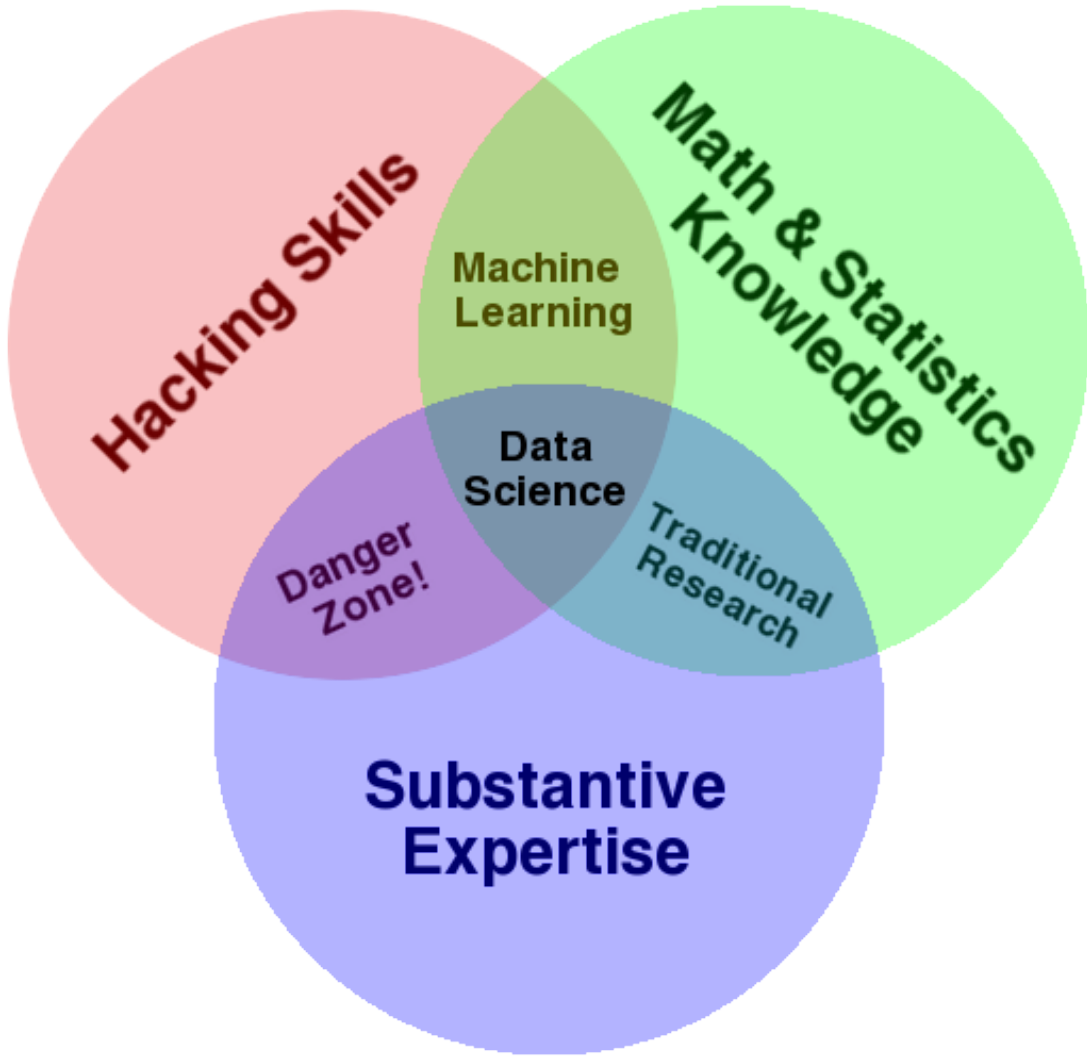
Machine Learning



http://drewconway.com/zia/2013/3/26/the-data-science-venn-diagram

- What is ML?
- Supervised Learning:
  - Regression
  - Classification
- Unsupervised Learning:
  - Clustering
  - Anomaly Detection
- Data Science Pipelines

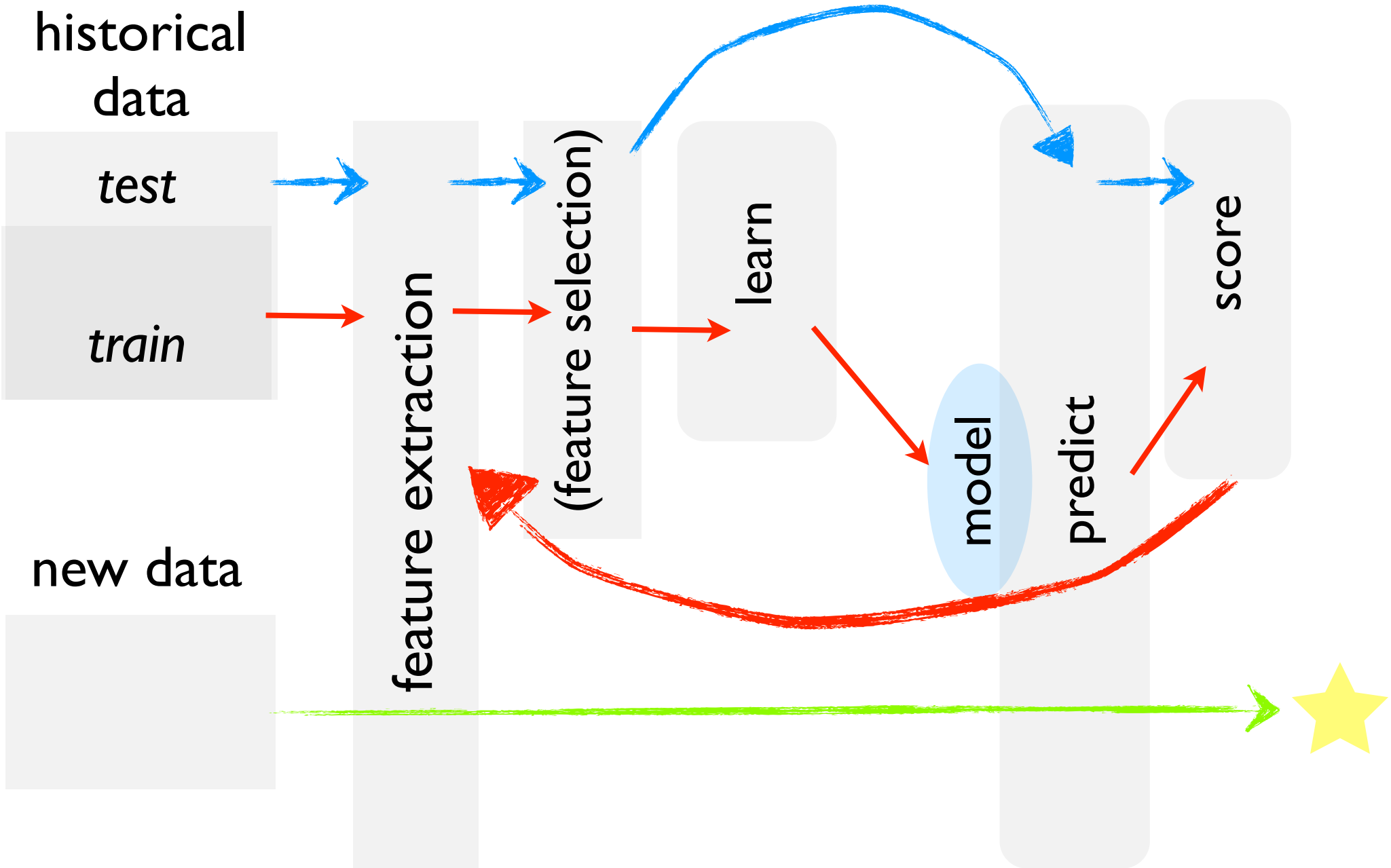
What is Machine Learning?

Short Answer: The offspring of Statistics and Computer Science

Better Answer: A set of models which aim to learn something about a data set to apply that knowledge to new data

- Using labels from *training* data to classify new objects (e.g. images, digits, webpages)
- Learning the relationship between explanatory *features* and response variable to predict for new data (e.g., stock market)
- Discovering natural clustering structure in data
- Detecting low-dimensional structure in high-dimensional data
- Finding outliers in large data sets

A Typical Machine Learning Workflow



Machine Learning with scikit-learn

Make sure you have version >= 0.13 installed

```
conda update scikit-learn
pip install scikit-learn
```

http://scikit-learn.org/stable/

also: http://mlpy.sourceforge.net/, http://orange.biolab.si/

Supervised Learning

Use *training* set of (***x***,y) pairs to learn to predict y for new ***x***

Regression - predicting continuous *outcome* (y) variable from a vector of input *features* (***x***)

- Linear Regression: `linear_model.LinearRegression`
- Lasso & Ridge Reg.: `linear_model.Lasso / linear_model.Ridge`
- Gaussian Process Regression: `gaussian_process.GaussianProcess`
- Nearest Neighbor Regression: `neighbors.KNeighborsRegressor`
- Support Vector Regression: `svm.SVR`
- Regression Trees: `tree.DecisionTreeRegressor`

... and more!

Notebook

archive.ics.uci.edu/ml/index.html

UCI

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Machine Learning Repository

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Center for Machine Learning and Intelligent Systems

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We currently maintain 253 data sets as a service to the machine learning community. You may **view all data sets** through our searchable interface. Our old web site is still available, for those who prefer the old format. For a general overview of the Repository, please visit our About page. For information about citing data sets in publications, please read our citation policy. If you wish to donate a data set, please consult our donation policy. For any other questions, feel free to contact the Repository librarians. We have also set up a mirror site for the Repository.

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Latest News:

2013-04-04: Welcome to the new Repository admins Kevin Bache and Moshe Lichman!

2010-03-01: Note from donor regarding Netflix data

2009-10-16: Two new data sets have been added.

2009-09-14: Several data sets have been added.

Newest Data Sets:

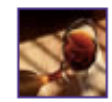
2013-09-06: Reuters RCV1 RCV2 Multilingual, Multiview Text Categorization Test collection

2013-09-04: Reuters RCV1/RCV2 Multilingual, Multiview Text

Most Popular Data Sets (hits since 2007):

473145:  Iris

329520:  Adult

285868:  Wine

Error Estimation & Model Selection

Q: How will our model perform on future data?

