Ensemble learning

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Ensemble learning

Definition 1

Ensemble learning - using multiple machine learning methods for a given problem and integrating their output to obtain final result.

Synonyms: committee-based learning, multiple classifier systems.

Applications:

- supervised methods: regression, classification
- unsupervised methods: clustering

Ensembles use cases

- solving C class classification with many binary classifiers
- underfitting, high model bias
  - existing model hypothesis space is too narrow to explain the true one
  - different oversimplified models have bias in different directions, mutually compensating each other.
- overfitting, high model variance
  - avoid local optima of optimization methods
  - too small dataset to figure out concretely the exact model hypothesis
- when task itself promotes usage of ensembles with features of different nature
  - E.g. computer security:
    - multiple sources of diverse information (password, face detection, fingerprint)
    - different abstraction levels need to be united (current action, behavior pattern during day, week, month)

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Multiclass classification with binary classifiers

- Solved problem: make C-class classification using many binary classifiers.
- Approaches:
  - one-versus-all
    - for each $c = 1, 2, ...C$ train binary classifier on all objects and output $\mathbb{I}[y_n = c]$,
    - assign class, getting the highest score in resulting C classifiers.
  - one-versus-one
    - for each $i, j \in [1, 2, ...C]$, $i \neq j$ learn on objects with $y_n \in \{i, j\}$ with output y_n
    - assign class, getting the highest score in resulting $C(C-1)/2$ classifiers.
  - error correcting codes

Error correcting codes

- Used in classification
- Each class ω_i is coded as a binary codeword W_i consisting of B bits:

$$\omega_i \rightarrow W_i$$

- Minimum sufficient amount of bits to code C classes is $\lceil \log_2 C \rceil$
- Given x, B binary classifiers predict each bit of the class codeword.
- Class is predicted as

$$\hat{c}(x) = \arg\min_c \sum_{b=1}^{B} |W_{cb} - \widehat{p}_b(x)|$$

- where W_{cb} is the b-th bit of codeword, corresponding to class c.
- More bits are used to make classification more robust to errors of individual binary classifiers.
- Codewords are selected to have maximum mutual Hamming distance or randomly.

