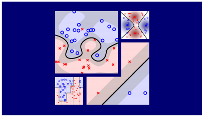
Machine Learning Techniques
(機器學習技法)



Lecture 7: Blending and Bagging

Hsuan-Tien Lin (林軒田)

htlin@csie.ntu.edu.tw

Department of Computer Science
& Information Engineering

National Taiwan University
(國立台灣大學資訊工程系)

Roadmap

1. Embedding Numerous Features: Kernel Models

Lecture 5: Support Vector Regression

kernel ridge regression (dense) via
ridge regression + **representer theorem**;
support vector regression (sparse) via
regularized **tube** error + **Lagrange dual**

2. Combining Predictive Features: Aggregation Models

Lecture 7: Blending and Bagging

- Motivation of Aggregation
- Uniform Blending
- Linear and Any Blending
- Bagging (Bootstrap Aggregation)

3. Distilling Implicit Features: Extraction Models

An Aggregation Story

Your T friends $g_1, \cdots, g_T$ predicts whether stock will go up as $g_t(\mathbf{x})$.

You can ...

- **select** the most trust-worthy friend from their **usual performance**
  —**validation!**
- **mix** the predictions from all your friends **uniformly**
  —let them **vote!**
- **mix** the predictions from all your friends **non-uniformly**
  —let them vote, but **give some more ballots**
- **combine** the predictions **conditionally**
  —if **[t satisfies some condition]** give some ballots to friend t
- ...

aggregation models: **mix** or **combine**
hypotheses (for better performance)

Aggregation with Math Notations

Your T friends $g_1, \cdots, g_T$ predicts whether stock will go up as $g_t(\mathbf{x})$.

- **select** the most trust-worthy friend from their **usual performance**
$$G(\mathbf{x}) = g_{t_*}(\mathbf{x}) \text{ with } t_* = \operatorname{argmin}_{t \in \{1,2,\cdots,T\}} E_{\text{val}}(g_t^-)$$
- **mix** the predictions from all your friends **uniformly**
$$G(\mathbf{x}) = \operatorname{sign}\left(\sum_{t=1}^{T} 1 \cdot g_t(\mathbf{x})\right)$$
- **mix** the predictions from all your friends **non-uniformly**
$$G(\mathbf{x}) = \operatorname{sign}\left(\sum_{t=1}^{T} \alpha_t \cdot g_t(\mathbf{x})\right) \text{ with } \alpha_t \geq 0$$
  - include **select**: $\alpha_t = [\![E_{\text{val}}(g_t) \text{ smallest}]\!]$
  - include **uniformly**: $\alpha_t = 1$
- **combine** the predictions **conditionally**
$$G(\mathbf{x}) = \operatorname{sign}\left(\sum_{t=1}^{T} q_t(\mathbf{x}) \cdot g_t(\mathbf{x})\right) \text{ with } q_t(\mathbf{x}) \geq 0$$
  - include **non-uniformly**: $q_t(\mathbf{x}) = \alpha_t$

aggregation models: a **rich family**

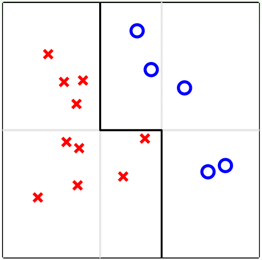
Recall: Selection by Validation

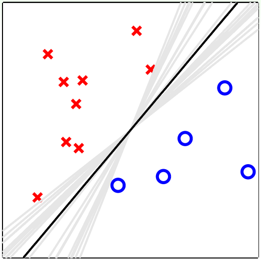
$$G(\mathbf{x}) = g_{t_*}(\mathbf{x}) \text{ with } t_* = \underset{t \in \{1,2,\cdots,T\}}{\operatorname{argmin}} E_{\text{val}}(g_t^-)$$

- **simple** and popular
- what if use $E_{\text{in}}(g_t)$ instead of $E_{\text{val}}(g_t^-)$?
  complexity price on d_{VC}, remember? :-)
- need **one strong** g_t^- to guarantee small E_{val} (and small E_{out})

selection:
rely on one strong hypothesis
aggregation:
can we do better with many
(possibly weaker) hypotheses?

Why Might Aggregation Work?