So far, we've split the data, using one set to ***train*** the model and the other to ***test*** its performance

scikit-learn can do cross-validation for us!

```
from sklearn import cross_validation
```

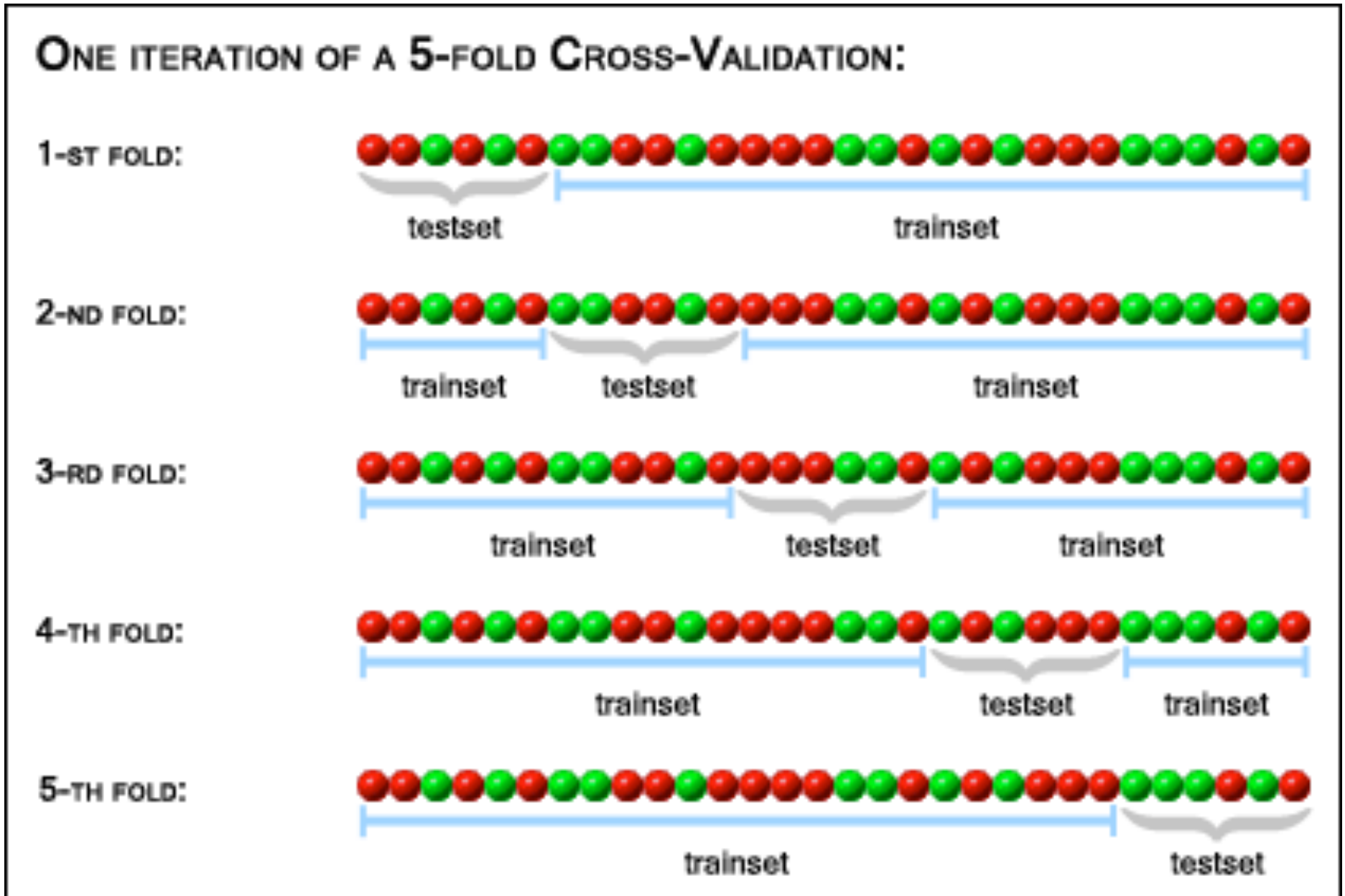
Better procedure:
Cross-Validation

K-fold CV - Randomly split the training data into K folds. For each k=1,...,K, train model only on the data not in fold k & predict for data in fold k. Compute performance metric over CV predictions.

Leave-one-out (LOO) CV - K-fold CV with K = number of training points.

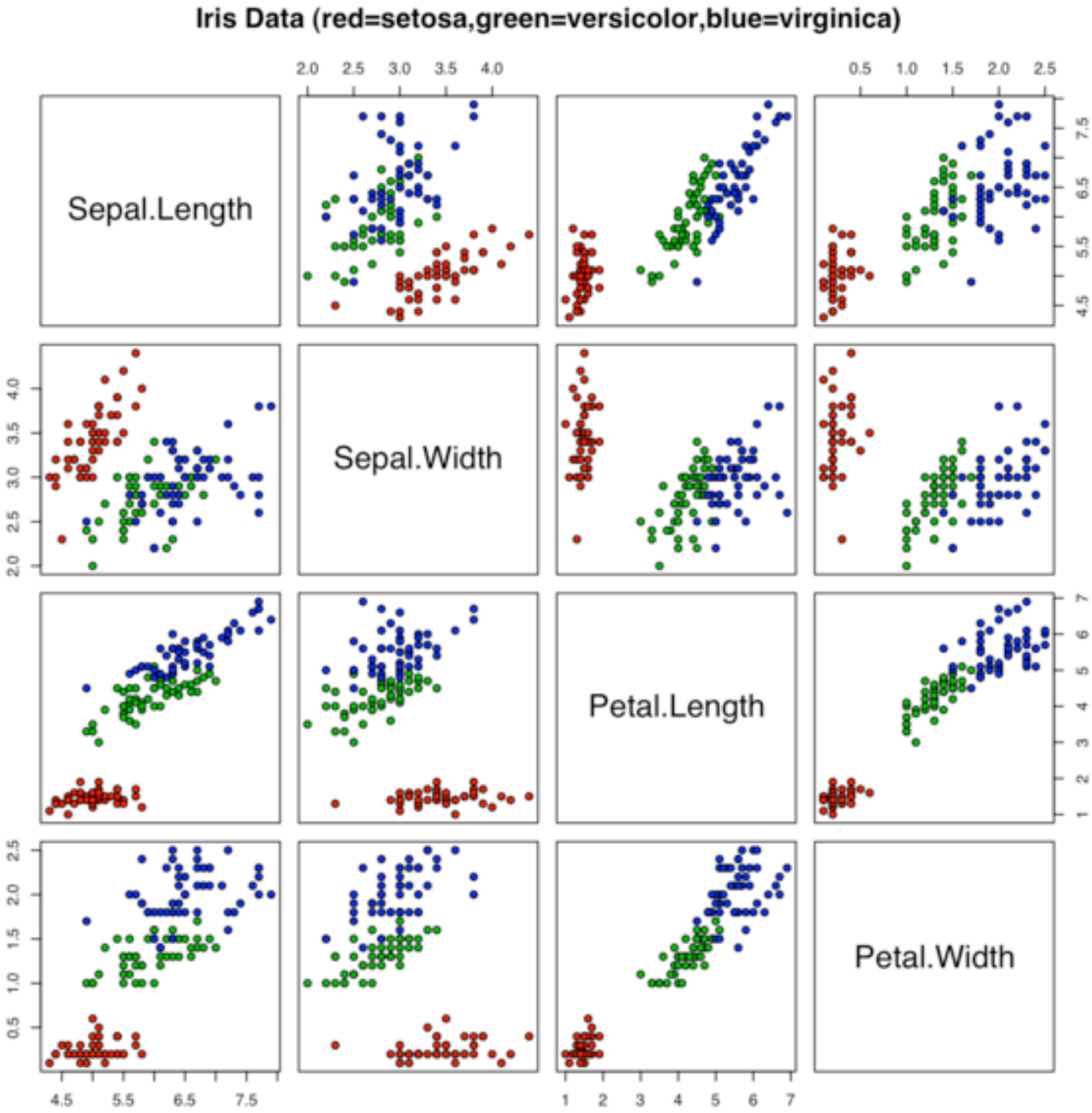
Cross-validation generators

`KFold` (n, k)	`StratifiedKFold` (y, k)	`LeaveOneOut` (n)	`LeaveOneLabelOut` (labels)
Split it K folds, train on K-1 and then test on left-out	It preserves the class ratios / label distribution within each fold.	Leave one observation out	Takes a label array to group observations



Supervised Learning

Classification - predicting the discrete class (y) of an object from a vector of input *features* (***x***)



setosa

veriscolor

virginica

Supervised Learning

Classification - predicting the discrete class (y) of an object from a vector of input *features* (**x**)

e.g. $\mathbf{x_i}$ = [5.1, 3.5, 1.4, 0.2]

[sepal length (cm), sepal width (cm), petal length (cm), petal width (cm)]

e.g. y_1 = "Iris-Setosa"

For Iris: Number of (**x,** y) "instances" = 150
Number of classes = 3

Notebook...

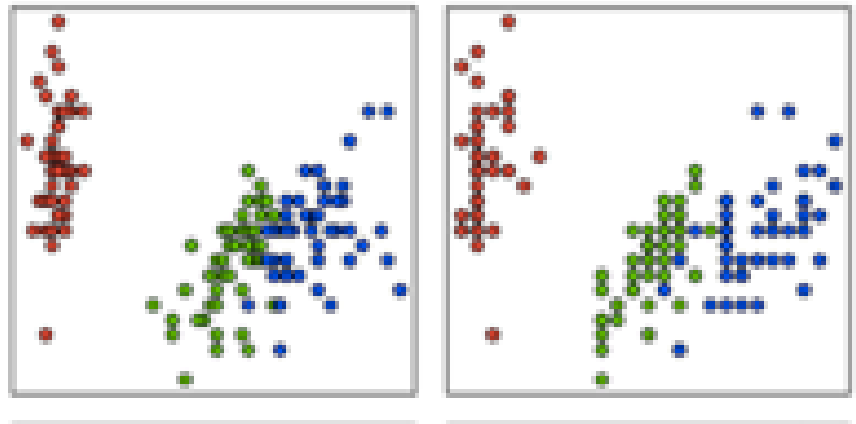
Supervised Learning, cont.

