CS109 – Data Science

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Announcements

- Story telling is important for data scientists
- Please make sure to target your audience as directed in the homework

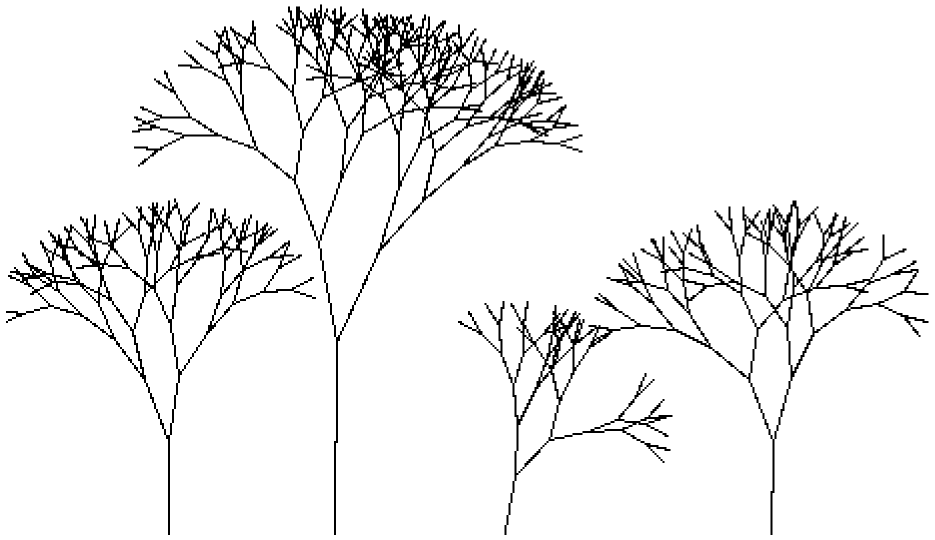
Next Topics

- Classifier wrapup:
  - Some RF things
  - Regression
- ML best practices
  - model choice
  - imbalanced data
  - missing values

- Recommender systems
  - collaborative filtering
  - content-based filtering

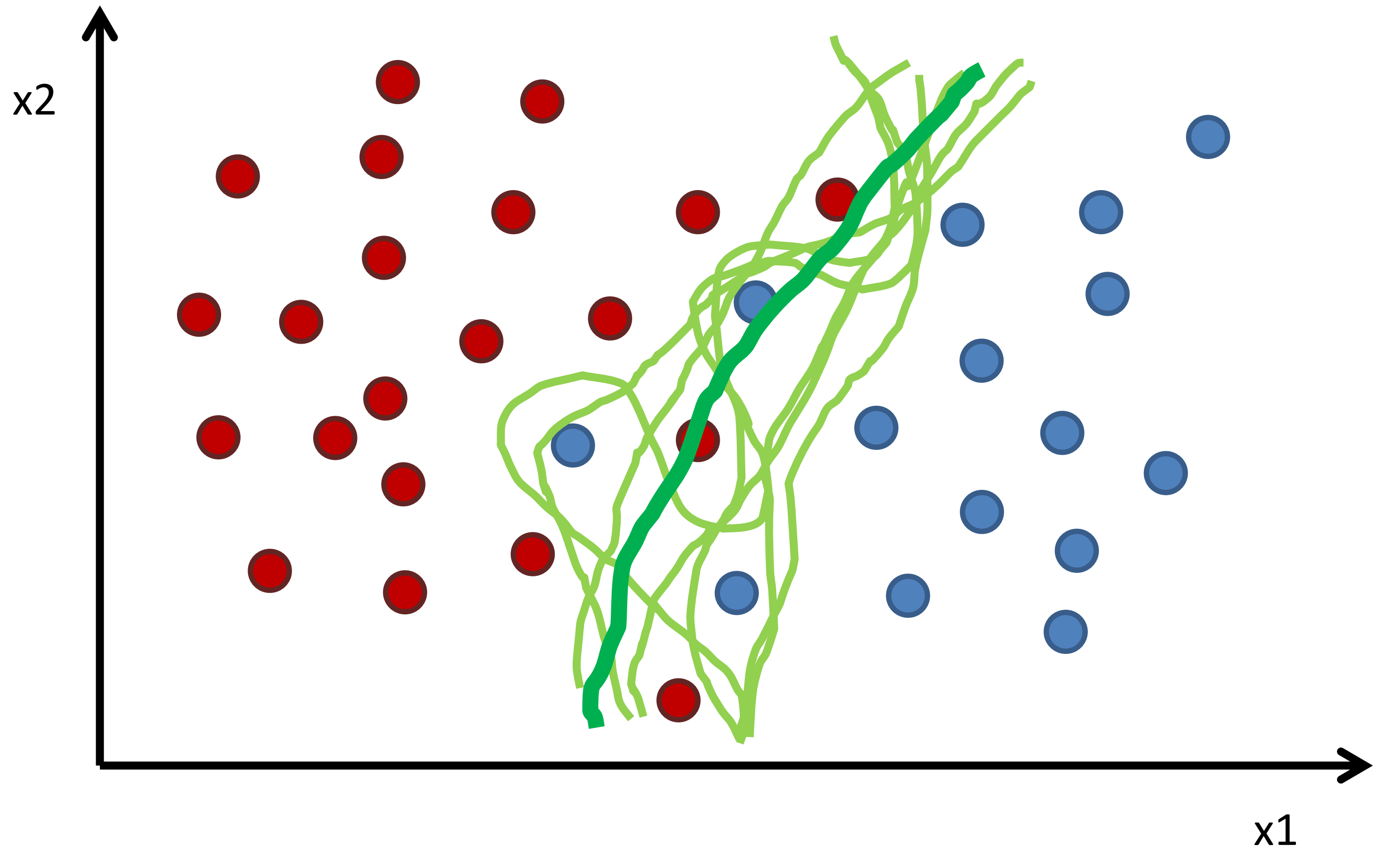
Random Forest

- Builds upon the idea of bagging
- Each tree build from bootstrap sample
- Node splits calculated from random feature subsets



http://www.andrewbuntine.com/articles/about/fun

Bagging Idea



Random Forest

- All trees are fully grown
- No pruning

- Two parameters
  - Number of trees
  - Number of features

What is the difference between Bagging and Random forest?

features

Random Forest Error Rate

- Error depends on:
  - Correlation between trees (higher is worse)
  - Strength of single trees (higher is better)

- Increasing number of features for each split:
  - Increases correlation
  - Increases strength of single trees

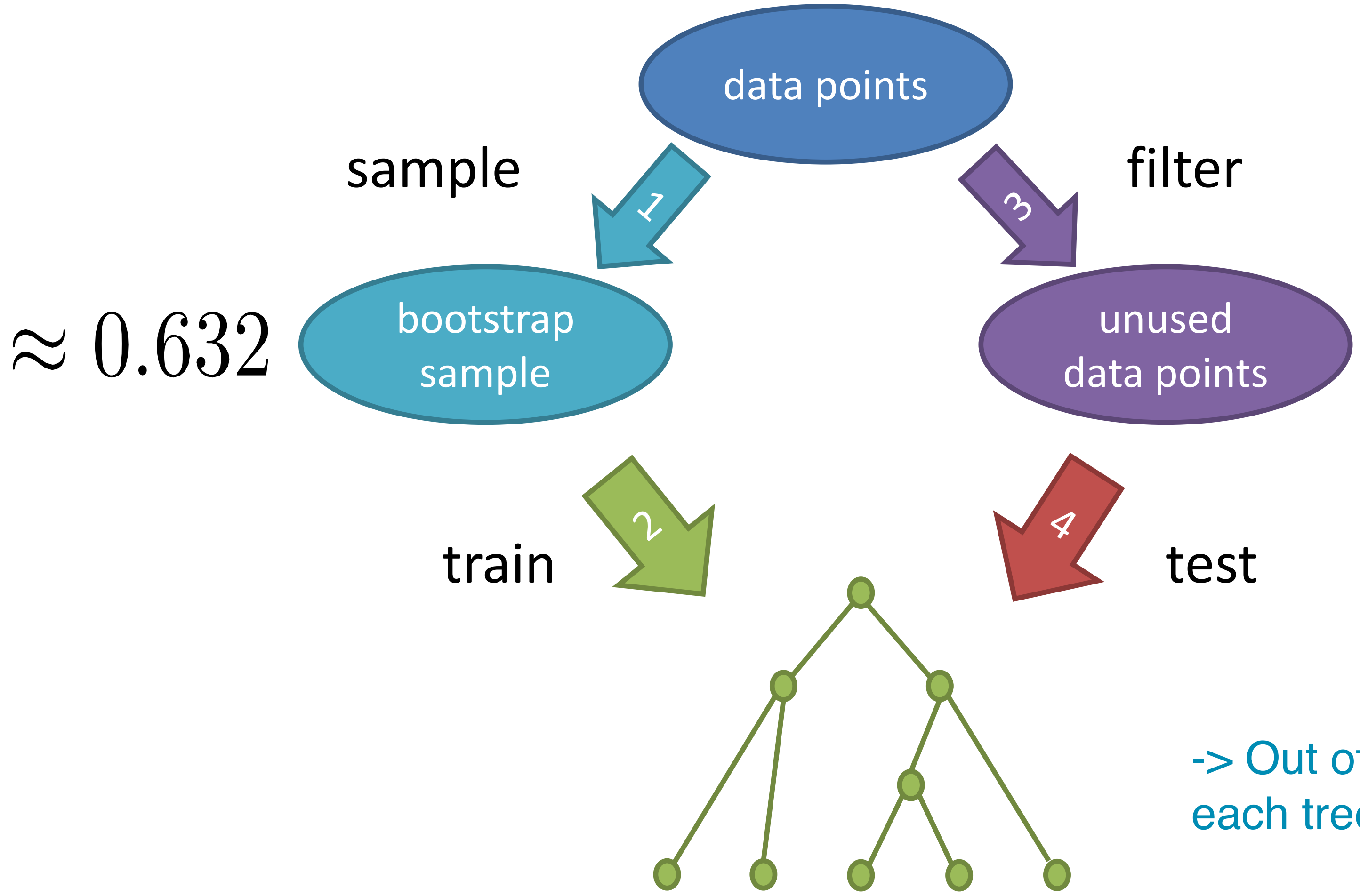
Extreme Scenario

y	x			
1	1	@	&	…
0	0	#	%	…
1	1	$	#	…
1	1	%	^	…
0	0	^	!	…
1	1	*	)	…
0	0	)	%	…
…	…	…	…	…

perfect tree only needs first column of x
all the rest is junk
- single fully grown tree computes genie measure for each column -> chooses x
- bagging: each tree would learn the same thing
- random forest with 1 feature: random noise, splits until completely overfit, high computation time AND wrong result

What would a single fully grown tree learn? How deep would it be?
What would Bagging learn? How would it differ from the single tree?
What would a Random Forest learn with max_feature=1?

Out of Bag Error



-> Out of bag error for each tree in the forest

Out of Bag Error

- Very similar to cross-validation
- Measured during training
- Can be too optimistic

so don't use it as evaluation of the classifier like with cross-validation

From a Kaggle Forum

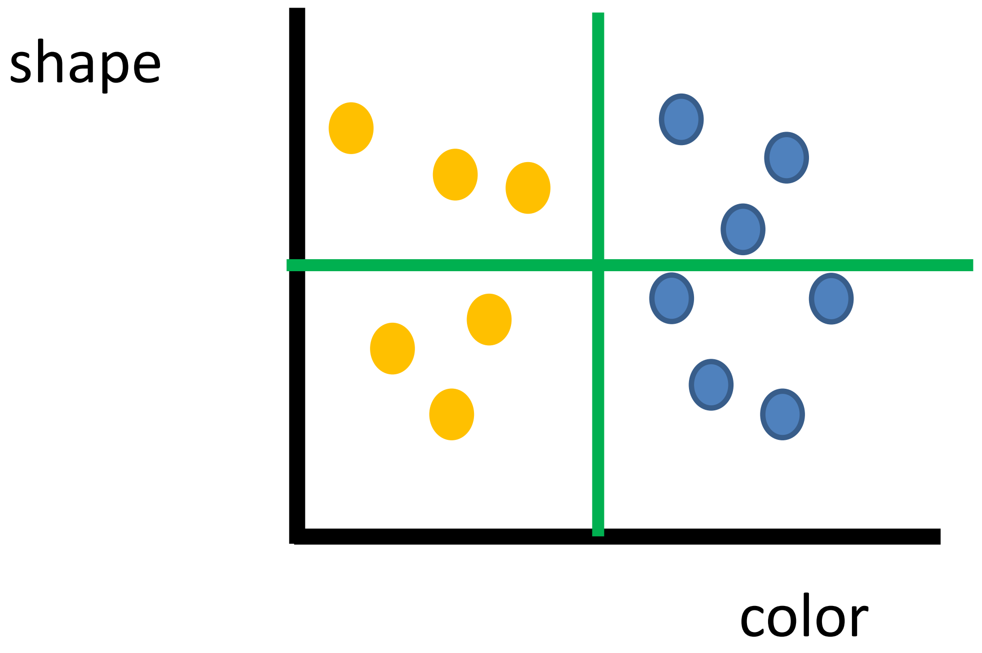
… it feels weird to be using cross-validation type methods with random forests since they are already an ensemble method using random samples with a lot of repetition. Using cross-validation on random forests feels redundant.

Without it, it doesn't work because very easy to overfit
This out of bag error is best way to battle it

Variable Importance - 1

- Again use out of bag samples
- Predict class for these samples
- Randomly permute values of one feature
- Predict classes again
- Measure decrease in accuracy

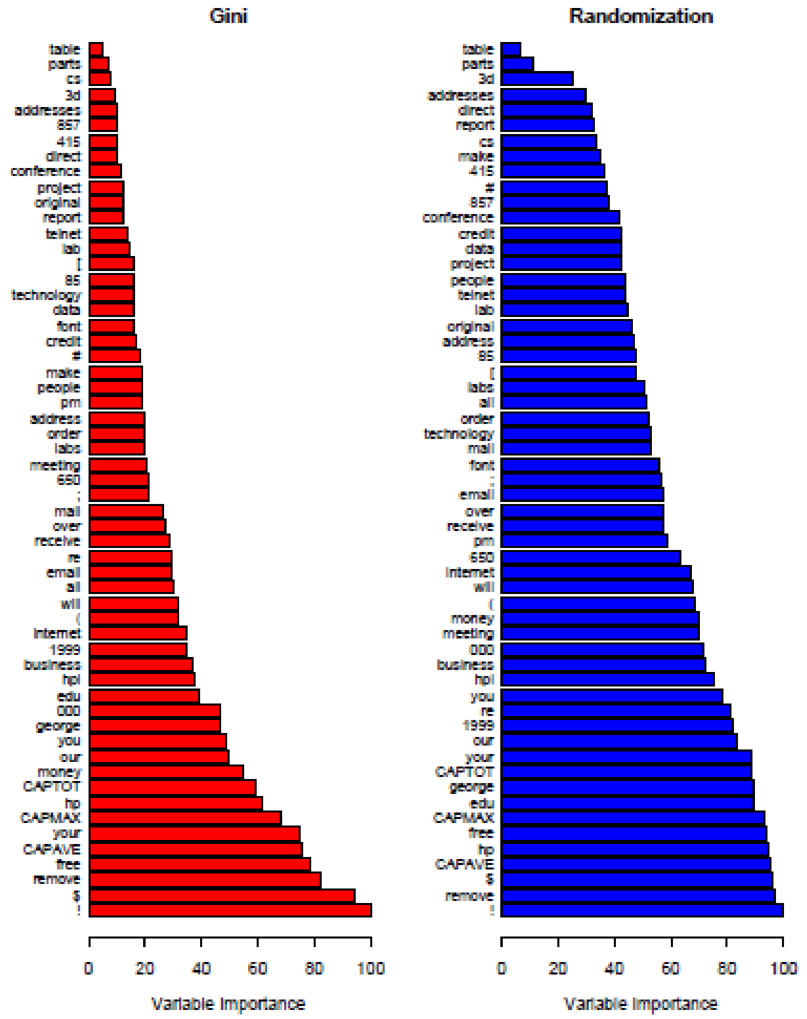
Variable Importance - 1



Variable Importance - 2

- Measure split criterion improvement Genie
- Record improvements for each feature
- Accumulate over whole ensemble

Example: Spam classification



Randomization tends to spread out the variable importance more uniformly.

Overall both methods mainly agree on what is important.

Hastie et al.,"The Elements of Statistical Learning: Data Mining, Inference, and Prediction", Springer (2009)

Regression

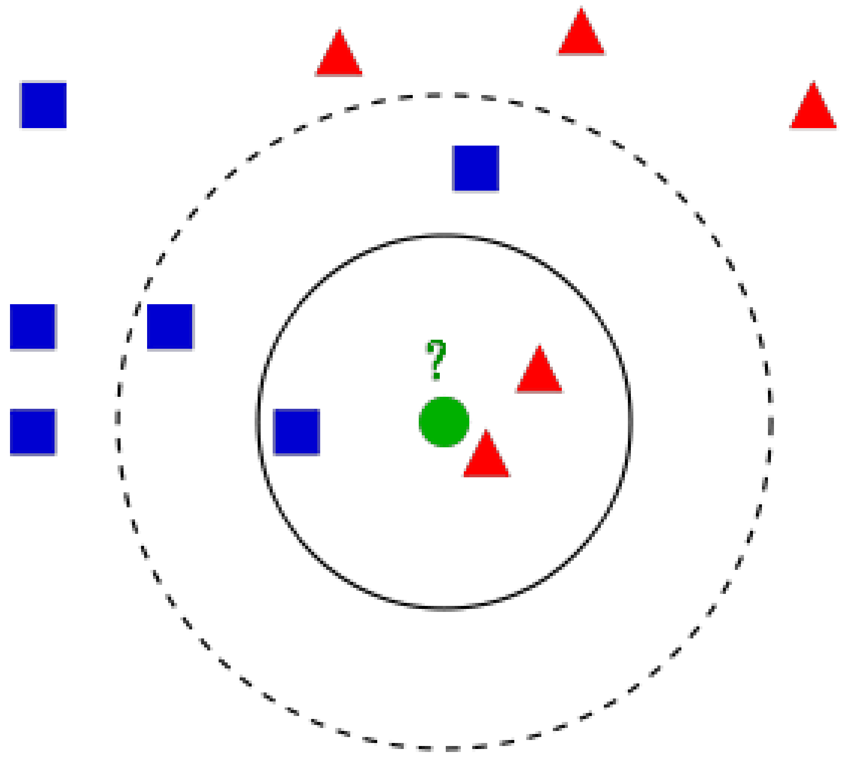
- What is the difference between regression and classification?