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- Accuracy improvement for classification
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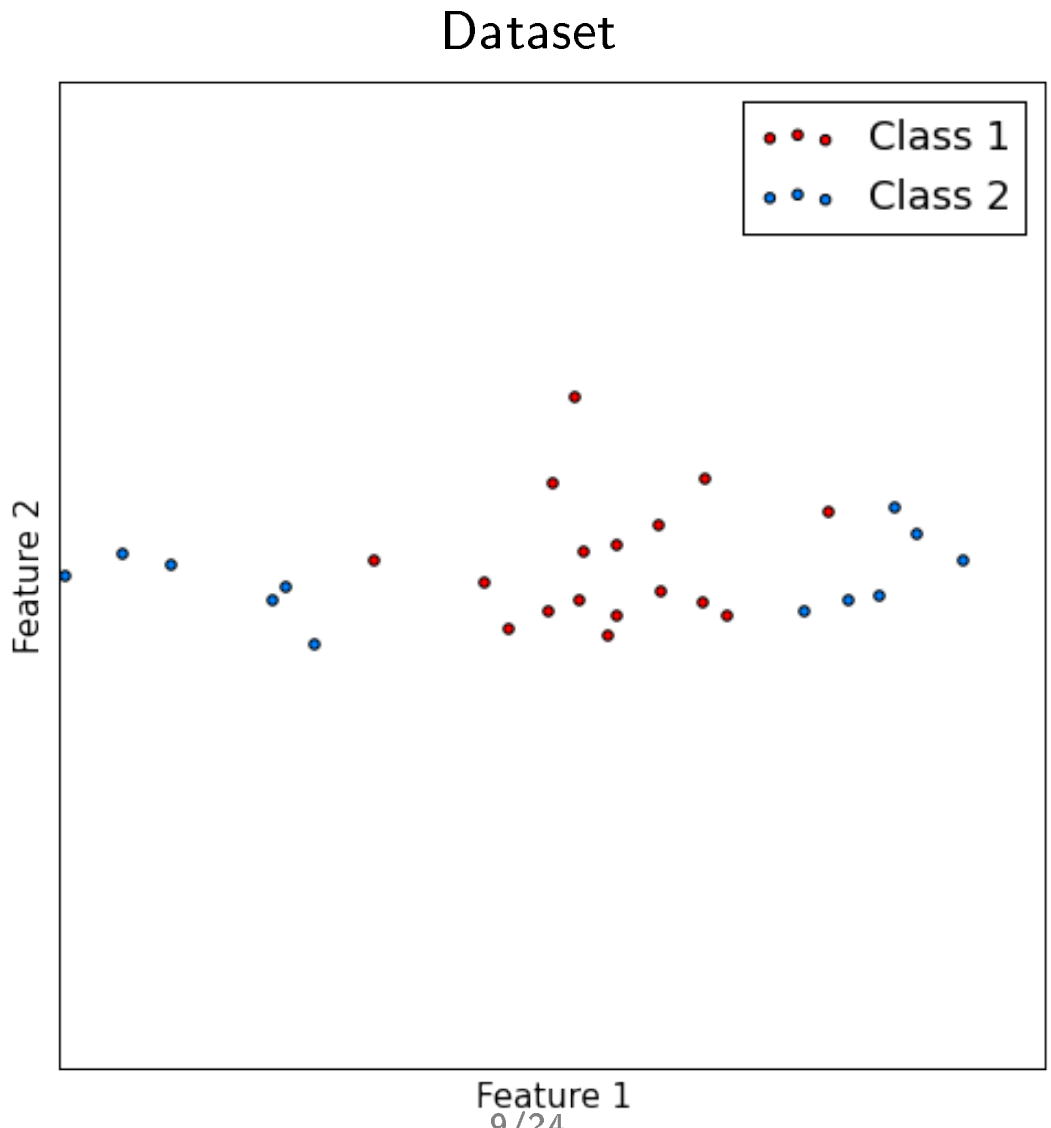
