Ensemble learning, bias-variance decomposition

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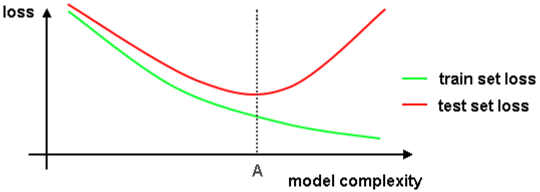
Loss vs. model complexity



Comments:

- expected loss on test set is always higher than on train set.
- left to A: model too simple, underfitting, high bias
- right to A: model too complex, overfitting, high variance

Bias-variance decomposition

- True relationship $y=f(x)+\varepsilon$
- This relationship is estimated using random training set $(X,Y)=\{(x_n,y_n),\ n=1,2...N\}$
- Recovered relationship $\widehat{f}(x)$, x-some fixed constant
- Noise ε is independent of any X, Y, $\mathbb{E}\varepsilon=0$

Bias-variance decomposition

$$\begin{aligned}\mathbb{E}_{X,Y,\varepsilon}\{[\widehat{f}(x)-y(x)]^2\} &= \left(\mathbb{E}_{X,Y}\{\widehat{f}(x)\}-f(x)\right)^2 \\ &\quad +\mathbb{E}_{X,Y}\left\{[\widehat{f}(x)-\mathbb{E}_{X,Y}\widehat{f}(x)]^2\right\}+\mathbb{E}\varepsilon^2\end{aligned}$$

- Intuition: $MSE = \text{bias}^2 + \text{variance} + \text{irreducible error}$
  - darts intuition

Proof of bias-variance decomposition

Define for brevity of notation $f=f(x)$, $\widehat{f}=\widehat{f}(x)$, $\mathbb{E}=\mathbb{E}_{X,Y,\varepsilon}$.

$$\begin{aligned}\mathbb{E}\left(\widehat{f}-f\right)^2 &= \mathbb{E}\left(\widehat{f}-\mathbb{E}\widehat{f}+\mathbb{E}\widehat{f}-f\right)^2=\mathbb{E}\left(\widehat{f}-\mathbb{E}\widehat{f}\right)^2+\left(\mathbb{E}\widehat{f}-f\right)^2\\ &\quad+2\mathbb{E}\left[(\widehat{f}-\mathbb{E}\widehat{f})(\mathbb{E}\widehat{f}-f)\right]\\ &=\mathbb{E}\left(\widehat{f}-\mathbb{E}\widehat{f}\right)^2+\left(\mathbb{E}\widehat{f}-f\right)^2\end{aligned}$$

We used that $(\mathbb{E}\widehat{f}-f)$ is a constant w.r.t. X,Y and hence $\mathbb{E}\left[(\widehat{f}-\mathbb{E}\widehat{f})(\mathbb{E}\widehat{f}-f)\right]=(\mathbb{E}\widehat{f}-f)\mathbb{E}(\widehat{f}-\mathbb{E}\widehat{f})=0$.

$$\begin{aligned}\mathbb{E}\left(\widehat{f}-y\right)^2 &= \mathbb{E}\left(\widehat{f}-f-\varepsilon\right)^2=\mathbb{E}\left(\widehat{f}-f\right)^2+\mathbb{E}\varepsilon^2-2\mathbb{E}\left[(\widehat{f}-f)\varepsilon\right]\\ &= \mathbb{E}\left(\widehat{f}-\mathbb{E}\widehat{f}\right)^2+\left(\mathbb{E}\widehat{f}-f\right)^2+\mathbb{E}\varepsilon^2\end{aligned}$$

Here $\mathbb{E}\left[(\widehat{f}-f)\varepsilon\right]=\mathbb{E}\left[(\widehat{f}-f)\right]\mathbb{E}\varepsilon=0$ since ε is independent of X,Y.