- mix **different weak hypotheses** uniformly —$G(\mathbf{x})$ 'strong'
- aggregation $\Longrightarrow$ **feature transform (?)**

- mix **different random-PLA hypotheses** uniformly —$G(\mathbf{x})$ 'moderate'
- aggregation $\Longrightarrow$ **regularization (?)**

proper aggregation $\Longrightarrow$ **better performance**

Fun Time

Consider three decision stump hypotheses from $\mathbb{R}$ to $\{-1, +1\}$: $g_1(x) = \text{sign}(1 - x)$, $g_2(x) = \text{sign}(1 + x)$, $g_3(x) = -1$. When mixing the three hypotheses uniformly, what is the resulting $G(x)$?

1. $2 [\![|x| \le 1]\!] - 1$
2. $2 [\![|x| \ge 1]\!] - 1$
3. $2 [\![x \le -1]\!] - 1$
4. $2 [\![x \ge +1]\!] - 1$

Fun Time

Consider three decision stump hypotheses from $\mathbb{R}$ to $\{-1, +1\}$: $g_1(x) = \text{sign}(1 - x)$, $g_2(x) = \text{sign}(1 + x)$, $g_3(x) = -1$. When mixing the three hypotheses uniformly, what is the resulting $G(x)$?

1. $2\,[\![|x| \le 1]\!] - 1$
2. $2\,[\![|x| \ge 1]\!] - 1$
3. $2\,[\![x \le -1]\!] - 1$
4. $2\,[\![x \ge +1]\!] - 1$

Reference Answer: 1

The 'region' that gets two positive votes from g_1 and g_2 is $|x| \le 1$, and thus $G(x)$ is positive within the region only. We see that the three decision stumps g_t can be aggregated to form a more sophisticated hypothesis G.

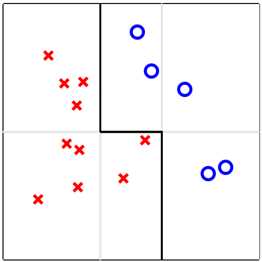
Uniform Blending (Voting) for Classification

uniform blending: known g_t, each with 1 ballot

$$G(\mathbf{x}) = \text{sign}\left(\sum_{t=1}^{T} 1 \cdot g_t(\mathbf{x})\right)$$

- same g_t (autocracy): as good as one single g_t
- very different g_t (**diversity** + **democracy**): majority can **correct** minority
- similar results with uniform voting for multiclass

$$G(\mathbf{x}) = \underset{1 \le k \le K}{\text{argmax}} \sum_{t=1}^{T} [\![g_t(\mathbf{x}) = k]\!]$$



how about **regression**?

Uniform Blending for Regression

$$G(\mathbf{x}) = \frac{1}{T}\sum_{t=1}^{T} g_t(\mathbf{x})$$

- same g_t (autocracy):
  as good as one single g_t
- very different g_t (**diversity** + **democracy**):
  some $g_t(\mathbf{x}) > f(\mathbf{x})$, some $g_t(\mathbf{x}) < f(\mathbf{x})$
  $\Longrightarrow$ average **could be** more accurate than individual

diverse hypotheses:

even simple uniform blending
can be better than any single hypothesis

Theoretical Analysis of Uniform Blending

$$G(\mathbf{x}) = \frac{1}{T}\sum_{t=1}^{T} g_t(\mathbf{x})$$

$$\begin{aligned}
\text{avg}\left((g_t(\mathbf{x}) - f(\mathbf{x}))^2\right) &= \text{avg}\left(g_t^2 - 2g_t f + f^2\right) \\
&= \text{avg}\left(g_t^2\right) - 2Gf + f^2 \\
&= \text{avg}\left(g_t^2\right) - G^2 + (G - f)^2 \\
&= \text{avg}\left(g_t^2\right) - 2G^2 + G^2 + (G - f)^2 \\
&= \text{avg}\left(g_t^2 - 2g_t G + G^2\right) + (G - f)^2 \\
&= \text{avg}\left((g_t - G)^2\right) + (G - f)^2
\end{aligned}$$

$$\begin{aligned}
\text{avg}\left(E_{\text{out}}(g_t)\right) &= \text{avg}\left(\mathcal{E}(g_t - G)^2\right) + E_{\text{out}}(G) \\
&\geq \qquad\qquad + E_{\text{out}}(G)
\end{aligned}$$