- Think about handling 5 star ratings as classification or as regression problem.

  regression preserves the ‘distance’ between labels

  classification doesn’t care about relationship between labels
  -> error is not weighted

KNN Recap



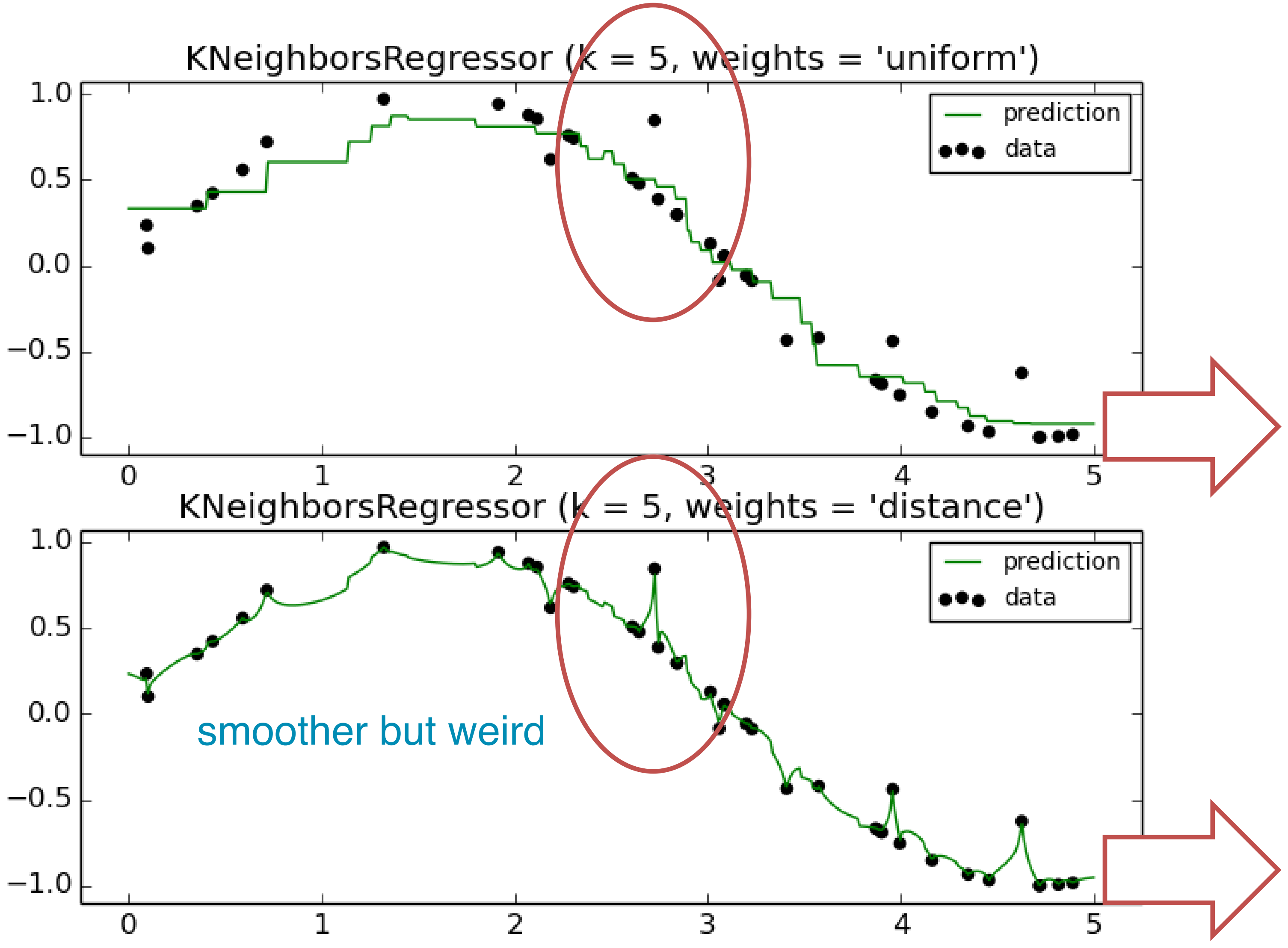
How would you modify KNN to do regression?

KNN for Regression

- Average the values of the K nearest neighbors

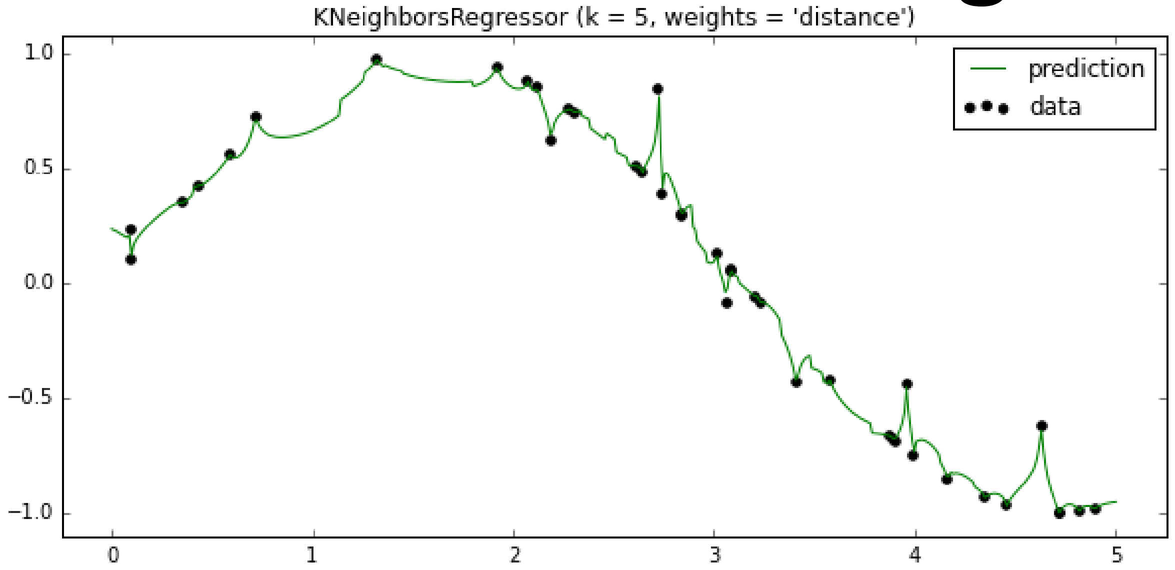
- Or build a weighted average of the K nearest neighbors

KNN Example (1D)

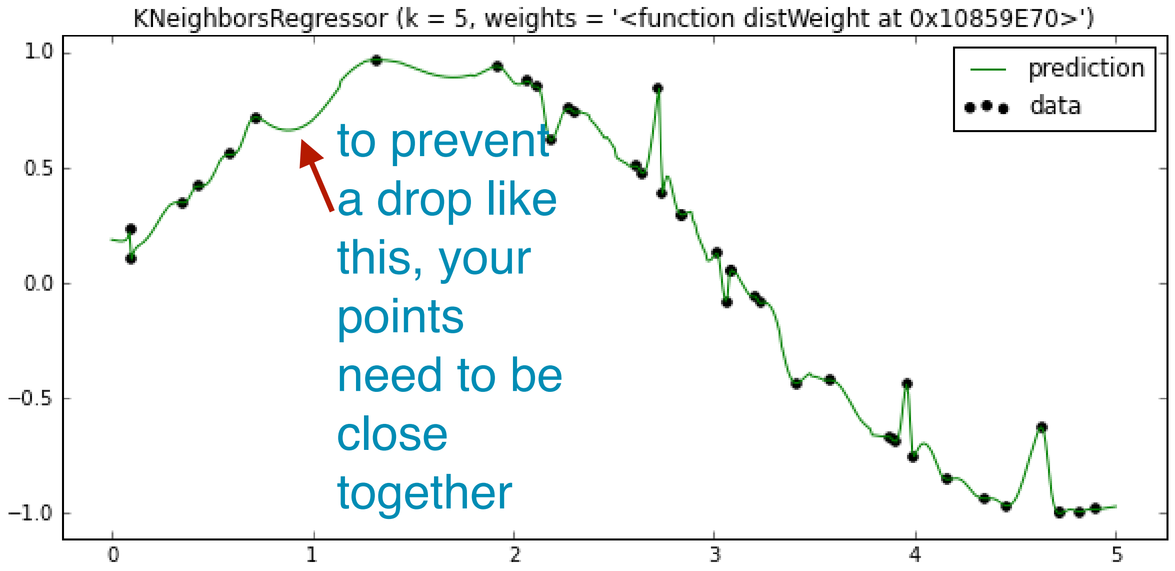


smoother but weird

Distance Weighting

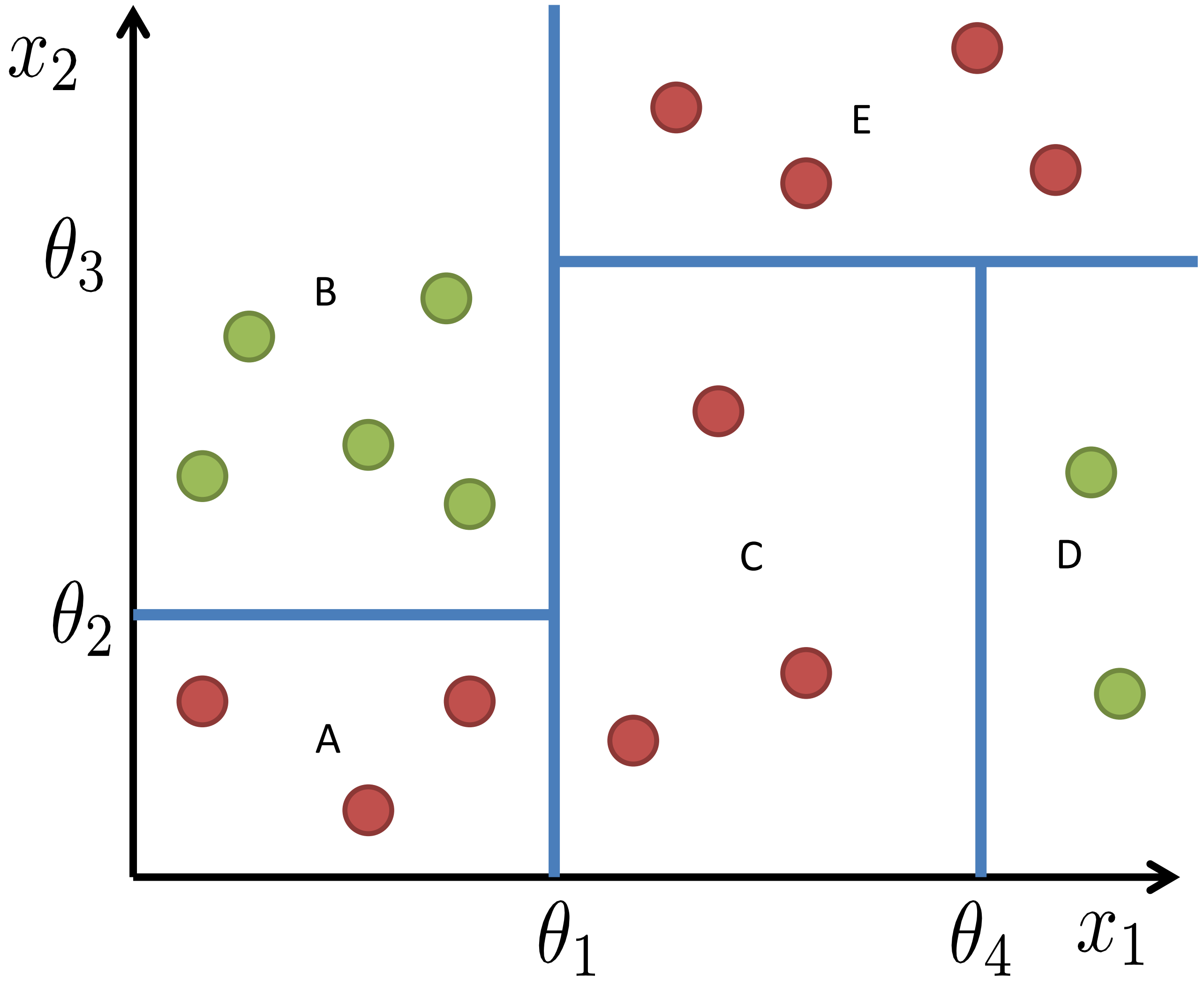


Linear weights

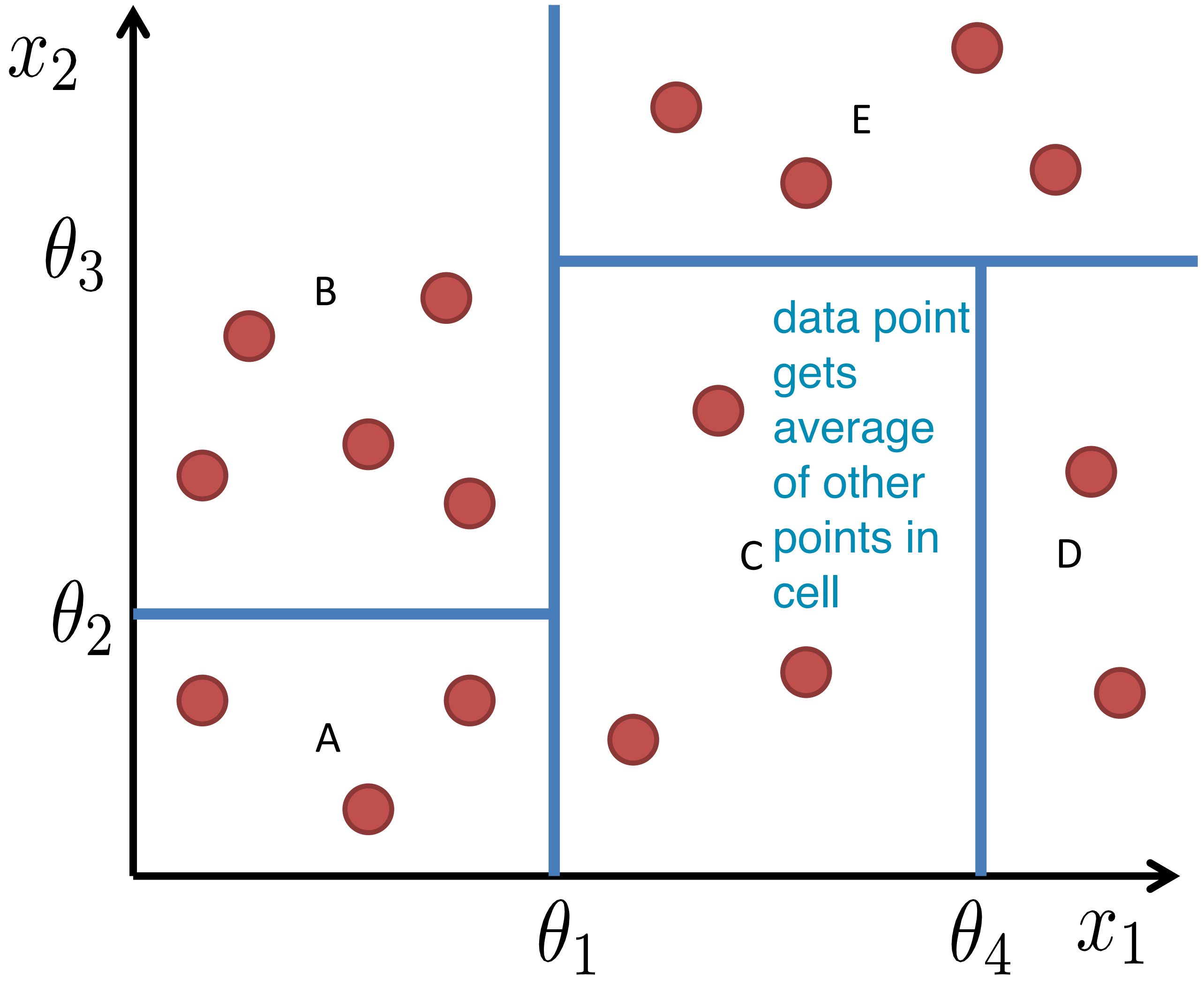


Quadratic weights

Decision Tree



Regression Tree

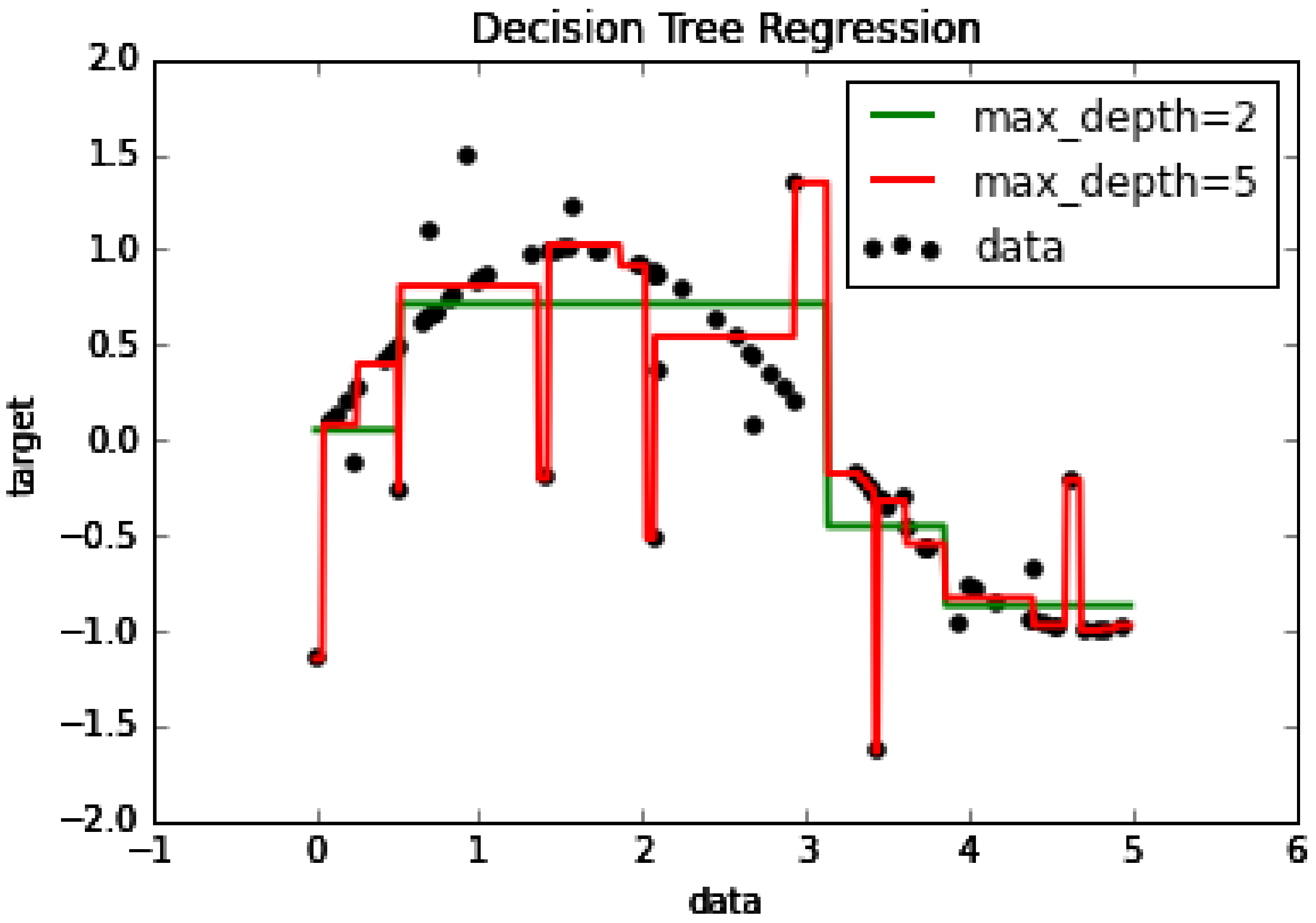


Regression Tree

- Again we average, this time over all points in one of the cells.
- During training, split in the way that reduces the squared error the most.

