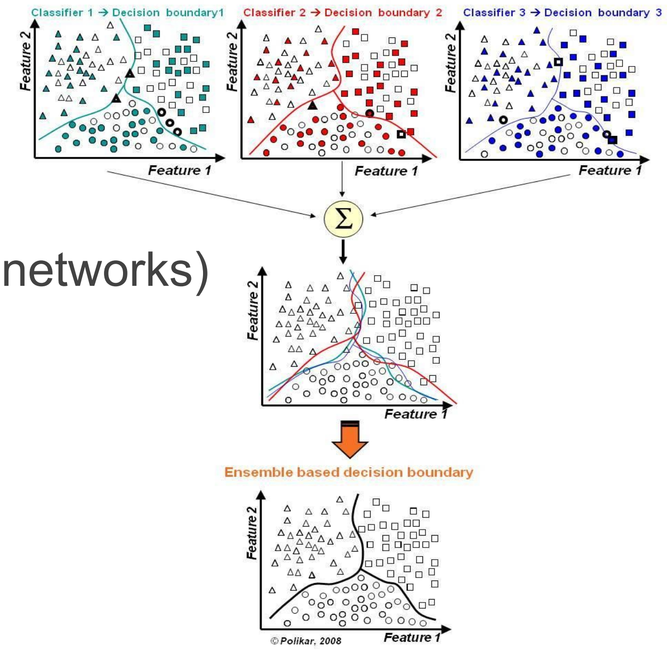
# Ensemble Learning

# What is Machine Learning Ensembles?

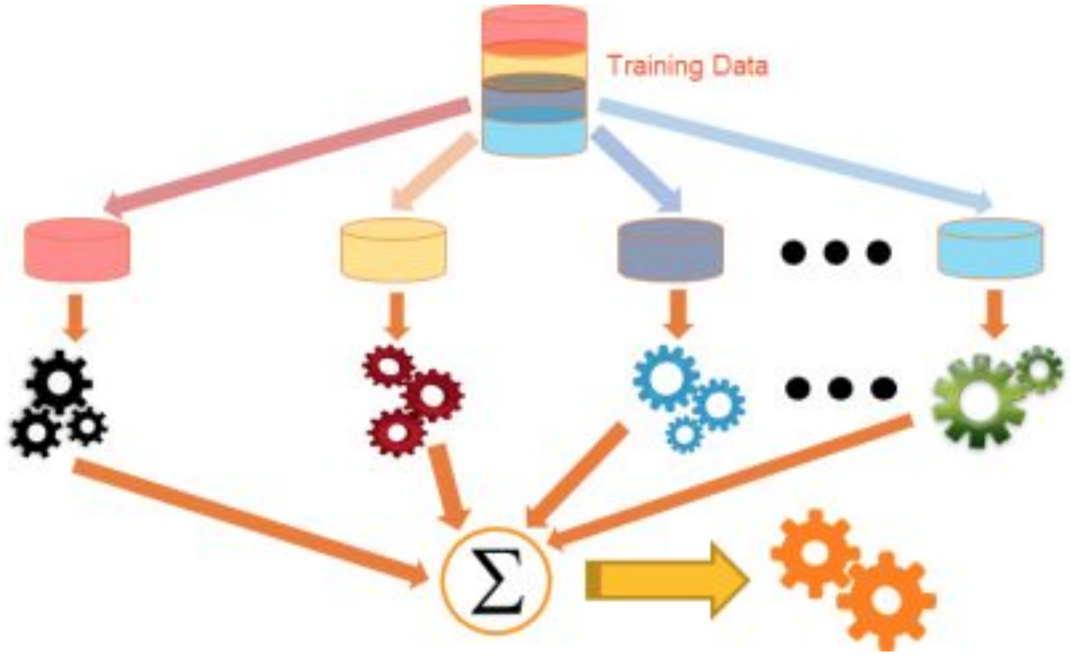
# Machine Learning Ensembles

- Techniques that generate a group of base learner with when combined have higher accuracy
- Strong v.s. Weak learner
- Stable (kNN) v.s. Unstable (decision trees, neural networks) machine learning algorithms.