Some Special g_t

consider a **virtual** iterative process that for $t = 1, 2, \ldots, T$

1. request size-N data $\mathcal{D}_t$ from P^N (i.i.d.)
2. obtain g_t by $\mathcal{A}(\mathcal{D}_t)$

$$\bar{g} = \lim_{T\to\infty} G = \lim_{T\to\infty} \frac{1}{T}\sum_{t=1}^{T} g_t = \mathop{\mathcal{E}}_{\mathcal{D}} \mathcal{A}(\mathcal{D})$$

$$\begin{aligned} \text{avg}\left(E_{\text{out}}(g_t)\right) &= \text{avg}\left(\mathcal{E}(g_t - \bar{g})^2\right) + E_{\text{out}}(\bar{g}) \\ \text{expected performance of } \mathcal{A} &= \text{expected deviation to consensus} \\ &\quad + \text{performance of consensus} \end{aligned}$$

- performance of consensus: called **bias**
- expected deviation to consensus: called **variance**

uniform blending:
reduces **variance** for more stable performance

Consider applying uniform blending $G(\mathbf{x}) = \frac{1}{T}\sum_{t=1}^{T} g_t(\mathbf{x})$ on linear regression hypotheses $g_t(\mathbf{x}) = \text{innerprod}(\mathbf{w}_t, \mathbf{x})$. Which of the following property best describes the resulting $G(\mathbf{x})$?

1. a constant function of $\mathbf{x}$
2. a linear function of $\mathbf{x}$
3. a quadratic function of $\mathbf{x}$
4. none of the other choices

Consider applying uniform blending $G(\mathbf{x}) = \frac{1}{T}\sum_{t=1}^{T} g_t(\mathbf{x})$ on linear regression hypotheses $g_t(\mathbf{x}) = \text{innerprod}(\mathbf{w}_t, \mathbf{x})$. Which of the following property best describes the resulting $G(\mathbf{x})$?

1. a constant function of $\mathbf{x}$
2. a linear function of $\mathbf{x}$
3. a quadratic function of $\mathbf{x}$
4. none of the other choices

Reference Answer: 2

$$G(\mathbf{x}) = \text{innerprod}\left(\frac{1}{T}\sum_{t=1}^{T}\mathbf{w}_t, \mathbf{x}\right)$$

which is clearly a linear function of $\mathbf{x}$. Note that we write 'innerprod' instead of the usual 'transpose' notation to avoid symbol conflict with T (number of hypotheses).

Linear Blending

linear blending: known g_t, each to be given α_t ballot

$$G(\mathbf{x}) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t \cdot g_t(\mathbf{x})\right) \text{ with } \alpha_t \geq 0$$

computing 'good' α_t : $\min_{\alpha_t \geq 0} E_{\text{in}}(\boldsymbol{\alpha})$

linear blending for regression

$$\min_{\alpha_t \geq 0} \frac{1}{N} \sum_{n=1}^{N} \left(y_n - \sum_{t=1}^{T} \alpha_t g_t(\mathbf{x}_n)\right)^2$$

LinReg + transformation

$$\min_{w_i} \frac{1}{N} \sum_{n=1}^{N} \left(y_n - \sum_{i=1}^{\tilde{d}} w_i \phi_i(\mathbf{x}_n)\right)^2$$

like two-level learning, remember? :-)

linear blending = LinModel + hypotheses as transform + constraints

Constraint on α_t

linear blending = LinModel + hypotheses as transform + constraints:

$$\min_{\alpha_t \geq 0} \quad \frac{1}{N}\sum_{n=1}^{N} \mathrm{err}\left(y_n, \sum_{t=1}^{T} \alpha_t g_t(\mathbf{x}_n)\right)$$

linear blending for binary classification

$$\text{if } \alpha_t < 0 \quad \Longrightarrow \quad \alpha_t g_t(\mathbf{x}) = |\alpha_t| \left(-g_t(\mathbf{x})\right)$$

- negative α_t for $g_t \equiv$ positive $|\alpha_t|$ for $-g_t$
- **if you have a stock up/down classifier with 99% error, tell me! :-)**

in practice, often
linear blending = LinModel + hypotheses as transform ~~+ constraints~~