Can’t use gini anymore -> squared error

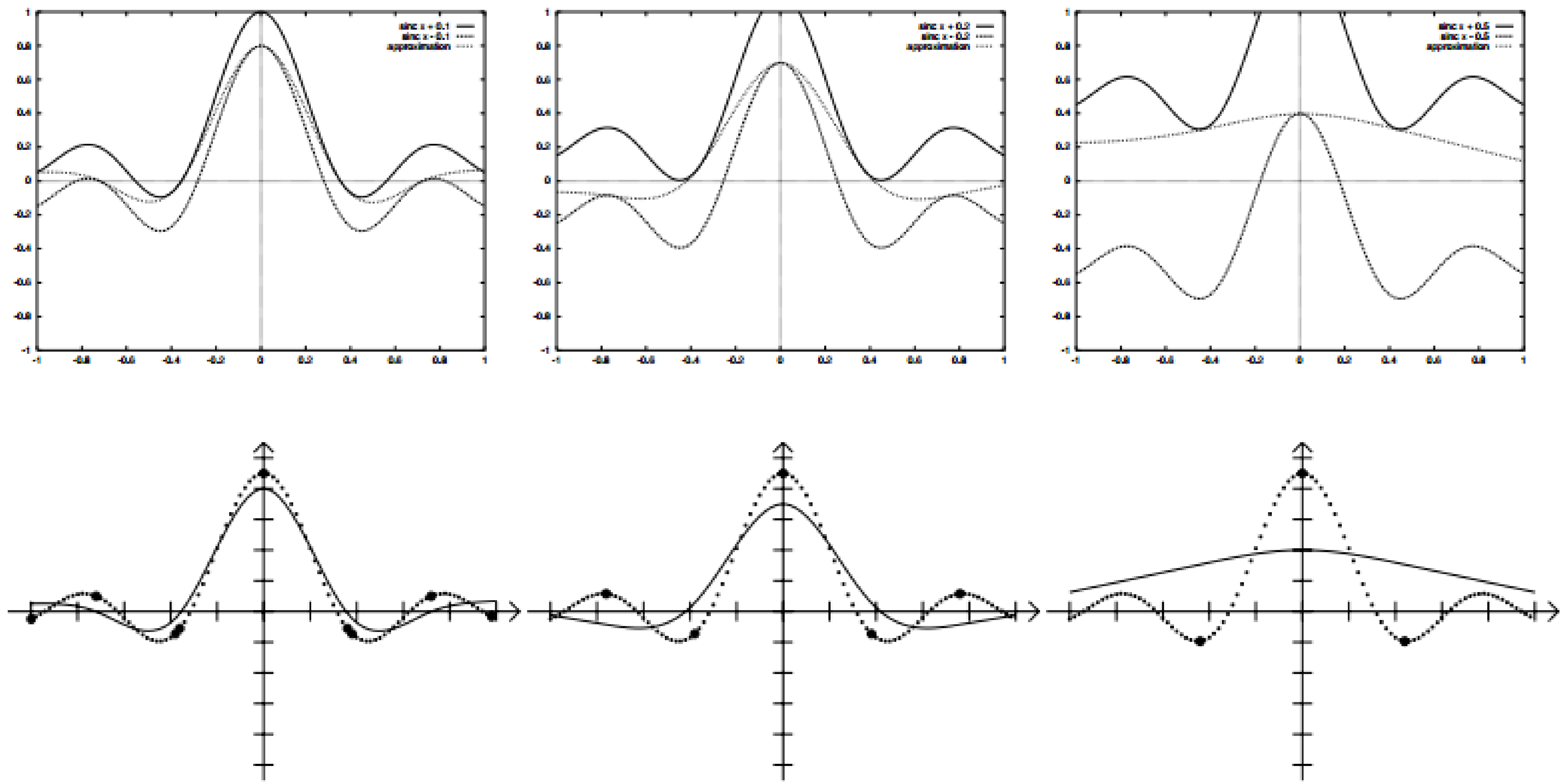
Regression Tree Training



Random Forest for Regression

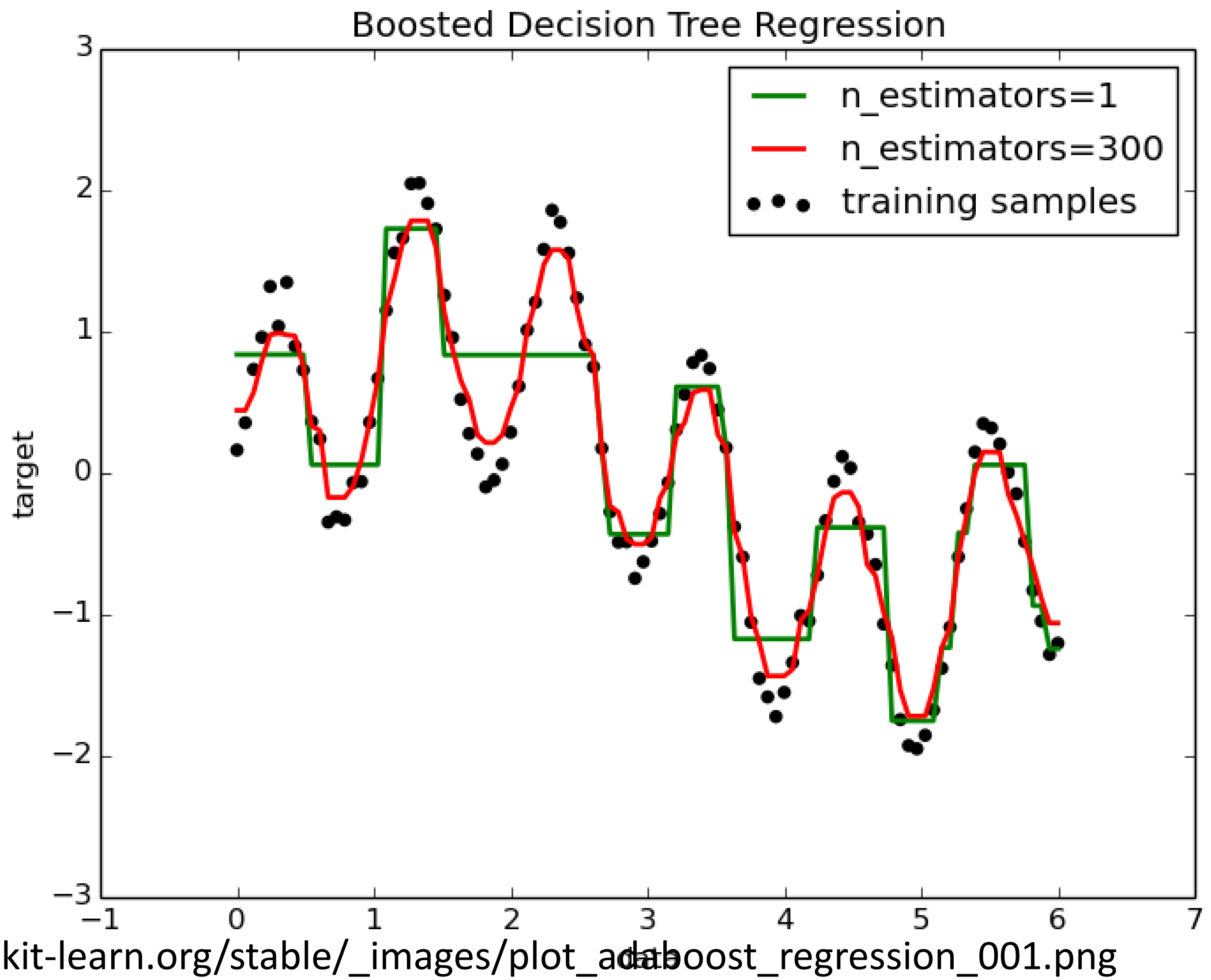
- Same idea as before
- Train multiple trees in parallel and average
- Different defaults
- max_features = n_features -> default = bagging
- square error in stead of gini

SVM for Regression



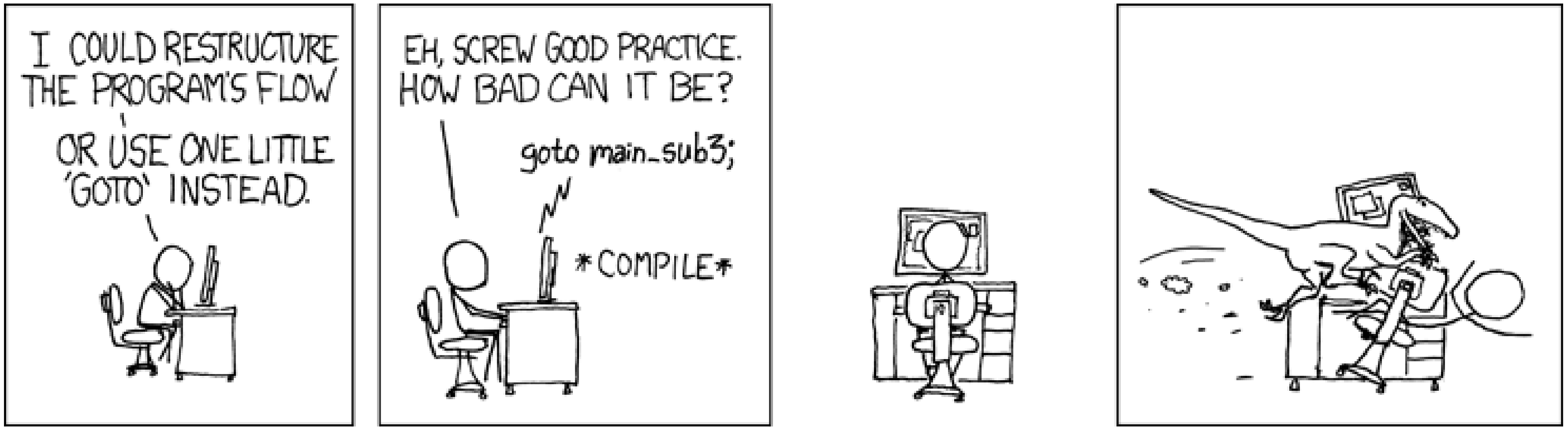
http://www2.cs.uh.edu/~ceick/ML/SVM-Regression.pdf

Boosting



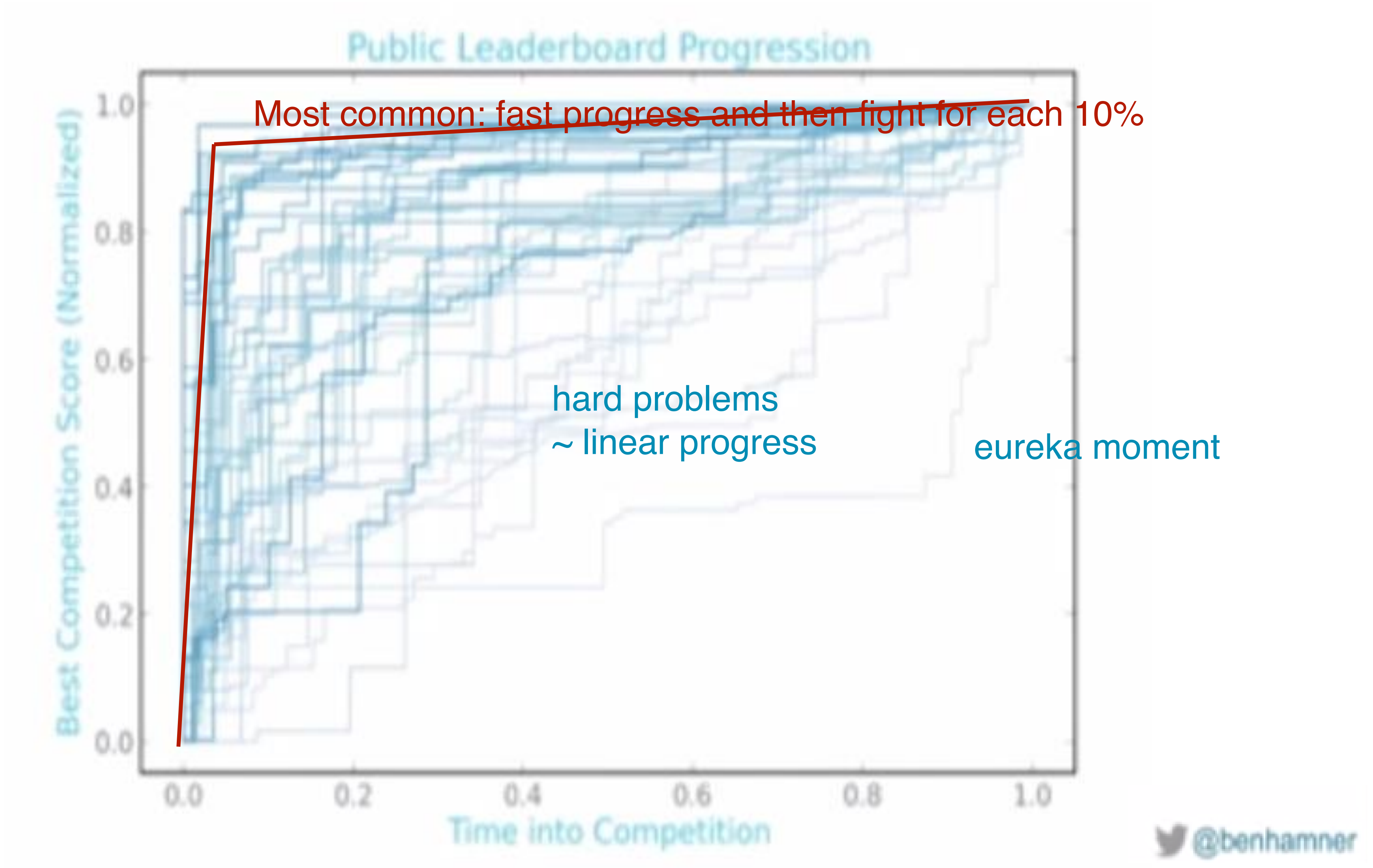
http://scikit-learn.org/stable/_images/plot_adaboost_regression_001.png