# Why Ensemble?

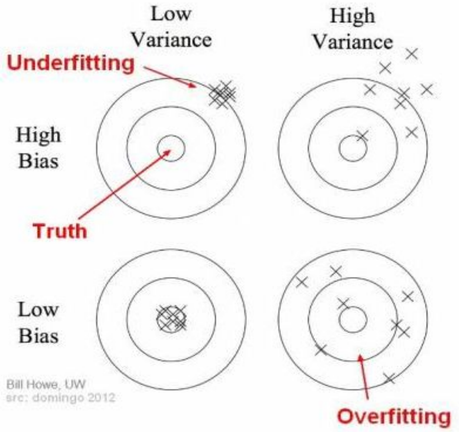
- Reduce Bias
- Reduce Variance
- Prediction Error:
  = Bias ^2
  + Variance
  + Irreducible Error



# Bias-Variance

- **Bias**: the difference between the average prediction of our model and the correct value which we are trying to predict

- **Variance**: the variability of model prediction for a given data point or a value which tells us spread of our data



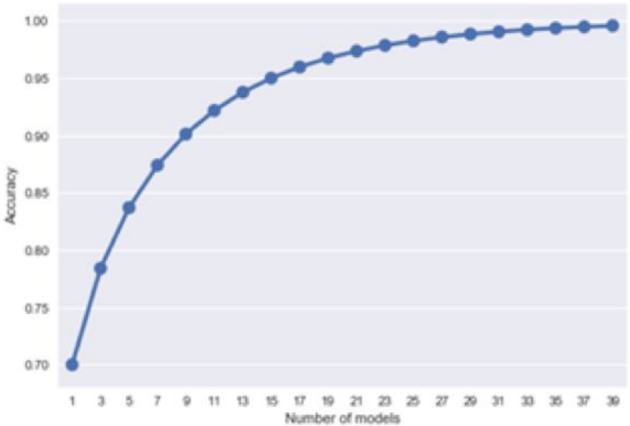
# Reduce Bias

- Assume a test set of 10 samples and k (assume k is odd) independent binary classifiers, where each classifier has p accuracy. By combining these k classifiers using majority voting, the improved accuracy will be

$$\sum_{i=0}^{\lfloor \frac{k}{2} \rfloor} \binom{k}{i} p^{k-i}(1-p)^{i}$$

If p = 0.7, then we have

| k | Ensemble Accuracy |
|---|---|
| 1 | 0.7 |
| 3 | 0.784 |
| 5 | 0.83692 |
| 11 | 0.92177520904 |
| 101 | 0.999987057446 |



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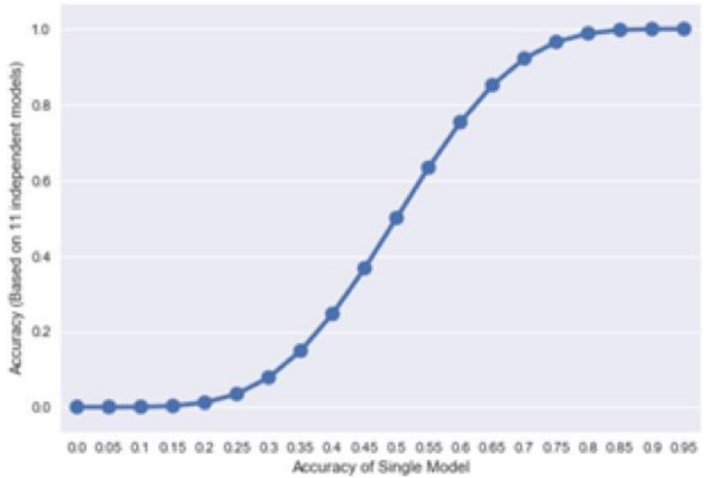
Fix # of classifiers to be 11