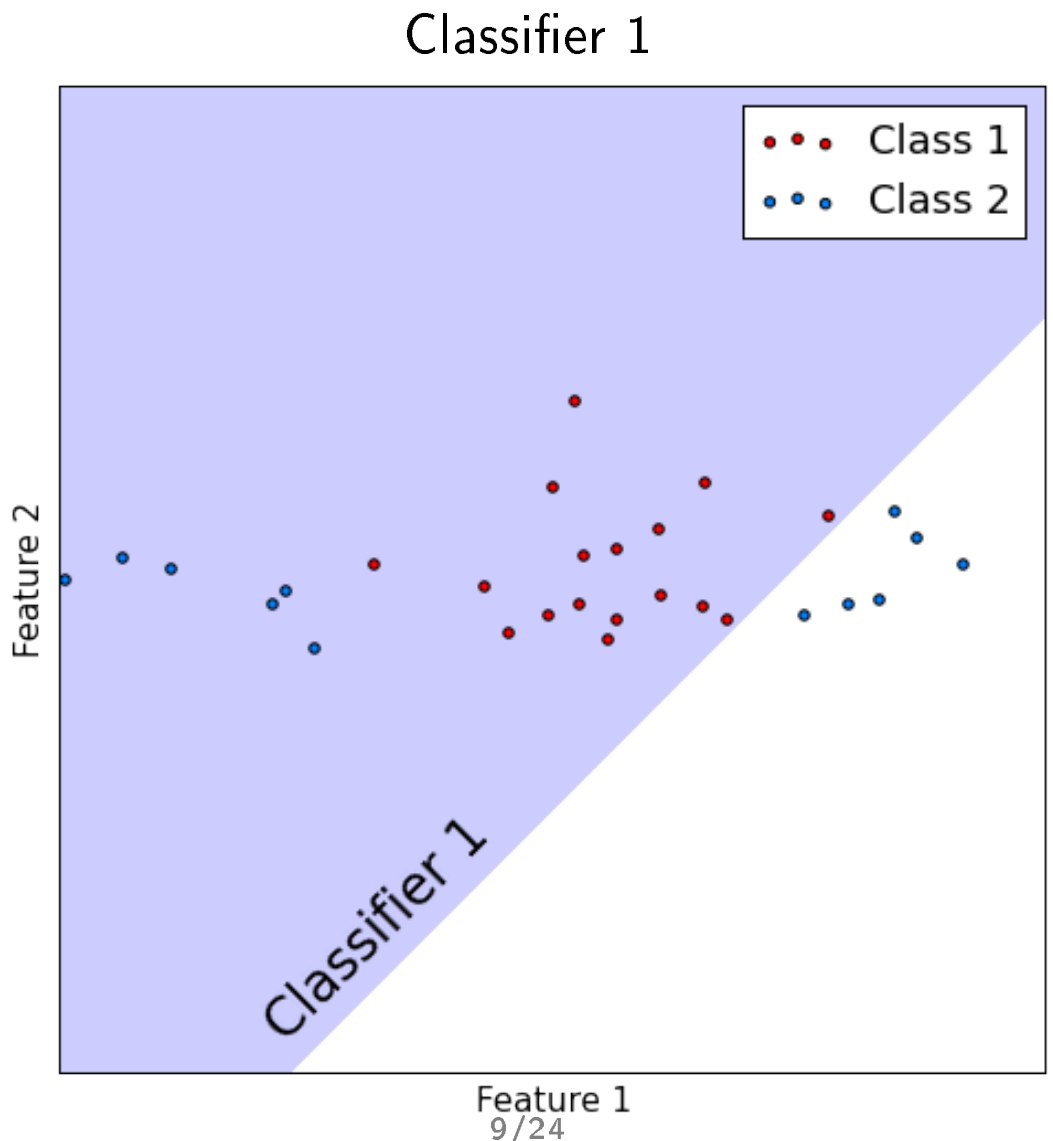
2 Accuracy improvement demos
- Accuracy improvement for classification
- Accuracy improvement for regression