Best Practices

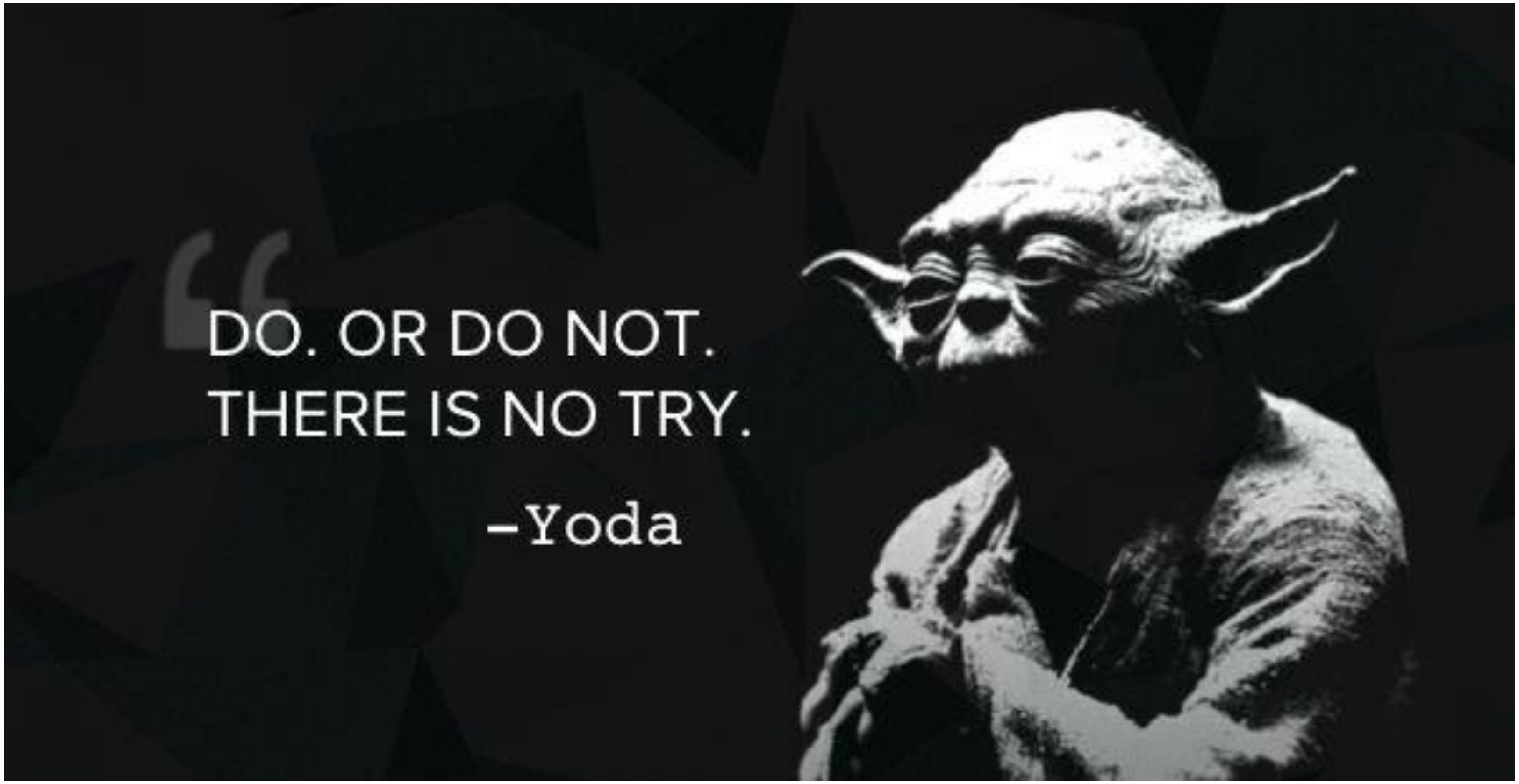

I COULD RESTRUCTURE THE PROGRAM'S FLOW
OR USE ONE LITTLE 'GOTO' INSTEAD.
EH, SCREW GOOD PRACTICE. HOW BAD CAN IT BE?
goto main_sub3;
COMPILE

https://xkcd.com/292/

Typical Progress

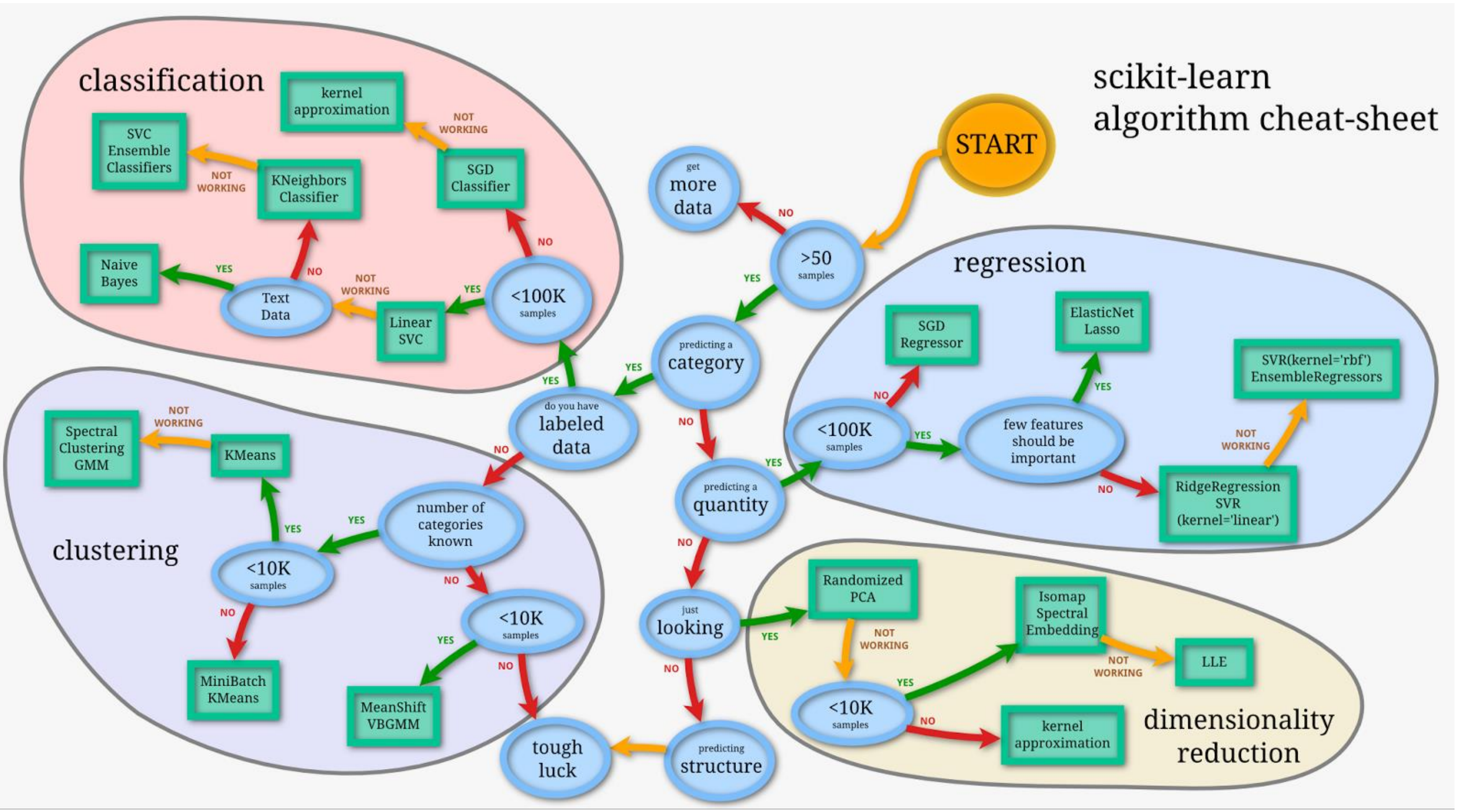


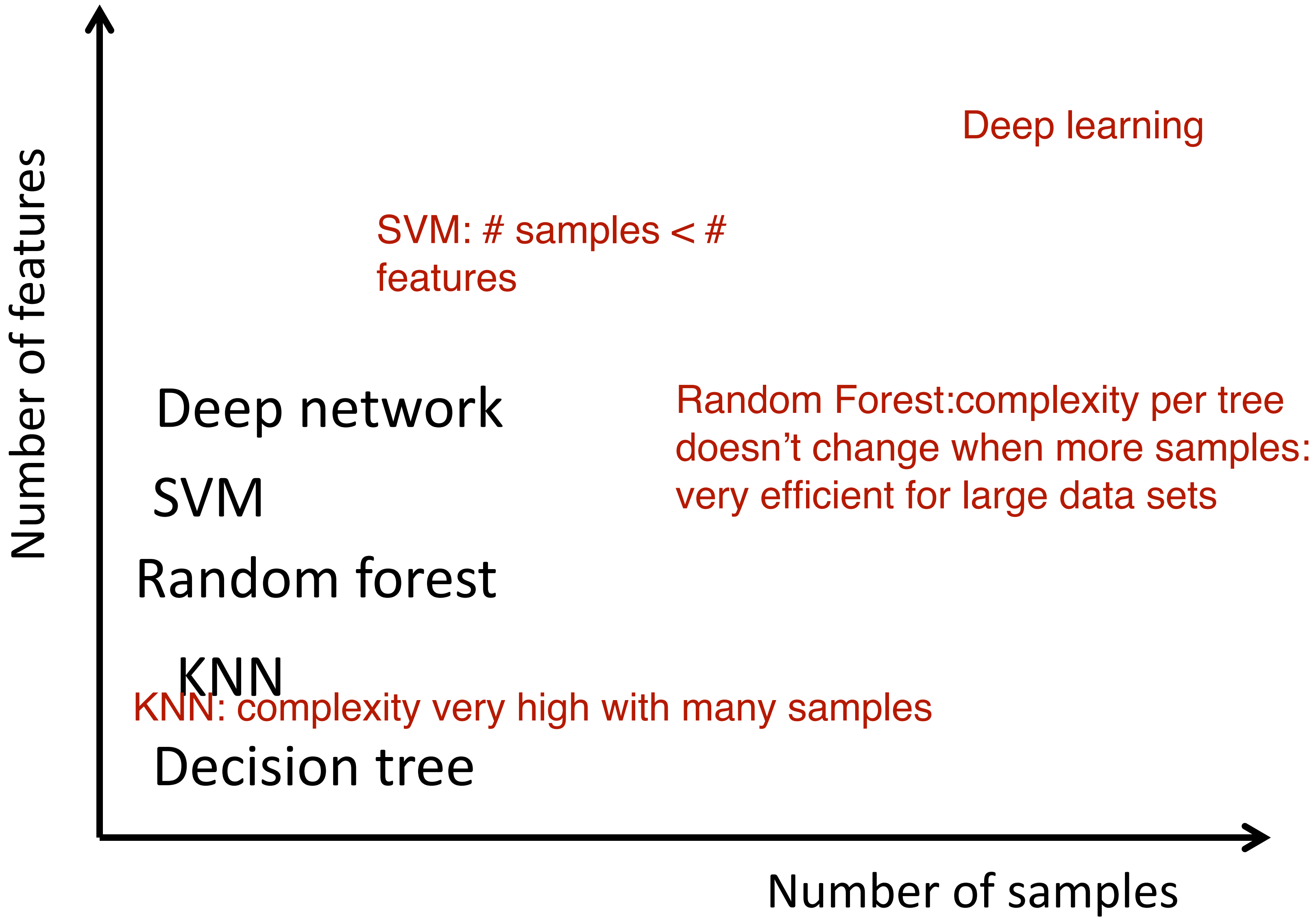
Under Promise, Over Deliver!



General Best Practices

- it will be harder than it looks
- know your application:
  - zero values
  - outliers
  - where do labels come from
- Document, document, document
  - for yourself! And for others
- commit, pull, push, repeat


scikit-learn
algorithm cheat-sheet
START
>50 samples
get more data
predicting a category
do you have labeled data
<100K samples
Linear SVC
Text Data
Naive Bayes
KNeighbors Classifier
SVC Ensemble Classifiers
SGD Classifier
kernel approximation
classification
number of categories known
<10K samples
KMeans
Spectral Clustering GMM
MiniBatch KMeans
MeanShift VBGMM
clustering
tough luck
predicting a quantity
few features should be important
SGD Regressor
ElasticNet Lasso
RidgeRegression SVR (kernel='linear')
SVR(kernel='rbf') EnsembleRegressors
regression
just looking
predicting structure
Randomized PCA
Isomap Spectral Embedding
LLE
dimensionality reduction
YES
NO
NOT WORKING



Deep learning

SVM: # samples < # features

Random Forest:complexity per tree doesn't change when more samples: very efficient for large data sets

KNN: complexity very high with many samples

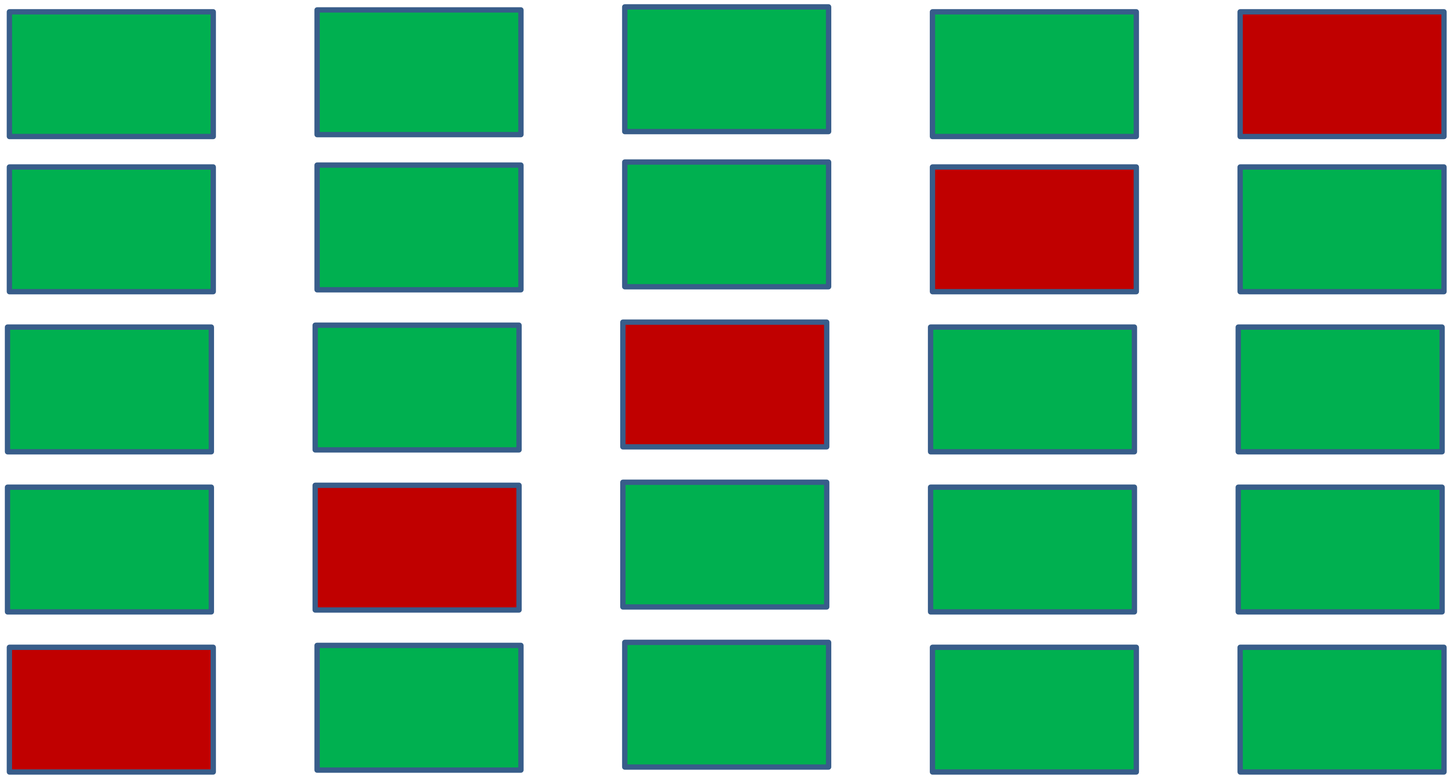
Cross Validation

training data
validation data
test data

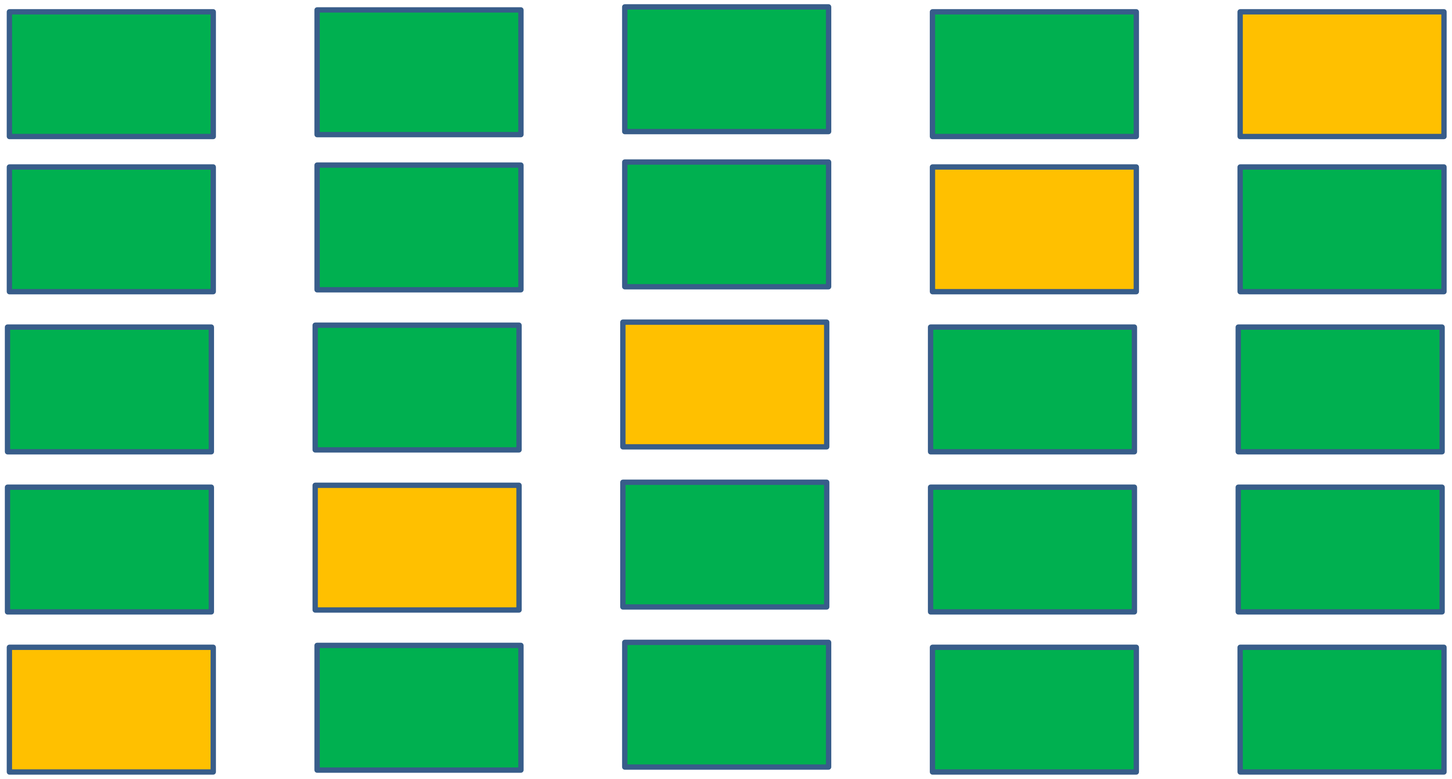
- Training data: train classifier
- Validation data: estimate hyper parameters
- Test data: estimate performance

- Be mindful of validation and test set, validation set might refer to test set in some papers.