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Ensemble learning

- Ensemble model - model using predictions of other models.
- Example: stacking
  - suppose we have base models $\widehat{y}_1 = f_1(x), ...\widehat{y}_M = f_M(x)$.
  - stacking: $\widehat{y}(x) = G(f_1(x), ...f_M(x))$
- Used in
  - supervised methods: regression, classification, collaborative filtering.
  - unsupervised methods: clustering, dimensionality reduction.

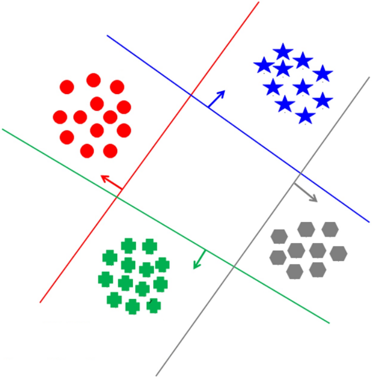
Motivation

- Many binary classifiers->multiclass classifier
- Features of different nature
- Iterated decision
- Solve overfitting
  - apply complex aggregating model
- Solve underfitting
  - e.g. majority voting, averaging
- Solve computational issues
  - e.g. kernel SVM on dataset subsets
- Do not rely on single model assumptions
  - ambiguity decomposition

2. Ensemble learning
    - Ensemble learning use cases

Multiclass classification using binary classifiers

Multiclass classification with one-vs-rest, one-vs-one, error correcting codes schemes:



Iterated decision, different features

Iterated decision

- Separate simple classes: 1,2,"3+4"
    - if "3+4" apply model to separate 3 from 4.
- Flat price prediction:
    - decide type: for living/for investment
    - purpose-for living: model depending on comfort, living tastes, etc.
    - purpose-for investment: another model depending on exchange rates, interest rates, stock growth, etc.
- Face detection on images:
    - detect view type: frontal/profile
    - one model detects face with frontal view
    - another model detects face with profile view

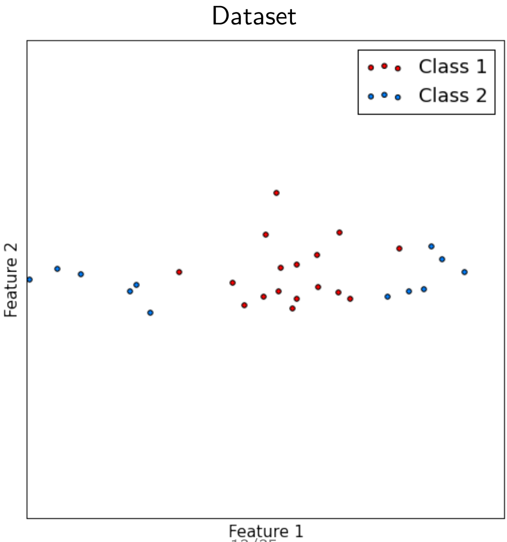
Features of different nature

- Person identification using diverse information:
  by voice, by face, by behavior patterns, etc.

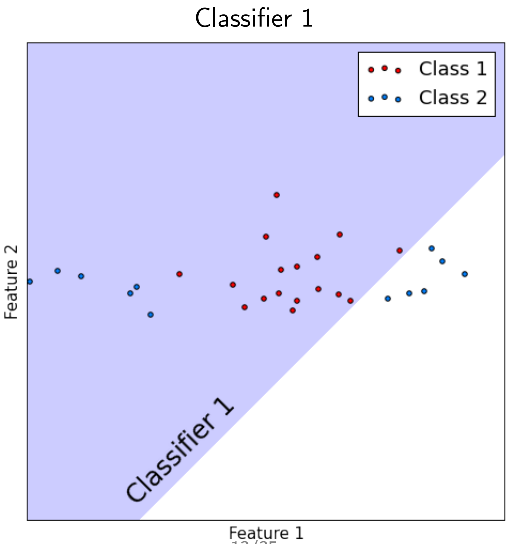
Solve underfitting

- Suppose $f_1(x), ...f_M(x)$ are too simple and underfit.
- May increase complexity by applying $G(f_1(x), ...f_M(x))$