Classification: original model space too narrow



Classification: original model space too narrow



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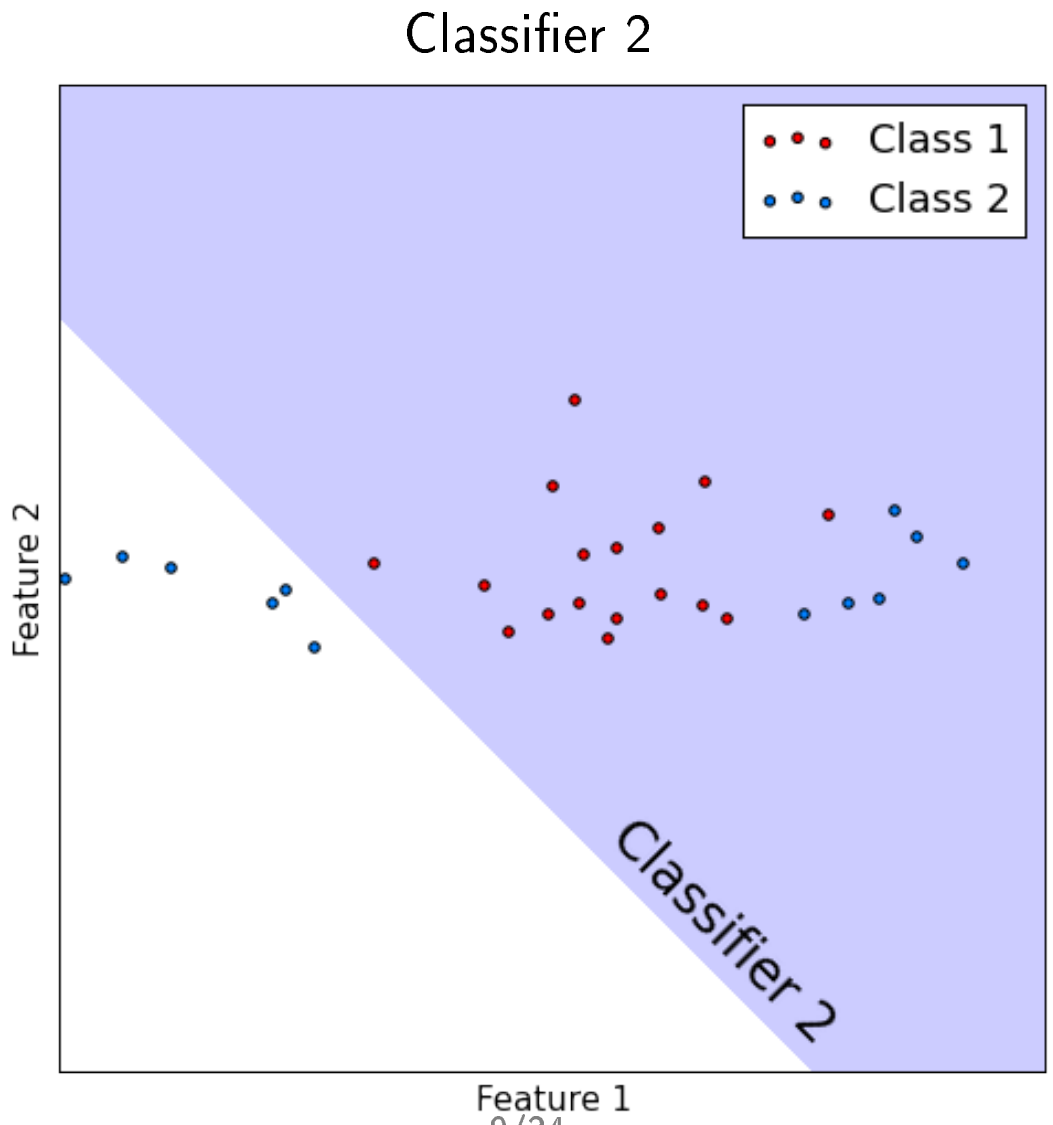
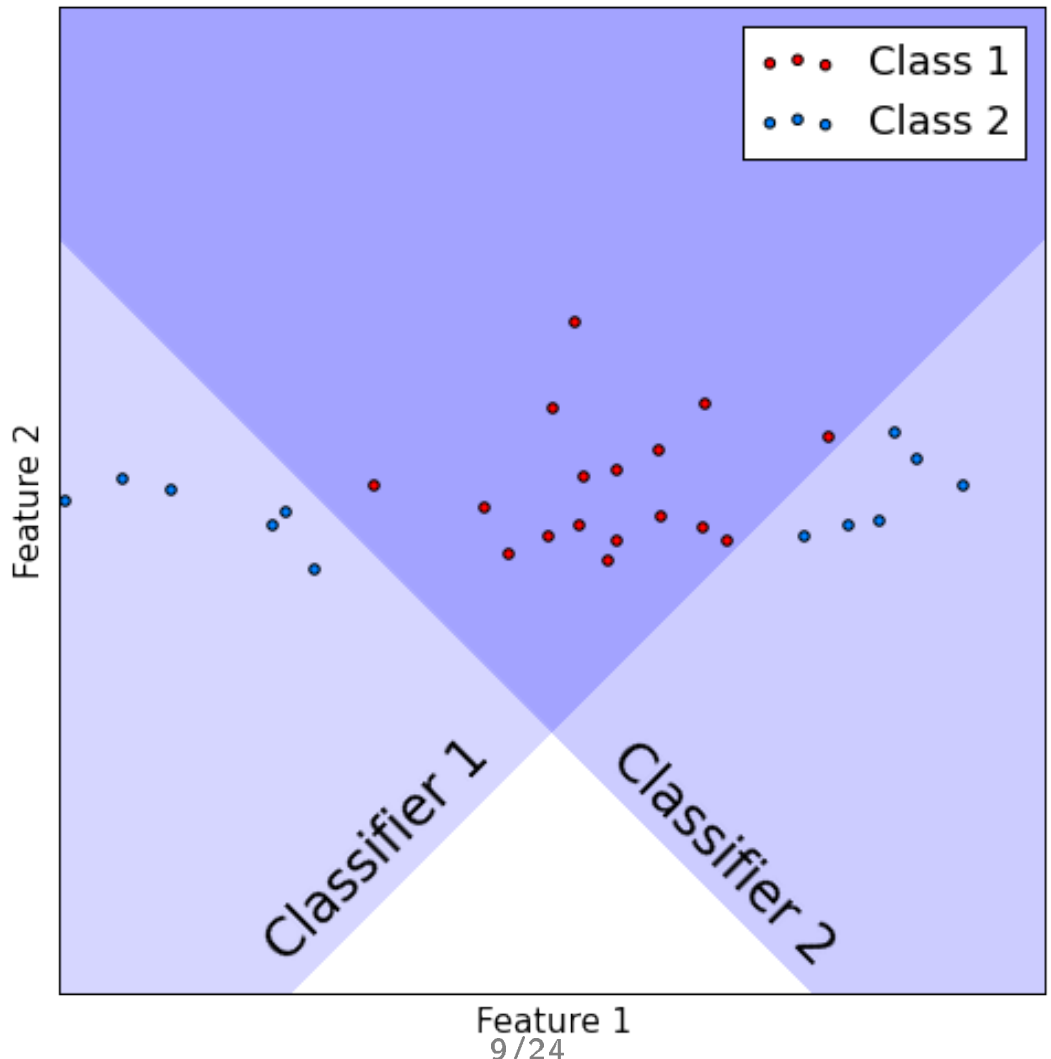