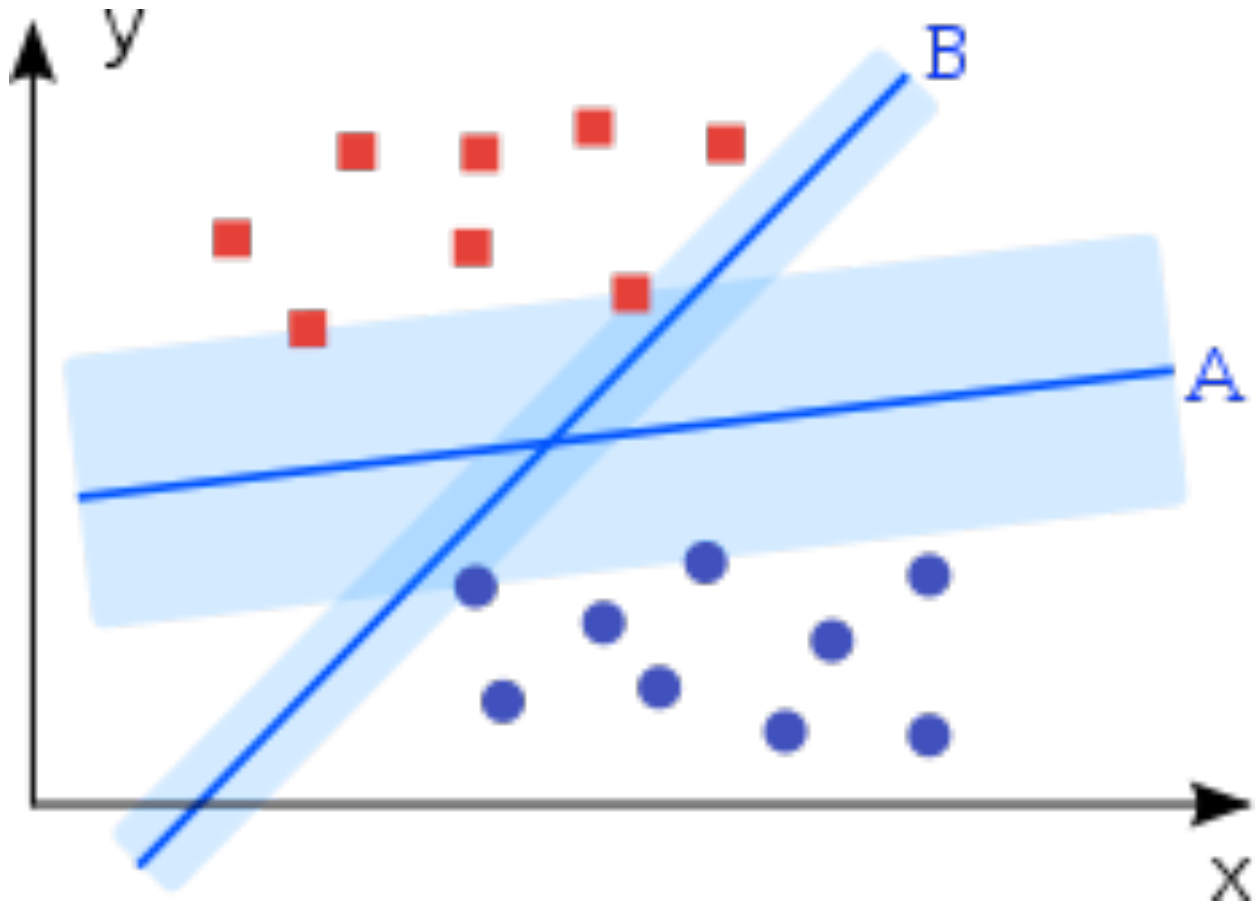
Classification - predicting the discrete class (y) of an object from a vector of input *features* (***x***)

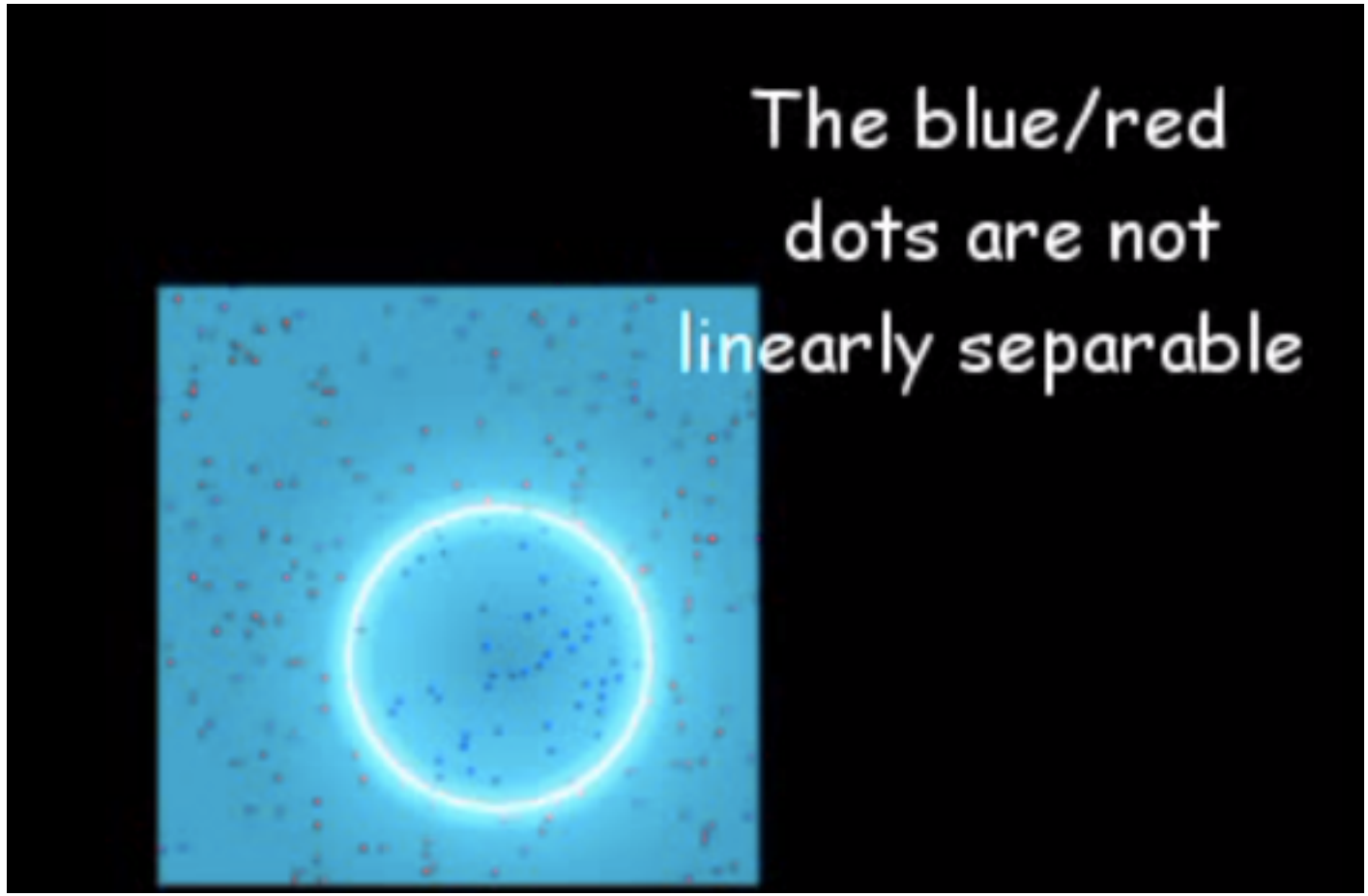
- Logistic Regression: `linear_model.LogisticRegression`
- KNN Classification: `neighbors.KNeighborsClassifier`
- LDA / QDA: `lda.LDA / lda.QDA`
- Naive Bayes: `naive_bayes.GaussianNB`
- Support Vector Machines: `svm.SVC`
- Classification Trees: `tree.DecisionTreeClassifier`
- Random Forest: `ensemble.RandomForestClassifier`
- Multi-class & multi-label Classification is supported: `multiclass.OneVsRest` `multiclass.OneVsOne`

- **`feature_selection:`** recursive, L1, and tree-based

Support Vector Machines
(1992)