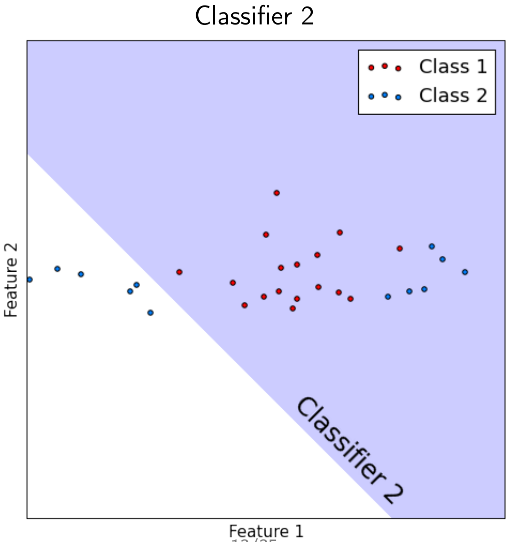
Example



Example

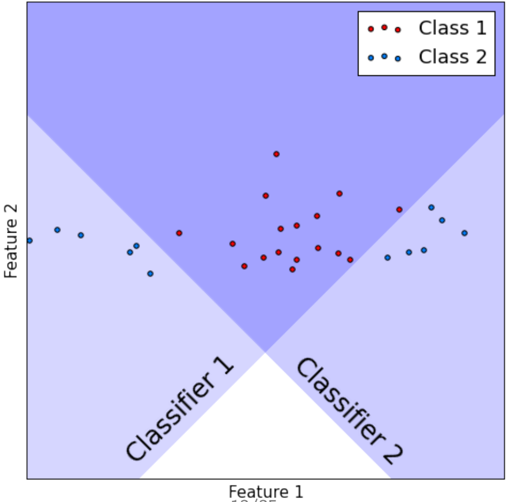

Classifier 1
Class 1
Class 2
Feature 2
Feature 1
Classifier 1

Example


Classifier 2
Class 1
Class 2
Classifier 2
Feature 2
Feature 1

Example

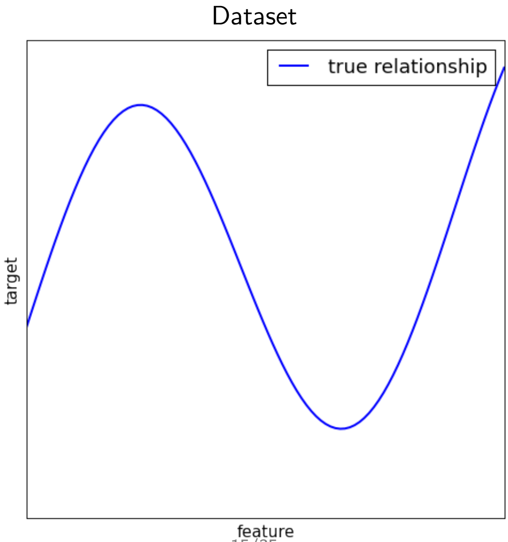
Classifier 1 and classifier 2 combined using AND rule



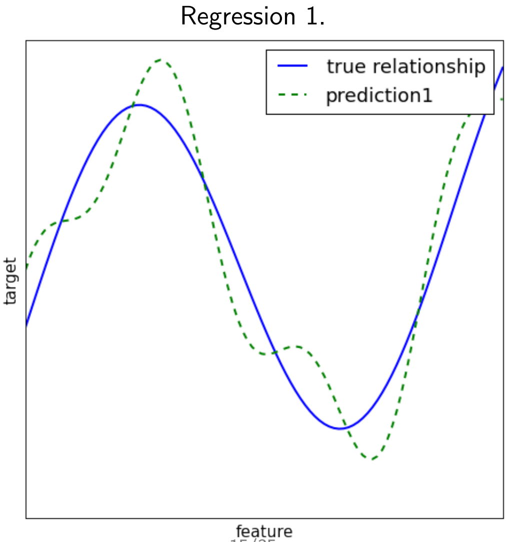
Solve overfitting

- $f_1(x), ...f_M(x)$ overfit (have high variance)
  - decision trees on different training sets
  - neural networks estimated with different initial conditions
- Regression: average their variability to get more robust estimate:
$$\widehat{y}(x) = \frac{1}{M}\sum_{m=1}^{M} f_m(x)$$
- Classification: majority voting.