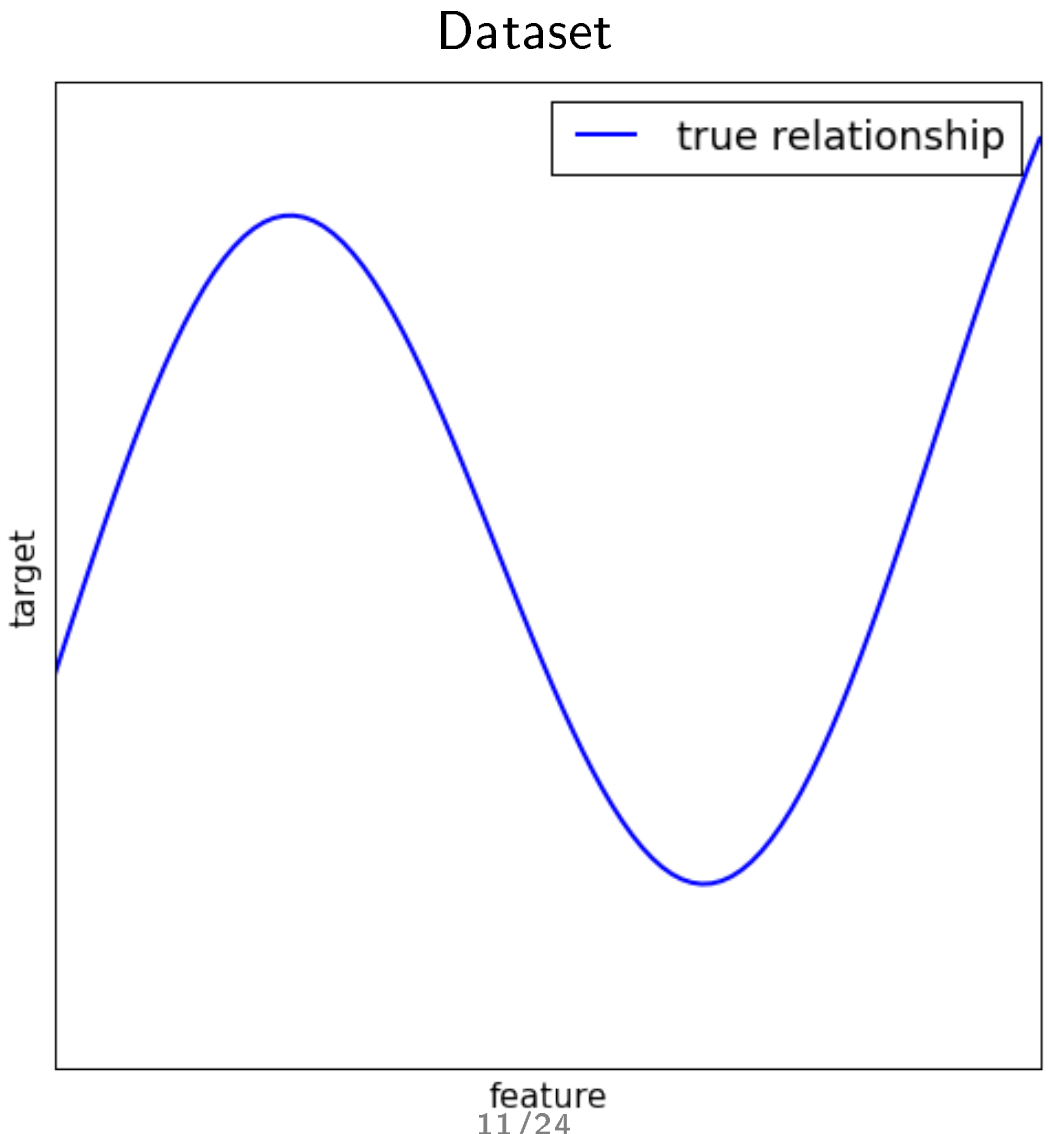
Classification: original model space too narrow

