previous analysis where Higgs boson was classified with Neural Networks. I chose to visualize the classification error along side with dimensionality reduction time to see the tradeoff between the speed and model accuracy.

```
In [408]: df_nn = nn.evaluate_nn_accuracy(higgs_data, reduced_higgs_dimension)
```

```
In [468]: nn.plot_evaluation(df_nn)
```



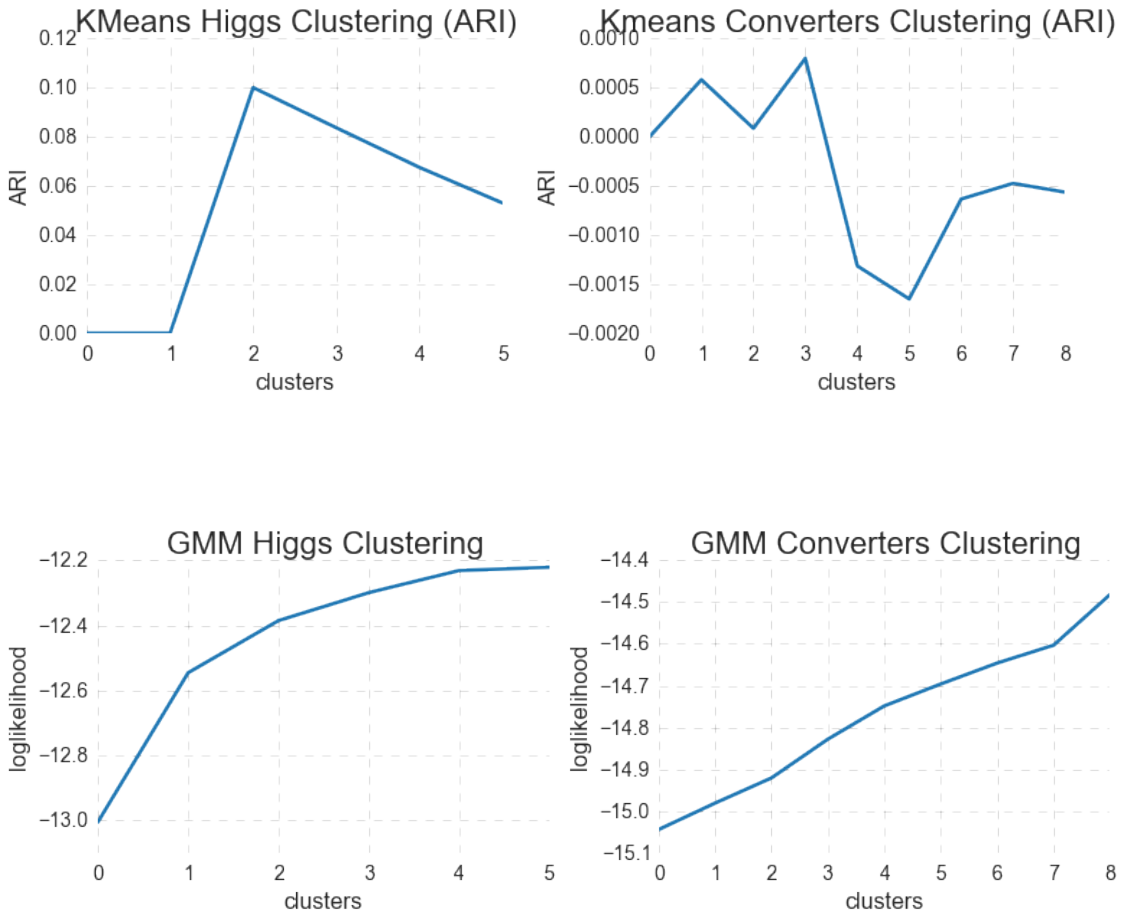
In addition to comparing the classification error between different dimensionality reduction algorithms, I added results from previous two algorithms (Backpropagation and Weights Learning with Genetic Algorithm) to be used as a baseline.

Very notable is the fact that **PCA** dimension reduction has improved classification error as compared to Backpropagation and is on par with Genetic Algorithm which performed best for learning weights. Reducing dimensions with randomized projection (**RCA**) does have not the best accuracy, however the speed of the algorithm is amazingly fast compared to all others and so it can be very beneficial in the cases accuracy could be sacrificed to avoid the curse of dimensionality.

1.8 Clustering post Dimensionality Reduction

Here I repeat the clustering experiments with projected data which in both dataset if smaller than the original dimensionality: Higgs (30 -> 7) and Converters (15 -> 10). Neither Kmeans or GMM showed a different structure on the projected datasets (see figure below), so the same insights about data distribution are preserved.

```
In [464]: df_higgs_dim = clustering.evaluate_higgs_clustering(higgs_data, reduced_higgs_dimension)

In [476]: df_conv_dim = clustering.evaluate_conv_clustering(bid_data, reduced_conv_dimension)

In [486]: clustering.plot_cluster_performance(df_higgs_dim, df_conv_dim)
```