5 – Fold Cross Validation



5 – Fold Cross Validation



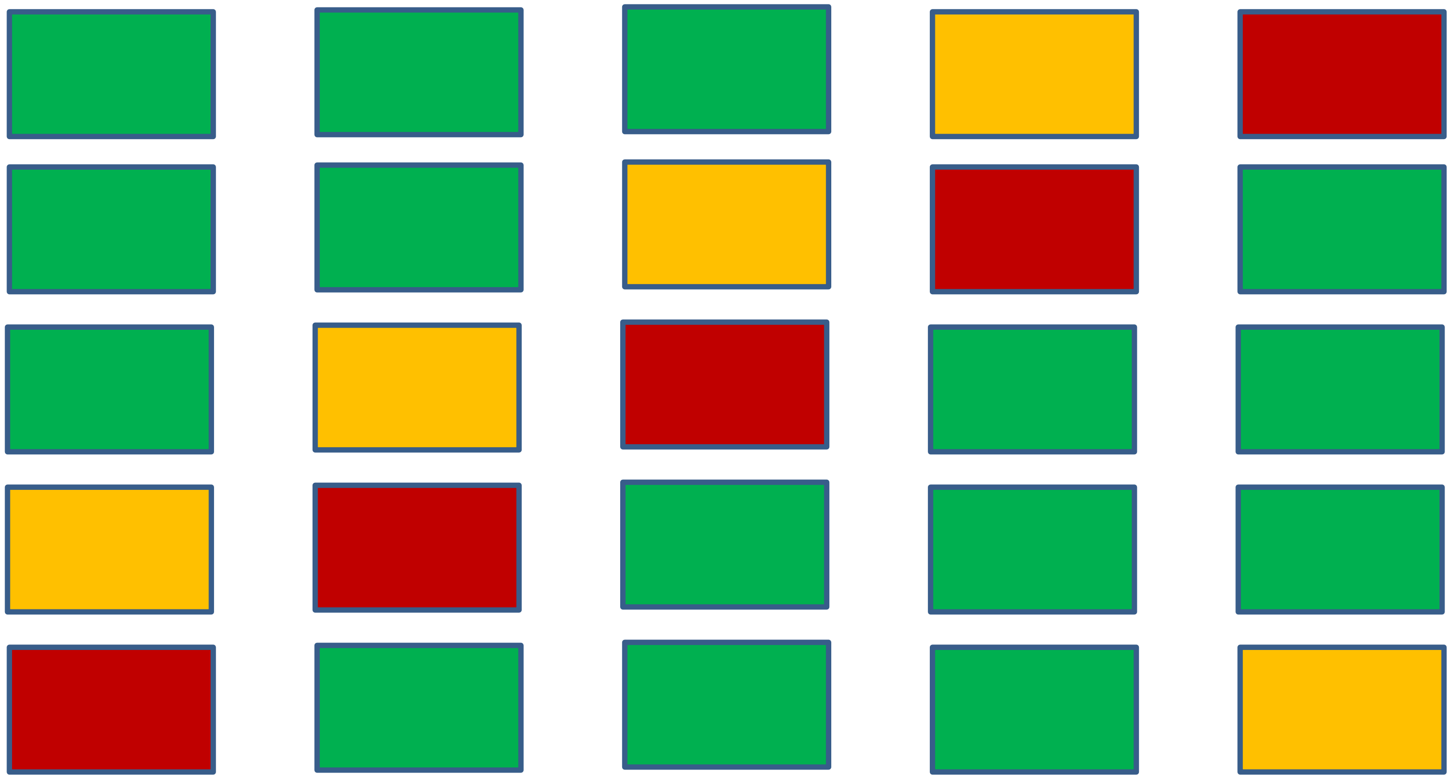
Then test

Last Step of Each Fold

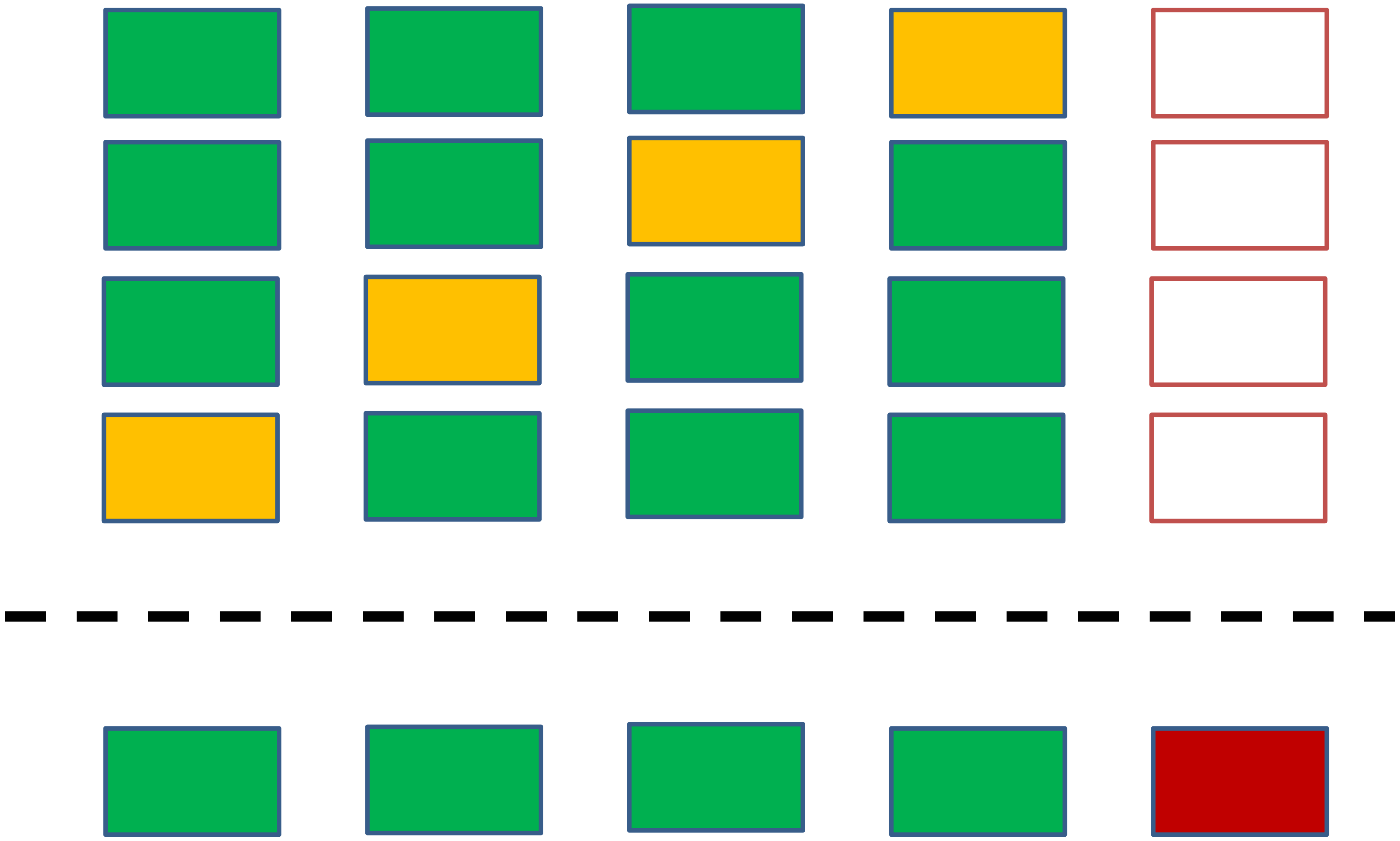
1. Take best parameters 🟨
2. Train on training data and validation data together 🟩 🟨
3. Test performance on test data 🟥

This is the **final** result of your method.

5 – Fold Cross Validation



5 – Fold Cross Validation



Things to Keep in Mind

- How do you aggregate the parameters?
- What if the hyperparameters are all over the place?
- What if the hyperparameters are at the border of your grid search window?

widen window and go again

Scenario - 1

- 1. Screen the predictors: find a subset of “good” predictors that show fairly strong (univariate) correlation with the class labels
- 2. Using just this subset of predictors, build a multivariate classifier.
- 3. Use cross-validation to estimate the unknown tuning parameters and to estimate the prediction error of the final model.

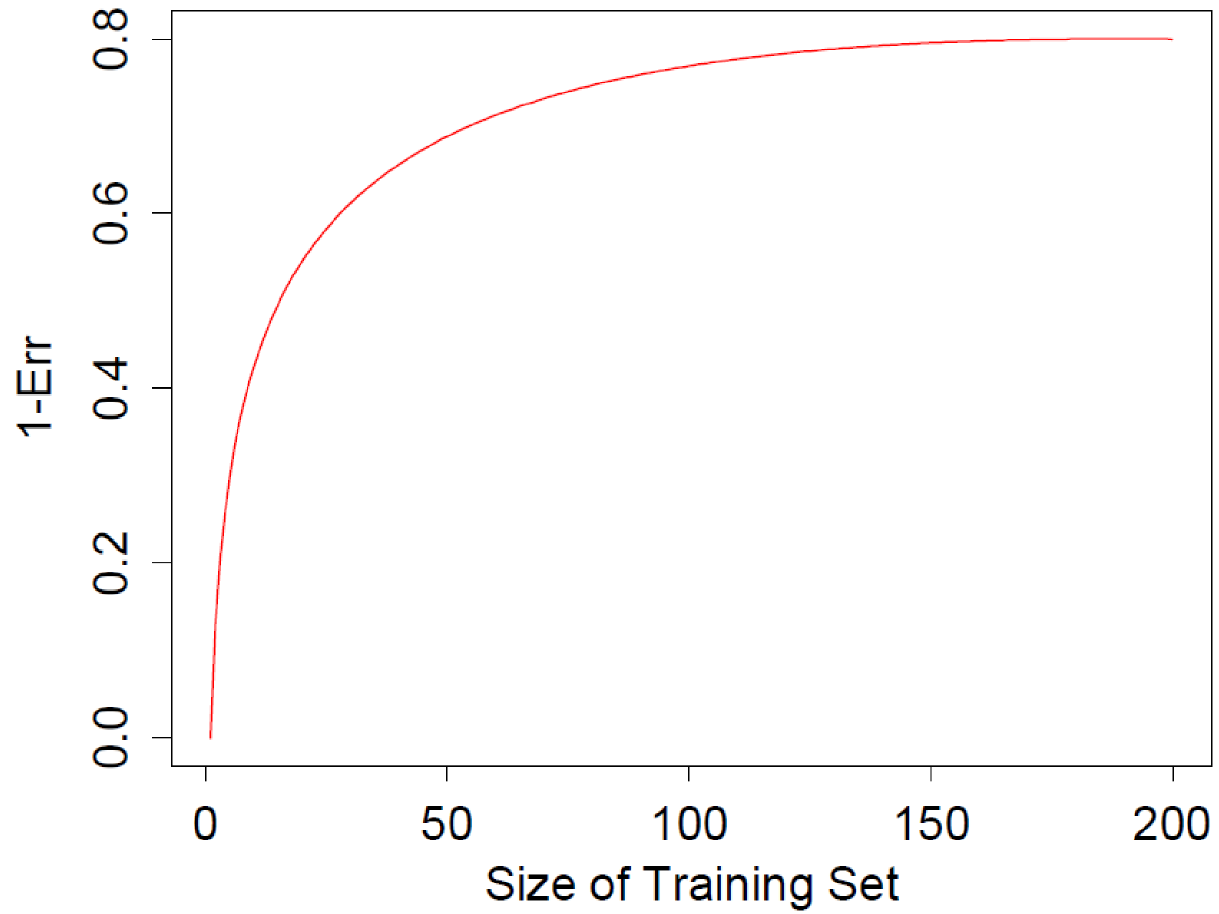
Hastie-Tibsherani_Friedman, “The Elements of Statistical Learning”

Scenario - 2

- 1. Divide the samples into K cross-validation folds (groups) at random.
- 2. For each fold k = 1, 2, . . . ,K
  - Find a subset of “good” predictors that show fairly strong (uni-variate) correlation with the class labels, using all of the samplesexcept those in fold k.
  - Using just this subset of predictors, build a multivariate classifier, using all of the samples except those in fold k.
  - Use the classifier to predict the class labels for the samples in fold k.

Hastie-Tibsherani_Friedman, “The Elements of Statistical Learning”

Effect of Sample Size

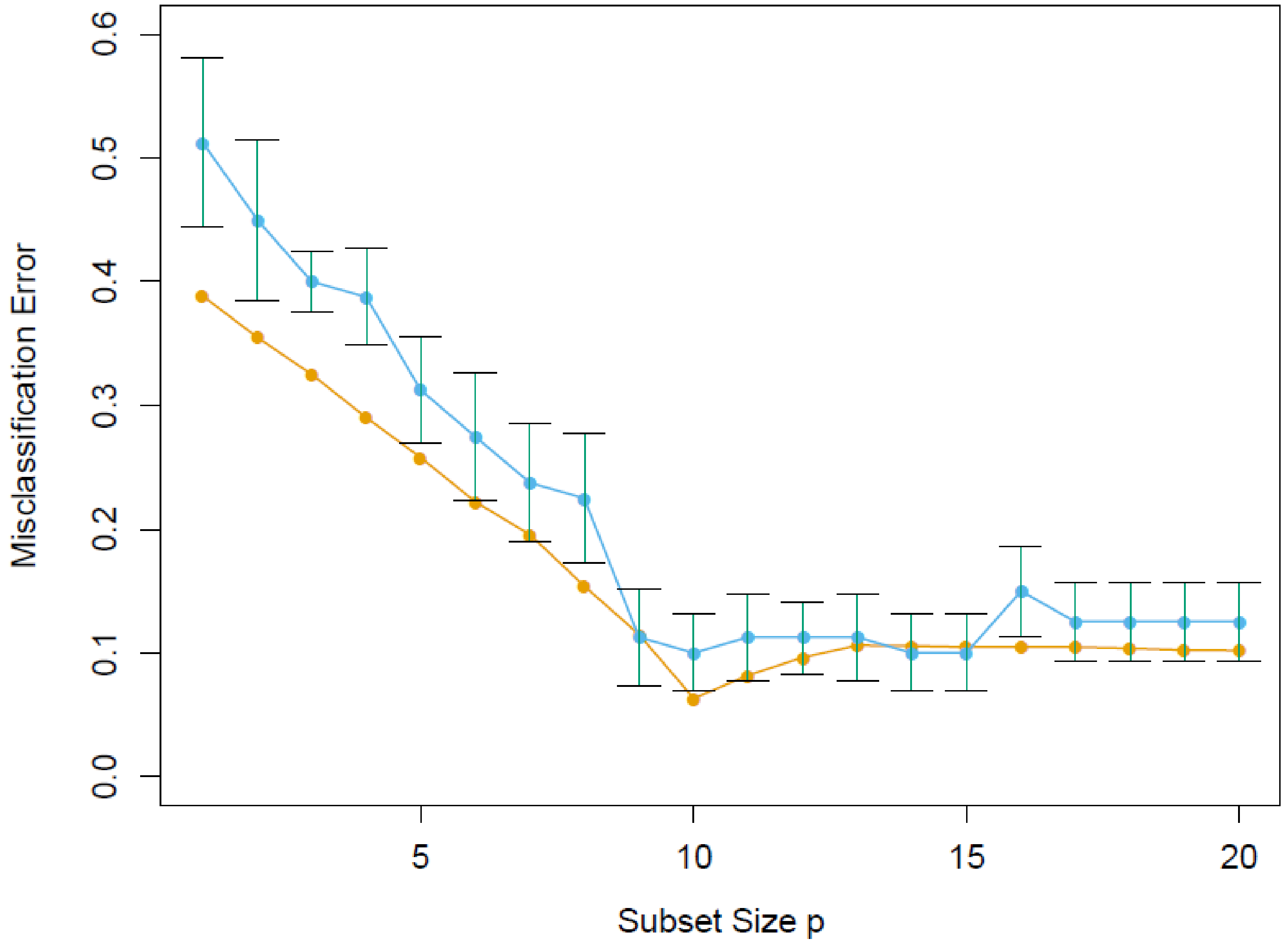


5-fold cross validation:

- n=200 => 160 samples
- n=50 => 40 samples

Hastie et al.,"The Elements of Statistical Learning: Data Mining, Inference, and Prediction"

Cross Validation Over Estimates Error

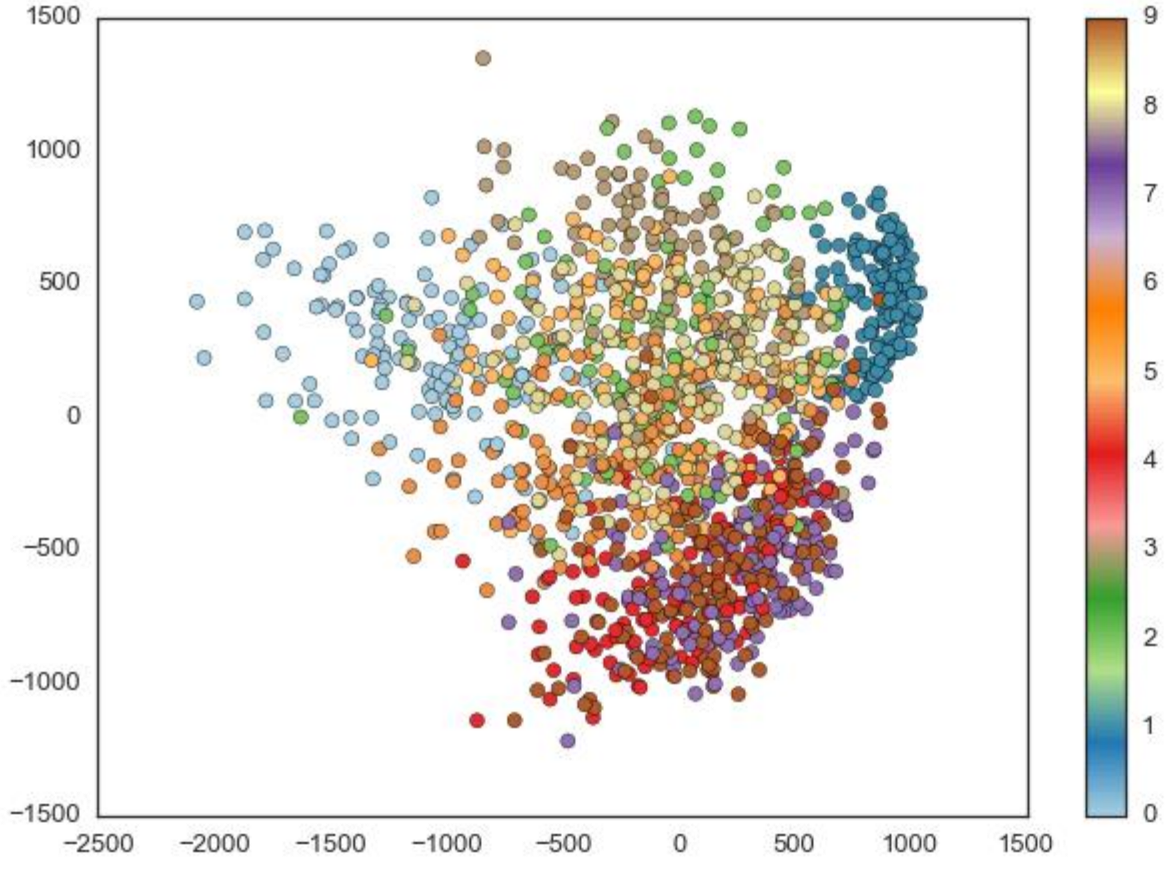


Hastie et al.,"The Elements of Statistical Learning: Data Mining, Inference, and Prediction"