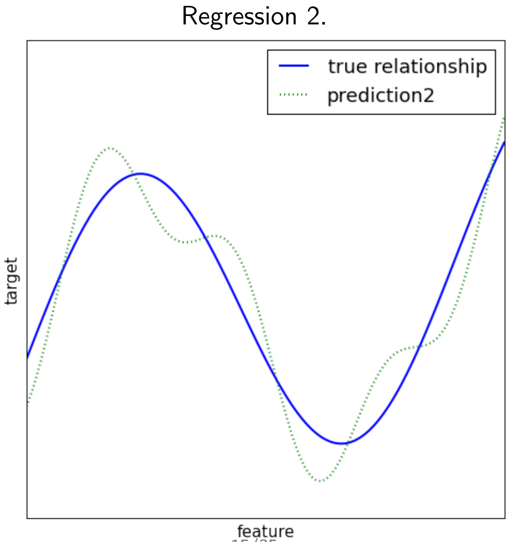
Regression: high variance



Regression: high variance

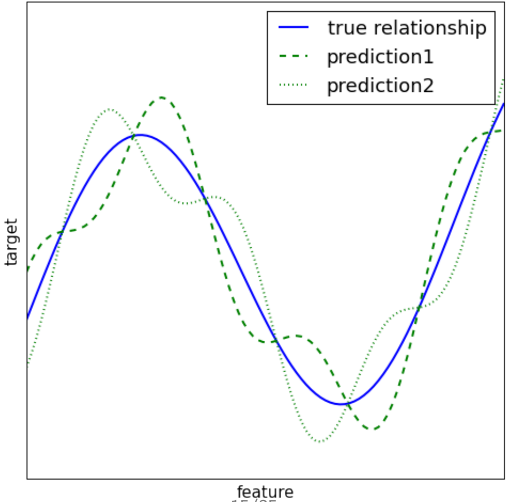


Regression: high variance



Regression: high variance

Average of regression 1 and regression 2 gives better prediction.



Majority voting of classifiers

- Consider M classifiers $f_1(x), ...f_M(x)$, performing binary classification.
- Let probability of mistake be constant $p \in (0, \frac{1}{2})$: $p(f_m(x) = y) = p \, \forall m$
- Suppose all models make mistakes or correct guesses independently of each other.
- Let $G(x)$ be majority voting combiner.
- Then $p(G(x) \neq y) \to 0$ as $M \to \infty$

Do not rely on single model assumptions

- Do not rely on single model assumptions, average risks.
- **Ambiguity decomposition:**
  consider predicting fixed (x, y) with ensemble for $F(x) = \sum_{m=1}^{M} w_m f_m(x)$, $w_m \geq 0$, $\sum_m w_m = 1$. Then

$$\underbrace{(F(x) - y)^2}_{\text{ensemble error}} = \underbrace{\sum_m w_m \left(f_m(x) - y\right)^2}_{\text{base learner error}} - \underbrace{\sum_m w_m \left(f_m(x) - F(x)\right)^2}_{\text{ambiguity}}$$

  - Ensemble is accurate when:
    - $f_m(x)$ are accurate
    - huge disagreement among $\{f_m(x)\}_m$.