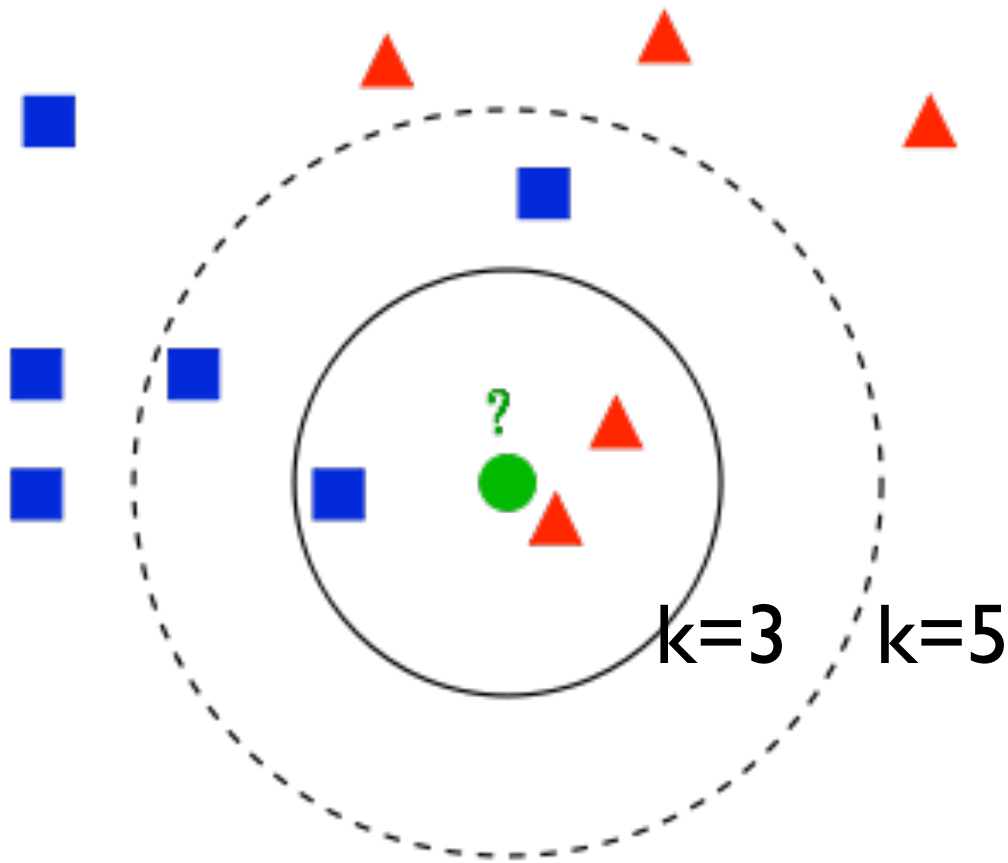


SVM with polynomial kernel visualization

http://www.youtube.com/watch?v=3liCbRZPrZA

Supervised Learning

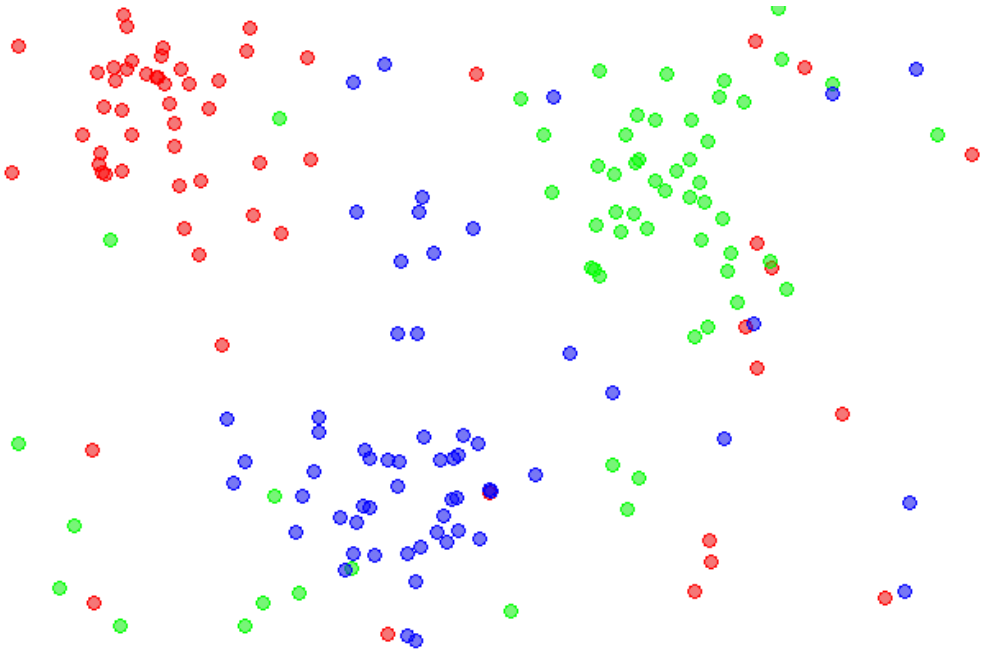
kNearestNeighbors (kNN)



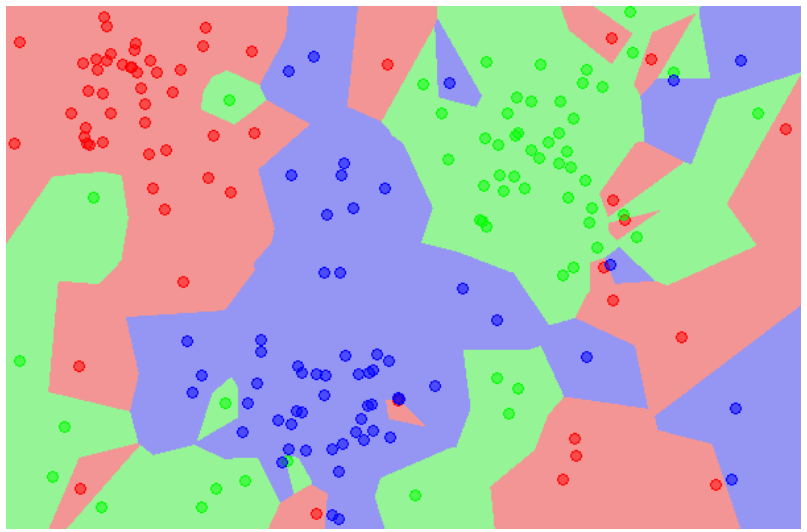
For each test point, **x** find the k-nearest instances in the training data

Classify the point according to the majority vote of their class labels

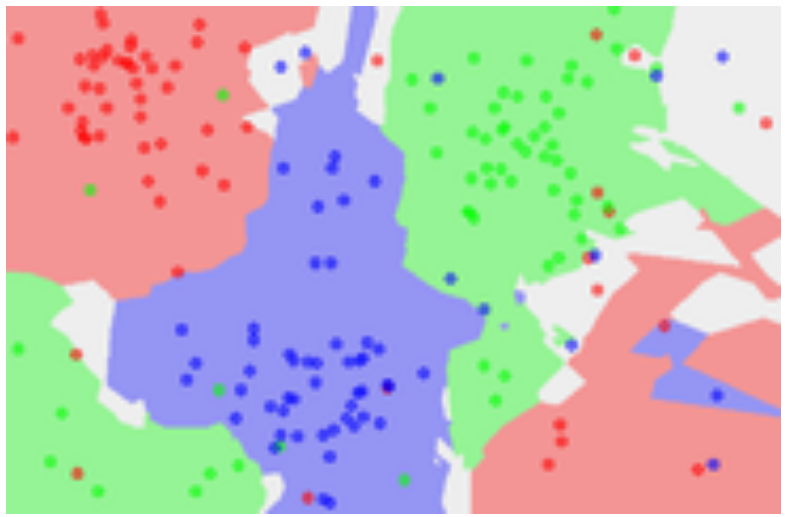
kNearestNeighbors (kNN)



