## MACHINE LEARNING QUICK REFERENCE: ALGORITHMS - 1

| Algorithm Type                      | Common Usage   | Suggested Usage   | Suggested Scale  | Interpretability | Common Concerns  |
|-------------------------------------|--|---|--|------------------|--|
| Penalized Regression                | Supervised regression     Supervised classification  | <ul> <li>Modeling linear or linearly separable phenomena</li> <li>Manually specifying nonlinear and explicit interaction terms</li> <li>Well suited for N &lt;&lt; p</li> </ul>   | Small to large data sets   | High             | <ul><li>Missing values</li><li>Outliers</li><li>Standardization</li><li>Parameter tuning</li></ul>   |
| Naïve Bayes                         | Supervised classification  | Modeling linearly separable phenomena in large data sets     Well-suited for extremely large data sets where complex methods are intractable  | Small to extremely large data sets   | Moderate         | Strong linear independence     assumption     Infrequent categorical levels  |
| Decision Trees                      | <ul> <li>Supervised regression</li> <li>Supervised classification</li> </ul>   | <ul> <li>Modeling nonlinear and nonlinearly separable phenomena in large, dirty data</li> <li>Interactions considered automatically, but implicitly</li> <li>Missing values and outliers in input variables handled automatically in many implementations</li> <li>Decision tree ensembles, e.g. random forests and gradient boosting, can increase prediction accuracy and decrease overfitting, but also decrease scalability and interpretability</li> </ul>   | Medium to large data sets  | Moderate         | <ul> <li>Instability with small training data sets</li> <li>Gradient boosting can be unstable with noise or outliers</li> <li>Overfitting</li> <li>Parameter tuning</li> </ul>                                   |
| k-Nearest Neighbors (kNN)           | <ul><li>Supervised regression</li><li>Supervised classification</li></ul>  | Modeling nonlinearly separable phenomena     Can be used to match the accuracy of more sophisticated techniques, but with fewer tuning parameters   | Small to medium data sets  | Low              | <ul> <li>Missing values</li> <li>Overfitting</li> <li>Outliers</li> <li>Standardization</li> <li>Curse of dimensionality</li> </ul>  |
| Support Vector<br>Machines (SVM)    | <ul> <li>Supervised regression</li> <li>Supervised classification</li> <li>Anomaly detection</li> </ul>  | <ul> <li>Modeling linear or linearly separable phenomena by using linear kernels</li> <li>Modeling nonlinear or nonlinearly separable phenomena by using nonlinear kernels</li> <li>Anomaly detection with one-class SVM (OSVM)</li> </ul>  | <ul> <li>Small to large data sets<br/>for linear kernels</li> <li>Small to medium data<br/>sets for nonlinear kernels</li> </ul> | Low              | Missing values     Overfitting     Outliers     Standardization     Parameter tuning     Accuracy versus deep neural networks depends on choice of nonlinear kernel; Gaussian and polynomial often less accurate |
| Artificial Neural<br>Networks (ANN) | <ul> <li>Supervised regression</li> <li>Supervised classification</li> <li>Unsupervised clustering</li> <li>Unsupervised feature extraction</li> <li>Anomalydetection</li> </ul> | <ul> <li>Modeling nonlinear and nonlinearly separable phenomena</li> <li>Deep neural networks (e.g. deep learning) are well suited for state-of-the-art pattern recognition in images, videos, and sound</li> <li>All interactions considered in fully connected, multilayer topologies</li> <li>Nonlinear feature extraction with autoencoder and restricted Boltzmann machine (RBM) networks</li> <li>Anomaly detection with autoencoder networks</li> <li>Clustering and visualization with self-organizing maps (SOMs)</li> </ul> | ,  | Low              | <ul> <li>Missing values</li> <li>Overfitting</li> <li>Outliers</li> <li>Standardization</li> <li>Parameter tuning</li> </ul>   |



## MACHINE LEARNING QUICK REFERENCE: ALGORITHMS - 2

| Algorithm Type                            | Common Usage   | Suggested Usage  | Suggested Scale  | Interpretability   | Common Concerns   |
|---|--|--|--|--|---|
| Association Rules                         | Supervised rule building     Unsupervised rule     building                  | Building sets of complex rules by using the co-occurrence of items or events in transactional data sets  | Medium to large transactional data sets  | Moderate   | <ul><li>Instability with small training data</li><li>Overfitting</li><li>Parameter tuning</li></ul>   |
| k-Means                                   | Unsupervised clustering  | <ul> <li>Creating a known a priori number of spherical, disjoint, equally sized clusters</li> <li>k-modes method can be used for categorical data</li> <li>k-prototypes method can be used for mixed data</li> </ul>   | Small to large data sets   | Moderate   | <ul> <li>Missing values</li> <li>Outliers</li> <li>Standardization</li> <li>Correct number of clusters is often unknown</li> <li>Highly sensitive to initialization</li> <li>Curse of dimensionality</li> </ul> |
| Hierarchical<br>Clustering                | Unsupervised clustering  | Creating a known a priori number of nonspherical, disjoint, or overlapping clusters of different sizes   | Small data sets  | Moderate   | Missing values     Standardization     Correct number of clusters is often unknown     Curse of dimensionality  |
| Spectral Clustering                       | Unsupervised clustering  | Creating a data-dependent number of arbitrarily-shaped, disjoint, or overlapping clusters of different sizes   | Small data sets  | Moderate   | <ul><li>Missing values</li><li>Standardization</li><li>Parameter tuning</li><li>Curse of dimensionality</li></ul>   |
| Principal<br>Components<br>Analysis (PCA) | Unsupervised feature extraction  | <ul> <li>Extracting a data-dependent number of linear, orthogonal features, where N &gt;&gt; p</li> <li>Extracted features can be rotated to increase interpretability, but orthogonality is usuallylost</li> <li>Singular value decomposition (SVD) is often used instead of PCA on wide or sparse data</li> <li>Sparse PCA can be used to create more interpretable features, but orthogonality is lost</li> <li>Kernel PCA can be used to extract nonlinear features</li> </ul> | Small to large data sets for traditional PCA and SVD Small to medium data sets for sparse PCA and kernel PCA | Generally low, but<br>higher for sparse<br>PCA or rotated<br>solutions | Missing values     Outliers   |
| Nonnegative Matrix<br>Factorization (NMF) | Unsupervised feature extraction  | Extracting a known a priori number of interpretable, linear, oblique, nonnegative features   | Small to large data sets   | High   | <ul> <li>Missing values</li> <li>Outliers</li> <li>Standardization</li> <li>Correct number of features is often unknown</li> <li>Presence of negative values</li> </ul>   |
| Random<br>Projections                     | Unsupervised feature extraction  | Extracting a data-dependent number of linear, uninterpretable, randomly-oriented features of equal importance  | Medium to extremely large data sets  | Low  | Missing values  |
| Factorization<br>Machines                 | Supervised regression and classification     Unsupervised feature extraction | Extracting a known a priori number of uninterpretable, oblique features from sparse or transactional data sets     Can automatically account for variable interactions     Creating models from a large number of sparse features; can outperform SVM for sparse data  | Medium to extremely large sparse or transactional data sets  | Moderate   | <ul> <li>Missing values</li> <li>Outliers</li> <li>Standardization</li> <li>Correct number of features is often unknown</li> <li>Less well suited for dense data</li> </ul>                                     |