Normalization

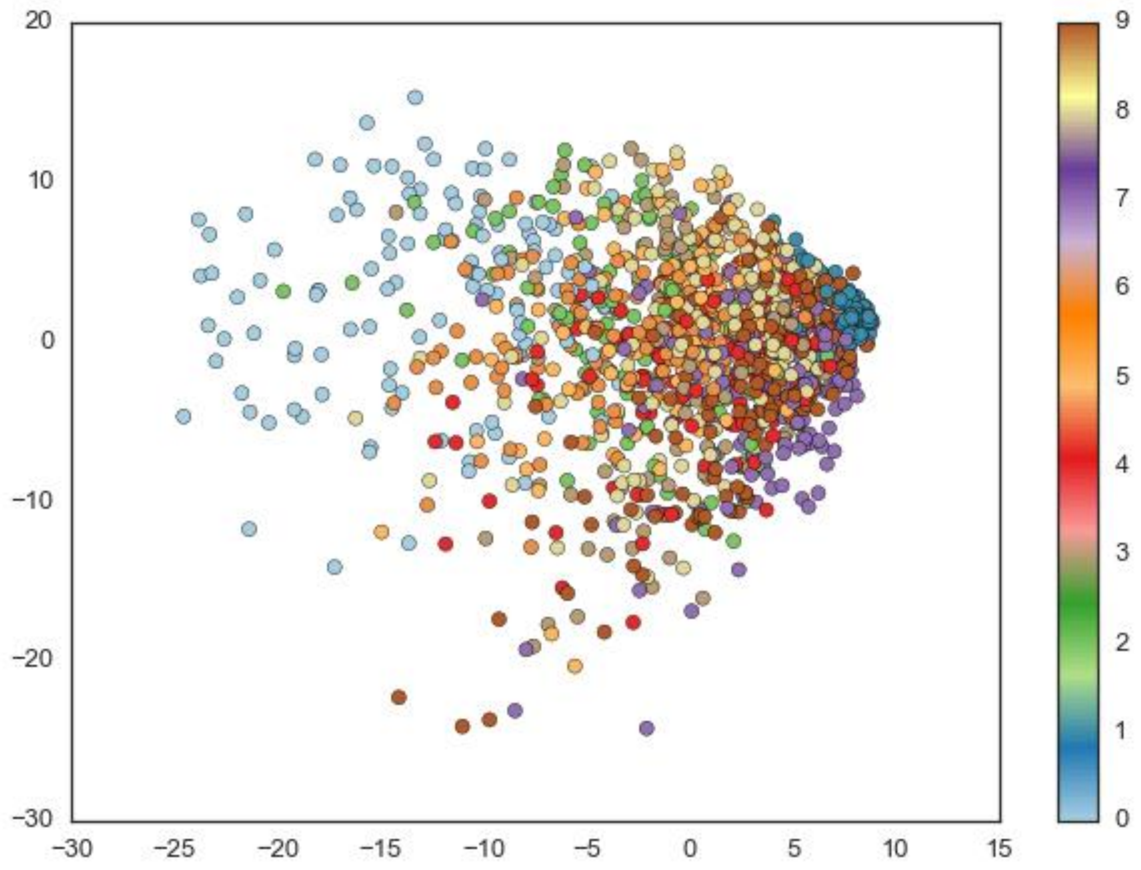
- Be very careful.
- Do not leak into the test data.
- Think about what is useful.

Example PCA on MNIST



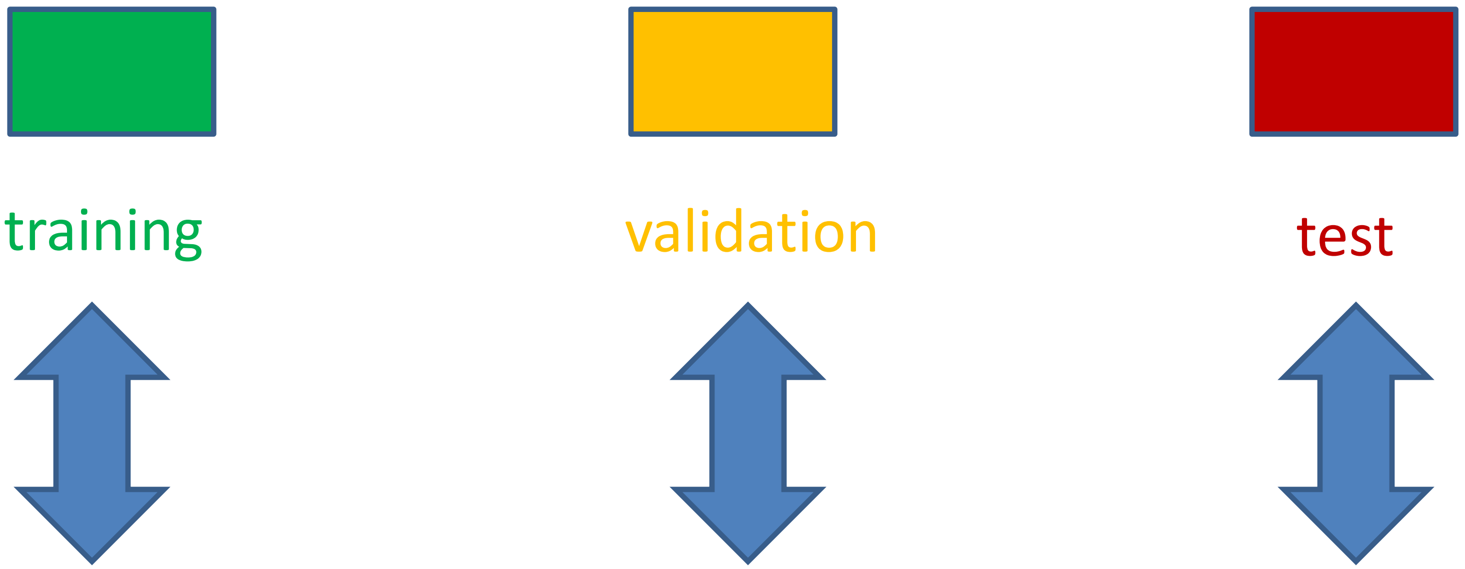
standard PCA

Example PCA on MNIST



PCA with normalized std dev

Normalization - 1

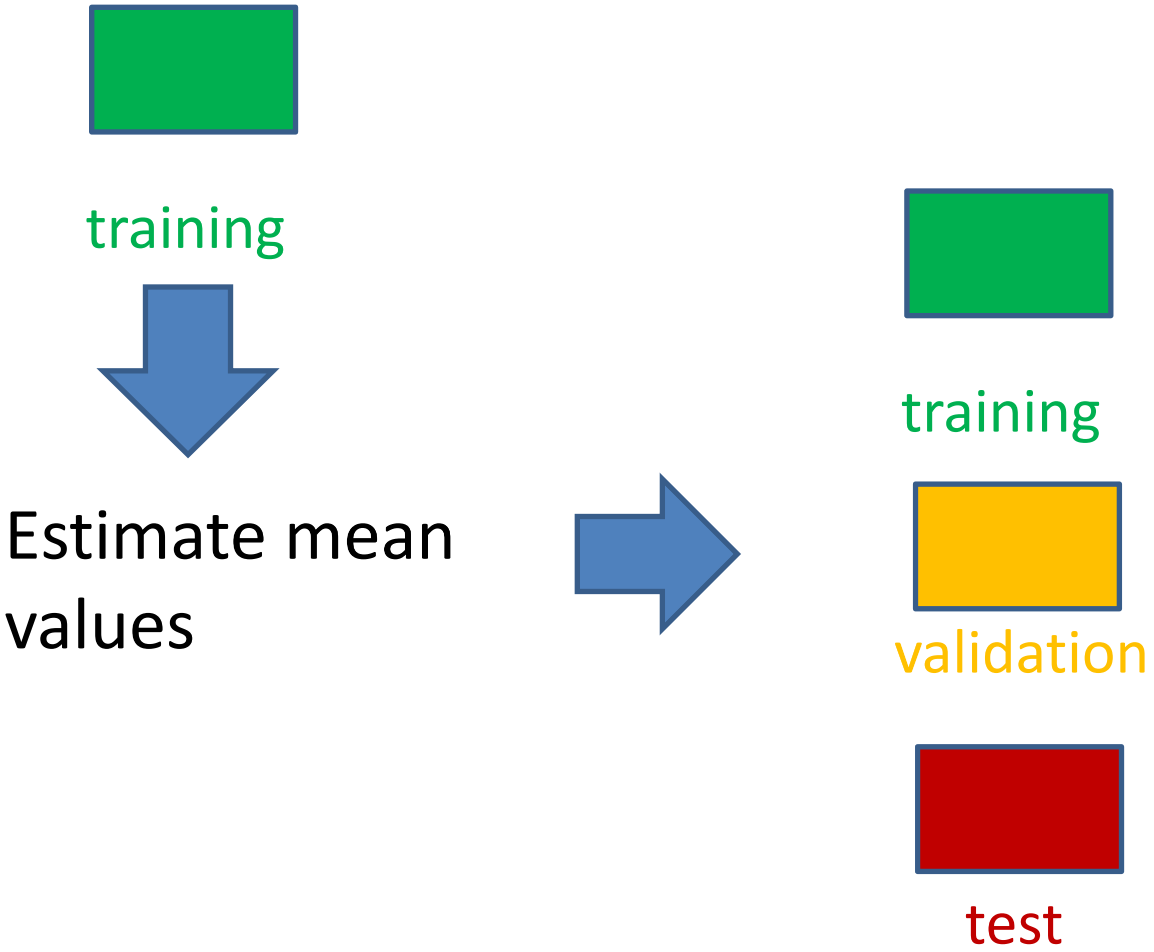


Estimate mean values and normalize.

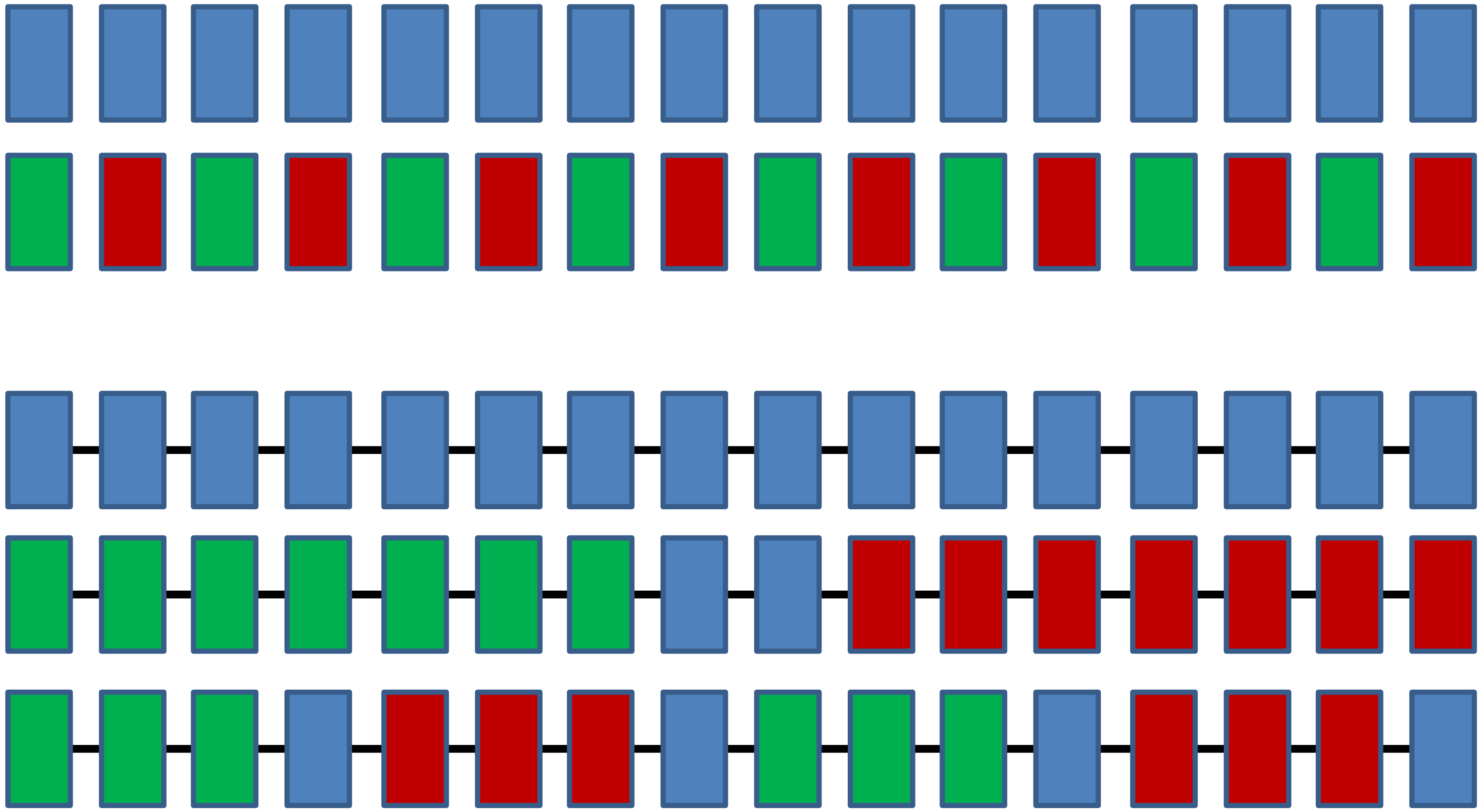
Estimate mean values and normalize.

Estimate mean values and normalize.

Normalization - 2



Know Your Data



Imbalanced Data

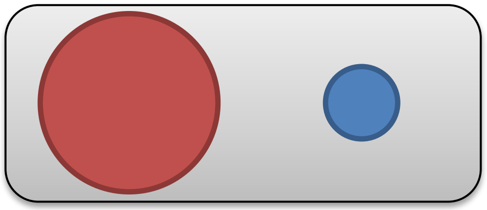
- subsample
- oversample
- re-weight sample points
- use clustering to reduce majority class

- re-calibrate classifier output

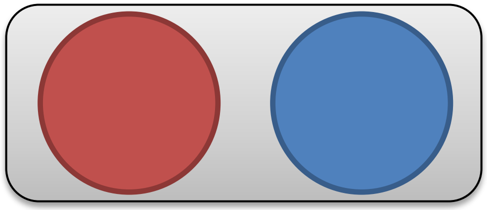
- Beware the easy true negatives

Imbalanced Classes

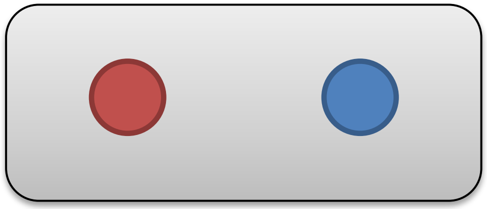
- The Problem:



- Oversample:

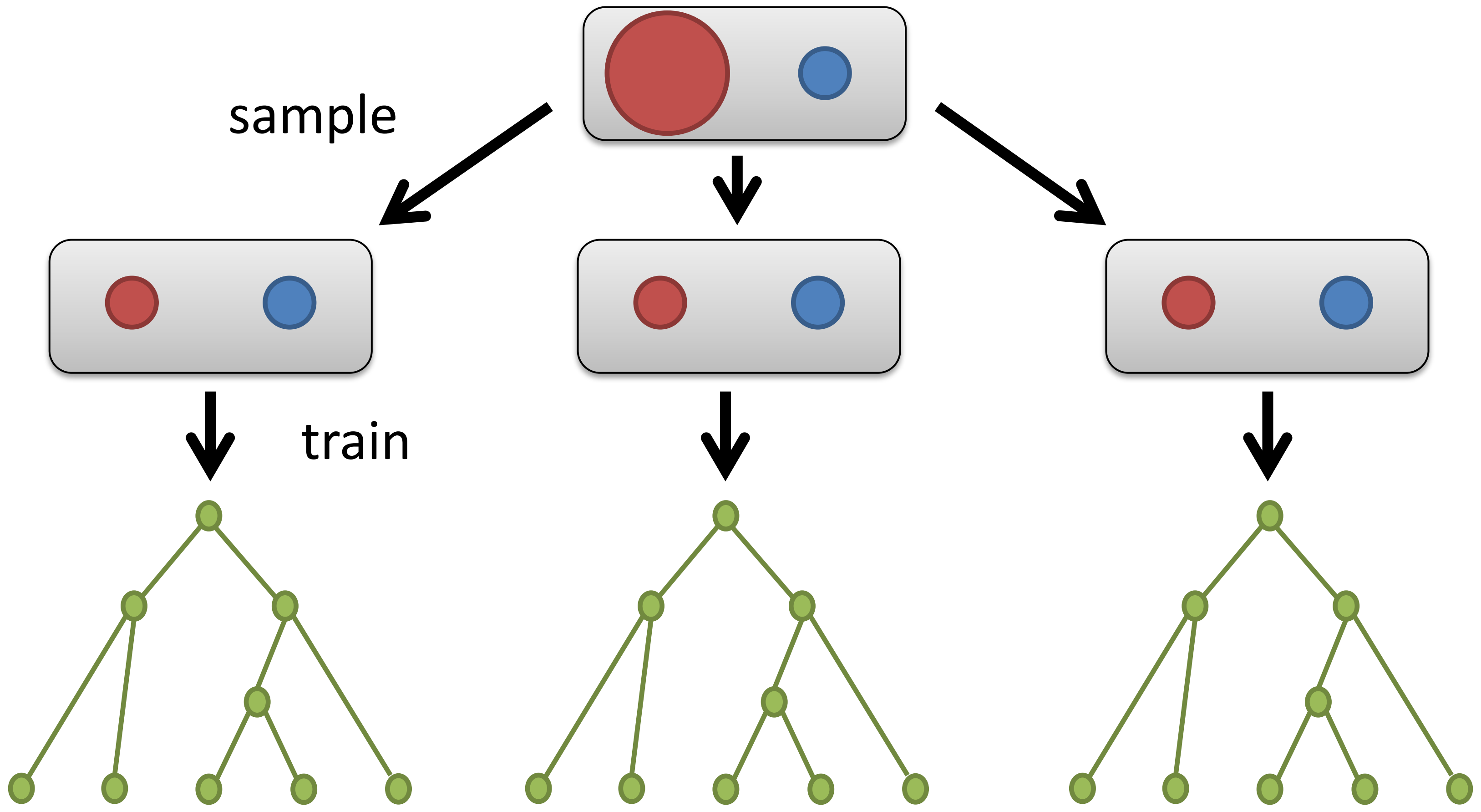


- Subsample:

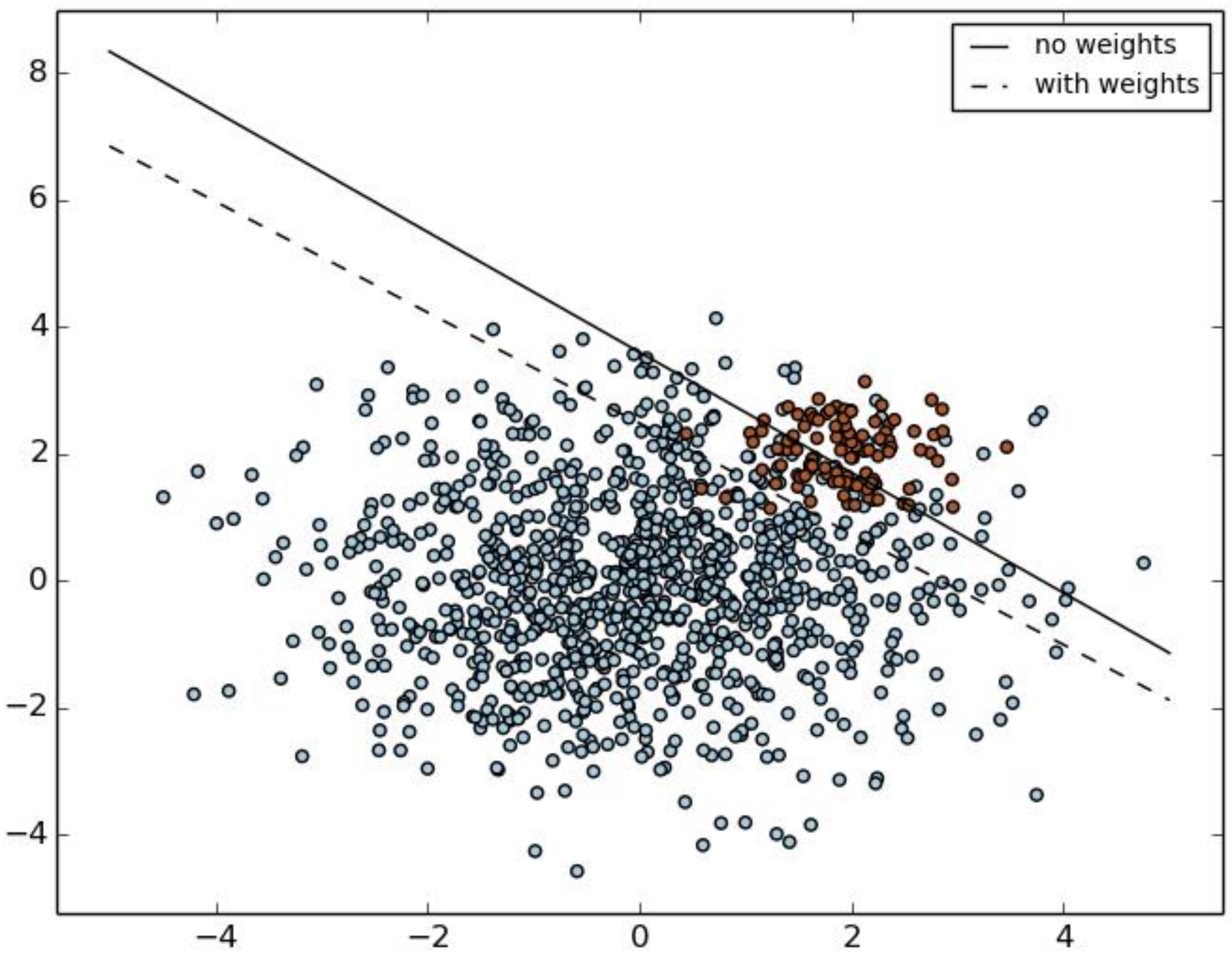


- Subsample for each tree in a random forest

Example: Random Forest Subsampling



Class Weights



http://scikit-learn.org/stable/_images/plot_separating_hyperplane_unbalanced_0011.png

Cross Validation with Imbalanced Classes

- Think about using stratified sampling to generate the folds
- The goal is to have the same class ratio in training, validation and test set.

Missing data

- Delete data points
  - Can cause sample size to be way too small
- Use the mean of the feature
  - Does not change the sample mean, but is independent of the other features.
- Use regression to estimate the value
  - Values will be deterministic

Recommender Systems

- We are already surrounded by them

Good Resources (also for this lecture)

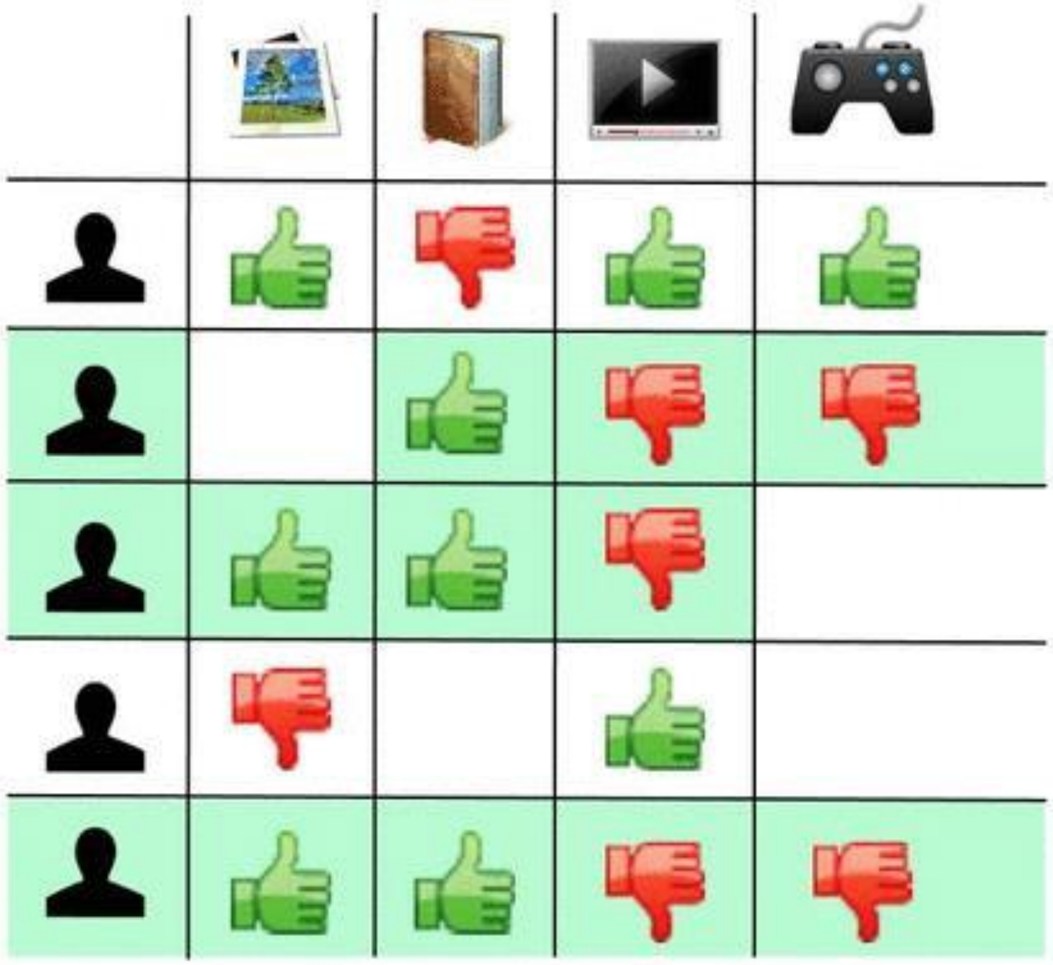
Survey on recommender systems by Michael D. Ekstrand et al.

- http://files.grouplens.org/papers/FnT%20CF%20Recsys%20Survey.pdf

Good slides from Stanford lecture by Lester Mackey

- http://web.stanford.edu/~lmackey/papers/cf_slides-pml09.pdf

Rating Matrix Completion Problem



	🖼	📕	▶	🎮
👤	👍	👎	👍	👍
👤		👍	👎	👎
👤	👍	👍	👎	
👤	👎		👍	
👤	👍	👍	👎	👎

https://en.wikipedia.org/wiki/Collaborative_filtering

Collaborative Filtering

Insight: Personal preferences are correlated

- If Jack loves A and B, and Jill loves A, B, and C, then Jack is more likely to love C

- Does not rely on item or user attributes (e.g. demographic info, author, genre)

Content-based Filtering

- Each item is described by a set of features
- Measure similarity between items
- Recommend items that are similar to the items the User liked

Comparison

- Collaborative filtering:
  - Items entirely described by user ratings
  - Good for new discoveries
  - People who like SciFi maybe also like Fantasy
- Content-based filtering:
  - Predictions are in users comfort zone
  - Can start with a single item
- Can do a hybrid approach

User Based Collaborative Filtering

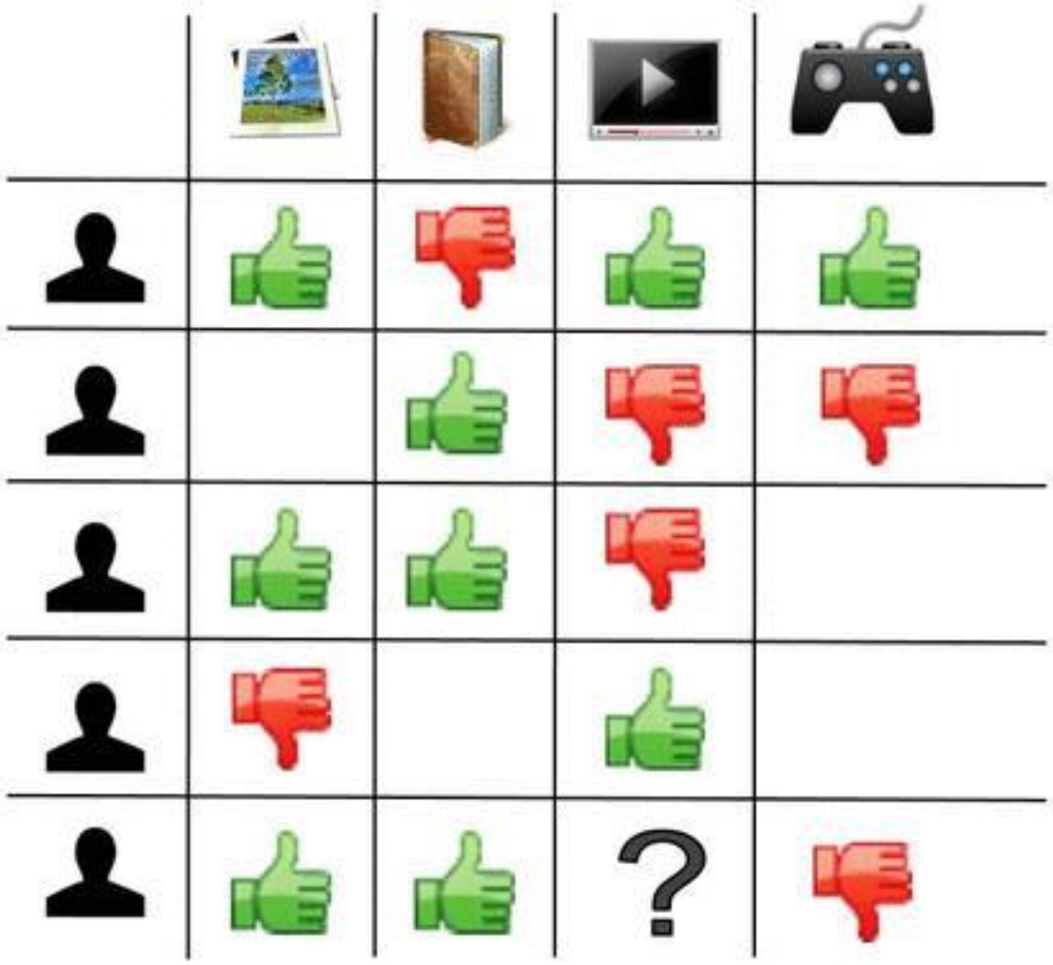
Intuition:

- I like what people similar to me like
- Users give ratings
- People with similar ratings in the past assumed to have similar ratings in the future

Item-based Collaborative Filtering

- Similar, but looks at the items instead of the users
- Useful if the user base is way larger than the number of items.
- More useful: Items are relatively stable in their rating, users vary more.

Short Recap of Terminology



https://en.wikipedia.org/wiki/Collaborative_filtering

We Could Use Missing Data Strategies

All that we talked about earlier:

- Omitting samples
- Using the mean rating of an item
- Doing regression

CF as Regression

- Choose favorite regression algorithm
- Train a predictor for each item
- Each user who rated that item provides one sample
- To predict rating of an item A, apply predictor for A to the user’s incomplete ratings vector.

Recommendation by Regression

- **Pros:**
  - Reduces recommendations to a well-studied problem
  - Many good prediction algorithms available

- **Cons:**
  - Have to handle tons of missing data
  - Training M predictors is expensive

KNN for Collaborative Filtering

- Widely used
- Item-based and User-based focus
- Represent each user as incomplete vector of item ratings
- Compute similarity between query user and all other users
- Find K most similar users who rated the query item
- Predict weighted average of ratings

Similarity Measures

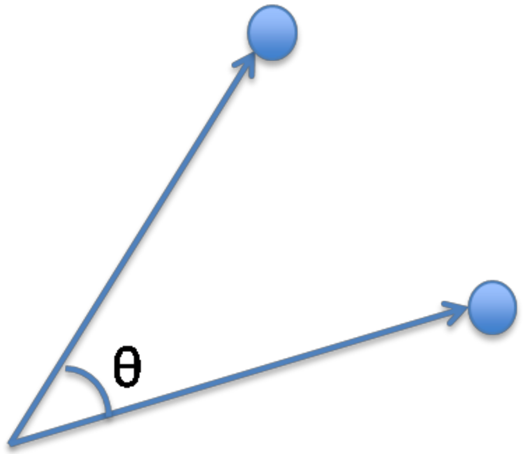
- Pearson Correlation Coefficient
  - bound between 1 and -1
  - suffers from computing high similarity between users with few ratings in common
  - set threshold for minimum number of co-rated itemssuffers from computing high similarity between users with few ratings in common

$$s(u,v) = \frac{\sum_{i \in I_u \cap I_v} (r_{u,i} - \bar{r}_u)(r_{v,i} - \bar{r}_v)}{\sqrt{\sum_{i \in I_u \cap I_v} (r_{u,i} - \bar{r}_u)^2} \sqrt{\sum_{i \in I_u \cap I_v} (r_{v,i} - \bar{r}_v)^2}}$$

Similarity Measures

- Cosine similarity
  - vector-space approach based on linear algebra
  - Unknown ratings are considered to be 0
  - this causes them to effectively drop out of the numerator

$$sim(A,B) = \cos(\theta) = \frac{A \cdot B}{\|A\|\|B\|}$$



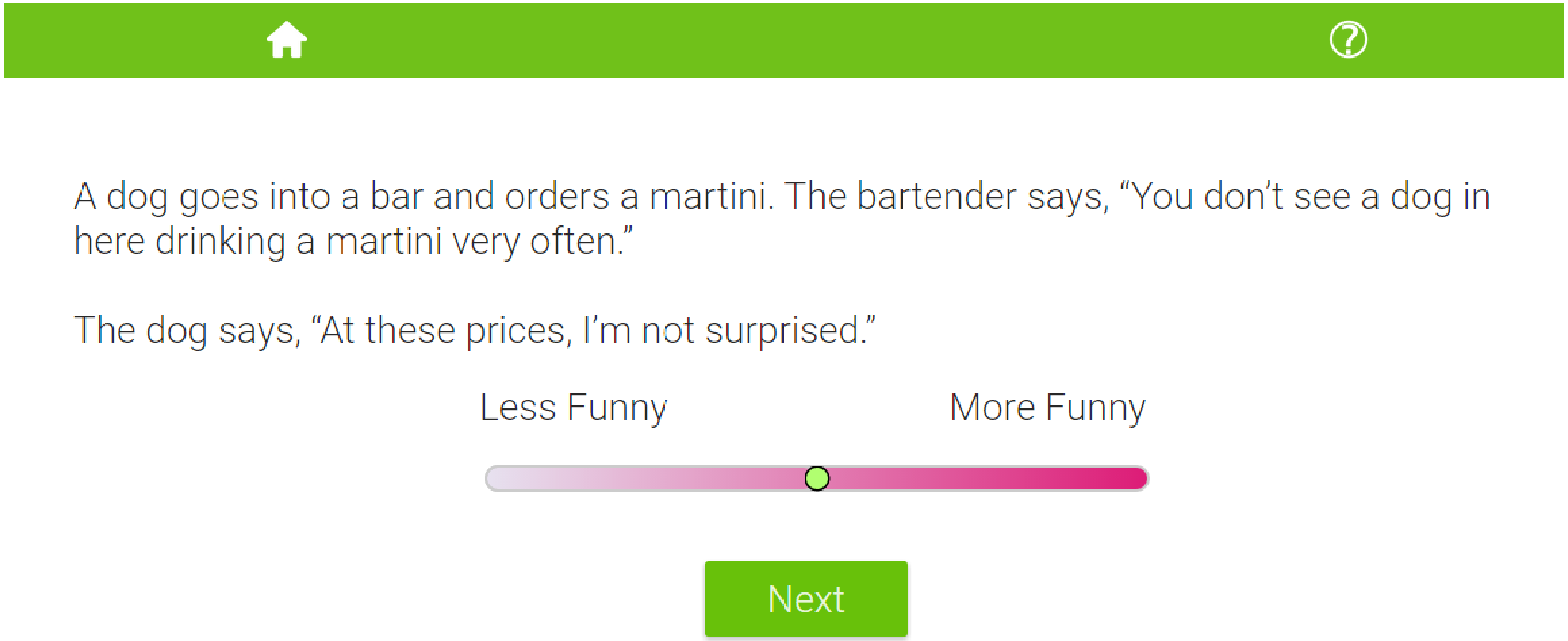
Dimensionality Reduction

- We have treated item or user ratings as vectors
- In many dimensions
- With lots of missing data

- Can we find a low-dimensional sub-space that captures our data?