Dataset



k=1

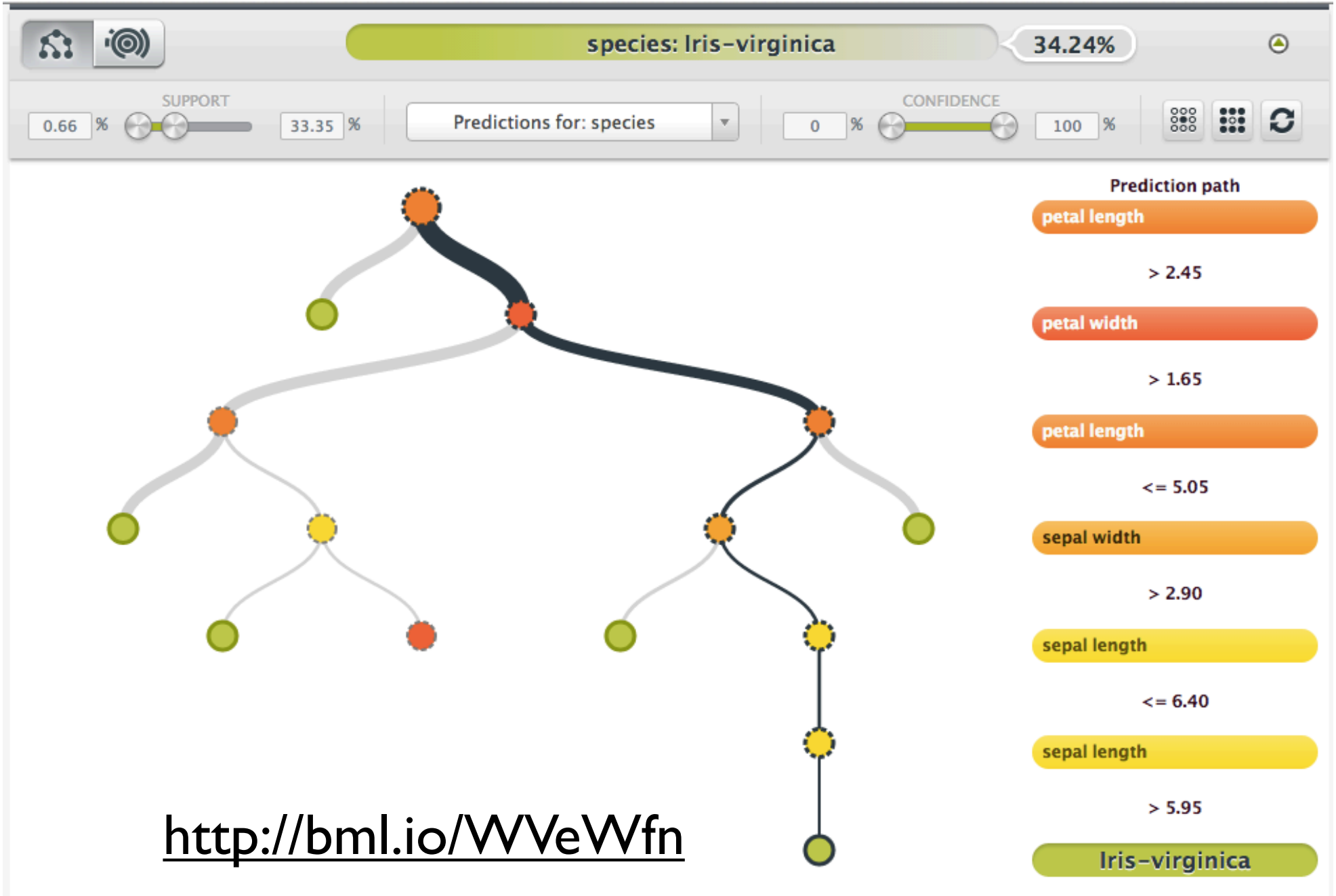


k=5

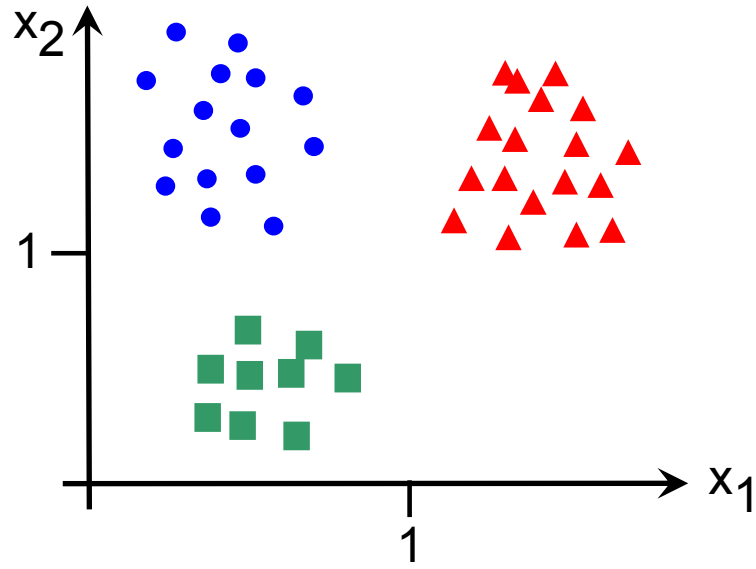
`neighbors.KNeighborsClassifier`

Decision Trees

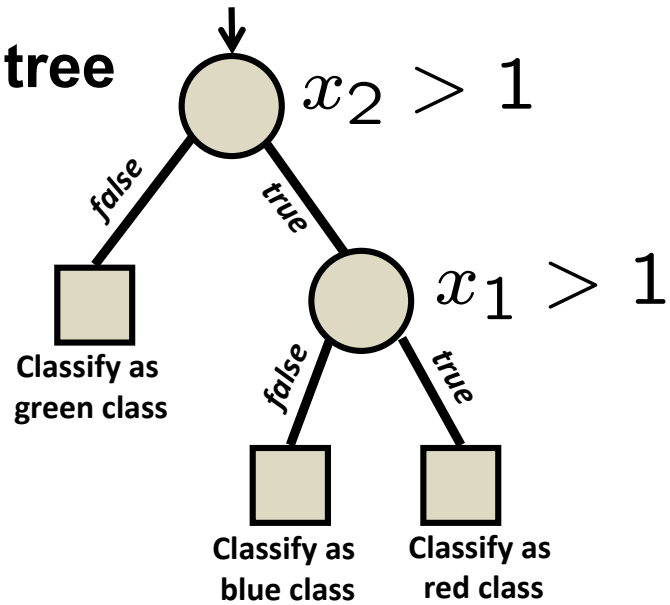
Classification and regression trees (CART)



http://bml.io/WVeWfn

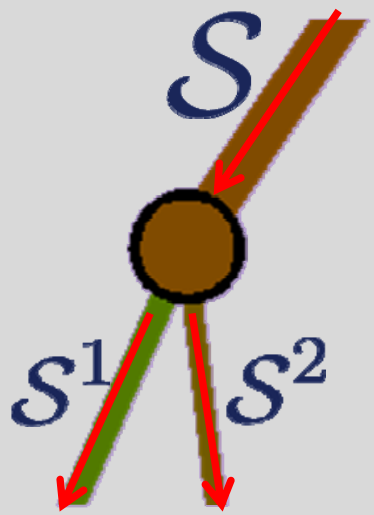


A decision tree



http://www.robots.ox.ac.uk/~az/lectures/ml/lect5.pdf

Building Trees Rigorously (Node Splitting Criteria)



Information gain

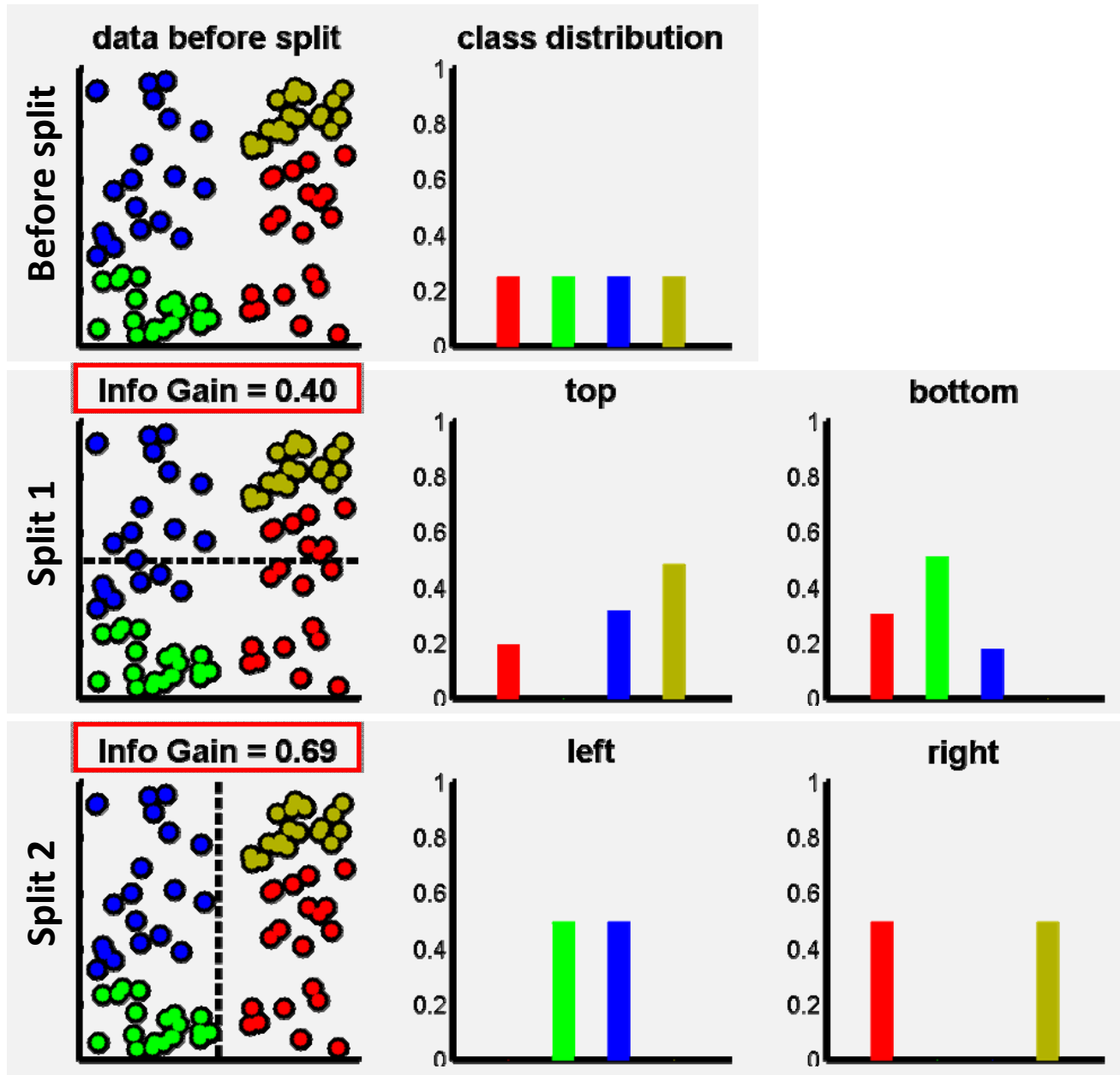
$$I = H(S) - \sum_{i \in \{1,2\}} \frac{|S^i|}{|S|} H(S^i)$$