**the weak learners should be better than random guess**

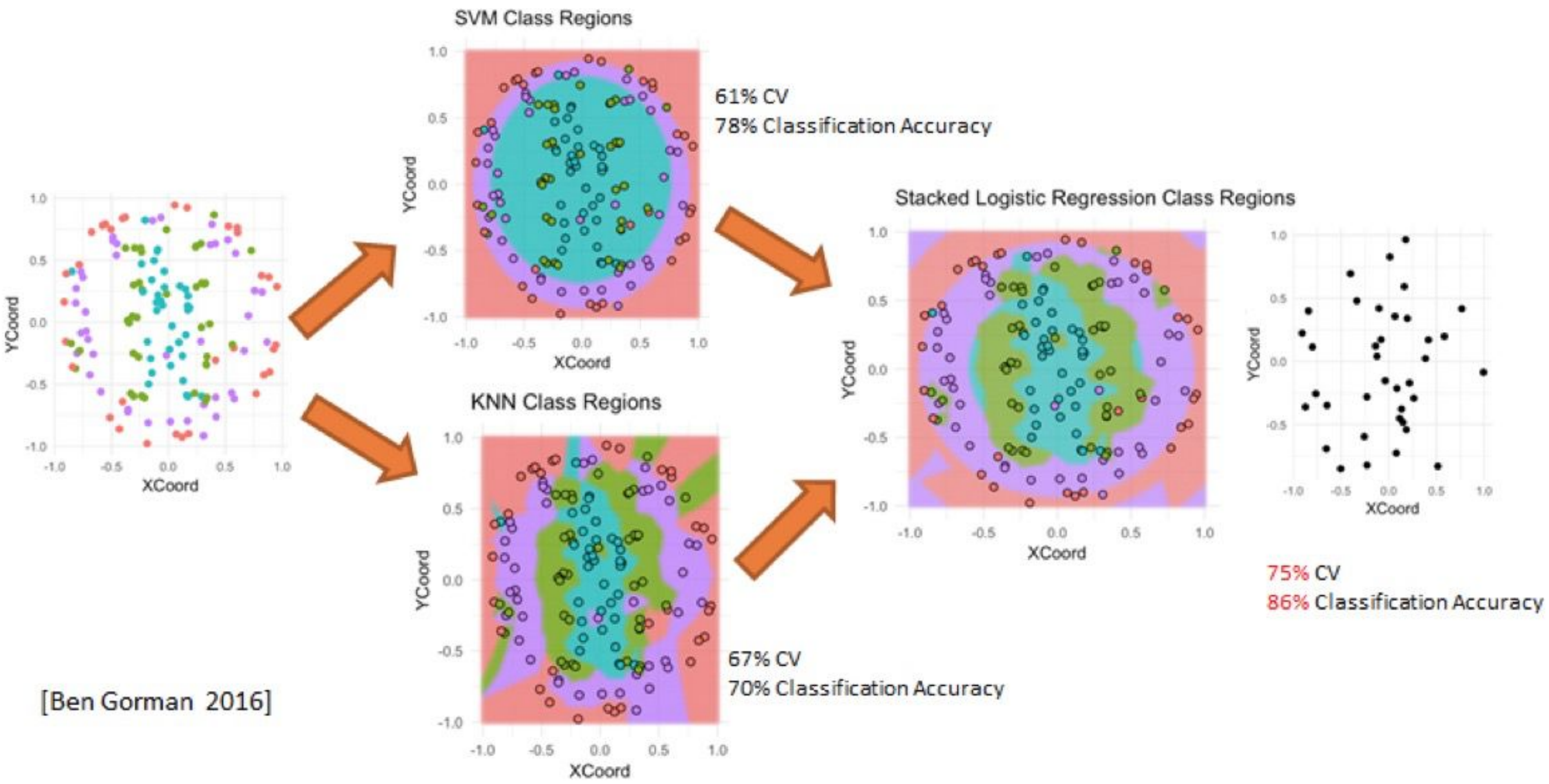


# Reduce Variance

- Suppose we have n independent models: M1, M2, …. Mn with the same variance σ ^2. The ensemble constructed from these models using averaging will have the variance as follows:

$$
\begin{aligned}
\mathrm{Var}(M^*) &= \mathrm{Var}\left(\frac{1}{n}\sum_i M_i\right) \\
&= \frac{1}{n^2}\mathrm{Var}\left(\sum_i M_i\right) \\
&= \frac{1}{n^2}\cdot n \cdot \mathrm{Var}(M_i) \\
&= \frac{\mathrm{Var}(M_i)}{n}
\end{aligned}
$$