Classifier 1 and classifier 2 combined using AND rule

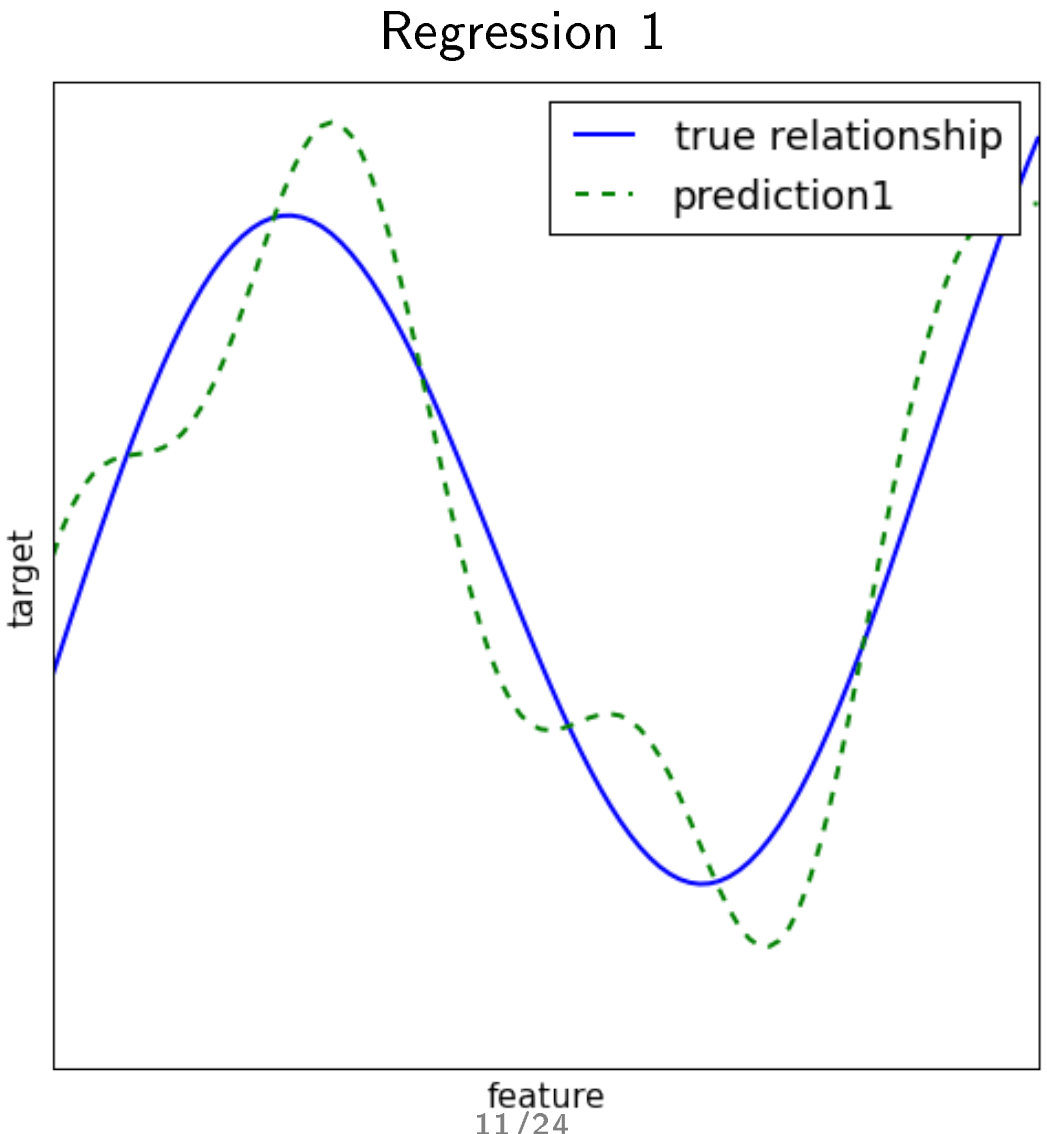


2 Accuracy improvement demos
- Accuracy improvement for classification
- Accuracy improvement for regression

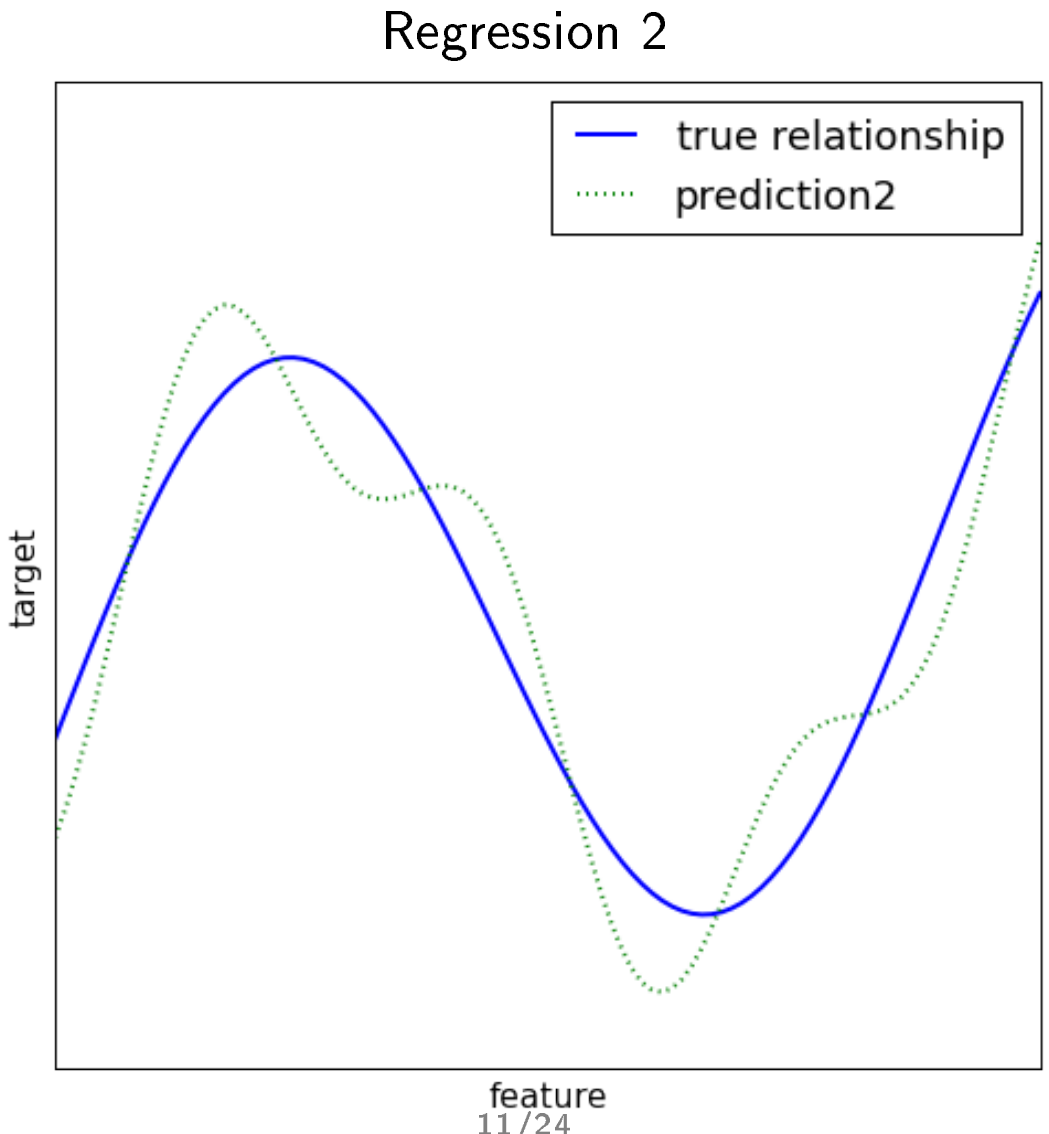
Regression: high variance



Regression: high variance