Shannon's entropy

$$H(S) = -\sum_{c \in C} p(c) \log(p(c))$$

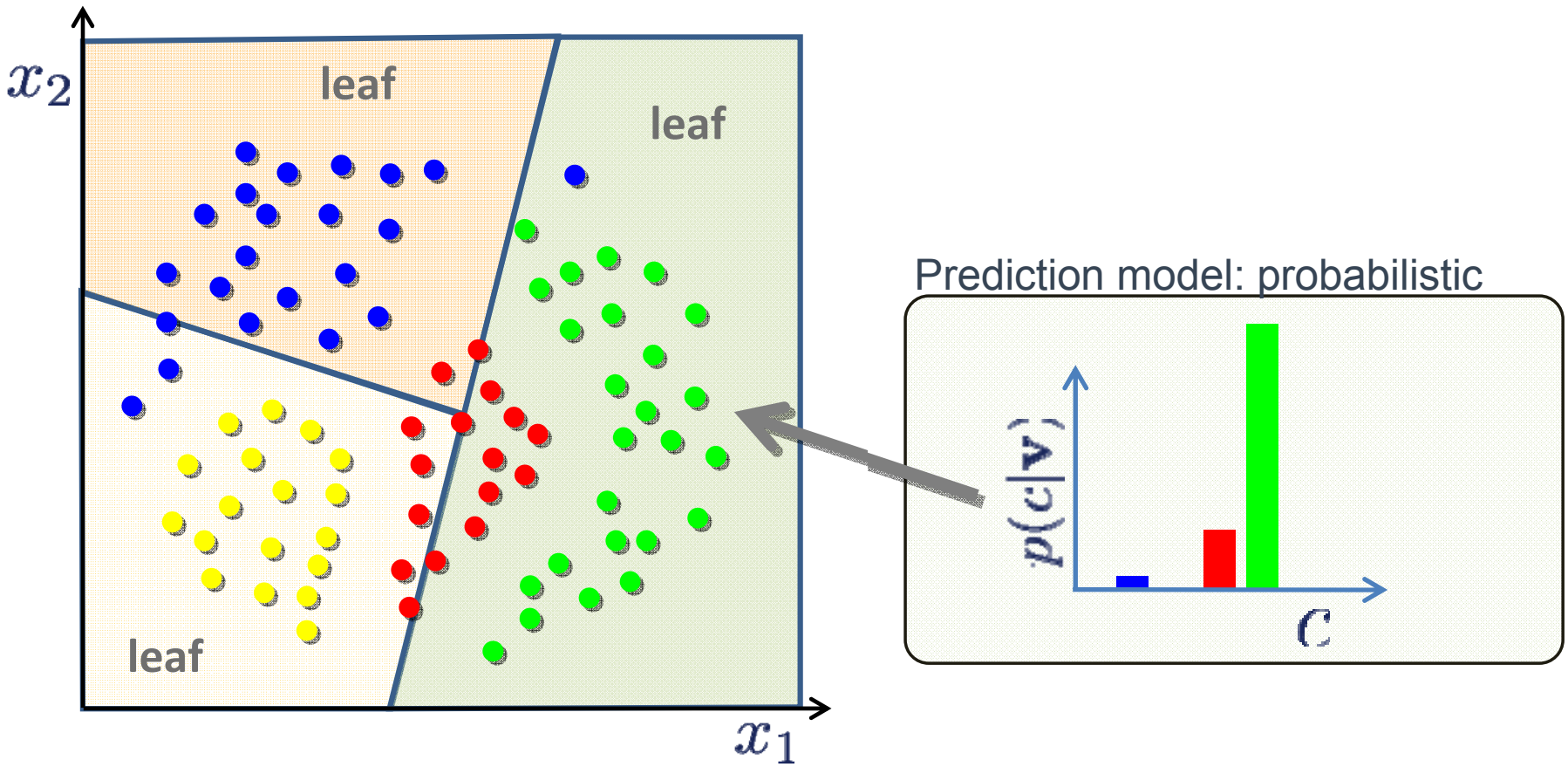
Node training

$$\theta^* = \arg\max_{\theta \in T} I$$



http://www.robots.ox.ac.uk/~az/lectures/ml/lect5.pdf

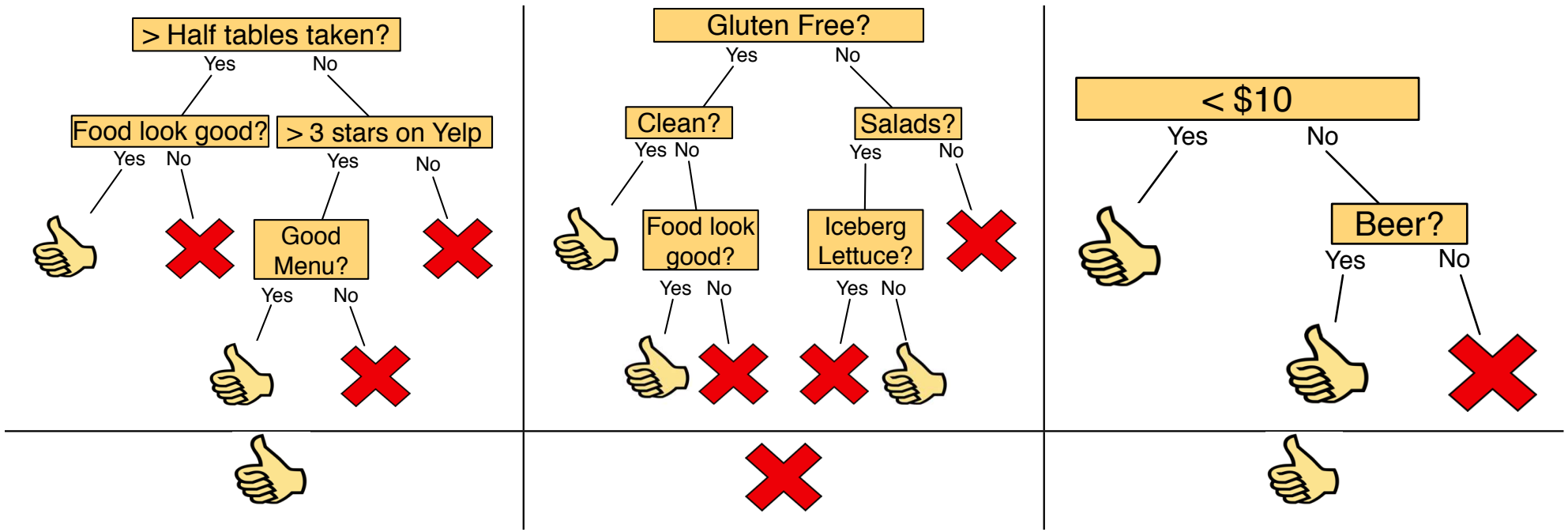
Making predictions from the Learned Tree



http://cs.stanford.edu/people/karpathy/svmjs/demo/

Collections of Trees ("Random Forests")

ensembles generally increase robustness



D. Eads

Error Estimation & Model Selection

Q: How do I choose which model and parameters to use?

KNN with what # of neighbors?
SVM which what kernel & bandwidth?
RF with how many trees and which mtry?
GP with what kernel & bandwidth?

Solution: use grid_search.GridSearchCV

`grid_search.`**`GridSearchCV`**(*estimator*, *param_grid*, *loss_func*, *n_jobs*, *cv=None*)

Computes *cv*-fold cross-validated *loss_func* (or *score_func*) of estimator over a *param_grid* on *n_jobs* cores, and returns the best model!

Error Estimation & Model Selection

Q: What evaluation metrics are available?

Loss Functions

metrics.zero_one(y_true, y_pred)
Zero-One classification loss
metrics.hinge_loss(y_true, pred_decision[, ...])
Cumulated hinge loss (non-regularized).
metrics.mean_square_error(y_true, y_pred)
Mean square error regression loss

Or write your own!!

Score Functions

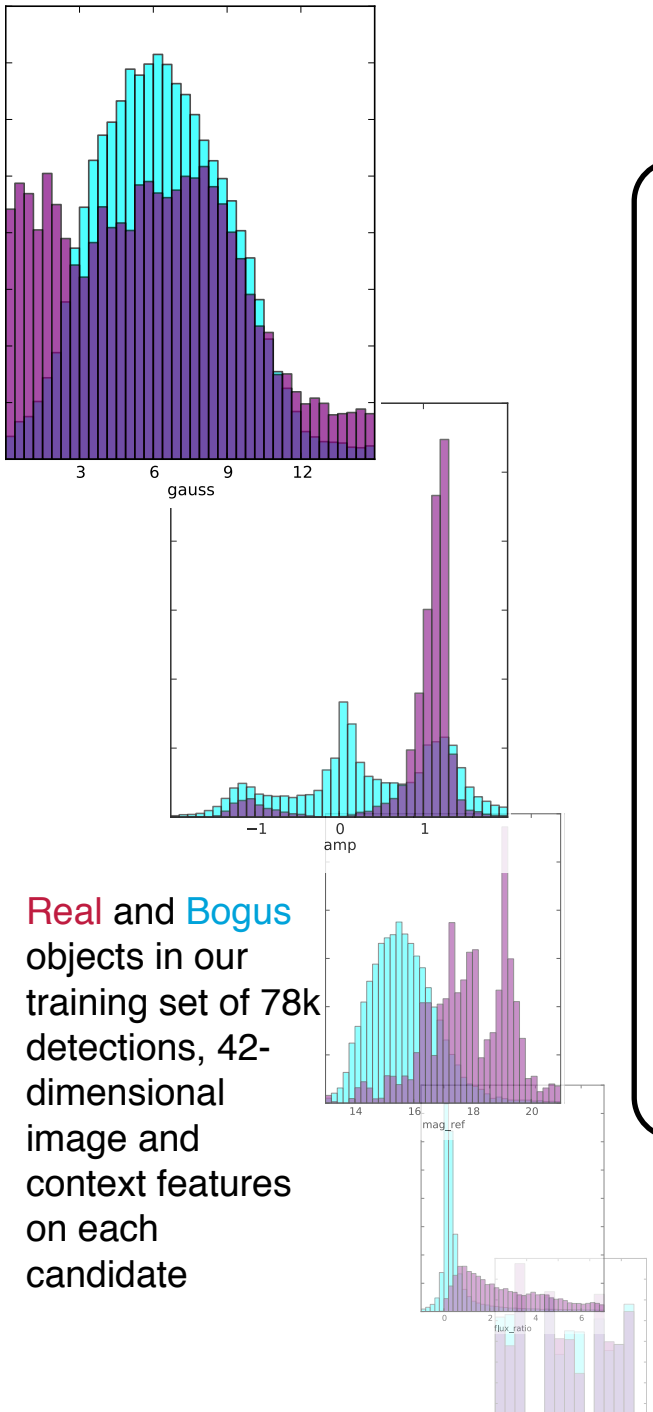
metrics.zero_one_score(y_true, y_pred)
Zero-One classification score
metrics.auc(x, y)
Compute Area Under the Curve (AUC)
metrics.precision_score(y_true, y_pred[, ...])
Compute the precision
metrics.recall_score(y_true, y_pred[, pos_label])
Compute the recall
metrics.fbeta_score(y_true, y_pred, beta[, ...])
Compute fbeta score
metrics.f1_score(y_true, y_pred[, pos_label])
Compute f1 score