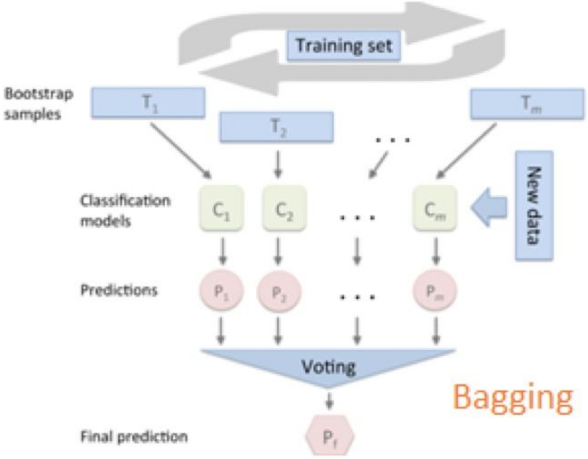
# Machine Learning Ensembles



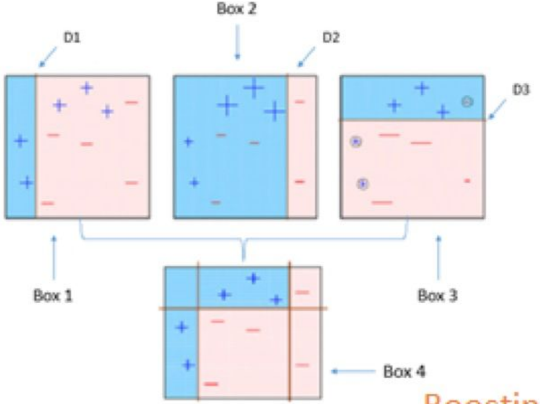

[Ben Gorman 2016]

# Common Ensemble Techniques

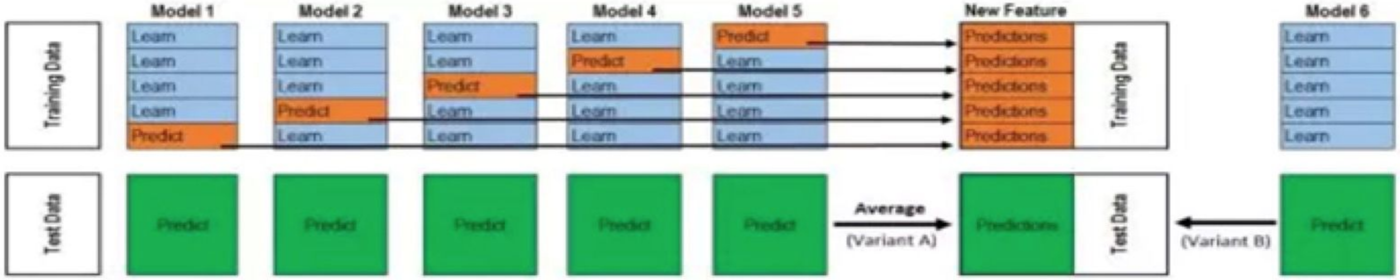
# Overview




Bagging




Boosting




Blending/Stacking

each data samples same weight

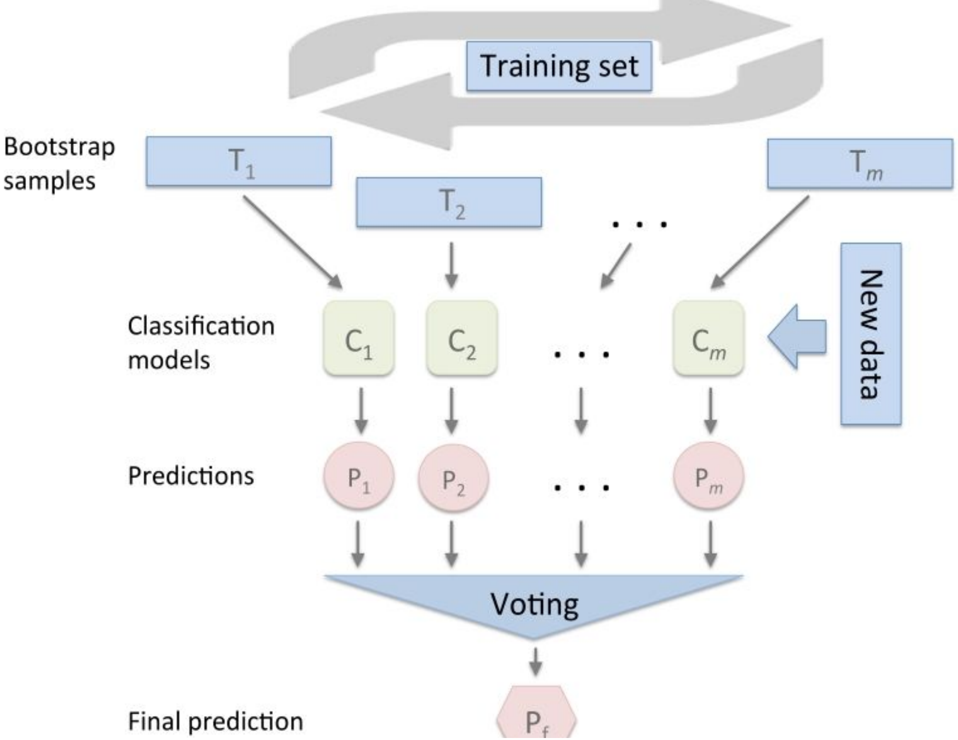
take the majority voting if it is a classification problem. take average if regression