Linear Blending versus Selection

in practice, often

$$g_1 \in \mathcal{H}_1, g_2 \in \mathcal{H}_2, \ldots, g_T \in \mathcal{H}_T$$

by minimum E_{in}

- recall: **selection by minimum E_{in}**
  —best of best, paying $d_{\text{VC}}\left(\bigcup_{t=1}^{T} \mathcal{H}_t\right)$
- recall: linear blending includes selection as special case
  —by setting $\alpha_t = \llbracket E_{\text{val}}(g_t^-) \text{ smallest} \rrbracket$
- complexity price of linear blending with E_{in} (aggregation of best):
  $\geq d_{\text{VC}}\left(\bigcup_{t=1}^{T} \mathcal{H}_t\right)$

like selection, blending practically done with
(E_{val} instead of E_{in}) + (g_t^- from minimum E_{train})

Any Blending

Given $g_1^-, g_2^-, \ldots, g_T^-$ from $\mathcal{D}_{\text{train}}$, transform $(\mathbf{x}_n, y_n)$ in $\mathcal{D}_{\text{val}}$ to $(\mathbf{z}_n = \boldsymbol{\Phi}^-(\mathbf{x}_n), y_n)$, where $\boldsymbol{\Phi}^-(\mathbf{x}) = (g_1^-(\mathbf{x}), \ldots, g_T^-(\mathbf{x}))$

Linear Blending

1. compute α = Lin$\left(\{(\mathbf{z}_n, y_n)\}\right)$
2. return $G_{\text{LINB}}(\mathbf{x})$ = LinH(innerprod$(\alpha, \boldsymbol{\Phi}(\mathbf{x}))$),

Any Blending (Stacking)

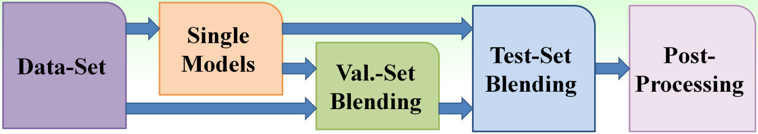
1. compute $\tilde{g}$ = **Any**$\left(\{(\mathbf{z}_n, y_n)\}\right)$
2. return $G_{\text{ANYB}}(\mathbf{x}) = \tilde{g}(\boldsymbol{\Phi}(\mathbf{x}))$,

where $\boldsymbol{\Phi}(\mathbf{x}) = (g_1(\mathbf{x}), \ldots, g_T(\mathbf{x}))$

any blending:

- **powerful**, achieves conditional blending
- but **danger of overfitting**, as always **:-(**

Blending in Practice



(Chen et al., A linear ensemble of individual and blended models for music rating prediction, 2012)

KDDCup 2011 Track 1: World Champion Solution by NTU

- validation set blending: a special any blending model

  $$E_{\text{test}} \text{ (squared)}: 519.45 \Longrightarrow 456.24$$

  —helped **secure the lead** in last two weeks

- test set blending: linear blending using $\tilde{E}_{\text{test}}$

  $$E_{\text{test}} \text{ (squared)}: 456.24 \Longrightarrow 442.06$$

  —helped **turn the tables** in last hour

blending 'useful' in practice,
despite the computational burden

Fun Time

Consider three decision stump hypotheses from $\mathbb{R}$ to $\{-1, +1\}$: $g_1(x) = \text{sign}(1 - x)$, $g_2(x) = \text{sign}(1 + x)$, $g_3(x) = -1$. When $x = 0$, what is the resulting $\mathbf{\Phi}(x) = (g_1(x), g_2(x), g_3(x))$ used in the returned hypothesis of linear/any blending?

1. $(+1, +1, +1)$
2. $(+1, +1, -1)$
3. $(+1, -1, -1)$
4. $(-1, -1, -1)$

Fun Time

Consider three decision stump hypotheses from $\mathbb{R}$ to $\{-1, +1\}$: $g_1(x) = \text{sign}(1 - x)$, $g_2(x) = \text{sign}(1 + x)$, $g_3(x) = -1$. When $x = 0$, what is the resulting $\mathbf{\Phi}(x) = (g_1(x), g_2(x), g_3(x))$ used in the returned hypothesis of linear/any blending?