Evaluation Plots

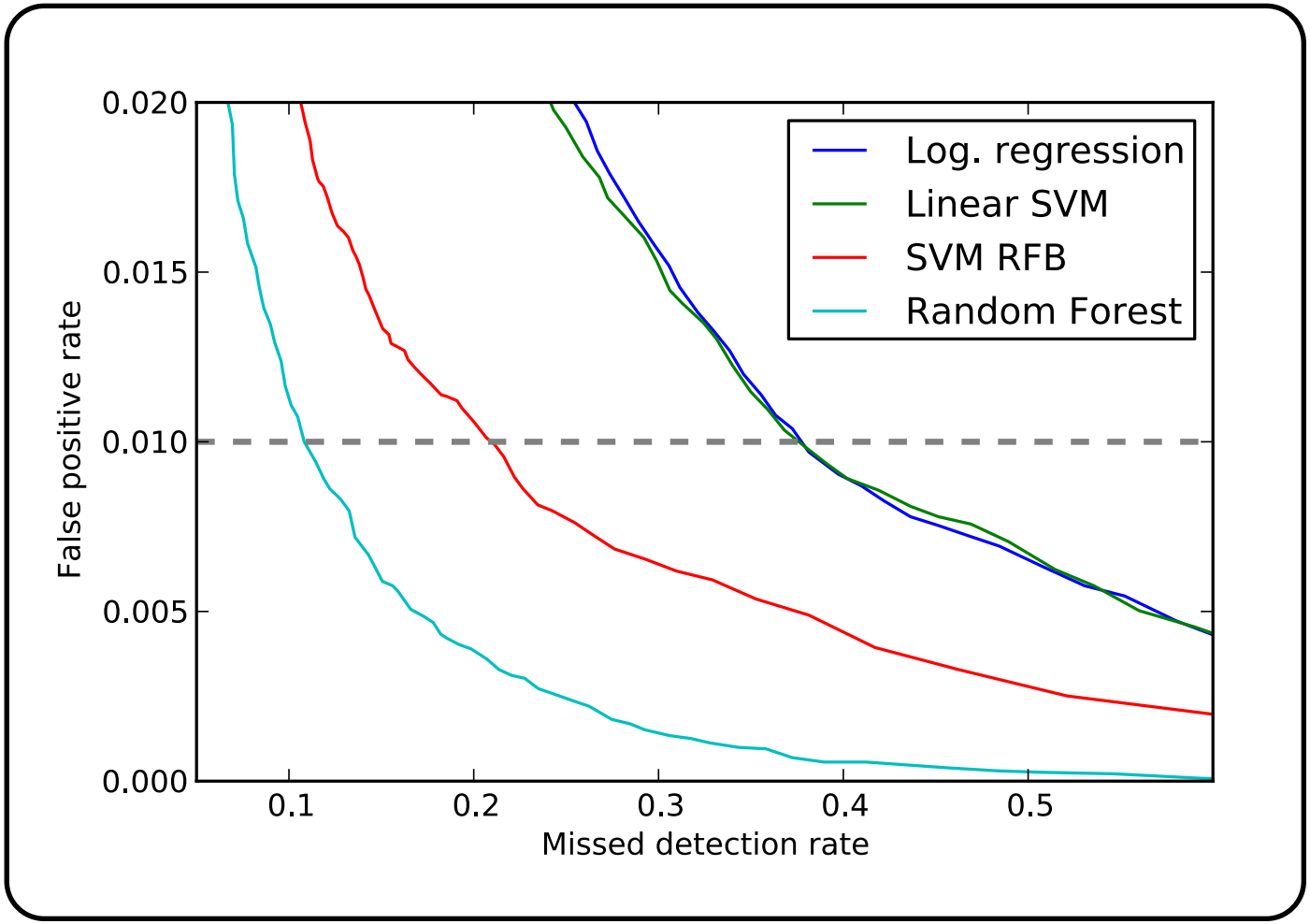
metrics.confusion_matrix(y_true, y_pred[, ...]) Compute confusion matrix to evaluate the accuracy of a classification
metrics.roc_curve(y_true, y_score) Compute Receiver operating characteristic (ROC)
metrics.precision_recall_curve(y_true, ...) Compute precision-recall pairs for different probability thresholds

Some classifiers work better than others

"ROC Curve"



Real and Bogus objects in our training set of 78k detections, 42-dimensional image and context features on each candidate



Brink+2012

arXiv.org > astro-ph > arXiv:1209.3775

To the Notebook!

Breakout #2

Classify the famous **Iris** data, first used by R.A Fisher.

To load in the data and split into training / testing sets:

```
iris = datasets.load_iris()
Xtr = iris.data[::2,:]
Xte = iris.data[1::2,:]
Ytr = iris.target[::2]
Yte = iris.target[1::2]
```

1. Choose your favorite classification model.
2. Find the parameters that minimize the 3-fold cross-validation misclassification rate over the training set.
3. Apply this optimized model to predict the class of each object in the held-out set.

a) What is your best 3-fold CV 0-1 score?

b) What is your 0-1 score when applying it to testing set?

Unsupervised Learning

Clustering: K-means, Hierarchical Clustering, Mixture Models, Affinity Propagation, Spectral Clustering and lots of evaluation metrics!

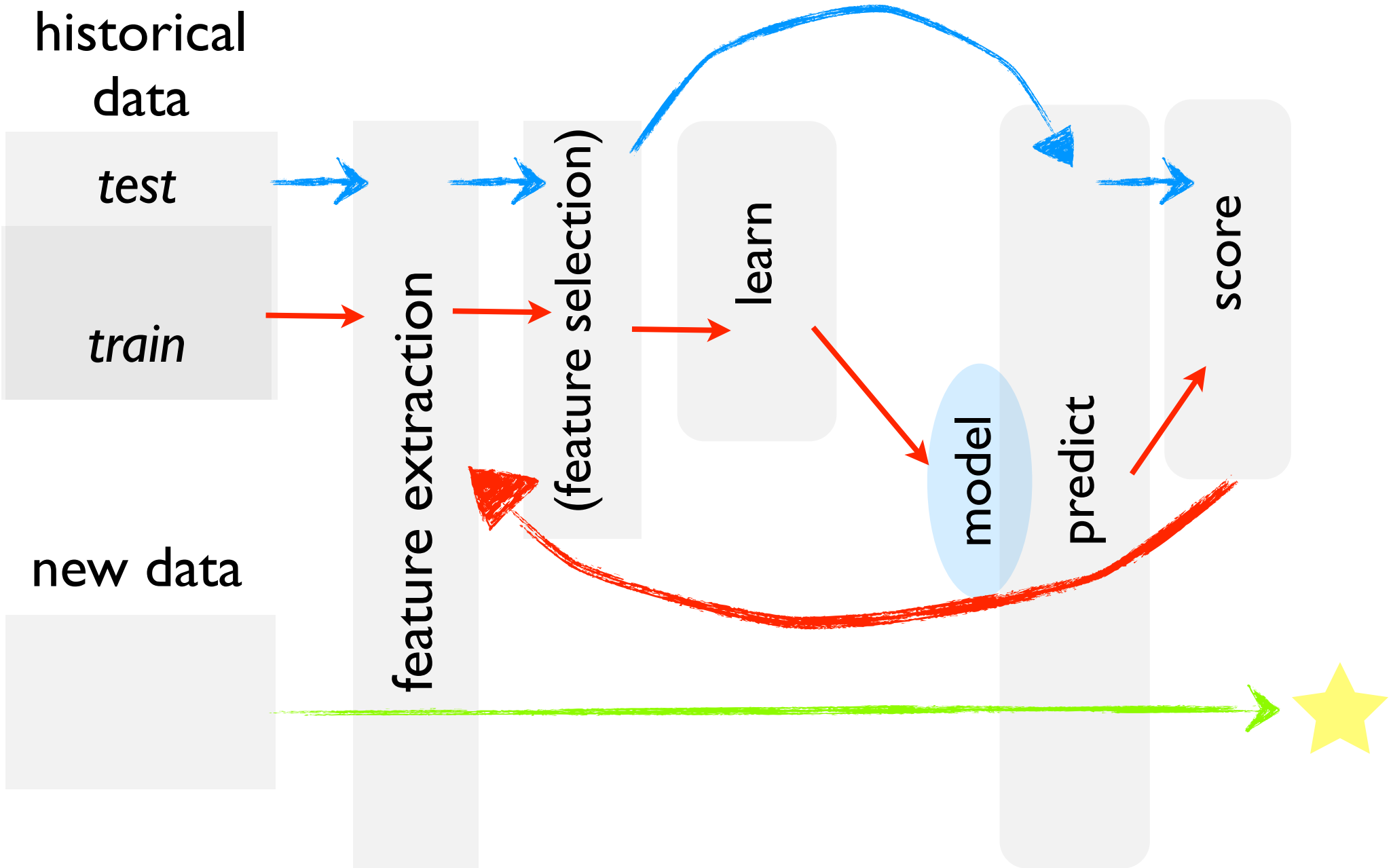
Manifold Learning: Isomap, Local Linear Embedding, Hessian Eigenmap, Local Tangent Space Alignment