Proof of ambiguity decomposition

Proof:

$$\sum_m w_m (f_m(x) - F(x))^2 = \sum_m w_m (f_m(x) - y + y - F(x))^2$$

$$= \sum_m w_m (f_m(x) - y)^2 + \sum_m w_m (y - F(x))^2 + 2 \sum_m w_m (f_m(x) - y)(y - F(x))$$

$$= \sum_m w_m (f_m(x) - y)^2 + (F(x) - y)^2 + 2(y - F(x)) \sum_m w_m (f_m(x) - y)$$

$$= \sum_m w_m (f_m(x) - y)^2 + (F(x) - y)^2 + 2(y - F(x))(F(x) - y)$$

$$= \sum_m w_m (f_m(x) - y)^2 + (F(x) - y)^2 - 2(F(x) - y)^2$$

$$= \sum_m w_m (f_m(x) - y)^2 - (F(x) - y)^2$$

Convex loss

Convex loss promotes the usage of averaged prediction instead of individual ones.

- Take convex loss $\mathcal{L}(\widehat{y}-y)$, such as absolute or square.
- Take $f_1(x),...f_M(x)$ with weights $p_1,...p_M$.
- For any fixed x consider 2 prediction strategies:

1. sample $m \sim Categorical(p_1,...p_M)$, $\widehat{y}(x)=f_m(x)$.
2. $\widehat{y}(x)=\sum_{m=1}^{M}p_m f_m(x)$

Which strategy is better (averaged over different sample outcomes m)?.

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Classifiers output **probabilities**

- Let $p_y^m(x)$ be probability of class y by classifier m.
- Possible final predictions:

$$p_y(x) = \frac{1}{M}\sum_{m=1}^{M} p_y^m(x)$$

$$p_y(x) = \text{median}_m\, p_y^m(x)$$

Allows weighted account of classifiers.

Classifiers output **labels**

- **Binary classification**: output +1 <=>
  - all classifiers predict +1 (AND rule)
  - at least one classifier predicts +1 (OR rule)
  - at least k classifiers predict +1 (k-out-of-N)
- **Multiclass classification**:
  - predict most popular class (majority vote)
- Extension - **weighted account for classifiers**:
  - weighted majority vote
  - weighted k-out-of-N

Classifiers output **scores**

- Let $g_y^m(x)$ be score of class y by model m.
- Problem: scores are incomparable across models.
- Solution:
  1. define ranking score: $s_c^m(x) = \sum_{c \neq i} \mathbb{I}[g_c^m(x) > g_i^m(x)]$
  2. since $s_c^m(x)$ are comparable, assign

$$\widehat{y}(x) = \arg\max_c \sum_{m=1}^{M} s_c^m(x)$$

Allows weighted account of classifiers. Called *Brier scores*.

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Stacking algorithm

- Consider training set $T = \{(x_n, y_n)\}_{n=1}^{N}$, base learners $f_1(x), ...f_M(x)$ and $G(\cdot)$.

Stacking algorithm

- Consider training set $T=\{(x_n,y_n)\}_{n=1}^N$, base learners $f_1(x),...f_M(x)$ and $G(\cdot)$.
- Training $f_1(x),...f_M(x)$, $G(\cdot)$ on the same data causes overfitting!

Stacking algorithm:

1. Set generated training set $T'=\{\}$
2. Split training set into K folds: T_1, T_2, ... T_K.
3. for k in 1,2,...K:
   train $f_1(x),...f_M(x)$ on $T\setminus T_k$
   for (x,y) in T_k:
   augment T' with sample $([f_1(x),...f_M(x)],y)$
4. Train $G(\cdot)$ on T'.
5. Retrain $f_1(x),...f_M(x)$ on T.

Comments

- Besides $f_1(x), ...f_M(x)$ $G(\cdot)$ may also depend on
  - original features x
  - internal representations inside f_m such as class scores, probabilities.