1. $(+1, +1, +1)$
2. $(+1, +1, -1)$
3. $(+1, -1, -1)$
4. $(-1, -1, -1)$

Reference Answer: 2

Too easy? :-)

What We Have Done

blending: aggregate after getting g_t;
learning: aggregate as well as getting g_t

aggregation type	blending	learning
uniform	voting/averaging	?
non-uniform	linear	?
conditional	stacking	?

learning g_t for uniform aggregation: diversity important

- diversity by different models: $g_1 \in \mathcal{H}_1, g_2 \in \mathcal{H}_2, \ldots, g_T \in \mathcal{H}_T$
- diversity by different parameters: GD with $\eta = 0.001, 0.01, \ldots, 10$
- diversity by algorithmic randomness:
  random PLA with different random seeds
- diversity by data randomness:
  within-cross-validation hypotheses g_v^-

next: diversity by data randomness without g^-

Revisit of Bias-Variance

$$\begin{aligned}\text{expected performance of } \mathcal{A} &= \text{expected deviation to consensus} \\ &\quad + \text{performance of consensus} \\ \text{consensus } \bar{g} &= \text{expected } g_t \text{ from } \mathcal{D}_t \sim P^N\end{aligned}$$

- consensus more stable than direct $\mathcal{A}(\mathcal{D})$, but comes from many more $\mathcal{D}_t$ than the $\mathcal{D}$ on hand
- want: approximate $\bar{g}$ by
  - finite (large) T
  - approximate $g_t = \mathcal{A}(\mathcal{D}_t)$ from $\mathcal{D}_t \sim P^N$ using only $\mathcal{D}$

bootstrapping: a statistical tool that re-samples from $\mathcal{D}$ to 'simulate' $\mathcal{D}_t$

Bootstrap Aggregation

bootstrapping

bootstrap sample $\tilde{D}_t$: re-sample N examples from $\mathcal{D}$ **uniformly with replacement**—can also use arbitrary N' instead of original N

virtual aggregation

consider a **virtual** iterative process that for $t = 1, 2, \ldots, T$

1. request size-N data $\mathcal{D}_t$ from P^N (i.i.d.)
2. obtain g_t by $\mathcal{A}(\mathcal{D}_t)$

$G = \text{Uniform}(g_t)$

bootstrap aggregation

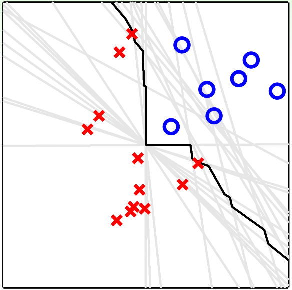
consider a **physical** iterative process that for $t = 1, 2, \ldots, T$

1. request size-N' data $\tilde{\mathcal{D}}_t$ from bootstrapping
2. obtain g_t by $\mathcal{A}(\tilde{\mathcal{D}}_t)$

$G = \text{Uniform}(g_t)$

bootstrap aggregation (BAGging):
a simple **meta algorithm**
on top of **base algorithm** $\mathcal{A}$

Bagging Pocket in Action



$T_{\text{POCKET}} = 1000$; $T_{\text{BAG}} = 25$

- very diverse g_t from bagging
- proper **non-linear** boundary after aggregating binary classifiers

bagging works reasonably well **if base algorithm sensitive to data randomness**

Fun Time

When using bootstrapping to re-sample N examples $\tilde{\mathcal{D}}_t$ from a data set $\mathcal{D}$ with N examples, what is the probability of getting $\tilde{\mathcal{D}}_t$ exactly the same as $\mathcal{D}$?

1. $0 \quad / N^N = 0$
2. $1 \quad / N^N$
3. $N! \ / N^N$
4. $N^N / N^N = 1$

Fun Time

When using bootstrapping to re-sample N examples $\tilde{\mathcal{D}}_t$ from a data set $\mathcal{D}$ with N examples, what is the probability of getting $\tilde{\mathcal{D}}_t$ exactly the same as $\mathcal{D}$?

1. $0 \;/N^N = 0$
2. $1 \;/N^N$
3. $N! \;/N^N$
4. $N^N/N^N = 1$

Reference Answer: 3

Consider re-sampling in an ordered manner for N steps. Then there are (N^N) possible outcomes $\tilde{D}_t$, each with equal probability. Most importantly, $(N!)$ of the outcomes are permutations of the original $\mathcal{D}$, and thus the answer.

Summary

1. Embedding Numerous Features: Kernel Models
2. Combining Predictive Features: Aggregation Models

Lecture 7: Blending and Bagging

- Motivation of Aggregation
  aggregated G strong and/or moderate
- Uniform Blending
  diverse hypotheses, 'one vote, one value'
- Linear and Any Blending
  two-level learning with hypotheses as transform
- Bagging (Bootstrap Aggregation)
  bootstrapping for diverse hypotheses

- **next: getting more diverse hypotheses to make G strong**

3. Distilling Implicit Features: Extraction Models