# Bagging

- A.k.a Bootstrap aggregation do sampling for the dataset
- Train m classifier from m bootstrap replica
- Combine outputs by voting
- Decreases error by decreasing the variance
- Random Forest (Randomly select features)
- ExtraTrees (Randomized top-down split)

based on the decision tree

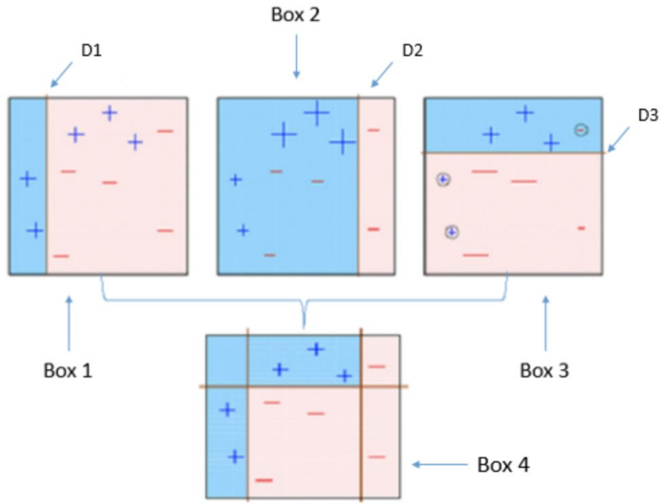
can be trained parallel



# Boosting

**different data weight will be given**

- Training samples are given weights (initially same weight)
- At each iteration, a new hypothesis is learned.
- Training samples are reweighted to focus the model on samples that the most recently learned classifier got wro
- Combine output by voting
- Gradient Boosting, Adaboost, XGBoost, LightGBM