Eigentaste

- http://eigentaste.berkeley.edu/index.html



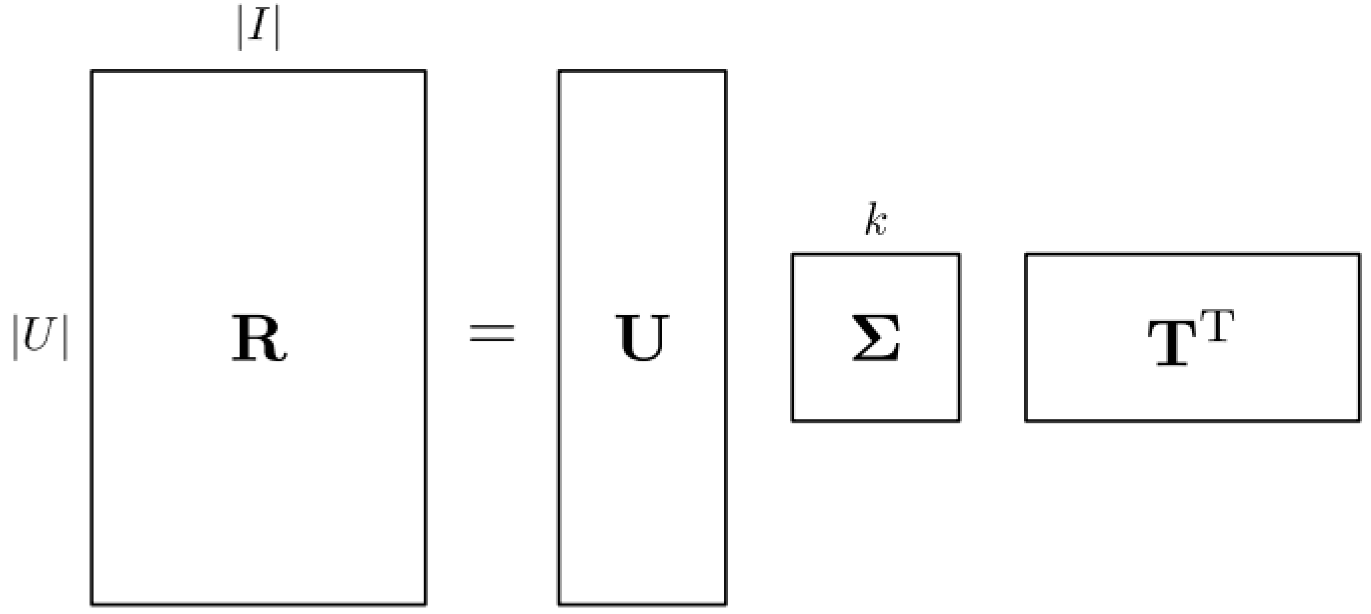
A dog goes into a bar and orders a martini. The bartender says, “You don’t see a dog in here drinking a martini very often.”

The dog says, “At these prices, I’m not surprised.”

PCA for Recomendations

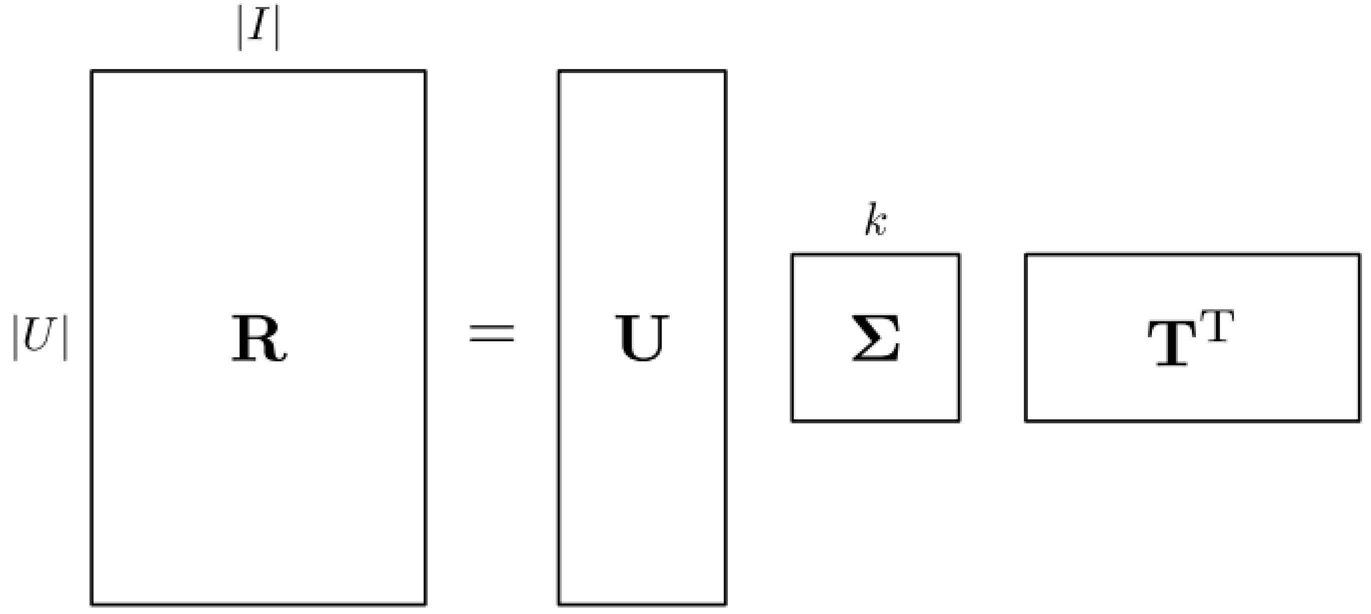
- Compute PCA of a dense rating matrix
- Keep the k largest components
- Project users into k-dimensional subspace
- Cluster users in k-dimensions
- Recommend jokes based on users cluster

Singular Value Decomposition



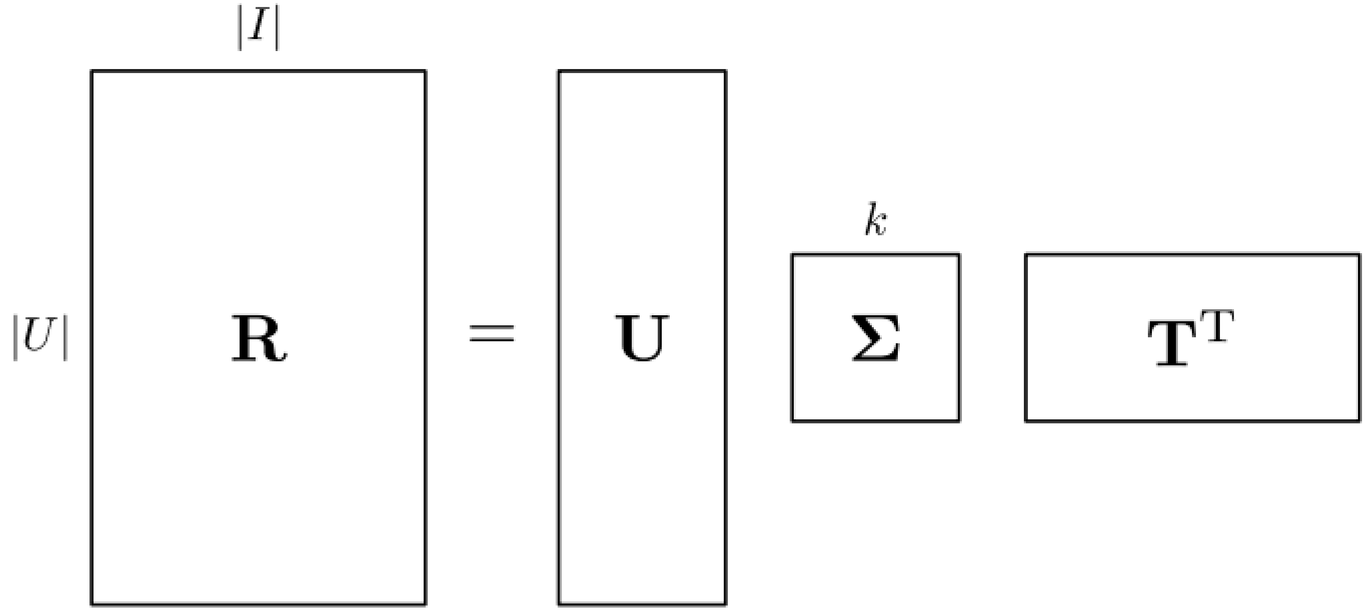
- This is what Simon Funk did for the Netflix prize: http://sifter.org/~simon/journal/20061027.2.html

Singular Value Decomposition



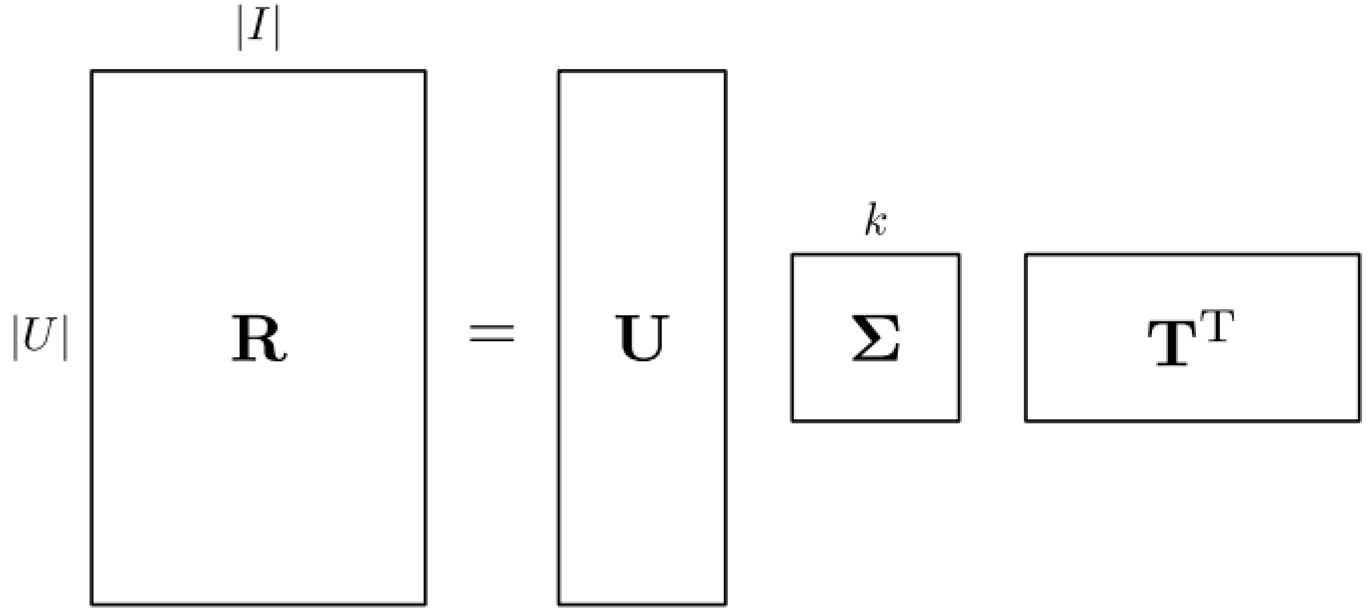
- Decomposes each matrix into three components
- Σ is diagonal and the entries are the singular values of the decomposition

Singular Value Decomposition



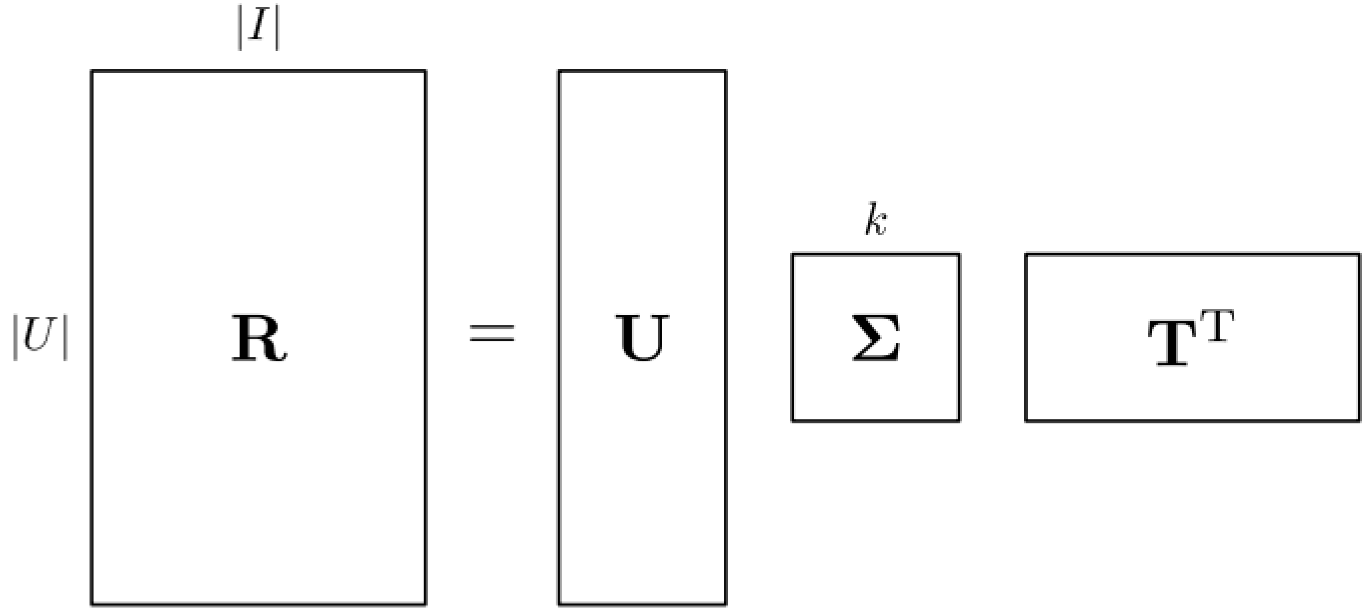
- U and T are orthogonal
- As in PCA we can truncate Σ to compute a lower rank approximation of R.

Singular Value Decomposition



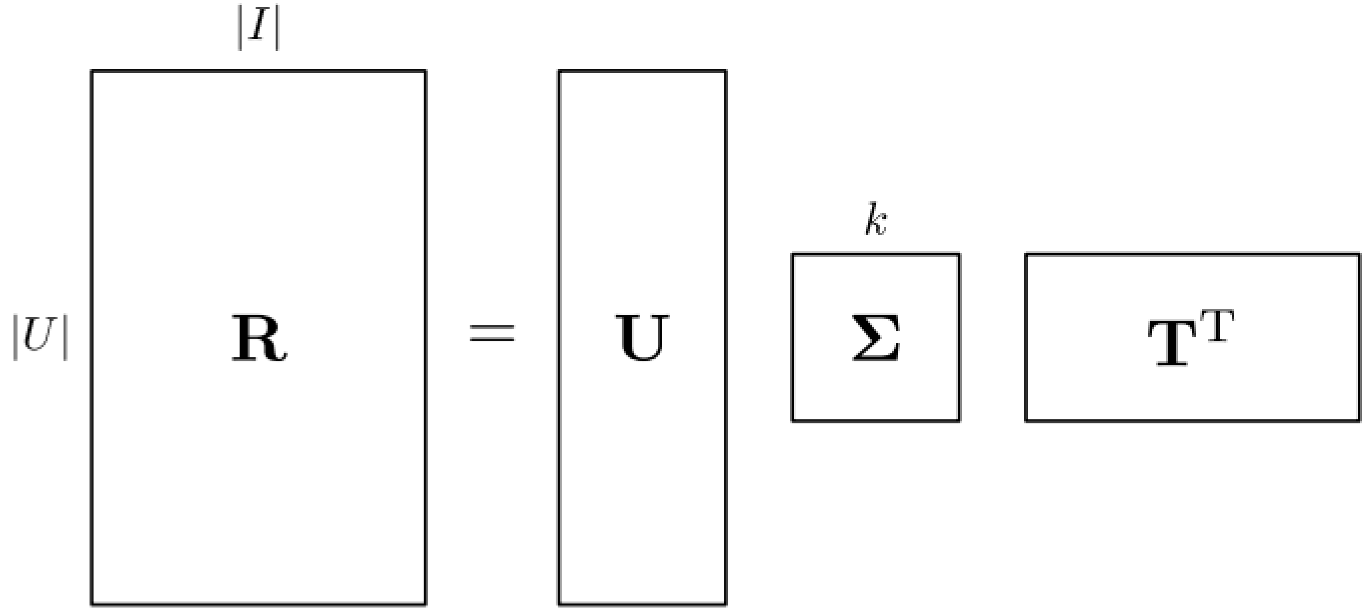
- Rows of U are users interest in the k inferred topics
- Rows of T are the items relevance for each topic

Singular Value Decomposition



- A user’s preference for an item, therefore, is the weighted sum of the user’s interest in each of the topics times that item’s relevance to the topic.

Singular Value Decomposition



- If we know the SVD, we could compute the missing values in R.
- Try to infer SVD from matrix with missing data, and reconstruct full matrix R