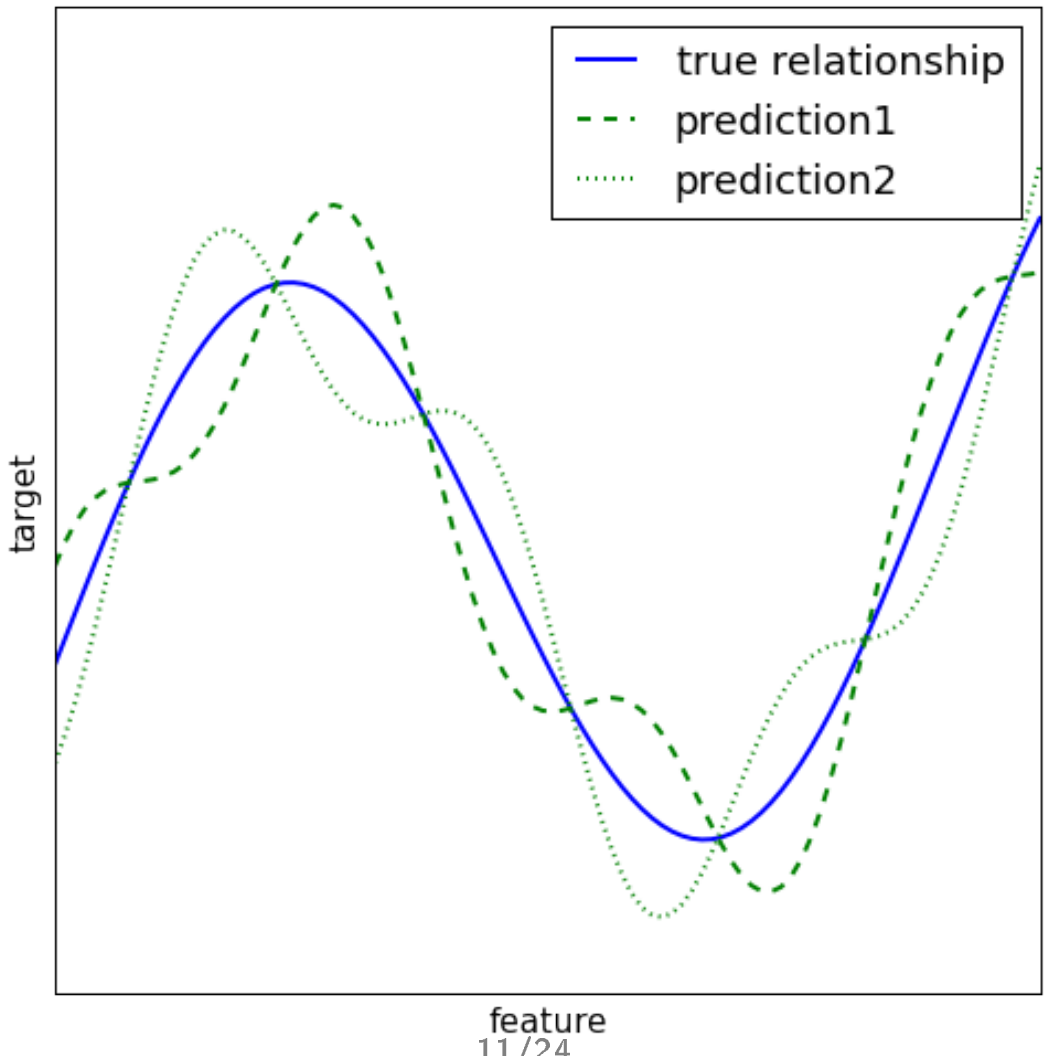


Regression: high variance



Regression: high variance

Regression 1 and regression 2 combined using averaging



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Fixed combiner at class level

Output of base learner k

Exact class: ω_1 or ω_2.