Runtime comparsion of the clustering time

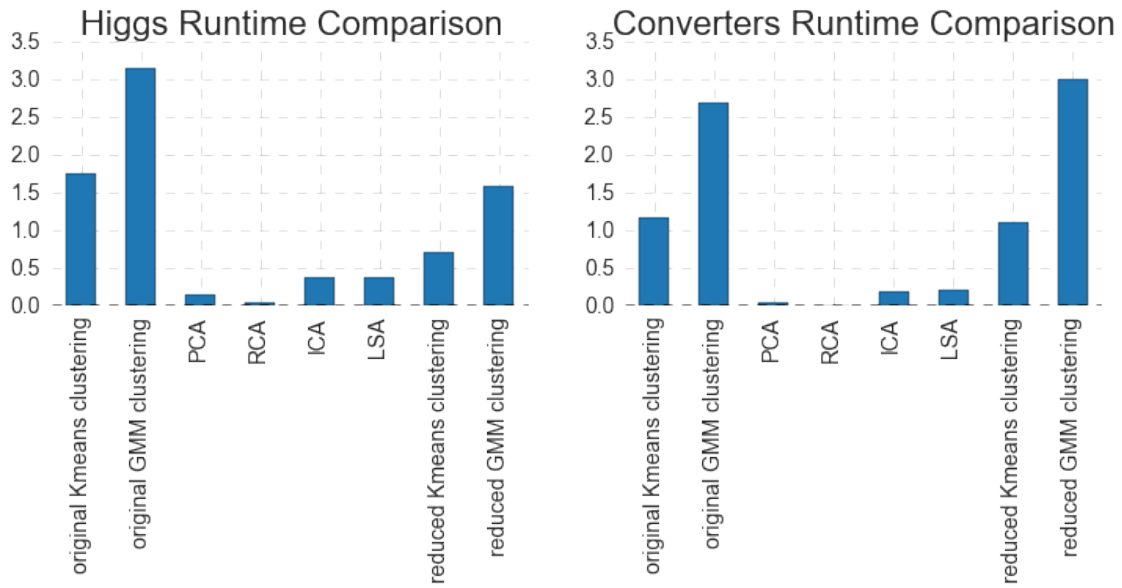
Another benefit of feature transformation algorithms (besides knowledge discovery) is the **speed** gain after projecting the original data to reduced dimensions.

Higgs clustering experiment: Reduce the data dimension from 30 to 7 and compare Kmeans and GMM clustering runtime before and after (2 clusters - signal and background). Both gained in speed improvement without loss of the data structure (even the slowest feature transformation algorithm proved to be beneficial to overal time saving)

Convertes clustering experiment: Reduce the data dimension from 15 to 10 and compare Kmeans and GMM clustering runtime before and after (3 clusters - converters, lead and non-converters). In order to preserve the original data structure (retaining 95% of variance), converters dataset dimensionality was not reduced as much as Higgs dataset. Note that in this case, projecting data to new dimensions and re-estimating the distribution is actually slower and thus there is no real benefit in transforming data other than visualization.

```
In [552]: higgs_time_df = clustering_dim_reduction.compare_cluster_runtime(higgs_data, 2, 7)

In [553]: conv_time_df = clustering_dim_reduction.compare_cluster_runtime(bid_data, 3, 10)
```

In [554]:
```
clustering_dim_reduction.plot_running_time(higgs_time_df, conv_time_df)
```



1.9 Neural Networks on Higgs dataset post Clustering as Dimensionality Reduction

To recapitulate this final experiment, following reductions were done:

- Project the original dataset of 30 features to new dataset of 7 features where 95% of data variance is retained.
- Run Kmeans Clustering with 2 clusters as suggested by model complexity analysis and add cluster-distance spaces as new features.
- Run GMM distribution estimation with 4 components as suggested by model analysis and add distribution estimation as a new feature to PCA projected set
- Rerun neural network classification with 9D (7 features + 2 cluster-distance space features) and 8D (7 features + 1 distribution assighment) data dimension

In [581]:
```
higgs_data_9d, _ = clustering_dim_reduction.kmeans_transform(higgs_data, 2, 7)
```

In [582]:
```
higgs_data_8d, _ = clustering_dim_reduction.gmm_transform(higgs_data, 4, 7)
```

In [583]:
```
_, _, err_9d = clustering_dim_reduction.neural_net_post_clustering(higgs_data_9d)
```

In [584]:
```
_, _, err_8d = clustering_dim_reduction.neural_net_post_clustering(higgs_data_8d)
```

In [592]:
```
err = pd.Series([28.739212, err_9d, err_8d], index=['Error on PCA reduced data',
                                                    'Error with new features added by KNN',
                                                    'Error with new features added by GMM'])
err
```

Out[592]:
```
Error on PCA reduced data                28.739212
Error with new features added by KNN     29.281965
Error with new features added by GMM     28.485630
dtype: float64
```

No significant error improvement is measured during this phase of the experiment, so the advantage here will be speed gain only.

If you used data that already had labels (for example data from a classification problem from assignment #1) did the clusters line up with the labels? Do they otherwise line up naturally? Why or why not? Compare and contrast the different algorithms. What sort of changes might you make to each of those algorithms to improve performance? How much performance was due to the problems you chose? Be creative and think of as many questions you can, and as many answers as you can. Take care to justify your analysis with data explictly. Can you describe how the data look in the new spaces you created with the various aglorithms? For PCA, what is the distribution of eigenvalues? For ICA, how kurtotic are the distributions? Do the projection axes for ICA seem to capture anything "meaningful"? Assuming you only generate k projections (i.e., you do dimensionality reduction), how well is the data reconstructed by the randomized projections? PCA? How much variation did you get when you re-ran your RP several times (I know I don't have to mention that you might want to run RP many times to see what happens, but I hope you forgive me)? When you reproduced your clustering experiments on the datasets projected onto the new spaces created by ICA, PCA and RP, did you get the same clusters as before? Different clusters? Why? Why not? When you re-ran your neural network algorithms were there any differences in performance? Speed? Anything at all? It might be difficult to generate the same kinds of graphs for this part of the assignment as you did before; however, you should come up with some way to describe the kinds of clusters you get. If you can do that visually all the better.