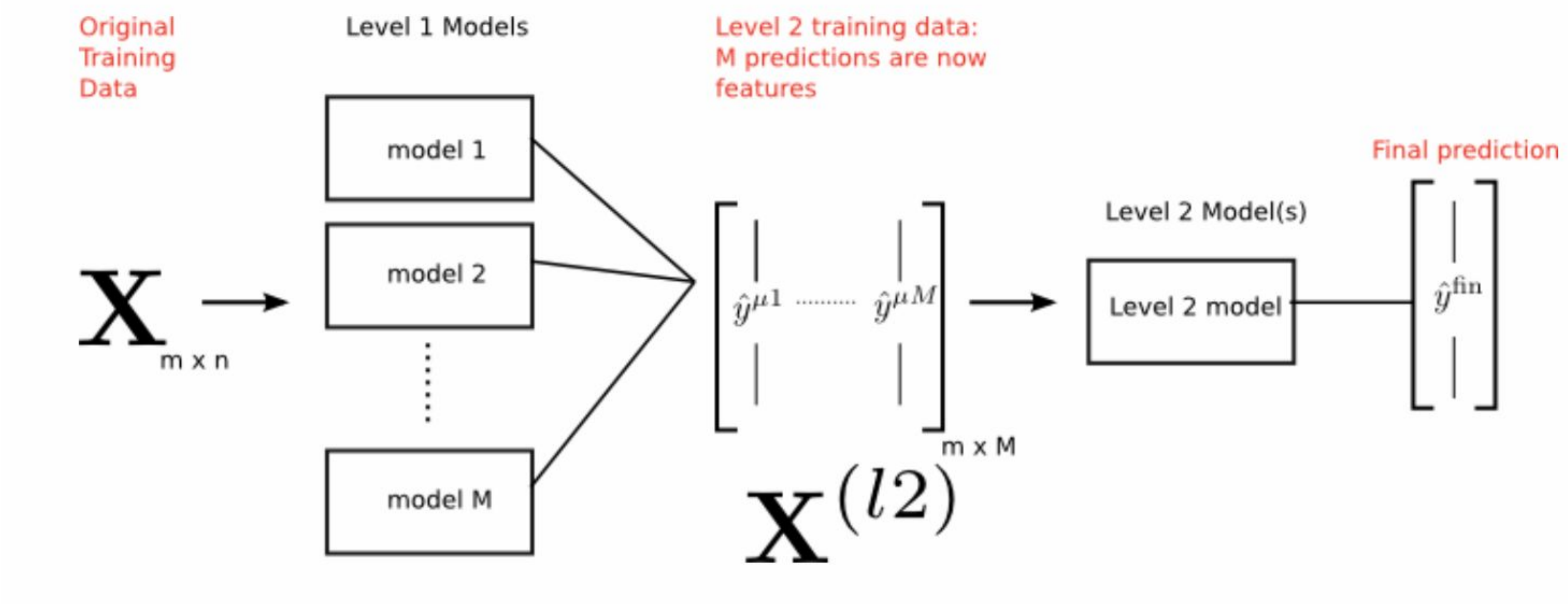

**should train the model sequentially**

# Stacking/Blending

use different models

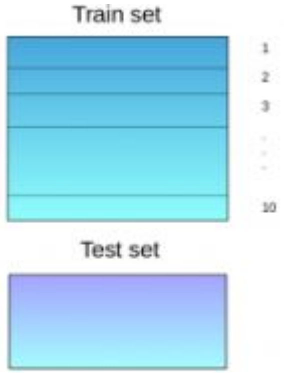
the level 1 prediction will be used as the features as level 2 model

- They are both ensemble learning technique that uses predictions from multiple models (such as KNN, SVM or Decision Tree) to build a new model.

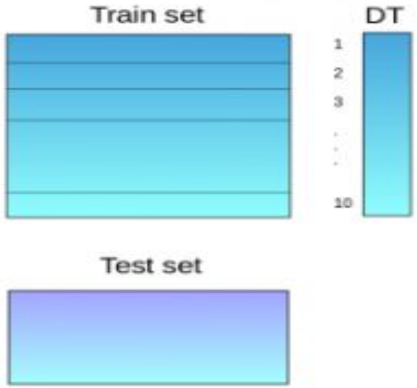


# Stacking

1 Train set is split into 10 parts

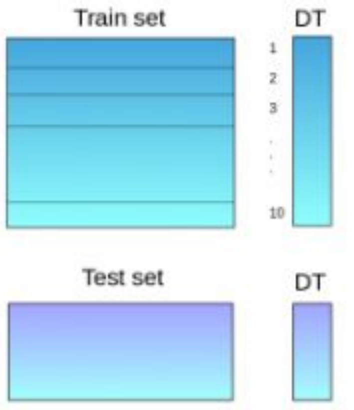



2 A base model is trained on 9 parts and predictions are made for the 10th part. It is looped for each part of data. And the prediction is regarded as new features.

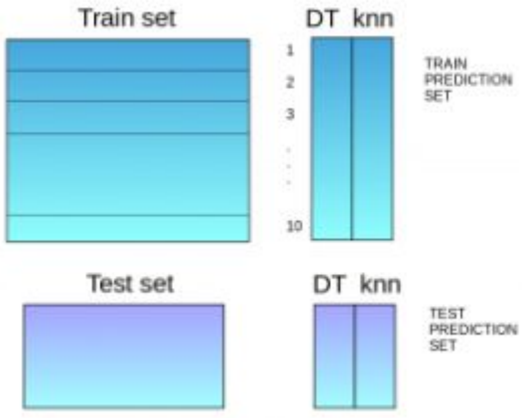


# Stacking

3 The based model is then fitted on the whole train dataset. Then, predictions are made on the test dataset as the new features.