Matrix Factorization: PCA, Kernel PCA, Sparse PCA, ICA, NMF, Dictionary Learning

Outlier Detection: Elliptic envelope, One-class SVM

Covariance Estimation: Sparse, Shrunk, and Robust estimators

A Typical Machine Learning Workflow



Kinect – random forest classifier

Input data for each frame

Output

RGB image

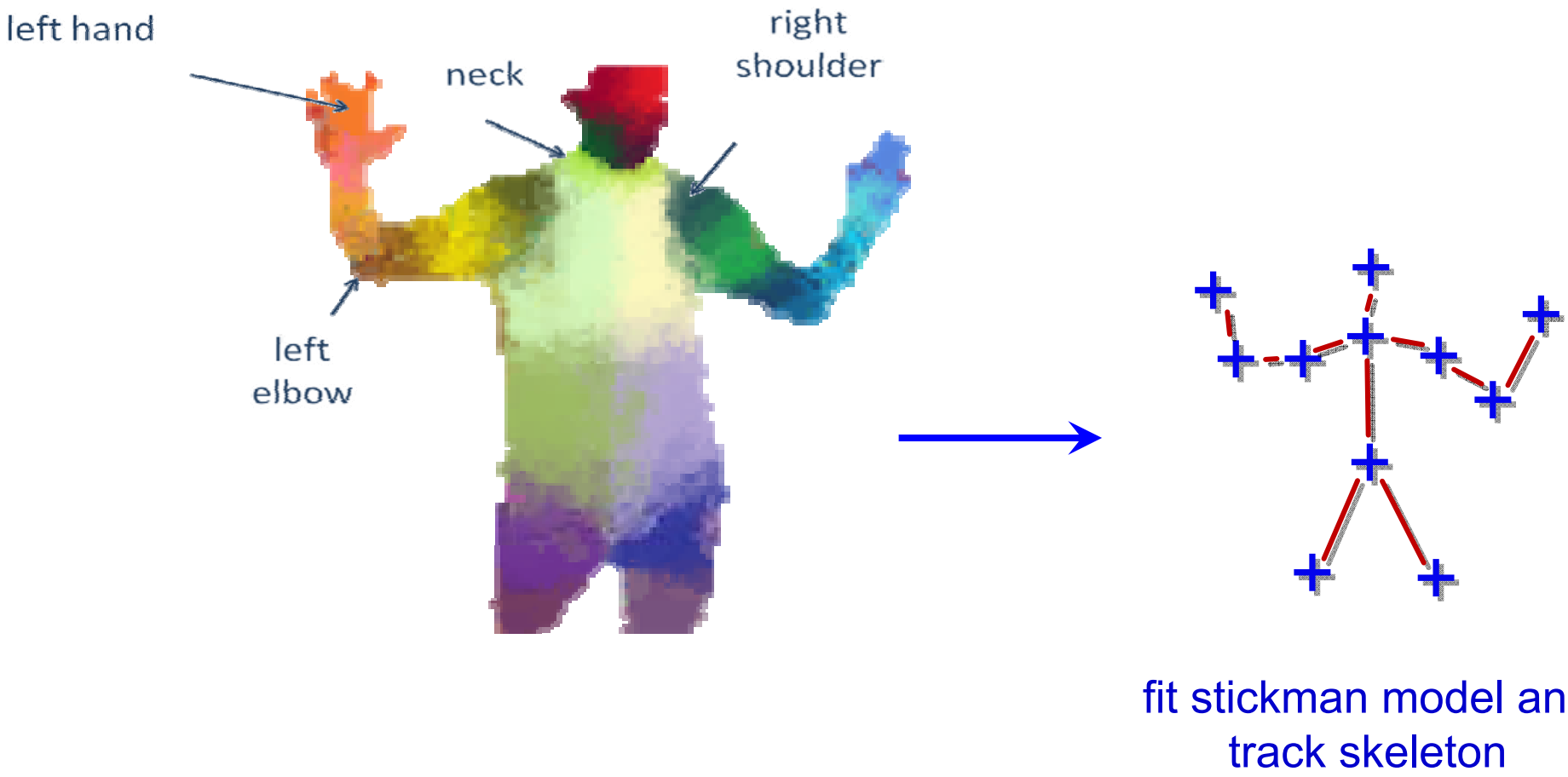
Depth image

Multi-class classification

inferred body parts

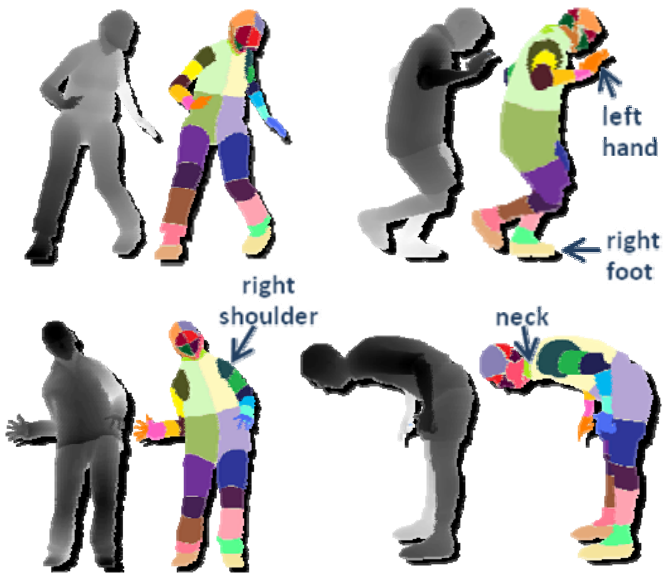
http://www.robots.ox.ac.uk/~az/lectures/ml/lect5.pdf

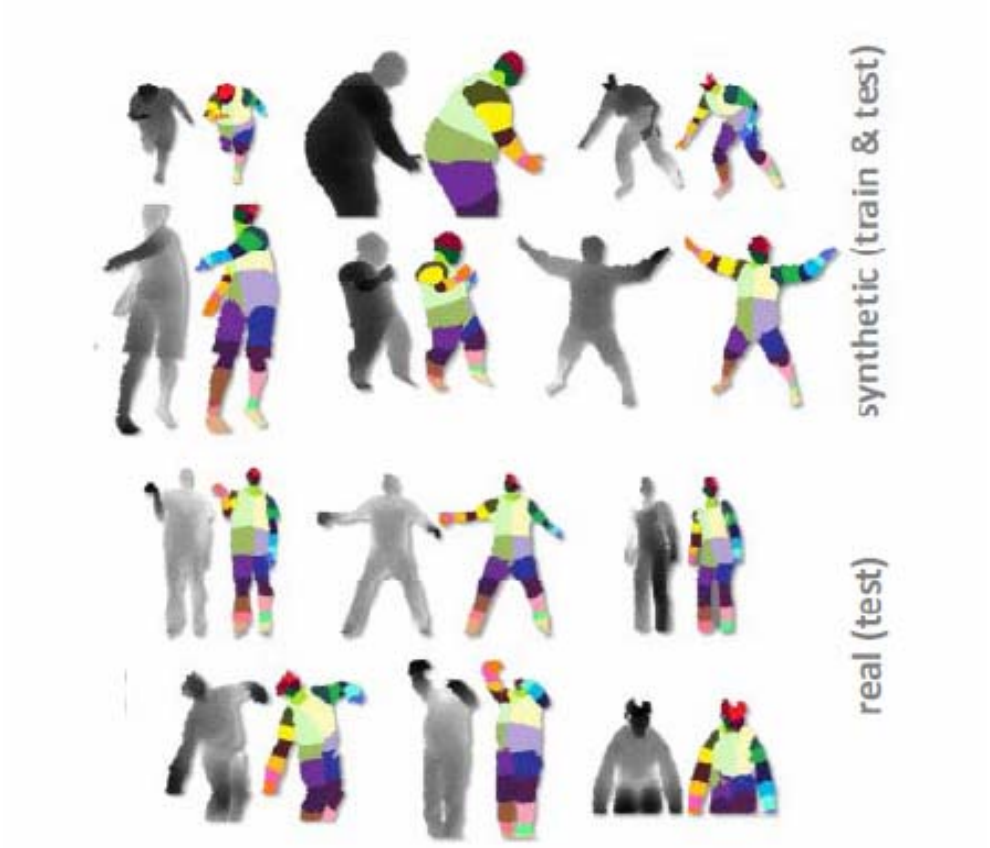
Goal: train a random forest classifier to predict body parts



Training/test Data

From motion capture system





e.g. 1 million training examples

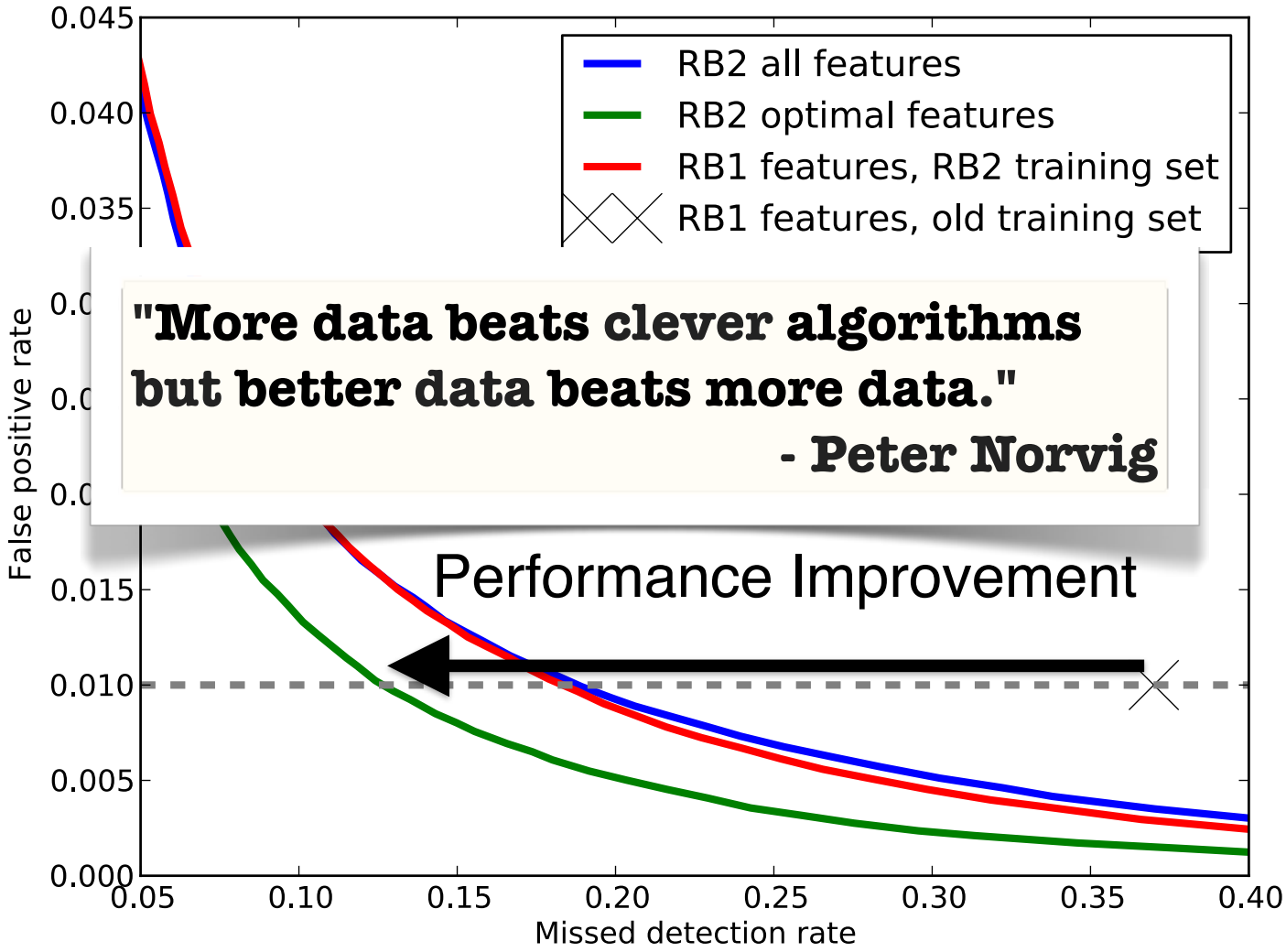
Example result

Input depth image (bg removed)

Inferred body parts (posterior)

body parts in 3D

Classification Improvements



Brink+2012

sklearn is missing a few things...

- Kernel smoothing / Loess
- Multivariate Adaptive Regression Splines (MARS)
- ~~Boosting~~
- ~~Multidimensional scaling (MDS)~~
- Neural Networks / Self-Organizing Maps
- Kalman Filtering / Particle Filtering
- ~~Hidden Markov Models~~
- Missing data imputation / surrogate splting
- Bayesian model fitting / non-parametrics

kNN:	http://bit.ly/1bfuoPn
Natural Language Processing:	http://www.ibm.com/developerworks/library/os-pythonnltk/