Combiner predicts ω_1 if:

- all classifiers predict ω_1 (AND rule)
- at least one classifier predicts ω_1 (OR rule)
- at least k classifiers predict ω_1 (k-out-of-N)
- majority of classifiers predict ω_1 (majority vote)

Each classifier may be assigned a weight, based on its performance:

- weighted majority vote
- weighted k-out-of-N (based on score sum)

Fixed combiner - ranking level

Output of base learner k

Ranking of classes:

$$\omega_{k_1} \succeq \omega_{k_2} \succeq \ldots \succeq \omega_{k_C}$$

Ranking is equivalent to scoring of each class (with incomparable scoring between classifiers).

Definition 2

Let $B_k(i)$ be the count of classes scored below ω_i by classifier k. **Borda count $B(i)$ of class** ω_i is the total number of classes scored below ω_i by all classifiers:

$$B(i) = \sum_{k=1}^{K} B_k(i)$$

Combiner predicts ω_i where $i = \arg\max_i B(i)$

Fixed combiner at class probability level

Output of base learner k

Vectors of class probabilities:

$$[p^k(\omega_1),\ p^k(\omega_2),\ \dots\ p^k(\omega_C)]$$

Combiner predicts ω_i if $i = \arg\max_i F(p^1(\omega_i), p^2(\omega_i), \dots p^K(\omega_i))$

- F = mean or median.

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Weighted averaging

Consider regression with K predictor models $f_k(x)$, $k = 1, 2, ...K$. (Alternatively we may consider K discriminant functions in classification)

Weighted averaging combiner

$$f(x) = \sum_{k=1}^{K} w_k f_k(x)$$

Naive fitting

$$\widehat{w} = \arg\min_{w} \sum_{i=1}^{N} \mathcal{L}(y_i, \sum_{k=1}^{K} w_k f_k(x_i))$$

will overfit. The mostly overfitted method will get the most weight.

Linear stacking

- Let training set $\{(x_i, y_i), i = 1, 2, ...N\}$ be split into M folds.
- Denote $fold(i)$ to be the fold, containing observation i
- Denote $f_k^{-fold(i)}$ be predictor k trained on all folds, except $fold(i)$.

Definition

Linear stacking is weighted averaging combiner, where weights are found using

$$\widehat{w} = \arg\min_w \sum_{i=1}^{N} \mathcal{L}(y_i, \sum_{k=1}^{K} w_k f_k^{-fold(i)}(x_i))$$

- For decreased overfitting we may add constraints $\{w_k \geq 0\}_{k=1}^K$ or regularizer $\sum_{k=1}^K \left(w_k - \frac{1}{K}\right)^2$.

General stacking

Definition

Generalized stacking is prediction

$$f(x) = A_\theta \left(f_1(x), f_2(x), \dots f_K(x) \right),$$

where A is some general form predictor and θ is a vector of parameters, estimated by

$$\widehat{\theta} = \arg\min_\theta \sum_{i=1}^{N} \mathcal{L} \left(y_i,\ A_\theta \left(f_1^{-fold(i)}(x), f_2^{-fold(i)}(x), \dots f_K^{-fold(i)}(x) \right) \right)$$

- Stacking is the most general approach
- It is a winning strategy in most ML competitions.
- $f_i(x)$ may be:
  - class number (coded using one-hot encoding).
  - vector of class probabilities
  - any initial or generated feature

4 Stacking
- Bagging and random forest

Bagging& random subspaces

- Bagging
  - random selection of samples (with replacement)[1][2]
  - efficient for methods with high variance w.r.t. X, Y.
- Random subspace method:
  - random selection of features (without replacement)
- We can apply both methods jointly
- Also we may sample different

[1] *what is the probability that observation will not belong to bootstrap sample?*

[2] *what is the limit of this probability with* $N \to \infty$*?*

Random forests

Input: training dataset $TDS = \{(x_i, y_i),\ 1 = 1, 2, ...N\}$; the number of trees B and the size of feature subsets m.
for $b = 1, 2, ...B$:

1. generate random training dataset TDS^b of size N by sampling (x_i, y_i) pairs from TDS with replacement.
2. build a tree using TDS^b training dataset with feature selection for each node from random subset of features of size m (generated **individually for each node**).

Output: B trees. Classification is done using majority vote and regression using averaging of B outputs.

Comments

- Random forests use random selection on both samples and features
- Step 1) is optional.
- Left out samples may be used for evaluation of model performance.
  - *Out-of-bag* prediction: assign output to x_i, $i = 1, 2, ...N$ using majority vote (classification) or averaging (regression) among trees with $b \in \{b : (x_i, y_i) \notin T^b\}$
  - *Out-of-bag* quality - lower bound for true model quality.[3]
- Less interpretable than individual trees
- +: Parallel implementation
- -: different trees are not targeted to correct mistakes of each other

[3] why *lower* bound?

Comments

- Extra-Random trees-random sampling of (feature,value) pairs
  - more bias and less variance for each tree
  - faster training of each tree
- RandomForest and ExtraRandomTrees do not overfit with increasing B
- Each tree should have high depth
  - otherwise averaging over oversimplified trees will also give oversimplified model!