**Eisner Results**

**Non-ensemble Results**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | **Plsda**  | **Gbm**  | **Svm**  | **Rf**  | **Glmnet**  | **pam**  |
| RPT  | .657 | .430 | .457 | .331 | .705 | .711 |
| Accuracy  | .757 | .557 | .871 | .957 | .786 | .771 |
| AUC-ROC | .685 | .773 | .933 | .975 | .958 | .744 |
| Stability  | .58 | .35 | .31 | .20 | .64 | .66 |

Output from feature.table

PAM Feature Table

|  |  |  |
| --- | --- | --- |
| features | consistency | frequency |
| Adipate | 10 | 1 |
| Creatine | 10 | 1 |
| Glucose | 10 | 1 |
| Succinate | 10 | 1 |
| X3.Hydroxyisovalerate | 10 | 1 |
| myo.Inositol | 9 | 0.9 |
| Betaine | 7 | 0.7 |
| Glutamine | 7 | 0.7 |
| Quinolinate | 6 | 0.6 |
| cis.Aconitate | 6 | 0.6 |
| Acetate | 5 | 0.5 |
| N.N.Dimethylglycine | 5 | 0.5 |
| Lysine | 3 | 0.3 |
| Leucine | 2 | 0.2 |

GLMNET Feature Table

|  |  |  |
| --- | --- | --- |
| features | consistency | frequency |
| Adipate | 10 | 1 |
| Glucose | 10 | 1 |
| Leucine | 10 | 1 |
| Quinolinate | 10 | 1 |
| Valine | 10 | 1 |
| X3.Hydroxyisovalerate | 10 | 1 |
| myo.Inositol | 9 | 0.9 |
| Succinate | 6 | 0.6 |
| Betaine | 4 | 0.4 |
| Glutamine | 4 | 0.4 |
| Lysine | 4 | 0.4 |
| Creatine | 3 | 0.3 |
| N.N.Dimethylglycine | 3 | 0.3 |
| Acetate | 3 | 0.3 |
| Alanine | 2 | 0.2 |
| Formate | 1 | 0.1 |
| Xylose | 1 | 0.1 |

**Abbreviated Ensemble Results**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | **Plsda**  | **Gbm**  | **Svm**  | **Rf**  | **Glmnet**  | **pam**  |
| RPT  | .696 | .486 | .612 | .433 | .572 | .721 |
| Accuracy  | .736 | .529 | .743 | .957 | .686 | .743 |
| AUC-ROC | .802 | .717 | .892 | 1.0 | .967 | .790 |
| Stability  | .66 | .45 | .52 | .28 | .49 | .70 |

Output from feature.table

PAM Feature Table

|  |  |  |
| --- | --- | --- |
| features | consistency | frequency |
| Adipate | 10 | 1 |
| Creatine | 10 | 1 |
| Glucose | 10 | 1 |
| Succinate | 10 | 1 |
| X3.Hydroxyisovalerate | 10 | 1 |
| myo.Inositol | 9 | 0.9 |
| N.N.Dimethylglycine | 9 | 0.9 |
| Quinolinate | 9 | 0.9 |
| Acetate | 7 | 0.7 |
| Glutamine | 5 | 0.5 |
| Betaine | 3 | 0.3 |
| Leucine | 2 | 0.2 |
| Sucrose | 2 | 0.2 |
| cis.Aconitate | 2 | 0.2 |
| X3.Hydroxybutyrate | 1 | 0.1 |
| Alanine | 1 | 0.1 |

PLSDA Feature Table

|  |  |  |
| --- | --- | --- |
| features | consistency | frequency |
| Glucose | 10 | 1 |
| Leucine | 10 | 1 |
| Quinolinate | 10 | 1 |
| Valine | 10 | 1 |
| X3.Hydroxyisovalerate | 10 | 1 |
| Adipate | 9 | 0.9 |
| Succinate | 9 | 0.9 |
| myo.Inositol | 7 | 0.7 |
| N.N.Dimethylglycine | 7 | 0.7 |
| Creatine | 5 | 0.5 |
| Glutamine | 4 | 0.4 |
| X3.Hydroxybutyrate | 2 | 0.2 |
| Betaine | 2 | 0.2 |
| Methylamine | 1 | 0.1 |
| Alanine | 1 | 0.1 |
| Pyroglutamate | 1 | 0.1 |
| Acetate | 1 | 0.1 |
| Formate | 1 | 0.1 |