Linear stacking (blending)

- Linear stacking:

$$f(x) = \sum_{m=1}^{M} w_m f_m(x)$$

$$\left(\sum_{m=1}^{M} w_m f_m(x_n) - y_n\right)^2 \to \min_{\mathbf{w}}$$

- $f_1(x), ...f_M(x)$ are correlated (predict the same y) => estimate unstable.
- For more robust estimate solve:

$$\begin{cases} \left(\sum_{m=1}^{M} w_m f_m(x_n) - y_n\right)^2 + \lambda \sum_{m=1}^{M} \left(w_m - \frac{1}{M}\right)^2 \to \min_{\mathbf{w}} \\ w_1 \geq 0, ...w_M \geq 0 \end{cases}$$

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Bagging & random subspaces

When model overfits to particular training set T, it is useful to generate many training sets $T_1, \ldots T_M$, estimate model on each of them and average.

- **Bagging**:
  - random selection of samples (with replacement)[1,2]
- **Random subspace method**:
  - random selection of features (without replacement)
- May apply both methods jointly.

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

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

Bagged trees

In CART trees we solve

$$\widehat{f},\widehat{h}=\arg\max_{f,h\in S(t)}\Delta I(t)$$

$S(t)$ for standard decision trees:

$S=\{\}$
for each f in $\{1,...,D\}$
  for each h in *unique* $\left\{x_n^f\right\}_{n:x_n\in t}$
    $S:=S\cup(f,h)$

Bagged decision trees - bagging applied to standard decision trees.

Random forest & extra random trees

- Random forest & extra random trees are bagged decision trees with restricted search through (f,h), controlled by $\alpha\in(0,1]$.
  - restricted search=>higher bias, smaller variance.

$S(t)$ for random forest:

```
S = {}, K = αD
sample d_1,...d_K randomly from {1,...,D} without replacement.
for each f in d_1,...d_K
    for each h in unique {x_n^f}_{n:x_n∈t}
        S := S ∪ (f,h)
```

$S(t)$ for extra random trees:

```
S = {}, K = αD
sample d_1,...d_K randomly from {1,...,D} without replacement.
for each f in d_1,...d_K
    sample h randomly from unique {x_n^f}_{n:x_n∈t}
    S := S ∪ (f,h)
```

Out-of-bag estimate

Training estimate (overfits, estimates loss from below)

$$L = \frac{1}{N}\sum_{n=1}^{N}\mathcal{L}\left(\frac{1}{M}\sum_{m=1}^{M}f_m(x_n), y_n\right)$$

Out-of-bag estimate

Training estimate (overfits, estimates loss from below)

$$L = \frac{1}{N}\sum_{n=1}^{N}\mathcal{L}\left(\frac{1}{M}\sum_{m=1}^{M} f_m(x_n), y_n\right)$$

Out-of-bag estimate (pessimistic, estimates loss from above)

$$L_{OOB} = \frac{1}{N}\sum_{n=1}^{N}\mathcal{L}\left(\frac{1}{|I_n|}\sum_{m\in I_n} f_m(x_n), y_n\right)$$

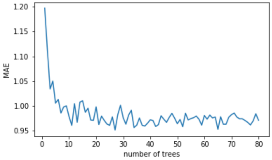
- $I_n \subset \{1, 2, ...M\}$- set of models that didn't use (x_n, y_n) for training.
- don't need for separate validation set!

Comments

- Bagged decision trees, RF, ERT:
    - have straightforward parallel implementation
    - but trees are not targeted to correct mistakes of each other
- Trees in RF, ERT may be built on the same training set T
    - due to stochastic $S(t)$ they will be different anyway

Comments

- Let M=# of base learners.
- ERT trains faster than RF, but on average requires higher M.
- Typical dependency between loss of bagging/RF/ERT depending on M:



- We average variability of tree to training set, what is more efficient for higher M.
- To find optimal hyperparameters set small M, find other parameters, then set high M back.

Conclusion

- Bias-variance decomposition gives 2 sources for poor accuracy:
  - bias: for underfitted models
  - variance: for overfitted models
- Stacking with complex aggregating model decreases bias.
  - may add variance
- Stacking with simple aggregating model (averaging, majority vote) decreases variance.