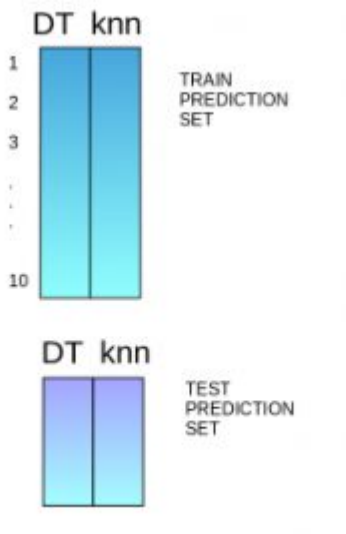



4. Steps 2-3 are repeated for another base model. Then, we are going to have another set of predictions for the train set and test set.



# Stacking

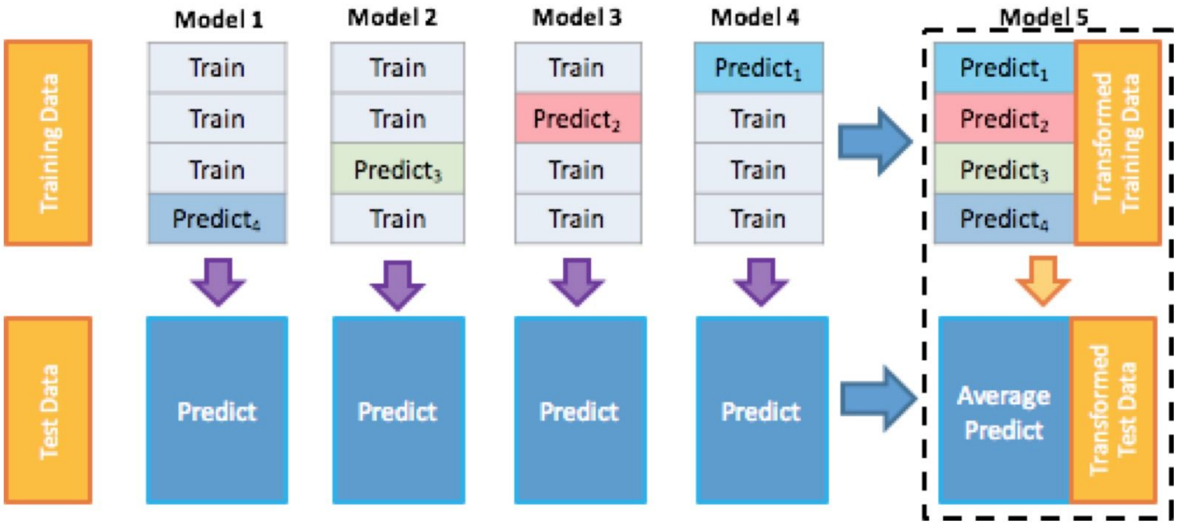
5 The predictions from the train set are used as features to build a new model.




6. This model is used to make final predictions on the test prediction set.

# Stacking

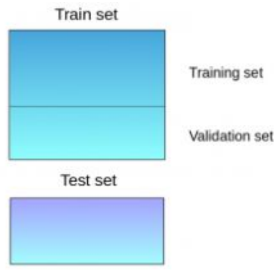
- Slightly different: in step 3, we just take the average predictions from one base model applied over different folders instead of re-training of the base model over the whole training dataset.



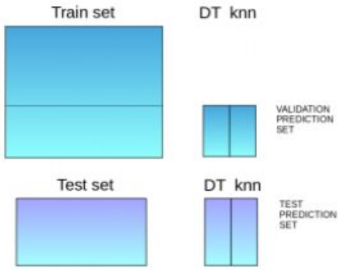
# Blending

- Different from stacking, blending does not perform cv. The holdout set and its predictions are used to build a model which is run on the test set.

1 The train set is split into training and validation sets.




2 Models are fitted on the training set. And the predictions are made on validation set and test set




3 The validation set and its predictions are used as features to build a new model (level-2).

4 This model is used to make final predictions on test dataset and meta-features.

# Some possible pitfalls

- Exponentially increasing training times and computational requirements
- Increase demand on infra. to  maintain and update these models.
- Greater chance of data leakage between models or stages in the whole training.

# In a nutshell

- **No Free Lunch Theorem**: There is no one algorithm that is always the most accurate.
- Our efforts should focus on obtaining base models which make different kinds of errors, rather than obtaining highly accurate base models
- What we need to do is to build weak learners that are at least more accurate than random guessing
- Feature Engineering !!!
- Keep trying (experimenting, tuning, etc.) !